Introduction to quantum optics

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These are the lecture notes for a course (PH260) that I am teaching at Zhiyuan College of Shanghai Jiao Tong University, though the first draft was created for a previous course I taught in Germany, so I will be updating and adapting the content to the level and interests of Zhiyuan students. It has been designed for students who have only had basic training on quantum mechanics, and hence, the course is suited for people at all levels (say, from the end of the bachelor all the way into the PhD).

Let me start with a few words about the topic of the lectures. Quantum optics treats the interaction between light and matter. We may think of light as the optical part of the electromagnetic spectrum, and matter as atoms. However, modern quantum optics covers a wild variety of systems, so that a more timely definition could be "quantum electrodynamics at low energies". Such scenario includes, for example, superconducting circuits, confined electrons, excitons in semiconductors, defects in solid state, or the center-of-mass motion of micro-, meso-, and macroscopic systems. Moreover, quantum optics is at the heart of the exponentially-growing field of quantum information processing and communication, both at the conceptual level and at the level of technological implementations. The ideas and experiments developed in quantum optics have also allowed us to take a fresh look at many-body problems of relevance for condensed matter and even high-energy physics. In addition, quantum optics holds the promise of testing foundational problems in quantum mechanics as well as physics beyond the standard model in table-sized experiments. One of the distinct features of quantum optics is that it deals with systems that are not isolated, that is, they leak out energy and information to their surrounding environment. While this is actually the most common situation in real physical systems, it is not the one students usually encounter in their standard quantum mechanics courses. A big part of this course is devoted to fill this gap: it goes through many of the tools and methods that have been developed to describe open quantum optical systems. Apart from their practical use, these methods also have deep physical interpretations which will make students understand quantum mechanics much better. Quantum optics and open systems are therefore topics that no future researcher in quantum physics should miss.

I cannot emphasize enough how important it is to read as much as possible about these topics in order to mature into the best version of a quantum physicist that one can be. Therefore, I conclude with a list of references that I have found especially useful at different points of my career [1–21].

I finish with a big note of warning: these notes are a work in progress, meaning that some proofs and many figures are still missing. However, I've tried my best to write everything in such a way that a reader can follow naturally all arguments and derivations even with these missing bits. Also two chapters are left to add, one on mathematical methods to analyze the dynamics of open systems, and another introducing the plethora of current experimental platforms where the tools and ideas developed in these notes are being currently implemented.

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I. BRIEF SUMMARY OF QUANTUM MECHANICS

In this short introductory chapter we will quickly review the basic elements of quantum mechanics required to follow the rest of the notes. This summary is just intended as a reminder for students who have already studied a course on quantum mechanics, as well as courses in linear algebra and classical mechanics. Nevertheless, in order to make the course self-contained and make sure that all students are familiar with all the concepts and notation used throughout the course, in Appendix A these are reviewed in full detail. It is advised that all students go slowly through that appendix, making sure they understand each and every concept that it introduces.

A. Quantum mechanics with pure states

Setting the stage: states and observables. Within the mathematical formalism of quantum mechanics, physical degrees of freedom are associated with a complex Hilbert space, that is, a vector space endorsed with an inner product (structure known as a *Euclidean space*), composed of *normalizable* vectors. We will denote Hilbert spaces with a calligraphic symbol, say $\mathcal{H}$, for example.

We will use the 'bra-ket' notation introduced by Dirac, where vectors are denoted by $|\psi\rangle \in \mathcal{H}$ (ket), and the inner product of two vectors $|\psi\rangle$ and $|\phi\rangle$ is denoted by $\langle\psi|\phi\rangle \in \mathbb{C}$ (bra-ket). Note that 'ψ' and 'ϕ' act just as labels for the vectors (their *names*, if you will).

The inner-product structure of the Hilbert space $\mathcal{H}$ allows us to define its dual, denoted by $\mathcal{H}^+$, whose elements are denoted by $\langle\psi| \in \mathcal{H}^+$ (bra). Whenever a bra meets a ket, a complex number is produced: $\langle\psi|\ |\phi\rangle \to \langle\psi|\phi\rangle$. Hence, ket-bra structures such as $|\psi\rangle\langle\phi|$ are operators, that is, objects that map kets onto kets: $|\psi\rangle\langle\phi|\ |\varphi\rangle \to \langle\phi|\varphi\rangle\ |\psi\rangle \in \mathcal{H}$ (and similarly for bras).

In quantum mechanics, the state of an isolated system is completely specified by a normalized vector in its Hilbert space, say $|\psi\rangle \in \mathcal{H}$ with $\langle\psi|\psi\rangle = 1$. Observables, on the other hand, are represented by self-adjoint operators, say $\hat{A} = \hat{A}^\dagger$ (we will always denote operators by a 'hat'). The spectral theorem tells us that the eigenvalues of such an operator are always real, while their eigenvectors form a basis of the Hilbert basis, that is,

$$\hat{A} = \sum_{j=1}^{d} a_j |a_j\rangle\langle a_j|, \tag{1}$$

with $a_j \in \mathbb{R}$ and

$$\sum_{j=1}^{d} |a_j\rangle\langle a_j| = \hat{I}, \text{ (resolution of the identity)} \tag{2a}$$

$$\langle a_j|a_l\rangle = \delta_{jl}, \text{ (orthonormality)} \tag{2b}$$

where $\hat{I}$ is the identity operator and we have denoted by d the dimension of the Hilbert space (which can be infinite, as we will discuss shortly). Applying (2a) to any vector $|\psi\rangle$, we obtain its expansion in the basis $\{|a_j\rangle\}_{j=1,...,d}$,

$$|\psi\rangle = \sum_{j=1}^{d} \psi_j |a_j\rangle, \qquad \text{with } \psi_j = \langle a_j|\psi\rangle. \tag{3}$$

The column vector with ψ_j as components, that is, $\vec{\psi} = (\psi_1, ..., \psi_d)^T$ is known as the representation of the ket $|\psi\rangle$ in the basis $\{|a_j\rangle\}_{j=1,...,d}$ (the upper index 'T' denotes 'transpose'). The representation of a bra $\langle\psi|$ is then given by the row vector $\vec{\psi}^\dagger = (\psi_1^*, ..., \psi_d^*)$. On the other hand, the representation of an operator $\hat{B}$ is a $d \times d$ matrix B with elements $B_{jl} = \langle a_j|\hat{B}|a_l\rangle$. Abstract expressions such as $\langle\phi|\hat{B}|\psi\rangle$ can then be evaluated as $\vec{\phi}^\dagger B \vec{\psi}$.

The case of a Hilbert space with infinite dimension, $d \to \infty$, deserves special attention. Since one can build infinite sequences that do not converge, there exist elements of the vector space underlaying the Hilbert space that are not normalizable. While these vectors are not elements of the Hilbert space itself, they can still be eigenvectors of operators acting on the Hilbert space. Specifically, one can find self-adjoint operators with a continuous spectrum, say,

$$\hat{X} = \int_{\mathbb{R}} dx\ x|x\rangle\langle x|, \tag{4}$$

where the eigenvectors are not normalizable, and therefore are not elements of the Hilbert space, $|x\rangle \notin \mathcal{H}$. Remarkably, one can still use these eigenvectors to build a resolution of the identity, provided that they are chosen to satisfy the so-called 'Dirac-delta orthonormalization condition'

$$\langle x|y\rangle = \delta(x-y) \quad \Rightarrow \quad \hat{I} = \int_{\mathbb{R}} dx\, |x\rangle\langle x|. \tag{5}$$

Using this property, we can now expand any vector $|\psi\rangle$ (belonging to the Hilbert space or not), as

$$|\psi\rangle = \int_{\mathbb{R}} dx \psi(x)|x\rangle, \qquad \text{with } \psi(x) = \langle x|\psi\rangle, \tag{6}$$

where now $\psi(x)$ is a continuous representation of the ket $|\psi\rangle$ in the *generalized* or *continuous basis* $\{|x\rangle\}_{x\in\mathbb{R}}$.

Note that while here we have discussed only operators with a purely continuous spectrum, in general, one can find observables with mixed spectrum, that is, part discrete and part continuous. The former are always normalizable while the latter are Dirac-delta normalizable, such that the collection of all eigenvectors forms a generalized basis that can be used to to form a resolution of the identity. Indeed, this is the case for most Hamiltonian operators of real systems. For example, atoms present a discrete set of low-energy states where the electrons are bound to the nucleus, but also a continuum of high-energy states where the atom is ionized and the electron is set free.

An important question is how to build observables in quantum mechanics, that is, how to define the self-adjoint operator associated to a physically measurable magnitude. In some cases, such as the spin of the electron, the observable isn't even present in classical physics, and it needs to be built based either on empirical observations or reasonable symmetry principles (for example, the electron's spin was postulated by Pauli to fit experiments, but it was finally shown to emerge naturally in quantum field theory by demanding the framework to be consistent with special relativity). However, for observables with a classical counterpart, quantum mechanics provides a well-defined prescription. In classical physics one can always describe the system through a set of generalized positions $\mathbf{q}$ and momenta $\mathbf{p}$, which define *phase space*. A classical state of the system is then associated with a point in phase space. On the other hand, observables are real functions on phase space, say, $A(\mathbf{q},\mathbf{p})$. Quantum mechanics then says that the corresponding observable is found by symmetrizing A with respect to the possible orderings of positions and momenta[1], what we denote by $A^{(s)}$, and then replacing them by operators $\hat{\mathbf{q}}$ and $\hat{\mathbf{p}}$, whose components satisfy *canonical commutation relations*

$$[\hat{q}_m, \hat{q}_n] = 0 = [\hat{p}_m, \hat{p}_n], \qquad [\hat{q}_m, \hat{p}_n] = \mathrm{i}\hbar\delta_{mn}. \tag{7}$$

The symmetrization ensures that the resulting operator $\hat{A} \equiv A^{(s)}(\hat{\mathbf{q}},\hat{\mathbf{p}})$ is self-adjoint. Note that it is the first time that we introduce Planck's constant, which plays a fundamental role in quantum mechanics. In this case, it prevents positions and momenta from commuting, if only by a little amount ($\hbar$ is very small 'by classical standards'), just enough to bring about a change of paradigm in physics!

Observing quantum systems. One of the most striking features of quantum mechanics concerns measurements of observables. When measuring an observable $\hat{A}$, quantum mechanics says that the outcome can be any of its eigenvalues $\{a_j\}_{j=1,\dots,d}$, which will appear with probability

$$\{p_j = |\langle a_j|\psi\rangle|^2\}_{j=1,\dots,d} \tag{8}$$

, where $|\psi\rangle$ is the state of the system. Hence, it is in general impossible to predict the outcome of a single measurement, but just the frequency with which the outcomes will appear when the experiment is repeated many times (e.g., either the process of state-preparation and measurement are repeated many times on a single system, or many copies of the same system in the same state are independently measured once).

Moreover, suppose that after the single measurement we obtain eigenvalue a_j as the outcome. Then, quantum mechanics says that right after the measurement, the state of the system *collapses* to $|a_j\rangle$. This is arguably the most radical difference with respect to classical physics: while observables can be measured without perturbing the state of classical systems, in quantum mechanics the measurement process irreversibly changes the state of the system. This collapse of the system's state is arguably the quantum-mechanical concept that has ignited the most fierce fights among physicists, and it keeps doing so [30].

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[1] For example, given $A = pq^2$, we write it in symmetric form as $A = \frac{1}{3}(q^2p + qpq + pq^2) \equiv A^{(s)}$, such that the expression contains all the possible orderings of pq^2 with equal weights.

On the practical side, there are two important statistical objects that roughly characterize what's to be expected from a state in a measurement process. First, the expectation value of the observable, defined as

$$\langle \hat{A} \rangle \equiv \langle \psi | \hat{A} | \psi \rangle = \sum_{j=1}^{d} a_j p_j, \tag{9}$$

which coincides with the statistical *mean* or *average* of the probability distribution, that is, the average of the outcomes expected after many repetitions of the measurement process. On the other hand, we also need a figure of the spread of the outcomes around the mean. Defining the *variance*

$$V(A) \equiv \langle \psi | \hat{A}^2 | \psi \rangle - \langle \psi | \hat{A} | \psi \rangle^2, \tag{10}$$

such a spread can be quantified by the *standard deviation* or *uncertainty* $\Delta A = \sqrt{V(A)}$. It is common to define the fluctuation operator $\delta \hat{A} = \hat{A} - \langle \hat{A} \rangle$, whose square gives us direct access to the variance as $V(A) = \langle (\delta \hat{A})^2 \rangle$. A shocking result is that of the *uncertainty relations*: given two observables $\hat{A}$ and $\hat{B}$, it is possible to prove that

$$\Delta A \Delta B \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|. \tag{11}$$

Hence, while in classical physics nothing prevents us from preparing states where we have perfect knowledge of all the observables of the system, the situation is radically different in quantum mechanics: a state with negligible variance in one observable, necessarily comes with a large variance in other observables that do not commute with the first one.

Unsupervised evolution. In the previous lines we discussed how the system behaves when it is observed. But what about the evolution of the system when it is not subject to any measurements? Quantum mechanics says that the evolution of a quantum system that is left *unsupervised* is completely characterized by the *evolution operator*, defined from the Hamiltonian $\hat{H}$ of the system as

$$\hat{U}(t) = e^{\hat{H} t / \mathrm{i}\hbar}, \tag{12}$$

where for simplicity we consider a time-independent Hamiltonian (in Section I C). Recall that the Hamiltonian is easy to construct from the classical one when that's available, but has to be formulated empirically or with reasonable theoretical arguments when the system involves degrees of freedom with no classical analog. In any case, the Hamiltonian is a self-adjoint operator, and therefore the evolution operator is unitary, $\hat{U}^\dagger(t) = \hat{U}^{-1}(t)$.

We can formulate the evolution induced by this operator in two apparently different, but equivalent ways:

- *Schrödinger picture.* In this formulation states evolve, while operators remain fixed in time. In particular, denoting by $|\psi(t)\rangle$ the state of the system at any time, quantum mechanics says

$$|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle \quad \Leftrightarrow \quad \mathrm{i}\hbar \partial_t |\psi\rangle = \hat{H} |\psi\rangle, \tag{13}$$

  where the latter is known as the *Schrödinger equation.*

- *Heisenberg picture.* An alternative formulation consists on the following one, where states remain fixed, and it is operators that evolve in time. Specifically, denoting by $\hat{A}(t)$ the time-evolved of an operator that is $\hat{A}(0)$ originally, quantum mechanics says that

$$\hat{A}(t) = \hat{U}^\dagger(t) \hat{A}(0) \hat{U}(t) \quad \Leftrightarrow \quad \mathrm{i}\hbar \partial_t \hat{A} = [\hat{A}, \hat{H}], \tag{14}$$

  where the latter is known as *Heisenberg equation.*

The equivalence between this two pictures is obvious from the following argument. In real experiments, states and operators are not directly observable. Instead, experimental observations are only sensible to expectation values of operators—note that even probabilities such as (13) can be written as expectation values $p_j = \langle \hat{P}_j \rangle$ of projectors $\hat{P}_j = |a_j\rangle\langle a_j|$—, which are written in both pictures as

$$\langle \psi(t) | \hat{A} | \psi(t) \rangle = \langle \psi(0) | \hat{U}^\dagger(t) \hat{A}(0) \hat{U}(t) | \psi(0) \rangle = \langle \psi | \hat{A}(t) | \psi \rangle. \tag{15}$$

Note that, for consistency, the original Heisenberg operator $\hat{A}(0)$ coincides with the one that remains fixed in the Schrödinger picture, simply denoted by $\hat{A}$ in the latter picture. Similarly, the original Schrödinger state $|\psi(0)\rangle$

coincides with the one that remains fixed in the Heisenberg picture, denoted in the latter picture by $|\psi\rangle$. Having these two alternative descriptions of quantum mechanics is very handy, as we will see throughout the notes.

Composite systems. Consider a system formed by two degrees of freedom or *subsystems*[2] (everything is trivially generalized to more subsystems). Can we build the Hilbert space $\mathcal{H}$ of the total system, just from knowledge of the individual Hilbert spaces $\mathcal{A}$ and $\mathcal{B}$ of its subsystems? Indeed we can, and quantum mechanics tells us that the total Hilbert space will be the tensor product of those spaces, that is, $\mathcal{H} = \mathcal{A} \otimes \mathcal{B}$.

The definition and properties of the tensor product map are reviewed in detail in Section A 2 d of Appendix A. Suffice here to say that:

- It puts in (unique) correspondence pairs of vectors ($|\psi_\mathcal{A}\rangle \in \mathcal{H}_\mathcal{A}, |\psi_\mathcal{B}\rangle \in \mathcal{H}_\mathcal{B}$), with a vector $|\psi\rangle \in \mathcal{H}$ in the total Hilbert space. We will denote such vector by $|\psi\rangle = |\psi_\mathcal{A}\rangle \otimes |\psi_\mathcal{B}\rangle$, or simply by the more economic way $|\psi\rangle = |\psi_\mathcal{A}, \psi_\mathcal{B}\rangle$ when there is no room for confusion.
- Of particular relevance is the correspondence between bases in the different Hilbert spaces. Given the bases $\{|e_j^\mathcal{A}\rangle\}_{j=1,\dots,d_\mathcal{A}}$ and $\{|e_j^\mathcal{B}\rangle\}_{j=1,\dots,d_\mathcal{B}}$ of $\mathcal{A}$ and $\mathcal{B}$, respectively, the set $\{|e_j^\mathcal{A}, e_l^\mathcal{B}\rangle = |e_j^\mathcal{A}\rangle \otimes |e_l^\mathcal{B}\rangle\}_{l=1,\dots,d_\mathcal{B}}^{j=1,\dots,d_\mathcal{A}}$ forms a basis of $\mathcal{H}$, which has then dimension $d = d_\mathcal{A} \times d_\mathcal{B}$.
- Given two kets $|\psi\rangle = |\psi_\mathcal{A}\rangle \otimes |\psi_\mathcal{B}\rangle$ and $|\phi\rangle = |\phi_\mathcal{A}\rangle \otimes |\phi_\mathcal{B}\rangle$, their inner product is defined as $\langle\phi|\psi\rangle = \langle\phi_\mathcal{A}|\psi_\mathcal{A}\rangle\langle\phi_\mathcal{B}|\psi_\mathcal{B}\rangle$.
- Given two operators $\hat{L}_\mathcal{A}$ and $\hat{L}_\mathcal{B}$, we define the action of their tensor product $\hat{L} = \hat{L}_\mathcal{A} \otimes \hat{L}_\mathcal{B}$ onto a vector $|\psi\rangle = |\psi_\mathcal{A}\rangle \otimes |\psi_\mathcal{B}\rangle$ by $\hat{L}|\psi\rangle = (\hat{L}_\mathcal{A}|\psi_\mathcal{A}\rangle) \otimes (\hat{L}_\mathcal{B}|\psi_\mathcal{B}\rangle)$. We will omit the tensor product between the operators when the notation makes it clear onto which Hilbert space they act. Hence, for example, we will simply write $\hat{L}_\mathcal{A}\hat{L}_\mathcal{B}|\psi\rangle = (\hat{L}_\mathcal{A}|\psi_\mathcal{A}\rangle) \otimes (\hat{L}_\mathcal{B}|\psi_\mathcal{B}\rangle)$ or $\hat{L}_\mathcal{A}|\psi\rangle = (\hat{L}_\mathcal{A}|\psi_\mathcal{A}\rangle) \otimes |\psi_\mathcal{B}\rangle$.

A remarkable concept appears in composite systems: *entanglement*. It refers to correlations between the subsystems that exploit the concept of quantum superposition, and cannot therefore appear in classical physics. As a concrete example, consider the state $|\psi\rangle = (|E_1^\mathcal{A}\rangle \otimes |E_1^\mathcal{B}\rangle + |E_2^\mathcal{A}\rangle \otimes |E_2^\mathcal{B}\rangle)/\sqrt{2}$, where $\left\{|E_j^\mathcal{S}\rangle\right\}_{j=1,2}^{\mathcal{S}=\mathcal{A},\mathcal{B}}$ are energy eigenstates of the corresponding subsystem (we assume that the subsystems do not interact after preparation of the state). Upon a measurement of the energy of subsystem $\mathcal{A}$, we cannot predict the outcome with certainty, which can be either $E_1^\mathcal{A}$ or $E_2^\mathcal{A}$ with 50% probability. However, we know that once one outcome appears, e.g., $E_1^\mathcal{A}$, then the full system collapses to the state $|E_1^\mathcal{A}\rangle \otimes |E_1^\mathcal{B}\rangle$, and therefore, we are now able to predict with certainty the outcome of an energy measurement on $\mathcal{B}$, without ever having interrogated $\mathcal{B}$ itself. Hence, $\mathcal{A}$ and $\mathcal{B}$ are correlated, since a measurement on one affects the state of the other. However, since the correlations are encoded in a quantum superposition, these are a purely quantum mechanical type of correlations that we cannot generate classically. This type of quantum correlations that make use of the superposition principle are known as entanglement, and are the heart of the field of quantum information that has emerged in recent decades, and holds great promise for technological applications in computation, communication, and sensing. Remarkably, this type of states have allowed us to show experimentally that nature is incompatible with determinism, unless we are willing to give up causality, and hence the probabilistic character of quantum mechanics is inherent to nature, not a product of our ignorance. You can learn a bit more about entanglement in Appendix A 3 h, and hopefully through some examples that we will study in the course.

B. Quantum mechanics with mixed states

Need for mixed states: noisy systems. Consider a system for which our state-preparation device is not perfect (as it often occurs in real experiments), and we cannot be sure that we prepared a given state $|\psi\rangle$, but only know that we prepared some state among a set $\{|\psi_m\rangle\}_{m=1,\dots,M}$ with associated probability distribution $\{w_m\}_{m=1,\dots,M}$, where $w_m \geq 0$ and $\sum_{m=1}^M w_m = 1$. We will call *ensemble* to the set $\{w_m, |\psi_m\rangle\}_{m=1,\dots,M}$. Note that the states of the ensemble do not need to be orthogonal, and actually M needs not be the dimension of the Hilbert space.

What will be the mean or expectation value of an operator $\hat{A}$ in this setup? The expectation value in a given state of the ensemble is $\langle\psi_m|\hat{A}|\psi_m\rangle$, so we simply need to average these over their probability distribution, that is

$$\langle\hat{A}\rangle = \sum_{m=1}^{M} w_m \langle\psi_m|\hat{A}|\psi_m\rangle. \tag{16}$$

[2] Here we speak about distinguishable subsystems, which is all we will care about in this course. The indistinguishable case is a bit more subtle. In particular, quantum mechanics says that, in such case, the Hilbert space of the total system is not all $\mathcal{A} \otimes \mathcal{B}$, but only the subspace composed by vectors which are either symmetric or antisymmetric under the exchange of the labels of the subsystems. In the first case we say we are dealing with bosons, and in the second with fermions. For example, the state $|e_j\rangle \otimes |e_{l\neq j}\rangle$, which is a basis state for distinguishable systems as we mention below, is not a basis state for indistinguishable subsystems. Instead, states $(|e_j\rangle \otimes |e_l\rangle \pm |e_l\rangle \otimes |e_j\rangle)/\sqrt{2}$ are correct basis states for bosons and fermions, respectively.

By defining an operator

$$\hat{\rho} = \sum_{m=1}^{M} w_m |\psi_m\rangle\langle\psi_m|, \tag{17}$$

we can rewrite (16) in the compact form

$$\langle \hat{A} \rangle = \mathrm{tr}\{\hat{\rho}\hat{A}\}, \tag{18}$$

where 'tr' is the trace operation, defined in terms of a basis $\{|e_j\rangle\}_{j=1...d}$ as $\mathrm{tr}\{\hat{D}\} = \sum_{j=1}^{d} \langle e_j|\hat{D}|e_j\rangle$ for any operator $\hat{D}$. It is very interesting to have been able to write expectation values in terms of a trace, since this is independent of the basis chosen to compute it, as is easily proved by using its cyclic property[3] $\mathrm{tr}\{\hat{D}_1\hat{D}_2...\hat{D}_N\} = \mathrm{tr}\{\hat{D}_2...\hat{D}_N\hat{D}_1\}$, and remembering that two bases are necessarily connected by a unitary transformation (see Appendix A 3 h for more details). Hence, this shows that the operator $\hat{\rho}$ is an important object on its own right, that contains all the information about the state of the *noisy* system. We then call it the *mixed state* of the system. Whenever $\hat{\rho}$ can be written as a rank[4]-1 projector $\hat{\rho} = |\psi\rangle\langle\psi|$, we say that the system is in *pure state* $|\psi\rangle$, and we can apply the formalism introduced in the previous section.

As a specific, instructive case of this type, consider the following situation. We are given a system in some known state $|\psi\rangle$, and we perform a measurement of some observable $\hat{A} = \sum_{j=1}^{d} a_j |a_j\rangle\langle a_j|$ as the initial step of some protocol that might involve some more operations later. Suppose, however, that the display of our measurement apparatus is broken, and doesn't show the outcome, what is known as a *non-selective measurement*. In other words, we know that a measurement took place, but we don't know the resulting outcome. Can we still describe the quantum statistics of the protocol? The answer is yes: even though we don't know the outcome, we know that after the measurement the state would have collapsed into state $|a_j\rangle$ with probability $p_j = |\langle a_j|\psi\rangle|^2$. This corresponds to the ensemble $\{p_j, |a_j\rangle\}_{j=1,...,d}$ or the mixed state $\hat{\rho} = \sum_{j=1}^{d} p_j |a_j\rangle\langle a_j|$. The only difference with the general case exposed above is that in this case the states of the ensemble form an orthonormal set, and hence the mixed state is diagonal in this basis.

Need for mixed states: state of a subsystem. Consider now a composite system such as the one introduced at the end of the previous section, and let it be in an arbitrary mixed state $\hat{\rho}$ acting on the full space $\mathcal{H} = \mathcal{A} \otimes \mathcal{B}$. Suppose that we hand in subsystem $\mathcal{A}$ to Alice, who is then allowed to perform experiments onto it, perhaps not even knowing that it is correlated with subsystem $\mathcal{B}$. The question now is: can Alice describe her experiments by using operators and states defined solely on $\mathcal{A}$? Below we prove that, indeed, all Alice needs to know in order to reproduce the statistics of her experiments is that her subsystem starts in the *reduced state*

$$\hat{\rho}_{\mathcal{A}} = \sum_{l=1}^{d_{\mathcal{B}}} \langle e_l^{\mathcal{B}}|\hat{\rho}|e_l^{\mathcal{B}}\rangle \equiv \mathrm{tr}_{\mathcal{B}}\{\hat{\rho}\}, \tag{19}$$

without having to make any reference to subsystem $\mathcal{B}$. The notation $\mathrm{tr}_{\mathcal{B}}$ means that we perform the trace only within the basis of subspace $\mathcal{B}$, operation known as *partial trace*, which leaves us with an operator acting on subspace $\mathcal{B}$. In more detail, if we expand the state of the full system as

$$\hat{\rho} = \sum_{mm'=1}^{d_{\mathcal{A}}} \sum_{nn'=1}^{d_{\mathcal{B}}} \rho_{mm';nn'} |e_m^{\mathcal{A}}\rangle\langle e_{m'}^{\mathcal{A}}| \otimes |e_n^{\mathcal{B}}\rangle\langle e_{n'}^{\mathcal{B}}|, \tag{20}$$

then, the reduced state (19) can be written as

$$\hat{\rho}_{\mathcal{A}} = \sum_{lnn'=1}^{d_{\mathcal{B}}} \left(\sum_{mm'=1}^{d_{\mathcal{A}}} \rho_{mm';nn'} |e_m^{\mathcal{A}}\rangle\langle e_{m'}^{\mathcal{A}}| \right) \underbrace{\langle e_l^{\mathcal{B}}|e_n^{\mathcal{B}}\rangle}_{\delta_{ln}} \underbrace{\langle e_{n'}^{\mathcal{B}}|e_l^{\mathcal{B}}\rangle}_{\delta_{ln'}} = \sum_{mm'=1}^{d_{\mathcal{A}}} \left(\sum_{l=1}^{d_{\mathcal{B}}} \rho_{mm';ll} \right) |e_m^{\mathcal{A}}\rangle\langle e_{m'}^{\mathcal{A}}|, \tag{21}$$

which is indeed an operator acting on $\mathcal{A}$ alone.

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[3] In finite dimension, the cyclic property of the trace always holds. However, in infinite dimension, the cyclic property (as presented in the main text) only holds when the operator $\hat{D}_1\hat{D}_2...\hat{D}_N$ has finite trace (indeed, one can end up mad trying to compute the trace of $[\hat{q},\hat{p}] = \mathrm{i}\hbar\hat{I}$; is it infinity or zero?). In practical terms, a finite trace is ensured when at least one of the operators is a mixed state $\hat{\rho}$.

[4] The rank of an operator is defined as its number of eigenvalues different than zero.

In order to prove that (19) is the correct 'local' state for Alice, let us compute the expectation value of an arbitrary operator $\hat{A}\otimes\hat{I}$, acting as the identity on subspace $\mathcal{B}$. According to (18), we can write the expectation value as

$$\begin{aligned}\langle\hat{A}\otimes\hat{I}\rangle &= \mathrm{tr}\{\hat{\rho}(\hat{A}\otimes\hat{I})\} = \sum_{j=1}^{d_\mathcal{A}}\sum_{l=1}^{d_\mathcal{B}}\left(\langle e_j^\mathcal{A}|\otimes\langle e_l^\mathcal{B}|\right)\hat{\rho}(\hat{A}\otimes\hat{I})\left(|e_j^\mathcal{A}\rangle\otimes|e_l^\mathcal{B}\rangle\right), \\ &= \sum_{j=1}^{d_\mathcal{A}}\sum_{l=1}^{d_\mathcal{B}}\left(\langle e_j^\mathcal{A}|\otimes\langle e_l^\mathcal{B}|\right)\hat{\rho}\left(\hat{A}|e_j^\mathcal{A}\rangle\otimes|e_l^\mathcal{B}\rangle\right) = \sum_{j=1}^{d_\mathcal{A}}\langle e_j^\mathcal{A}|\underbrace{\left(\sum_{l=1}^{d_\mathcal{B}}\langle e_l^\mathcal{B}|\hat{\rho}|e_l^\mathcal{B}\rangle\right)}_{\hat{\rho}_\mathcal{A}}\hat{A}|e_j^\mathcal{A}\rangle = \mathrm{tr}\{\hat{\rho}_\mathcal{A}\hat{A}\}.\end{aligned} \tag{22}$$

Hence, Alice is able to refer any of her observables $\hat{A}$ acting on $\mathcal{A}$, to expectation values $\langle\hat{A}\rangle = \mathrm{tr}\{\hat{\rho}_\mathcal{A}\hat{A}\}$ in which $\hat{\rho}_\mathcal{A}$ is the state of her subsystem.

Consider now the special case in which the full system is in some pure state $|\psi\rangle$, that is, $\hat{\rho} = |\psi\rangle\langle\psi|$. Referred to some basis $\{|e_j^\mathcal{B}\rangle\}_{j=1,\ldots,d_\mathcal{B}}$ of subsystem $\mathcal{B}$, the state of the full system can always be written in the form

$$|\psi\rangle = \sum_{m=1}^{d_\mathcal{B}}\sqrt{w_m}|\psi_m\rangle\otimes|e_m^\mathcal{B}\rangle, \tag{23}$$

where $\{w_m\}_{m=1,\ldots,d_\mathcal{B}}$ is a probability distribution, and $\{|\psi_m\rangle\}_{m=1,\ldots,d_\mathcal{B}}$ are some states in $\mathcal{A}$ (as above, they do not need to be orthogonal). The reduced state (19) then reads

$$\hat{\rho}_\mathcal{A} = \sum_{lmm=1}^{d_\mathcal{B}}\sqrt{w_m w_{m'}}|\psi_m\rangle\langle\psi_{m'}|\underbrace{\langle e_l^\mathcal{B}|e_m^\mathcal{B}\rangle}_{\delta_{lm}}\underbrace{\langle e_{m'}^\mathcal{B}|e_l^\mathcal{B}\rangle}_{\delta_{lm'}} = \sum_{m=1}^{d_\mathcal{B}} w_m|\psi_m\rangle\langle\psi_m|, \tag{24}$$

which is of the same form as the mixed state we defined in (17) for noisy systems. Hence, even though the state $|\psi\rangle$ of the whole system is pure, in general we need to describe the reduced state of the subsystems by a mixed state.

This situation allows us to discuss an important property of mixed states: their ensemble decomposition is not unique. In particular, note that we could have chosen any other basis of subspace $\mathcal{B}$, for example, a basis $\{|d_k^\mathcal{B}\rangle\}_{k=1,\ldots,d_\mathcal{B}}$, related to the previous basis by a unitary matrix U with elements U_{jl}, that is, $\{|e_m^\mathcal{B}\rangle = \sum_{k=1}^{d_\mathcal{B}}U_{mk}|d_k^\mathcal{B}\rangle\}_{j=1,\ldots,d_\mathcal{B}}$. In terms of this new basis, state (23) is written as

$$|\psi\rangle = \sum_{m=1}^{d_\mathcal{B}}\sqrt{w_m}|\psi_m\rangle\otimes\left(\sum_{k=1}^{d_\mathcal{B}}U_{mk}|d_k^\mathcal{B}\rangle\right) = \sum_{k=1}^{d_\mathcal{B}}\sqrt{v_k}|\phi_k\rangle\otimes|d_k^\mathcal{B}\rangle, \tag{25}$$

where we have defined

$$\sqrt{v_k}|\phi_k\rangle = \sum_{m=1}^{d_\mathcal{B}}U_{mk}\sqrt{w_m}|\psi_m\rangle, \tag{26}$$

where $|\phi_k\rangle\in\mathcal{A}$ are states, and the new probability distribution $\{v_k\}_{k=1,\ldots,d_\mathcal{B}}$ is found by taking the norm square of the last expression:

$$v_k\underbrace{\langle\phi_k|\phi_k\rangle}_{1} = \sum_{mm'=1}^{d_\mathcal{B}}U_{mk}^*U_{m'k}\underbrace{\sqrt{w_m w_{m'}}\langle\psi_m|\psi_{m'}\rangle}_{\text{define it as } S_{mm'}} = (USU^\dagger)_{kk}, \tag{27}$$

and is easily shown to be normalized (note that we use the cyclic property of the trace in the second step)

$$\sum_{k=1}^{d_\mathcal{B}}v_k = \mathrm{tr}\{USU^\dagger\} = \mathrm{tr}\{S\} = \sum_{k=1}^{d_\mathcal{B}}w_k\underbrace{\langle\psi_k|\psi_k\rangle}_{1} = 1. \tag{28}$$

Hence, taking the partial trace with respect to the new basis, the reduced state reads now

$$\hat{\rho}_\mathcal{A} = \sum_{k=1}^{d_\mathcal{B}}v_k|\phi_k\rangle\langle\phi_k|, \tag{29}$$

which is formed from an ensemble $\{v_k, |\phi_k\rangle\}_{k=1,\ldots,d_{\mathcal{B}}}$ different than that of (24).

Informational interpretation and quantification of mixedness. There is a common thread to both the case of a noisy system and a subsystem of a composite system: in both cases, the mixture appears because we are not monitoring some degree of freedom that our system shares correlations with (the noise in the first case, subsystem $\mathcal{B}$ in the second case). In other words, the *mixture* simply *reflects* our *ignorance* about some information of the system that has 'leaked' into another system that we cannot interrogate. This suggests an interpretation of mixedness as lack of information, making the concept more intuitive.

Given this informational interpretation of mixed states, it is fairly natural to ask which is the state that is *maximally mixed*, that is, that has leaked out the maximum amount of information. Let us consider here a Hilbert space $\mathcal{H}$ with finite dimension d (we will consider the infinite dimensional case in the next chapter, when discussing states of the harmonic oscillator). It is easy to argue that the maximally-mixed state in this case corresponds to

$$\hat{\rho}_{\mathrm{MM}} = \frac{\hat{I}}{d}. \tag{30}$$

Indeed, when the state of the system is $\hat{\rho}_{\mathrm{MM}}$ and an arbitrary observable $\hat{A}$ is measured, all its eigenvalues are equally likely to appear as an outcome of the measurement, that is,

$$p_j = \langle a_j|\hat{\rho}_{\mathrm{MM}}|a_j\rangle = \frac{1}{d} \quad \forall j. \qquad \text{(flat distribution)} \tag{31}$$

Hence, this state maximizes the overall uncertainty of the system's observables, as expected for a maximally-mixed state. In other words: with the system in such state, the outcome of any measurement is completely random!

The mixedness of a state $\hat{\rho}$ can be quantified by the *von Neumann entropy*, which is defined as

$$S[\hat{\rho}] = -\mathrm{tr}\{\hat{\rho}\log\hat{\rho}\}. \tag{32}$$

Given the diagonal representation of the state

$$\hat{\rho} = \sum_{j=1}^{d} \lambda_j |r_j\rangle\langle r_j|, \tag{33}$$

where its eigenvectors $\{|r_j\rangle\}_{j=1,2,\ldots,d}$ form an orthonormal basis of the Hilbert space $\mathcal{H}$, the von Neumann entropy reads then (proven from the spectral theorem)

$$S[\hat{\rho}] = -\sum_{j=1}^{d} \lambda_j \log\lambda_j. \tag{34}$$

This is just the Shannon entropy of the distribution $\{\lambda_j\}_{j=1,2,\ldots,d}$, which is one of the most fundamental quantities in classical information theory. You can easily check that the entropy is 0 for a pure state, while it has a maximum $\log d$ for the maximally-mixed state.

It is interesting to note (and easy to prove mathematically [45]) that the entropy does not change by unitary evolution, cannot decrease by non-selective measurements, and cannot increase by selective measurements (indeed, when no degeneracies are present, it collapses to zero, as the state becomes pure). These properties are indeed expected from a purely informational point of view: while evolving unsupervised, the system does not exchange any information with any other system; when we perform a selective measurement indeed we gain information about the system and its post-measurement state; and when the measurement is non-selective, not only we don't gain any information, but it can scramble the information that was contained in the state.

Reformulation of quantum mechanics for mixed states. The previous discussions have served to illustrate how incredibly useful mixed states are when dealing with quantum systems. For this reason, it is important to take a step back, and reformulate the basic laws of quantum mechanics that we saw in the previous section, but with a formalism adapted to mixed states.

Let us start by enunciating that: the state of a general quantum system is completely specified by a *density operator* $\hat{\rho}$ acting on its Hilbert space, that is, a self-adjoint operator ($\hat{\rho} = \hat{\rho}^\dagger$), with non-negative eigenvalues ($\hat{\rho} \geq 0$), and unit trace ($\mathrm{tr}\{\hat{\rho}\} = 1$). Because projectors are positive, self-adjoint operators, density operators always allow for an ensemble decomposition of the type (17), which is not unique as explained above. The condition for two ensemble decompositions $\{w_m, |\psi_m\rangle\}_{m=1,\ldots,M}$ and $\{v_k, |\phi_k\rangle\}_{k=1,\ldots,K}$ to represent the same density operator, is that they are connected by a unitary matrix U (with elements U_{km}) through

$$\sqrt{v_k}|\phi_k\rangle = \sum_{m=1}^{M} U_{km}\sqrt{w_m}|\psi_m\rangle, \tag{35}$$

where if $N \neq M$ we can add $|N - M|$ arbitrary states with zero probability to the ensemble with smaller number of elements, so that U is a square matrix.

The combination of the three properties that define density operators ensure that the diagonal entries of the representation of $\hat{\rho}$ form a probability distribution in any basis. In fact, when measuring an observable with eigenexpansion $\hat{A} = \sum_{j=1}^{d} a_j |a_j\rangle\langle a_j|$, the probability of obtaining outcome a_j is given by

$$p_j = \langle a_j|\hat{\rho}|a_j\rangle = \mathrm{tr}\{\hat{\rho}|a_j\rangle\langle a_j|\}, \tag{36}$$

that is, by the corresponding diagonal element of the state's representation in the observable's eigenbasis. The expectation value of any operator $\hat{A}$ is then given by

$$\langle \hat{A}\rangle = \sum_{j=1}^{d} a_j p_j = \mathrm{tr}\{\hat{\rho}\hat{A}\}. \tag{37}$$

Note that we have written all observable quantities in terms of traces of operators multiplied by the density operator. This is very useful because traces do not depend on the basis, as mentioned above. The property $\mathrm{tr}\{\hat{\rho}|\psi\rangle\langle\phi|\} = \langle\phi|\hat{\rho}|\psi\rangle$ is sometimes useful in this context.

Finally, in the Schrödinger picture, states of unsupervised systems evolve according to

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t) \quad \Leftrightarrow \quad \mathrm{i}\hbar\partial_t\hat{\rho} = [\hat{H}, \hat{\rho}], \tag{38}$$

where $\hat{U}(t)$ is the time-evolution operator defined in (12), and the latter is known as the *von Neumann equation*. Note that (38) is trivial to prove by writing the initial state in some initial ensemble, and letting each state of the ensemble evolve according the Schrödinger-picture expression (13).

These are the laws of quantum mechanics as we will used them throughout the lectures, where we will see that mixed states appear very naturally in many interesting situations.

C. Change of picture and time-dependent Hamiltonians

As we have seen, unsupervised evolution in quantum mechanics admits two alternative, but equivalent descriptions: one in which states evolve (Schrödinger picture) and another where operators evolve (Heisenberg picture). Having these two alternatives is actually quite useful, both from the conceptual and practical points of view. Here, however, we will discuss how these are just two limits of an infinite number of equivalent or *intermediate pictures*, in which both states and operators evolve.

In order to see this, consider a completely general unitary operator $\hat{U}_\mathrm{c}(t)$, which might even be time dependent. The 'c' subindex stands for 'change' (of picture). As we have stressed several times already, in quantum mechanics, all connections to observable phenomena are made through expectation values. On the other hand, starting from the Schrödinger picture, we can rewrite the expectation value of a generic operator $\hat{A}$ at any time as

$$\langle \hat{A}\rangle(t) = \mathrm{tr}\{\hat{\rho}(t)\hat{A}\} = \mathrm{tr}\Big\{\hat{U}_\mathrm{c}^\dagger(t)\hat{\rho}(t)\hat{U}_\mathrm{c}(t)\hat{U}_\mathrm{c}^\dagger(t)\hat{A}\hat{U}_\mathrm{c}(t)\Big\}, \tag{39}$$

where we have used $\hat{U}_c(t)\hat{U}_c^\dagger(t) = \hat{I}$ and the cyclic property of the trace. This is a very suggestive expression that allows us to define new pictures for quantum dynamics as follows. Let's define the state and operator in the new picture as

$$\hat{\rho}_\mathrm{I}(t) = \hat{U}_\mathrm{c}^\dagger(t)\hat{\rho}(t)\hat{U}_\mathrm{c}(t), \tag{40a}$$

$$\hat{A}_\mathrm{I}(t) = \hat{U}_\mathrm{c}^\dagger(t)\hat{A}\hat{U}_\mathrm{c}(t), \tag{40b}$$

where the 'I' subindex stands for 'intermediate' (picture). The interpretation of these operators is very interesting. Recall that $\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t)$, where $\hat{U}(t)$ is the time-evolution operator of the system. We see that the state (40a) in the new picture can be written as $\hat{\rho}_\mathrm{I}(t) = \hat{U}_\mathrm{I}(t)\hat{\rho}(0)\hat{U}_\mathrm{I}^\dagger(t)$, in terms of a unitary $\hat{U}_\mathrm{I}(t) = \hat{U}_\mathrm{c}^\dagger(t)\hat{U}(t)$, which can be interpreted as the time-evolution operator of the state in the new picture (with the subtlety that we might have $\hat{U}_\mathrm{c}(0) \neq \hat{I}$). Moreover, the form of $\hat{U}_\mathrm{I}(t)$ allows us to interpret the new picture in a very intuitive way: we are simply removing some part $\hat{U}_\mathrm{c}(t)$ from the total evolution $\hat{U}(t)$ of the system. And since we are removing it from the state, we add it to the operators, as shown in (40b), in order for expectation values to remain unaffected, that is,

$$\langle \hat{A}\rangle(t) = \mathrm{tr}\{\hat{\rho}_\mathrm{I}(t)\hat{A}_\mathrm{I}(t)\}. \tag{41}$$

As you may imagine, it is very interesting to have a tool like this, that allows us to remove parts of the evolution of the system that we are not interested in, for example because they induce trivial fast dynamics that simply overshadow more subtle slowly-varying phenomena. Note also that taking $\hat{U}_\mathrm{c} = \hat{I}$ we remain in the Schrödinger picture, while taking $\hat{U}_c(t) = \hat{U}(t)$ we move all the way to the Heisenberg picture.

It's interesting to write down the evolution equation of the state in the new intermediate picture. Taking the time derivative of (40a), and denoting the Hamiltonian of the system by $\hat{H}(t)$, where we even allow for some explicit time dependence, so that $\mathrm{i}\hbar\partial_t\hat{\rho} = [\hat{H}(t), \hat{\rho}]$, we easily obtain

$$\mathrm{i}\hbar\partial_t\hat{\rho}_\mathrm{I} = [\hat{H}_\mathrm{I}(t), \hat{\rho}_\mathrm{I}], \quad \text{with } \hat{H}_\mathrm{I}(t) = \hat{U}_\mathrm{c}^\dagger(t)\hat{H}(t)\hat{U}_\mathrm{c}(t) - \mathrm{i}\hbar\hat{U}_\mathrm{c}^\dagger(t)\partial_t\hat{U}_\mathrm{c}(t), \tag{42}$$

where we have used $\partial_t(\hat{U}_\mathrm{c}^\dagger\hat{U}_\mathrm{c}) = 0$, so that $(\partial_t\hat{U}_\mathrm{c}^\dagger)\hat{U}_\mathrm{c} = -\hat{U}_\mathrm{c}^\dagger\partial_t\hat{U}_\mathrm{c}$. Hence, states still evolve according to the von Neumann equation, but with a modified Hamiltonian $\hat{H}_\mathrm{I}(t)$. Note that this Hamiltonian is in general time dependent, even if the original one $\hat{H}$ is not. The case in which we choose $\hat{U}_\mathrm{c}(t) = \exp(\hat{H}_\mathrm{c}t/\mathrm{i}\hbar)$, with $\hat{H}_\mathrm{c}$ an arbitrary Hermitian time-independent operator with energy units, is especially interesting, since in that case the Hamiltonian in the new picture takes the form

$$\hat{H}_\mathrm{I}(t) = \hat{U}_\mathrm{c}^\dagger(t)\hat{H}(t)\hat{U}_\mathrm{c}(t) - \hat{H}_\mathrm{c}. \tag{43}$$

Moreover, in such case, operators evolve according to a Heisenberg equation, $\mathrm{i}\hbar\partial_t\hat{A} = [\hat{A}, \hat{H}_\mathrm{c}]$.

As mentioned, it is clear that Hamiltonians in intermediate pictures are time dependent, even if the original Hamiltonian is not. It is then interesting to consider which form the time-evolution operator takes in such a case. In order to find a compact expression, we will combine the so-called Dyson expansion with the time-ordering symbol. The Dyson expansion is just a formal solution of the von Neumann equation (42), or its equivalent Schrödinger equation $\mathrm{i}\hbar\partial_t|\psi\rangle_\mathrm{I} = \hat{H}_\mathrm{I}(t)|\psi\rangle_\mathrm{I}$. In particular, we are looking for the unitary operator that connects the states at times 0 and t, that is, $|\psi(t)\rangle_\mathrm{I} = \hat{U}_\mathrm{I}(t)|\psi(0)\rangle_\mathrm{I}$. Inserting this expression in the Schrödinger equation, and noting that it should be satisfied for all initial states $|\psi(0)\rangle_\mathrm{I}$, we then see that the time-evolution operator itself satisfies the Schrödinger equation

$$\mathrm{i}\hbar\partial_t\hat{U}_\mathrm{I}(t) = \hat{H}_\mathrm{I}(t)\hat{U}_\mathrm{I}(t), \qquad \text{with } \hat{U}_\mathrm{I}(0) = \hat{I}. \tag{44}$$

The formal integration of this equation reads

$$\hat{U}_\mathrm{I}(t) = \hat{I} + \frac{1}{\mathrm{i}\hbar}\int_0^t dt_1 \hat{H}_\mathrm{I}(t_1)\hat{U}_\mathrm{I}(t_1). \tag{45}$$

Iterating this solution, by plugging it in $\hat{U}_\mathrm{I}(t_1)$ on the right-hand-side, we obtain

$$\hat{U}_\mathrm{I}(t) = \hat{I} + \frac{1}{\mathrm{i}\hbar}\int_0^t dt_1 \hat{H}_\mathrm{I}(t_1) + \frac{1}{(\mathrm{i}\hbar)^2}\int_0^t dt_1 \int_0^{t_1} dt_2 \hat{H}_\mathrm{I}(t_1)\hat{H}_\mathrm{I}(t_2)\hat{U}_\mathrm{I}(t_2). \tag{46}$$

Iterating this process an infinite number of times, we find the formal expression of the time-evolution operator in the form of the following *Dyson series* expansion

$$\hat{U}_\mathrm{I}(t) = \hat{I} + \sum_{n=1}^{\infty}\frac{1}{(\mathrm{i}\hbar)^n}\int_0^t dt_1 \int_0^{t_1} dt_2 ... \int_0^{t_{n-1}} dt_n \hat{H}_\mathrm{I}(t_1)\hat{H}_\mathrm{I}(t_2)...\hat{H}_\mathrm{I}(t_n). \tag{47}$$

This is not a very practical expression, except for perturbation theory, where the series can be truncated to a desired order. However, it can be written in a very compact and useful form by making use of the time-ordering symbol $\mathcal{T}$, which is defined as the operation that reorders products of time-dependent operators in chronological order (from right to left). For example, for a product of two operators, we have

$$\mathcal{T}\left\{\hat{A}(t)\hat{B}(t')\right\} = \begin{cases} \hat{A}(t)\hat{B}(t') & \text{for } t > t' \\ \hat{B}(t')\hat{A}(t) & \text{for } t < t' \end{cases}. \tag{48}$$

The Dyson series can then be written in the simpler form

$$\hat{U}_\mathrm{I}(t) = \mathcal{T}\left\{e^{\int_0^t dt' \hat{H}_\mathrm{I}(t')/\mathrm{i}\hbar}\right\}, \tag{49}$$

which is specially useful if we know the explicit time dependence of the Hamiltonian, so the integral can be carried out, after which the time-ordering symbol is not required anymore. We have an example of this far along the course,

see Eq. (370). Note also that the time-ordering symbol can also be removed if the Hamiltonian commutes with itself at all times, $[\hat{H}_{\rm I}(t), \hat{H}_{\rm I}(t')] = 0 \ \forall (t, t')$.

Let us finally remark that, in the literature, what we have called 'intermediate' pictures are sometimes called 'interaction' pictures. However, we will reserve such name for the specific situation of starting from a Hamiltonian $\hat{H} = \hat{H}_0(t) + \hat{H}_{\rm int}(t)$, in which $\hat{H}_0(t)$ contains the free evolution of two subsystems interacting through $\hat{H}_{\rm int}(t)$, and moving to an intermediate picture defined by $\hat{U}_{\rm c}(t) = \mathcal{T}\left\{e^{\int_0^t dt' \hat{H}_0(t')/{\rm i}\hbar}\right\}$, that is, a picture where free evolution is 'discounted' in the sense described above, and the Hamiltonian in the new picture simply reads as $\hat{H}_{\rm I}(t) = \hat{U}_{\rm c}^\dagger(t) \hat{H}_{\rm int}(t) \hat{U}_{\rm c}(t)$.

II. QUANTIZATION OF THE ELECTROMAGNETIC FIELD AS A COLLECTION OF HARMONIC OSCILLATORS.

The main goal of this chapter is the quantization of the electromagnetic field. We will follow a heuristic, but physically intuitive approach in which, starting from Maxwell equations, the electromagnetic field is put in correspondence with a mechanical model consisting of collection of harmonic oscillators. Given the connection between the electromagnetic field and the harmonic oscillator, we also study in detail here the latter. We first explain how the one-dimensional harmonic oscillator is described in a classical context by a trajectory in phase space. The first step in the quantum description will be finding the Hilbert space by which it is described. We will then introduce a convenient way of representing the quantum state of the oscillator in phase space, the so-called Wigner function, and then put forward a few important states: coherent, squeezed, and thermal states.

A. Light as an electromagnetic wave

Nowadays it feels quite natural to say that *light* is an *electromagnetic wave*. Arriving to this conclusion, however, was not trivial at all. The history of such a discovery starts in the first half of the XIX century with Faraday, who showed that the polarization of light can change when subject to a magnetic field; this was the first hint suggesting that there could be a connection between light and electromagnetism, and he was the first to propose that light could be an electromagnetic disturbance of some kind, able to propagate without the need of a reference medium. However, this qualitative idea did not find a rigorous mathematical formulation until the second half of the century, when Maxwell developed a consistent theory of electromagnetism, and showed how the theory was able to predict the existence of electromagnetic waves propagating at a speed which was in agreement with the speed measured for light at the time [56]. A couple of decades after his proposal, the existence of electromagnetic waves was experimentally demonstrated by Hertz [57], and the theory of light as an electromagnetic wave found its way towards being accepted.

Our starting point are Maxwell's equations formulated as partial differential equations for the *electric* and *magnetic*[5] vector *fields* $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$, respectively, where $\mathbf{r}$ (t) is the position (time) where (when) the fields are observed. This formulation is due to Heaviside [58], as Maxwell originally proposed his theory in terms of *quaternions*. The theory consists of four equations. The first two are called the *homogeneous Maxwell equations* and read

$$\boldsymbol{\nabla}\cdot\mathbf{B}=0 \quad \text{and} \quad \boldsymbol{\nabla}\times\mathbf{E}=-\partial_t\mathbf{B}, \tag{50}$$

where $\boldsymbol{\nabla}=(\partial_x,\partial_y,\partial_z)$. The other two are called the *inhomogeneous Maxwell equations* and are written as

$$\boldsymbol{\nabla}\cdot\mathbf{E}=\rho/\varepsilon_0 \quad \text{and} \quad \boldsymbol{\nabla}\times\mathbf{B}=\mu_0\varepsilon_0\partial_t\mathbf{E}+\mu_0\mathbf{j}, \tag{51}$$

where any electric or magnetic source is introduced in the theory by a *charge density* function $\rho(\mathbf{r},t)$ and a *current distribution* vector $\mathbf{j}(\mathbf{r},t)$, respectively; the parameters $\varepsilon_0=8.8\times10^{-12}$ F/m and $\mu_0=1.3\times10^{-6}$ H/m are the so-called *electric permittivity* and the *magnetic permeability* of vacuum, respectively.

We will show the process of quantization of the electromagnetic field in the absence of sources ($\rho=0$ and $\mathbf{j}=\mathbf{0}$). Under these circumstances, the inhomogeneous equations are simplified to

$$\boldsymbol{\nabla}\cdot\mathbf{E}=0 \quad \text{and} \quad c^2\boldsymbol{\nabla}\times\mathbf{B}=\partial_t\mathbf{E}, \tag{52}$$

where $c=1/\sqrt{\varepsilon_0\mu_0}\simeq3\times10^8$m/s.

The homogeneous equations (50) allow us to derive the fields from a *scalar potential* $\phi(\mathbf{r},t)$ and a *vector potential* $\mathbf{A}(\mathbf{r},t)$ as

$$\mathbf{B}=\boldsymbol{\nabla}\times\mathbf{A} \quad \text{and} \quad \mathbf{E}=-\boldsymbol{\nabla}\phi-\partial_t\mathbf{A}, \tag{53}$$

hence reducing to four the degrees of freedom of the electromagnetic field. These potentials, however, are not unique: we can always use an arbitrary function $\Lambda(\mathbf{r},t)$ to change them as

$$\mathbf{A}\to\mathbf{A}+\boldsymbol{\nabla}\Lambda \quad \text{and} \quad \phi\to\phi-\partial_t\Lambda, \tag{54}$$

what is known as the *gauge invariance* of Maxwell's equations.

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[5] *As we won't deal with materials sensitive to the magnetic field, we will use the term "magnetic field" for the* $\mathbf{B}$*-field, which is usually denoted by "magnetic induction field" when it needs to be distinguished from the* $\mathbf{H}$*-field (which we won't be using in this notes).*

Introducing (53) into the inhomogeneous equations we get the equations satisfied by the potentials

$$\left(c^2\boldsymbol{\nabla}^2 - \partial_t^2\right)\mathbf{A} = \partial_t\boldsymbol{\nabla}\phi + c^2\boldsymbol{\nabla}\left(\boldsymbol{\nabla}\cdot\mathbf{A}\right), \tag{55a}$$

$$\boldsymbol{\nabla}^2\phi + \partial_t\boldsymbol{\nabla}\cdot\mathbf{A} = 0. \tag{55b}$$

The problem is highly simplified if we exploit the gauge invariance and choose $\boldsymbol{\nabla}\cdot\mathbf{A} = 0$, as the second equation becomes the Laplace equation, which can be shown to further imply that $\phi = 0$ for physical fields vanishing at infinity. Hence the only equations left are

$$\left(c^2\boldsymbol{\nabla}^2 - \partial_t^2\right)\mathbf{A} = \mathbf{0} \tag{56}$$

which are wave equations with speed c for the components of the vector potential. Note that the condition $\boldsymbol{\nabla}\cdot\mathbf{A} = 0$ (known as the *Coulomb condition*) relates the three components of $\mathbf{A}$, and hence, only two degrees of freedom of the initial six (the electric and magnetic vector fields) remain.

It is finally important to note that the wave equation (56) has a unique solution inside a given spatio-temporal region only if both the vector potential and its derivative along the direction normal to the boundary of the region are specified at any point of the boundary [59]; these are known as *Dirichlet* and *Neumann* conditions, respectively. In general, however, physical problems do not impose so many constraints, and hence there coexist several solutions of the wave equation, which we will call *spatiotemporal modes*.

B. Quasi-1D approximation and quantization inside a cavity

In order to simplify the derivations and get to the core of the physical problem without many spurious technicalities, we will consider a simplified one-dimensional model for the light field[6]. In particular, we assume that the field propagates along the z direction, with neither its polarization nor its transverse profile along the x and y directions changing upon propagation. Moreover, we take the transverse profile as homogeneous, that is, independent of x and y, and a linear polarization along the x axis. Under such conditions, the vector potential can be expanded in terms of linearly polarized plane waves $\mathbf{e}_x e^{\mathrm{i}kz}$ with $k \in \mathbb{R}$ and $\mathbf{e}_x$ the unit vector along the x direction. Hence, we can generally write

$$\mathbf{A}(z,t) = \mathcal{N}\mathbf{e}_x \sum_k q_k(t) e^{\mathrm{i}kz}, \tag{57}$$

where from now on we omit the dependence on x and y in the argument of the fields, $\mathcal{N}$ is an appropriate normalization factor that we will choose later, q_k are the expansion coefficients, and the sum runs over all the allowed wave vectors, which are all the real numbers in free space, but get restricted whenever the boundary conditions are not open. Specifically, let us consider a simple cavity consisting on two perfectly conducting plane mirrors facing each other, see Fig. 1. The components of the electric field parallel to the conducting mirrors must vanish [59, 61]. Taking $z = 0$ at the mirror on the left, and $z = L$ at the mirror on the right, and focusing on a pair of $\pm k$ components, the $z = 0$ boundary conditions imply

$$\mathbf{E}(0,t) = -\partial_t\mathbf{A}(0,t) = 0 \Rightarrow \dot{q}_k(t) = -\dot{q}_{-k}(t) \Rightarrow q_k(t) = b - q_{-k}(t),$$

where furthermore $q_k(t) \in \mathbb{R}$ and $b = 0$, because otherwise $\mathbf{A}(z,t)$ is not real in all spacetime. On the other hand, the boundary conditions at $z = L$ imply

$$\mathbf{E}(L,t) = -\partial_t\mathbf{A}(L,t) = 0 \Rightarrow \dot{q}_k(t)\sin(kL) = 0 \Rightarrow kL = n\pi, \text{with } n \in \mathbb{N}.$$

Putting everything together, we obtain the relation $q_k(t) = -q_{-k}(t) \in \mathbb{R}$ between the expansion coefficients, and $k = \pi n/L \equiv k_n$ with $n \in \mathbb{N}$ as the only allowed wave vectors. The vector potential, and the electric and magnetic

[6] Quantization in three dimensions and in a realistic cavity with spherical dielectric mirrors can be found in [60].

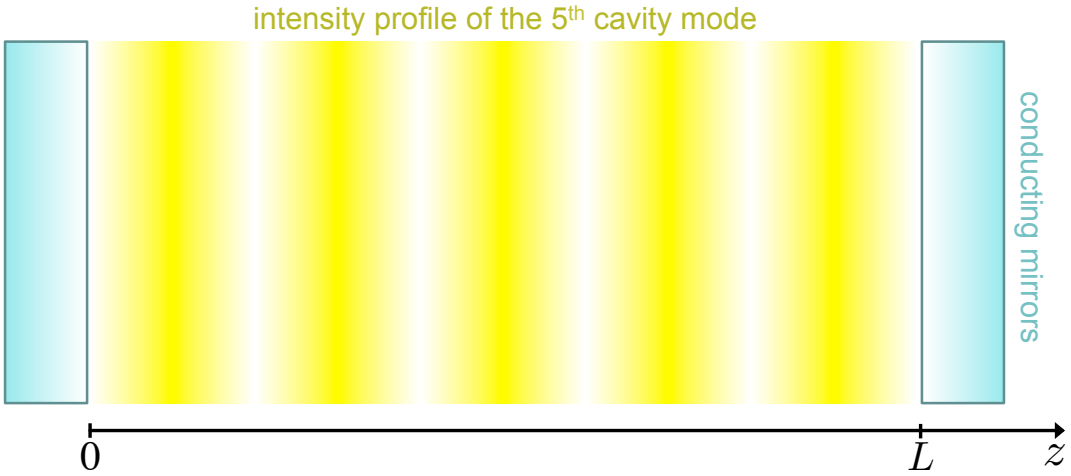

Figure 1. Simplified cavity used in the notes. It is formed by two perfectly conducting plane mirrors facing each other. We neglect variations in polarization or transverse (x,y) profile, while the vanishing of the electric field at the mirror's surface provides the cavity mode structure. We show the intensity pattern corresponding to the 5^{th} mode, proportional to $\sin^2 5\pi z/L$.

fields are then written as

$$\mathbf{A}(z,t) = \mathcal{N}\mathbf{e}_x \sum_{n=1}^{\infty} q_n(t) \sin(k_n z)\,, \tag{58a}$$

$$\mathbf{E}(z,t) = -\partial_t \mathbf{A}(z,t) = -\mathcal{N}\mathbf{e}_x \sum_{n=1}^{\infty} \dot{q}_n(t) \sin(k_n z)\,, \tag{58b}$$

$$\mathbf{B}(z,t) = \boldsymbol{\nabla} \times \mathbf{A}(z,t) = \mathcal{N}\mathbf{e}_y \sum_{n=1}^{\infty} k_n q_n(t) \cos(k_n z)\,, \tag{58c}$$

so that the electric field vanishes at $z = 0$ and $z = L$ as required. Note that we have changed the notation slightly from q_k to q_n, since the wave vectors are specified by the integer n. Also, note that we have introduced an irrelevant factor 2i into $\mathcal{N}$, since it is an arbitrary normalization factor that we will conveniently choose later.

It is interesting to note that the choices $q_k(t) = -q_{-k}(t)$ and $k = \pi n/L$ can be understood from a different point of view, more general than the boundary conditions imposed by the conducting mirrors. The choice for the amplitudes $q_{\pm k}$ simply reflects the fact that inside a cavity there is no reason why we should distinguish left moving and right moving waves, as they cannot be excited separately (if we excite one, the other will appear by reflection in the mirror, picking up a π phase). On the other hand, the quantization of the wave number appears from the natural requirement that a cavity mode has to reproduce itself after a cavity roundtrip, so that the phase accumulated after a roundtrip, $2kL$, must be an integer multiple of 2π.

At this point it is important to highlight the following orthogonality relations between the cavity mode functions

$$\int_0^L dz \sin(k_n z)\sin(k_m z) = \int_0^L dz \cos(k_n z)\cos(k_m z) = \frac{L}{2}\delta_{nm}. \tag{59}$$

Introducing (58a) in the wave equation and acting with $\int_0^L dz \sin(k_n z)$ from the left, we get

$$\int_0^L dz \sin(k_n z)\left(c^2\partial_z^2 - \partial_t^2\right)\mathbf{A} = -\mathcal{N}\mathbf{e}_x \sum_{m=1}^{\infty} \int_0^L dz \sin(k_n z)\sin(k_m z)\left(k_m^2 c^2 q_m(t) + \ddot{q}_m(t)\right) = \mathbf{0}, \tag{60}$$

which using the previous orthogonality relations leads us the following evolution equations for the amplitudes $q_n(t)$:

$$\ddot{q}_n + \omega_n^2 q_n = 0, \tag{61}$$

with $\omega_n = ck_n$. This is precisely the evolution equation for a harmonic oscillator of frequency ω_n. Hence, this suggests that the modes of the electromagnetic field behave as harmonic oscillators, so that field quantization can be carried out simply by quantizing each of these oscillators.

In order to prove that this is indeed the case, we need to prove that the Hamiltonian of the electromagnetic field can be written as the corresponding sum of harmonic oscillator Hamiltonians. In order to show that this is indeed the case, let us next evaluate the electromagnetic energy contained in the cavity at time t, which reads [59, 61]

$$E_{\rm em}(t) = \frac{1}{2}\int_{\rm cavity} d^3\mathbf{r}\left[\varepsilon_0 \mathbf{E}^2(z,t) + \frac{1}{\mu_0}\mathbf{B}^2(z,t)\right]. \tag{62}$$

Introducing the expansions (58) in this expression, and using the orthogonality relations (59), we obtain

$$\begin{aligned} E_{\rm em}(t) &= \frac{\mathcal{N}^2}{2}\int_{\rm cavity} dxdy \sum_{n,m=1}^{\infty}\left[\varepsilon_0 \dot{q}_n(t)\dot{q}_m(t)\int_0^L dz \sin(k_n z)\sin(k_m z) + \frac{k_n k_m}{\mu_0} q_n(t) q_m(t)\int_0^L dz \cos(k_n z)\cos(k_m z)\right] \\ &= \frac{\mathcal{N}^2 \varepsilon_0 L}{4}\int_{\rm cavity} dxdy \sum_{n=1}^{\infty}\left[\dot{q}_n^2(t) + c^2 k_n^2 q_n^2(t)\right]. \end{aligned} \tag{63}$$

Let us now assume that the transverse integral contributes with a finite area $\int_{\rm cavity} dxdy = S$ (as would happen in a physical scenario where the electromagnetic field is confined also laterally). Choosing a normalization constant $\mathcal{N} = \sqrt{2/\varepsilon_0 L S}$, and defining $p_n = \dot{q}_n$, we get

$$E_{\rm em}(t) = \sum_{n=1}^{\infty}\left[\frac{1}{2}p_n^2(t) + \frac{\omega_n^2}{2}q_n^2(t)\right], \tag{64}$$

which is precisely the Hamiltonian of a collection of unit-mass harmonic oscillators with positions q_n, momenta p_n, and frequencies ω_n.

Since we have managed to make a correspondence between a classical model described by a set of generalized positions and momenta, and the electromagnetic field, we can quantize the latter by following the quantization prescription that we learned in Section I A. In particular, we just need to replace positions and momenta with self-adjoint operators $\hat{q}_n$ and $\hat{p}_n$ satisfying canonical commutation relations $[\hat{q}_n, \hat{p}_m] = \mathrm{i}\hbar\delta_{nm}$ and $[\hat{q}_n, \hat{q}_m] = 0 = [\hat{p}_n, \hat{p}_m]$.

Let us finally remark that, while we have presented the highly idealized and simplified situation of a perfect optical cavity within the quasi 1-D approximation, quantization in more realistic settings proceeds in a similar way. In particular, it's always a matter of finding the normal modes of Maxwell's equations and mapping them to a collection of harmonic oscillators, which can be technically challenging, but is conceptually the same we have done. Moreover, even in the context of general quantum field theory one proceeds exactly in the same fashion, just with a few important subtleties. For example, when dealing with fields with half-integer spin (fermions), canonical *anticommutation* relations must be used in order to obtain a bounded Hamiltonian (spin-statistics theorem). Also, at high energies, one needs to use a formalism that explicitly shows Lorentz invariance, in order to make sure that the theory is free of incompatibilities with special relativity. While Maxwell equations are indeed Lorentz invariant, the Coulomb-gauge condition $\boldsymbol{\nabla}\cdot\mathbf{A} = 0$ is not, which is fine for our low-energy (optical) purposes, but would not hold in higher-energy contexts. If you are interested on the quantization of the electromagnetic field in a relativistic setting and/or in the presence of matter, [2] is a good place to start.

C. Classical analysis of the harmonic oscillator

We thus see that there exists a direct relation between the electromagnetic field and the one-dimensional harmonic oscillator. Let us then discuss along the next sections the physics of the latter. We start here by its classical description (remember that Section A 1 offers a review of the required classical mechanics).

Consider the basic mechanical model of a *one-dimensional harmonic oscillator*: A particle of mass m is at rest at some equilibrium position which we take as $x = 0$; when displaced from this position by some amount a, a restoring force $F = -kx$ starts acting on the particle, trying to bring it back to $x = 0$. Newton's equation of motion for the particle is therefore $m\ddot{x} = -kx$, which together with the initial conditions $x(0) = a$ and $\dot{x}(0) = v$ gives the solution $x(t) = a\cos\omega t + (v/\omega)\sin\omega t$, being $\omega = \sqrt{k/m}$ the so-called *angular frequency*. Therefore the particle will be bouncing back and forth between positions $-\sqrt{a^2 + v^2/\omega^2}$ and $\sqrt{a^2 + v^2/\omega^2}$ with time period $2\pi/\omega$ (hence the name 'harmonic oscillator').

Let us study now the problem from a Hamiltonian point of view. For this one-dimensional problem with no constraints, we can take the position of the particle and its momentum as the generalized coordinate and momentum,

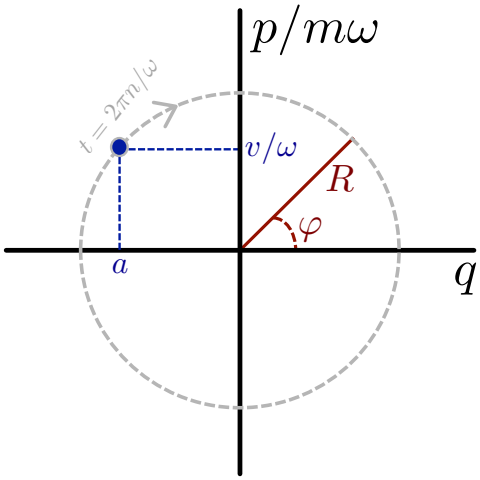

Figure 2. Phase space trajectory of the classical harmonic oscillator. It starts at a point $(a, v/\omega)$ and describes a circular trajectory of radius R coming back to this initial point at times t_n. Defining the amplitude and phase of the oscillator, the motion is described by a fixed amplitude and a phase φ which decreases linearly with time, as explained in the main text.

that is, $q = x$ and $p = m\dot{x}$. The restoring force derives from a potential $V(x) = kx^2/2$, and hence the Hamiltonian takes the form

$$H_{\mathrm{o}} = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2. \tag{65}$$

The canonical equations read

$$\dot{q} = \frac{p}{m} \qquad \text{and} \qquad \dot{p} = -m\omega^2 q, \tag{66}$$

which together with some initial conditions $q(0) = a$ and $p(0) = mv$ give the trajectory

$$\left(q, \frac{p}{m\omega}\right) = \left(a\cos\omega t + \frac{v}{\omega}\sin\omega t, \frac{v}{\omega}\cos\omega t - a\sin\omega t\right), \tag{67}$$

where we normalize the momentum to $m\omega$ for convenience. Starting at the phase space point $(a, v/\omega)$ the system evolves periodically drawing a circle of radius $R = \sqrt{a^2 + v^2/\omega^2}$ as shown in Fig. 2, returning to its initial point at times $t_n = 2\pi n/\omega$, with $n \in \mathbb{N}$. This circular trajectory could have been derived without even solving the equations of motion, as the conservation of the Hamiltonian $H_{\mathrm{o}}(t) = H_{\mathrm{o}}(0)$ leads directly to $q^2 + p^2/m^2\omega^2 = R^2$, which is exactly the circumference of Fig. 2. This is a simple manifestation of the power of the Hamiltonian formalism. The trajectory is most easily represented by defining the so-called *normal* variable $\nu(t) = q(t) + \mathrm{i}p(t)/m\omega = R\exp[\mathrm{i}\varphi(t)]$, which in this case has a constant amplitude $|\nu|$ and a phase that decreases linearly with time, $\varphi(t) = \varphi(0) - \omega t$.

D. The quantum harmonic oscillator: number states, energy quantization, and quadrature eigenstates

The harmonic oscillator is the prototype of a system described quantum mechanically by an infinite-dimensional Hilbert space. In order to see this, we just find the eigenstates of its Hamiltonian, which is given by the operator

$$\hat{H}_{\mathrm{o}} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2, \tag{68}$$

by virtue of the discussion after Principle III in Section A, with the *position* $\hat{q}$ and *momentum* $\hat{p}$ satisfying the commutation relation

$$[\hat{q}, \hat{p}] = \mathrm{i}\hbar. \tag{69}$$

We will always work with dimensionless versions of them, the so-called X and P *quadratures* (although we may keep using the names 'position' and 'momentum' most of the time)

$$\hat{X} = \hat{q}/q_{\mathrm{zpf}} \qquad \text{and} \qquad \hat{P} = \hat{p}/p_{\mathrm{zpf}}, \tag{70}$$

with $q_{\rm zpf} = \sqrt{\hbar/2\omega m}$ and $p_{\rm zpf} = \sqrt{\hbar\omega m/2}$, which satisfy the commutation relation

$$[\hat{X}, \hat{P}] = 2\mathrm{i}, \tag{71}$$

and therefore the uncertainty relation

$$\Delta X \Delta P \geq 1. \tag{72}$$

We will see later that $q_{\rm zpf}$ and $p_{\rm zpf}$ provide the uncertainty of position and momentum when the oscillator is in its ground state, the so-called *zero-point fluctuations*. In terms of these quadratures, the Hamiltonian reads

$$\hat{H}_{\rm o} = \frac{\hbar\omega}{4}\left(\hat{X}^2 + \hat{P}^2\right). \tag{73}$$

In order to find the eigensystem of this operator, we decompose the quadratures as

$$\hat{X} = \hat{a}^\dagger + \hat{a} \qquad \text{and} \qquad \hat{P} = \mathrm{i}(\hat{a}^\dagger - \hat{a}), \tag{74}$$

where the operators $\hat{a}$ and $\hat{a}^\dagger$, known as the *annihilation* and *creation operators*, satisfy the commutation relation

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{75}$$

In terms of these operators, the Hamiltonian is rewritten as

$$\hat{H}_{\rm o} = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2), \tag{76}$$

and hence the problem has been reduced to finding the eigensystem of the so-called *number operator* $\hat{N} = \hat{a}^\dagger\hat{a}$.

Let us denote by n a generic real number contained in the spectrum of $\hat{N}$, whose corresponding eigenvector we denote by $|n\rangle$, so that, $\hat{N}|n\rangle = n|n\rangle$. The eigensystem of $\hat{N}$ is readily found from the following four properties:

- $\hat{N}$ is a positive semidefinite operator, as for any vector $|\psi\rangle$ it is satisfied $\langle\psi|\hat{N}|\psi\rangle = |\hat{a}|\psi\rangle|^2 \geq 0$. When applied to its eigenvectors, $|\psi\rangle = |n\rangle$, this property forbids the existence of negative eigenvalues, that is,

$$n \geq 0. \tag{77}$$

- Applying the commutation relation[7] $[\hat{N}, \hat{a}] = -\hat{a}$ to $|n\rangle$, it is straightforward to show that the vector $\hat{a}|n\rangle$ is also an eigenvector of $\hat{N}$ with eigenvalue $n-1$. Similarly, from the commutation relation $[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$ it is found that the vector $\hat{a}^\dagger|n\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue $n+1$.
  Hence, we have $\hat{a}|n\rangle = k_1|n-1\rangle$ and $\hat{a}^\dagger|n\rangle = k_2|n+1\rangle$, with some constants k_1 and k_2 that can be found as follows. We just calculate the absolute value squared of these expressions, obtaining

$$|k_1|^2\langle n-1|n-1\rangle = \langle n|\hat{a}^\dagger\hat{a}|n\rangle = n\langle n|n\rangle, \tag{78a}$$

$$|k_2|^2\langle n+1|n+1\rangle = \langle n|\underbrace{\hat{a}\hat{a}^\dagger}_{\hat{a}^\dagger\hat{a}+1}|n\rangle = (n+1)\langle n|n\rangle. \tag{78b}$$

  Assuming that the eigenvectors can be normalized (which is another of the properties that we introduce next), and taking the constants positive for definiteness, we then obtain $k_1 = \sqrt{n}$ and $k_2 = \sqrt{n+1}$, and finally

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \qquad \text{and} \qquad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{79}$$

- The identities $\langle n|\hat{N}|m\rangle = n\langle n|m\rangle = m\langle n|m\rangle$, allow us to write $(n-m)\langle n|m\rangle = 0$, hence showing that eigenvectors corresponding to different eigenvalues are arthogonal, that is,

$$\langle n|m\rangle = 0 \quad \text{when } n \neq m. \tag{80}$$

- We will show later that the eigenstate with $n = 0$ is normalizable, and hence, so are all the other eigenvectors with $n \in \mathbb{N}$ by virtue of (79).

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[7] This is straightforward to find by using the property $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$, valid for any three operators $\hat{A}$, $\hat{B}$, and $\hat{C}$.

These four properties are compatible only with a spectrum formed by non-negative integers $n = 0, 1, 2, 3, ...$; otherwise (79) would allow us to find negative eigenvalues, which are not allowed by the first property. Note that (79) ensures that $\hat{a}|0\rangle = 0$. Thus, the set of eigenvectors $\{|n\rangle\}_{n=0,1,...}$ is an infinite, countable set of orthonormal eigenvectors, that is, $\langle n|m\rangle = \delta_{nm}$. Finally, according to the principles of quantum mechanics only the vectors normalized to one are physically accessible states, and hence we conclude that the vector space spanned by the eigenvectors of $\hat{N}$ is an infinite-dimensional Hilbert space (it is isomorphic to $l^2(\infty)$, the prototype of infinite-dimensional Hilbert space, see Section A 2 c). The orthonormal basis $\{|n\rangle\}_{n=0,1,...}$ is known as *Fock basis*.

Let us now explain some physical consequences. The vectors $\{|n\rangle\}_{n=0,1,...}$ are eigenvectors of the energy (the Hamiltonian) with eigenvalues $\{E_n = \hbar\omega(n + 1/2)\}_{n=0,1,...}$, and hence quantum theory predicts that the energy of the oscillator is quantized: Only a discrete set of energies separated by $\hbar\omega$ can be measured in an experiment. The number of *quanta* or *excitations* is given by n, and that's why $\hat{n}$ is called the 'number' operator, as it 'counts' the number of excitations. Similarly, the creation and annihilation operators receive their names because they add and subtract excitations. As these vectors have a well defined number of excitations, $\Delta N = 0$, we will call them *number states*. Consequently, $|0\rangle$ will be called the *vacuum state* of the oscillator, as it has no quanta.

On the other hand, while in classical mechanics the harmonic oscillator can have zero energy (what happens when it is resting in its equilibrium position), quantum mechanics predicts that the minimum energy that the oscillator can have is $E_0 = \hbar\omega/2 > 0$. One way to understand where this *zero–point* energy comes from is by minimizing the expectation value of the Hamiltonian, which can be written as

$$\langle \hat{H}_{\rm o}\rangle = \frac{\hbar\omega}{4}\left(\Delta X^2 + \Delta P^2 + \langle \hat{X}\rangle^2 + \langle \hat{P}\rangle^2\right), \tag{81}$$

subject to the constraint $\Delta X \Delta P \geq 1$ imposed by the uncertainty principle. It is easy to argue that the minimum value of $\langle \hat{H}_{\rm o}\rangle$ is obtained for the state satisfying $\Delta X = \Delta P = 1$ and $\langle \hat{X}\rangle = \langle \hat{P}\rangle = 0$, which corresponds, not surprisingly, to the vacuum state $|0\rangle$. Hence, the energy present in the ground state of the oscillator comes from the fact that the uncertainty principle does not allow its position and momentum to be exactly zero, they have some fluctuations even in the vacuum state, and this *vacuum* or *zero-point fluctuations* contribute to the energy of the oscillator. Indeed, since the quadrature fluctuations are equal to 1 with our normalization of position and momentum, see (70), this means that $q_{\rm zpf} = \sqrt{\hbar/2\omega m}$ and $p_{\rm zpf} = \sqrt{\hbar\omega m/2}$ are the real position and momentum zero-point fluctuations for the particular oscillator we work with.

In contrast to the number operator, which has a discrete spectrum, the quadrature operators possess a pure continuous spectrum. Let us focus on the $\hat{X}$ operator, whose eigenvectors we denote by $\{|x\rangle\}_{x\in\mathbb{R}}$ with corresponding eigenvalues $\{x\}_{x\in\mathbb{R}}$, that is,

$$\hat{X}|x\rangle = x|x\rangle. \tag{82}$$

In order to prove that $\hat{X}$ has a pure continuous spectrum, just note that, from the relation

$$e^{\frac{\rm i}{2}y\hat{P}}\hat{X}e^{-\frac{\rm i}{2}y\hat{P}} = \hat{X} + y, \tag{83}$$

which is easily found via the Baker-Campbell-Haussdorf lemma[8], it follows that if $|x\rangle$ is an eigenvector of $\hat{X}$ with x eigenvalue, then the vector $\exp(-{\rm i}y\hat{P}/2)|x\rangle$ is also an eigenvector of $\hat{X}$ with eigenvalue $x + y$. Now, as this holds for any real y, we conclude that the spectrum of $\hat{X}$ is the whole real line. Moreover, as a self-adjoint operator, one can use its eigenvectors as a continuous basis of the Hilbert space of the oscillator by using the Dirac normalization $\langle x|y\rangle = \delta(x - y)$. The same results can be obtained for the $\hat{P}$ operator, whose eigenvectors we denote[9] by $\{|p\rangle\}_{p\in\mathbb{R}}$ with corresponding eigenvalues $\{p\}_{p\in\mathbb{R}}$, that is,

$$\hat{P}|p\rangle = p|p\rangle. \tag{85}$$

Note that this results rely only on the canonical commutation relations, and hence are completely general, valid for any system, not only for the harmonic oscillator. Note also that not being vectors contained in the Hilbert space of the oscillator (they cannot be properly normalized), the position and momentum eigenvectors cannot correspond to

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[8] This lemma reads

$$e^{\hat{B}}\hat{A}e^{-\hat{B}} = \sum_{n=0}^{\infty}\frac{1}{n!}[\underbrace{\hat{B},[\hat{B},...[\hat{B}}_{n},\underbrace{\hat{A}]...]}_{n}], \tag{84}$$

and is valid for two general operators $\hat{A}$ and $\hat{B}$.

[9] Truth is that it doesn't look very smart to differentiate eigenstates of different operators ($\hat{N}$, $\hat{X}$, $\hat{P}$,...) just by the label (n, x, p,...), but it will always be clear which state we are referring to from the context.

physical states. Nevertheless, we will see that they can be understood as an unphysical limit of some physical states (the squeezed states).

Let us now prove that the vacuum state can be normalized. We will proceed by constructing explicitly its representation in the position eigenbasis (*wave function*). Let us first prove that there exists a Fourier transform relation between the position and momentum bases, that is,

$$|p\rangle = \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{4\pi}} \exp\left(\frac{\mathrm{i}}{2}px\right)|x\rangle \qquad \Longleftrightarrow \qquad |x\rangle = \int_{-\infty}^{+\infty} \frac{dp}{\sqrt{4\pi}} \exp\left(-\frac{\mathrm{i}}{2}px\right)|p\rangle. \tag{86}$$

To this aim we now prove that

$$\langle x|p\rangle = \frac{1}{\sqrt{4\pi}} \exp(\mathrm{i}xp/2). \tag{87}$$

First note that the commutator $[\hat{X}, \hat{P}] = 2\mathrm{i}$ implies that

$$\langle x|\hat{P}|x'\rangle = \frac{2\mathrm{i}\delta\left(x - x'\right)}{x - x'}, \tag{88}$$

and hence

$$\begin{aligned} \langle x|\hat{P}|\psi\rangle &= \int_{\mathbb{R}} dx' \langle x|\hat{P}|x'\rangle\langle x'|\psi\rangle = \int_{\mathbb{R}} dx' \frac{2\mathrm{i}\delta(x - x')}{x - x'}\langle x'|\psi\rangle \\ &= \int_{\mathbb{R}} dx' \frac{2\mathrm{i}\delta\left(x - x'\right)}{x - x'}\left[\langle x|\psi\rangle + (x' - x)\frac{d\langle x|\psi\rangle}{dx} + \sum_{n=2}^{\infty} \frac{(x' - x)^n}{n!}\frac{d^n\langle x|\psi\rangle}{dx^n}\right]. \end{aligned} \tag{89}$$

The order zero of the Taylor expansion is zero because the kernel is antisymmetric around x, while the terms of order two or above give zero as well after integrating them. This means that

$$\langle x|\hat{P}|\psi\rangle = -2\mathrm{i}\frac{d\langle x|\psi\rangle}{dx}, \tag{90}$$

which applied to $|\psi\rangle = |p\rangle$ yields the differential equation

$$p\langle x|p\rangle = -2\mathrm{i}\frac{d\langle x|p\rangle}{dx}, \tag{91}$$

with solution $\langle x|p\rangle = C\exp(\mathrm{i}xp/2)$. We find the normalization constant C by demanding the states to satisfy the Dirac-delta normalization[10]:

$$\langle x|x'\rangle = \int_{\mathbb{R}} dp\langle x|p\rangle\langle p|x'\rangle = |C|^2 \int_{\mathbb{R}} dp e^{\mathrm{i}(x-x')p/2} = 4\pi|C|^2\delta(x - x') \Rightarrow C = 1/\sqrt{4\pi},$$

which leads to (87).

As an example of the use of these continuous representations, we now find the position representation of the number states, which we write as

$$|n\rangle = \int_{\mathbb{R}} dx\psi_n(x)|x\rangle. \tag{93}$$

As a first step we find the projection of vacuum onto a position eigenstate, the so-called *ground state wave function* $\psi_0(x) = \langle x|0\rangle$. We do it from

$$0 = \langle x|\hat{a}|0\rangle = \frac{1}{2}\langle x|(\hat{X} + \mathrm{i}\hat{P})|0\rangle = \frac{1}{2}\left(x + 2\frac{d}{dx}\right)\psi_0(x), \tag{94}$$

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[10] When working with quadratures, the following form of the Dirac delta is useful:

$$\delta(x) = \int_{\mathbb{R}} \frac{dz}{2\pi} e^{\mathrm{i}zx} = \int_{\mathbb{R}} \frac{dp}{4\pi} e^{\mathrm{i}px/2}. \tag{92}$$

where we have used (90), which is a simple differential equation for $\psi_0(x)$ having

$$\psi_0(x) = \frac{1}{(2\pi)^{1/4}} e^{-x^2/4}, \tag{95}$$

as its solution. The factor $(2\pi)^{-1/4}$ is found by imposing the normalization

$$\langle 0|0\rangle = \langle 0| \underbrace{\int_{\mathbb{R}} dx |x\rangle\langle x|}_{\hat{I}} |0\rangle = \int_{\mathbb{R}} dx |\psi_0(x)|^2 = 1, \tag{96}$$

which proves that the vacuum state is normalizable.

Let us also write explicit wave functions for an arbitrary number state $|n\rangle$ (the n^{th} *excited wave function*). This is found from the ground state wave function as

$$\psi_n(x) = \langle x|n\rangle = \frac{1}{\sqrt{n!}}\langle x|\hat{a}^{\dagger n}|0\rangle = \frac{1}{\sqrt{n!}2^n}\langle x|\left(\hat{X} - \mathrm{i}\hat{P}\right)^n|0\rangle = \frac{1}{\sqrt{n!}2^n}\left(x - 2\frac{d}{dx}\right)^n \psi_0(x), \tag{97}$$

which, reminding the Rodrigues formula for the Hermite polynomials

$$H_n\left(\frac{x}{\sqrt{2}}\right) = 2^{-n/2} e^{x^2/4}\left(x - 2\frac{d}{dx}\right)^n e^{-x^2/4}, \tag{98}$$

leads to the simple expression

$$\psi_n(x) = \frac{1}{\sqrt{2^{n+1/2}\pi^{1/2} n!}} H_n\left(\frac{x}{\sqrt{2}}\right) e^{-x^2/4}. \tag{99}$$

E. Visualizing quantum states in phase space: The Wigner function

As the position and momentum do not have common eigenstates, and moreover, their eigenvectors cannot correspond to physical states of the oscillator, one concludes that these observables cannot take definite values in quantum mechanics. Given the state $\hat{\rho}$, the best one can offer are *probability density functions* that will dictate the statistics of a measurement of these observables, that is, $\langle x|\hat{\rho}|x\rangle$ and $\langle p|\hat{\rho}|p\rangle$. In other words, quantum mechanically, well defined trajectories in phase space do not exist: the position and momentum of the oscillator are always affected by some (*quantum*) *noise*.

The following question arises naturally: is it then possible to describe quantum mechanics as a probability distribution in phase space which simply blurs classical trajectories? As we are about to see, the answer is only partially positive, as quantum noise is much more subtle than common classical noise.

Let us denote such probability distribution by $W_\rho(\mathbf{r})$, where we combine all phase-space variables into the vector $\mathbf{r} = (x, p)^T$ and the subindex indicates the quantum state $\hat{\rho}$ it corresponds to. A logical way of building this distribution is as that having the position and momentum probability density functions as its marginals, that is,

$$\langle x|\hat{\rho}|x\rangle = \int_{\mathbb{R}} dp W_\rho(\mathbf{r}) \qquad \text{and} \qquad \langle p|\hat{\rho}|p\rangle = \int_{\mathbb{R}} dx W_\rho(\mathbf{r}). \tag{100}$$

It's possible to show that these conditions uniquely define $W_\rho(\mathbf{r})$, which receives the name of *Wigner function*.

Before presenting it, let us combine the quadrature operators in the vector $\hat{\mathbf{R}} = (\hat{X}, \hat{P})^T$, so that the canonical commutation relations can be combined into the single expression

$$[\hat{R}_m, \hat{R}_n] = 2\mathrm{i}\Omega_{mn}, \quad \text{where } \Omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

is the so-called *symplectic form*, which satisfies $\Omega^T = -\Omega = \Omega^{-1}$. It is also convenient to define the so-called *displacement operator*

$$\hat{D}(\mathbf{r}) = \exp\left[\frac{\mathrm{i}}{2}\hat{\mathbf{R}}^T\Omega\mathbf{r}\right] = \exp\left[\frac{\mathrm{i}}{2}(p\hat{X} - x\hat{P})\right], \tag{101}$$

of which we will learn a lot more later, and its expectation value

$$\chi_\rho(\mathbf{s}) = \mathrm{tr}\{\hat{\rho}\hat{D}(\mathbf{s})\} = \langle \hat{D}(\mathbf{s})\rangle. \tag{102}$$

which is known as *quantum characteristic function*. Consider then the distribution defined as the Fourier transform of the characteristic function

$$W_\rho(\mathbf{r}) = \int_{\mathbb{R}^2} \frac{d^2\mathbf{s}}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{s}}\chi_\rho(\mathbf{s}), \tag{103}$$

which is dubbed the *Wigner function* of state $\hat{\rho}$. In the next section we prove that this distribution satisfies the following properties:

1. It has the right marginals, as defined by (100).
2. It is real at all points in phase space, that is, $W_\rho(\mathbf{r}) \in \mathbb{R}$ for all $\mathbf{r}$ and $\hat{\rho}$.
3. It is normalized, that is,

$$\int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho(\mathbf{r}) = 1. \tag{104}$$

4. Averages in phase space correspond to quantum expectation values of symmetrically-ordered operators, that is,

$$\langle (\hat{X}^m\hat{P}^n)^{(s)}\rangle = \int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho(\mathbf{r}) x^m p^n, \tag{105}$$

   where we remind that $(\hat{X}^m\hat{P}^n)^{(s)}$ refers to the symmetrized version of the corresponding product with respect to position and momentum, e.g., $(\hat{X}^2\hat{P})^{(s)} = (\hat{X}^2\hat{P} + \hat{P}\hat{X}^2 + \hat{X}\hat{P}\hat{X})/3$. Taking into account that a reasonable prescription for finding the quantum operator associated to a classical observable $A(x,p)$ consists precisely of symmetrizing it with respect to x and p, and then change the position and momentum by the corresponding self-adjoint operators (what guarantees the self-adjointness of the remaining operator, as explained in Secs. I A and A 3 e), this result seems to reinforce the interpretation of $W_\rho(\mathbf{r})$ as a probability density function dictating how quantum fluctuations are distributed in phase space.

5. The Wigner function admits the following alternative expression in terms of the transition amplitude $\langle x_2|\hat{\rho}|x_1\rangle$ between positions x_1 and x_2:

$$W_\rho(\mathbf{r}) = \int_{\mathbb{R}} \frac{dy}{4\pi} e^{-\frac{\mathrm{i}}{2}py} \left\langle x + \frac{y}{2}\right| \hat{\rho} \left| x - \frac{y}{2}\right\rangle. \tag{106}$$

   This is indeed the original form first introduced by Wigner [9], and it is sometimes useful for calculations.

6. The trace product of two states can be written as the overlap between their corresponding Wigner functions, that is,

$$\mathrm{tr}\{\hat{\rho}_1\hat{\rho}_2\} = 4\pi \int_{\mathbb{R}^2} d^2\mathbf{r} W_{\rho_1}(\mathbf{r}) W_{\rho_2}(\mathbf{r}). \tag{107}$$

7. When particularizing this expression to two orthogonal pure states, that is, $\hat{\rho}_j = |\psi_j\rangle\langle\psi_j|$ with $\langle\psi_1|\psi_2\rangle = 0$, we obtain[11]

$$\int_{\mathbb{R}^2} d^2\mathbf{r} W_{|\psi_1\rangle}(\mathbf{r}) W_{|\psi_2\rangle}(\mathbf{r}) = \frac{1}{4\pi}|\langle\psi_1|\psi_2\rangle|^2 = 0. \tag{108}$$

   This identity is only possible if the Wigner function is negative at some points of phase space, as otherwise the product of two Wigner functions would always add positively to the integral. Hence, in general, the Wigner function is not a true probability density function in the classical-statistical sense!

---

[11] At this point, it is interesting to remind that for any vector $|\psi\rangle$ and operator $\hat{A}$, the following identity holds $\mathrm{tr}\{|\psi\rangle\langle\psi|\hat{A}\} = \langle\psi|\hat{A}|\psi\rangle$. This is easy to prove just by writing the trace in a basis of the Hilbert space, and using that the sum of the corresponding projectors is a resolution of the identity.

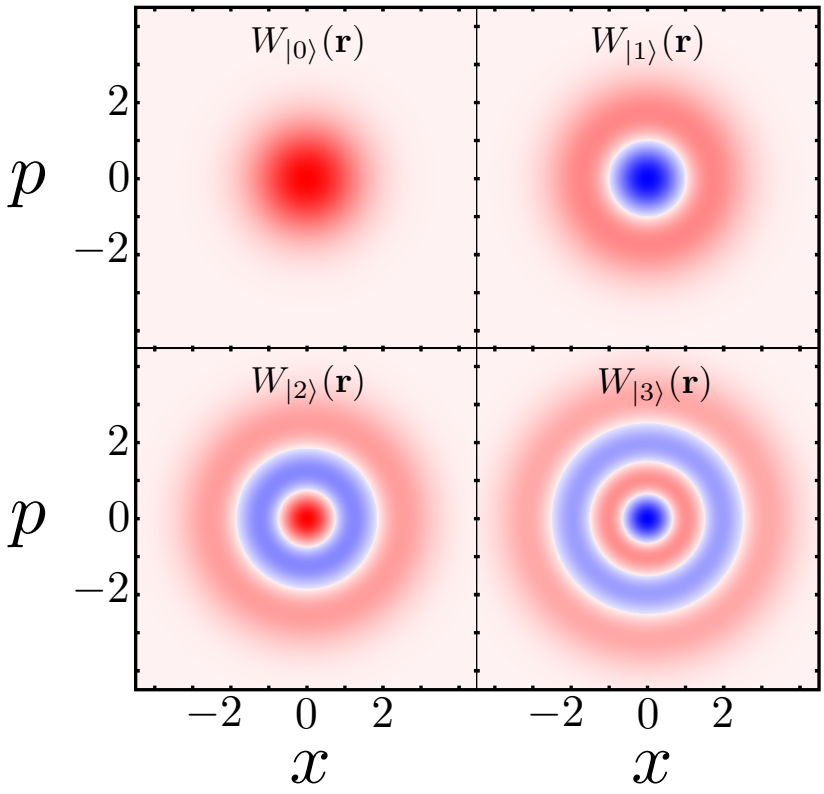

Figure 3. Density plot of the Wigner functions corresponding to the first 4 Fock states. Red and blue regions correspond to positive and negative values of the function, respectively. In both cases regions with higher contrast correspond to larger absolute value.

8. When particularizing the trace-product expression to $\hat{\rho}_1 = \hat{\rho}_2 \equiv \hat{\rho}$, we get

$$\int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho^2(\mathbf{r}) = \frac{1}{4\pi}\mathrm{tr}\{\hat{\rho}^2\} \leq \frac{1}{4\pi}, \tag{109}$$

where the last inequality follows from $\mathrm{tr}\{\hat{\rho}^2\} \leq 1$, a condition satisfied by all density operators, since they have positive eigenvalues smaller than or equal to one. This expression shows that the Wigner function cannot have divergences, and hence, it can always be plotted in phase space to visualize quantum states.

9. It uniquely determines the quantum state $\hat{\rho}$ of the system as

$$\hat{\rho} = \int_{\mathbb{R}^2} \frac{d^2\mathbf{s}}{4\pi} \hat{D}^\dagger(\mathbf{s}) \chi_\rho(\mathbf{s}), \tag{110}$$

and hence the Wigner function contains the same information as the quantum state, providing an alternative representation of the latter.

These properties show that the Wigner function has almost all the right properties expected from a probability density function in phase space. In fact, it only differs from it in the fact that it can be negative. This is indeed crucial, as it means that quantum mechanics cannot be simulated with classical means, and therefore, it really goes beyond anything we could predict with classical physics. Despite not being a true probability density function in general, the Wigner function is still a very useful and rigorous way of visualizing quantum fluctuations in phase space. Moreover, as we will see, most of the easily experimentally accessible states of the harmonic oscillator have a positive Wigner function, and therefore, for these states we can apply all the intuition behind standard probability theory to how quantum fluctuations are distributed in phase space. In addition, whenever negativities appear in an experiment, these offer a smoking gun that something genuinely quantum is happening, something that cannot be simulated by adding classical noise in the system.

To conclude this section, let us evaluate the Wigner function of a number state $\hat{\rho} = |n\rangle\langle n|$ as an example. It is not difficult to do so by using expression (106) for the Wigner function, together with the wave function (99) that we

found for that state, obtaining

$$
\begin{aligned}
W_{|n\rangle}(\mathbf{r}) =& \int_{\mathbb{R}} \frac{dy}{4\pi} e^{-\frac{\mathrm{i}}{2}py} \langle x+y/2|n\rangle\langle n|x-y/2\rangle = \int_{\mathbb{R}} \frac{dy}{4\pi} e^{-\frac{\mathrm{i}}{2}py} \psi_n(x+y/2)\psi_n^*(x-y/2) \\
=& \frac{1}{2^{n+1/2}\pi^{1/2}n!} \int_{\mathbb{R}} \frac{dy}{4\pi} e^{-\frac{\mathrm{i}}{2}py - \frac{(x+y/2)^2+(x-y/2)^2}{4}} H_n\left(\frac{x+y/2}{\sqrt{2}}\right) H_n\left(\frac{x-y/2}{\sqrt{2}}\right) \\
=& \frac{1}{2^{n+1/2}\pi^{1/2}n!} e^{-\frac{x^2}{2}} \int_{\mathbb{R}} \frac{dy}{4\pi} e^{-\frac{\mathrm{i}}{2}py - \frac{y^2}{8}} H_n\left(\frac{x+y/2}{\sqrt{2}}\right) H_n\left(\frac{x-y/2}{\sqrt{2}}\right) \\
=& \frac{1}{2^{n+1/2}\pi^{1/2}n!} e^{-\frac{x^2+p^2}{2}} \int_{\mathbb{R}} \frac{dy}{4\pi} e^{-\frac{1}{8}(y+2\mathrm{i}p)^2} H_n\left(\frac{x+y/2}{\sqrt{2}}\right) H_n\left(\frac{x-y/2}{\sqrt{2}}\right),
\end{aligned}
\tag{111}
$$

where in the last step we have just completed the square in the exponential. Let us now make the variable change $y = 2(z - \mathrm{i}p)$, which is a shift of the integration variable along the imaginary line, so that the integral now is still performed parallel to the real line in the complex-y plane. The previous expression is then turned into

$$
\begin{aligned}
W_{|n\rangle}(\mathbf{r}) &= \frac{1}{2^{n+1/2}\pi^{1/2}n!} e^{-\frac{x^2+p^2}{2}} \int_{\mathrm{i}p-\infty}^{\mathrm{i}p+\infty} \frac{dz}{2\pi} e^{-z^2/2} H_n\left(\frac{x+z-\mathrm{i}p}{\sqrt{2}}\right) H_n\left(\frac{x-z+\mathrm{i}p}{\sqrt{2}}\right) \\
&= \frac{(-1)^n}{2^{n+1/2}\pi^{1/2}n!} e^{-\frac{x^2+p^2}{2}} \int_{\mathrm{i}p-\infty}^{\mathrm{i}p+\infty} \frac{dz}{2\pi} e^{-z^2/2} H_n\left(\frac{z+x-\mathrm{i}p}{\sqrt{2}}\right) H_n\left(\frac{z-x-\mathrm{i}p}{\sqrt{2}}\right),
\end{aligned}
\tag{112}
$$

where in the second equality we have used $H_n(-x) = (-1)^n H_n(x)$. Finally, using the following relation between the Hermite and Laguerre polynomials

$$
\int_{\mathrm{i}p-\infty}^{\mathrm{i}p+\infty} dz e^{-z^2/2} H_n\left(\frac{z+\xi_1}{\sqrt{2}}\right) H_n\left(\frac{z-\xi_2}{\sqrt{2}}\right) = 2^n\sqrt{2\pi}n! L_n(\xi_1\xi_2),
\tag{113}
$$

where the Laguerre polynomial of order n is defined by the Rodrigues formula

$$
L_n(z) = \frac{\exp(z)}{n!}\frac{d^n}{dz^n}\left[z^n \exp(-z)\right],
\tag{114}
$$

we arrive to the simple expression

$$
W_{|n\rangle}(\mathbf{r}) = \frac{(-1)^n}{2\pi} L_n(x^2+p^2) e^{-\frac{x^2+p^2}{2}}.
\tag{115}
$$

For any $n > 0$, this function has negative regions. For example, for odd n it is always negative at the origin of phase space, since $L_n(0) = 1 \ \ \forall n$. The Wigner functions of the first 4 Fock states are plotted in Fig. 3.

F. Proof of the Wigner function properties

In this section we prove the properties of the Wigner function introduced above. Let us start with property 1. In particular, we next prove that integrating the Wigner function over momenta leads to the probability density function associated to position measurements. We start from

$$
\int_{\mathbb{R}} dp W_\rho(\mathbf{r}) = \int_{\mathbb{R}^2} \frac{d^2\mathbf{r}}{(4\pi)^2} \underbrace{\left[\int_{\mathbb{R}} dp e^{\frac{\mathrm{i}}{2}x'p}\right]}_{4\pi\delta(x')} e^{-\frac{\mathrm{i}}{2}p'x} \chi(\mathbf{r}') = \int_{\mathbb{R}} \frac{dp'}{4\pi} e^{-\frac{\mathrm{i}}{2}p'x} \underbrace{\chi(0,p')}_{\mathrm{tr}\{\hat{\rho}\hat{D}(0,p')\}},
\tag{116}
$$

and then write the trace in the position eigenbasis obtaining

$$
\int_{\mathbb{R}} dp W_\rho(\mathbf{r}) = \int_{\mathbb{R}} dy \int_{\mathbb{R}} \frac{dp'}{4\pi} e^{-\frac{\mathrm{i}}{2}p'x} \langle y|\hat{\rho}e^{\frac{\mathrm{i}}{2}p'\hat{X}}|y\rangle = \int_{\mathbb{R}} dy \underbrace{\left[\int_{\mathbb{R}} \frac{dp'}{4\pi} e^{-\frac{\mathrm{i}}{2}p'(x-y)}\right]}_{4\pi\delta(x-y)} \langle y|\hat{\rho}|y\rangle = \langle x|\hat{\rho}|x\rangle,
\tag{117}
$$

just as we wanted to prove. Similarly, you can prove that the integration of the Wigner function over position leads to the probability density function for momentum measurements.

Property 3, that the Wigner function is normalized, is proven immediately from the previous expression, since

$$\int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho(\mathbf{r}) = \int_{\mathbb{R}} dx \underbrace{\int_{\mathbb{R}} dp W_\rho(\mathbf{r})}_{\langle x|\hat{\rho}|x\rangle} = \mathrm{tr}\left\{\hat{\rho}\int_{\mathbb{R}} dx|x\rangle\langle x|\right\} = \mathrm{tr}\{\hat{\rho}\} = 1. \tag{118}$$

On the other hand, the Wigner function is real (property 2) by construction, since using $\hat{D}^\dagger(\mathbf{r}) = \hat{D}(-\mathbf{r})$, we get

$$W_\rho^*(\mathbf{r}) = \int_{\mathbb{R}^2} \frac{d^2\mathbf{r}'}{(4\pi)^2} e^{\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{r}'}\langle\hat{D}(\mathbf{r}')\rangle^* = \int_{\mathbb{R}^2} \frac{d^2\mathbf{r}'}{(4\pi)^2} e^{\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{r}'}\langle\hat{D}(-\mathbf{r}')\rangle = \int_{\mathbb{R}^2} \frac{d^2\mathbf{r}''}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{r}''}\langle\hat{D}(\mathbf{r}'')\rangle = W_\rho(\mathbf{r}) \tag{119}$$

where in the second to last step we made the integration variable change $\mathbf{r}' = -\mathbf{r}''$.

In order to prove property 4 regarding expectation values of operators in symmetric order, we need some preliminary results. First, note that the exponentiation of a linear combination of position and momentum follows Newton's binomial expansion, but with products of operators in symmetric order, that is,

$$(a\hat{X} + b\hat{P})^n = \sum_{k=0}^{n} \binom{n}{k} a^{n-k}b^k \left(\hat{X}^{n-k}\hat{P}^k\right)^{(s)}. \tag{120}$$

You can easily convince yourself by trying out some values of n. This leads to the following expansion of the displacement operator

$$\hat{D}(\mathbf{r}) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{\mathrm{i}}{2}\right)^n \left(p\hat{X} - x\hat{P}\right)^n = \sum_{n=0}^{\infty}\left(\frac{\mathrm{i}}{2}\right)^n \sum_{k=0}^{n} \frac{p^{n-k}(-x)^k}{k!(n-k)!}\left(\hat{X}^{n-k}\hat{P}^k\right)^{(s)}. \tag{121}$$

Then, we will also need to keep in mind the action of derivatives of the Dirac delta function,

$$\int_{-\infty}^{+\infty} dx \left[\frac{d^n\delta(x)}{dx^n}\right] f(x) = (-1)^n \int_{-\infty}^{+\infty} dx\delta(x)\frac{d^n f(x)}{dx^n}, \tag{122}$$

which is easily proven integrating by parts and using the fact that the delta function and its derivatives to all orders vanish at infinity, that is, $[d^n\delta(x)/dx^n]|_{x=\pm\infty} = 0 \quad \forall n$. Using these properties, we can then prove the property we seek as

$$\begin{aligned}\int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho(\mathbf{r}) x^m p^r &= \int_{\mathbb{R}^2} d^2\mathbf{r} \int_{\mathbb{R}^2} \frac{d^2\mathbf{r}'}{(4\pi)^2}\left[\left(-\frac{2}{i}\right)^m\left(\frac{2}{i}\right)^r \partial_{p'}^m\partial_{x'}^r e^{\frac{\mathrm{i}}{2}(x'p-p'x)}\right]\langle\hat{D}(\mathbf{r}')\rangle \\ &= \left(-\frac{2}{i}\right)^m\left(\frac{2}{i}\right)^r \int_{\mathbb{R}^2} d^2\mathbf{r}'\left\langle\hat{D}(\mathbf{r}')\right\rangle \partial_{p'}^m\partial_{x'}^r \underbrace{\int_{\mathbb{R}^2}\frac{d^2\mathbf{r}}{(4\pi)^2} e^{\frac{\mathrm{i}}{2}(x'p-p'x)}}_{\delta(x')\delta(p')} \\ &= \left(-\frac{2}{i}\right)^m\left(\frac{2}{i}\right)^r (-1)^{r+m}\int_{\mathbb{R}^2} d^2\mathbf{r}'\delta(x')\delta(p')\partial_{p'}^m\partial_{x'}^r\langle\hat{D}(\mathbf{r}')\rangle,\end{aligned} \tag{123}$$

where in the last step we have integrated by parts in order to bring the derivatives to the characteristic function. The derivatives acting on the expansion (121) for the displacement operator, together with the action of the delta functions, force $n = m + r$ and $k = r$ in that expression, leading to the desired expression

$$\int_{\mathbb{R}^2} d^2\mathbf{r} p W_\rho(\mathbf{r}) x^m p^r = \left(\hat{X}^m\hat{P}^r\right)^{(s)}. \tag{124}$$

Next we prove that the definition of the Wigner function in terms of a quantum characteristic function (103) coincides with Wigner's original formulation (106). For this, we will rely on some additional properties of the displacement and translation operators. In the case of the displacement operator, we use the weaker (sometimes called *disentangling*) form of the Baker-Campbell-Haussdorf lemma[12] (125) to write it as

$$\hat{D}(\mathbf{r}) = e^{\frac{\mathrm{i}}{4}xp}e^{-\frac{\mathrm{i}}{2}x\hat{P}}e^{\frac{\mathrm{i}}{2}p\hat{X}}, \tag{126}$$

---

[12] This form says that given two operators $\hat{A}$ and $\hat{B}$ that commute with their commutator, we can "disentangle" the exponential of their sum as

$$e^{\hat{A}+\hat{B}} = e^{-[\hat{A},\hat{B}]/2}e^{\hat{A}}e^{\hat{B}}. \tag{125}$$

proven by setting $\hat{A} = -\mathrm{i}x\hat{P}/2$ and $\hat{B} = \mathrm{i}p\hat{X}/2$ in (125). In the case of the translation operator, we need its action on the position eigenstates

$$e^{-\frac{\mathrm{i}}{2}y\hat{P}}|x\rangle = |x+y\rangle, \tag{127}$$

which is easily proven by inserting a representation of the identity in the momentum basis and using (87),

$$e^{-\frac{\mathrm{i}}{2}y\hat{P}}|x\rangle = \int_{\mathbb{R}} dp\langle p|x\rangle e^{-\frac{\mathrm{i}}{2}y\hat{P}}|p\rangle = \int_{\mathbb{R}} dp \underbrace{\frac{1}{\sqrt{4\pi}}e^{-\frac{\mathrm{i}}{2}(x+y)p}}_{\langle p|x+y\rangle}|p\rangle = |x+y\rangle. \tag{128}$$

With this properties at hand, we can now turn our definition of the Wigner function (103) into Wigner's original definition (106). For this, we simply write the trace in the position eigenbasis, obtaining

$$\begin{aligned} W_\rho(\mathbf{r}) &= \int_{\mathbb{R}^2} \frac{d^2\mathbf{r}'}{(4\pi)^2} e^{\frac{\mathrm{i}}{2}(x'p-p'x)} \int_{\mathbb{R}} dy\langle y|\hat{\rho}e^{\frac{\mathrm{i}}{4}x'p'}e^{-\frac{\mathrm{i}}{2}x'\hat{P}}e^{\frac{\mathrm{i}}{2}p'\hat{X}}|y\rangle = \int_{\mathbb{R}} \frac{dx'}{4\pi}e^{\frac{\mathrm{i}}{2}x'p}\int_{\mathbb{R}} dy \underbrace{\int_{\mathbb{R}} \frac{dp'}{4\pi}e^{\frac{\mathrm{i}}{2}p'(y-x+x'/2)}}_{\delta(y-x+x'/2)}\langle y|\hat{\rho}|y+x'\rangle \\ &= \int_{\mathbb{R}} \frac{dx'}{4\pi}e^{\frac{\mathrm{i}}{2}x'p}\langle x-x'/2|\hat{\rho}|x+x'/2\rangle, \end{aligned} \tag{129}$$

which making the integration variable change $x' = -y$ leads to the desired expression (106).

The next property, specifically the trace product rule of expression (107), is easily proven by using Wigner's original formulation (106). In particular, we write

$$\begin{aligned} \int_{\mathbb{R}^2} d^2\mathbf{r}W_{\rho_1}(\mathbf{r})W_{\rho_2}(\mathbf{r}) &= \int_{\mathbb{R}} dx \int_{\mathbb{R}} \frac{dy_1}{4\pi}\int_{\mathbb{R}} \frac{dy_2}{4\pi}\underbrace{\int_{\mathbb{R}} dp e^{-\frac{\mathrm{i}}{2}(y_1+y_2)p}}_{4\pi\delta(y_1+y_2)}\langle x+y_1/2|\hat{\rho}_1|x-y_1/2\rangle\langle x+y_2/2|\hat{\rho}_2|x-y_2/2\rangle \\ &= \frac{1}{4\pi}\int_{\mathbb{R}} dx\int_{\mathbb{R}} dy\langle x+y/2|\hat{\rho}_1|x-y/2\rangle\langle x-y/2|\hat{\rho}_2|x+y/2\rangle, \end{aligned} \tag{130}$$

so that making the variable changes $\{x_+ = x+y/2, x_- = x-y/2\}$, we prove the desired result

$$\int_{\mathbb{R}^2} d^2\mathbf{r}W_{\rho_1}(\mathbf{r})W_{\rho_2}(\mathbf{r}) = \frac{1}{4\pi}\int_{\mathbb{R}^2} dx_+dx_-\langle x_+|\hat{\rho}_1|x_-\rangle\langle x_-|\hat{\rho}_2|x_+\rangle = \frac{1}{4\pi}\int_{\mathbb{R}} dx_+\langle x_+|\hat{\rho}_1\hat{\rho}_2|x_+\rangle = \frac{1}{4\pi}\mathrm{tr}\{\hat{\rho}_1\hat{\rho}_2\}. \tag{131}$$

In order to prove the last property, which allows us to recover the quantum state $\hat{\rho}$ from the characteristic function through expression (110), we simply need two more useful properties of the displacement operator. The first one is

$$\mathrm{tr}\{\hat{D}(\mathbf{r})\} = 4\pi\delta^{(2)}(\mathbf{r}), \tag{132}$$

easily proven by using the form (126) of the displacement operator, performing the trace in the position eigenbasis, using the translation property (127), and the fact that position eigenstates are Dirac-delta orthonormal:

$$\mathrm{tr}\{\hat{D}(\mathbf{r})\} = e^{\frac{\mathrm{i}}{4}xp}\mathrm{tr}\left\{e^{-\frac{\mathrm{i}}{2}x\hat{P}}e^{\frac{\mathrm{i}}{2}p\hat{X}}\right\} = e^{\frac{\mathrm{i}}{4}xp}\int_{\mathbb{R}} dy\langle y|e^{-\frac{\mathrm{i}}{2}x\hat{P}}e^{\frac{\mathrm{i}}{2}p\hat{X}}|y\rangle = e^{\frac{\mathrm{i}}{4}xp}\underbrace{\int_{\mathbb{R}} dy e^{\frac{\mathrm{i}}{2}py}}_{4\pi\delta(p)}\underbrace{\langle y|\underbrace{e^{-\frac{\mathrm{i}}{2}x\hat{P}}|y\rangle}_{|y+x\rangle}}_{\delta(x)} = 4\pi\delta^{(2)}(\mathbf{r}). \tag{133}$$

The second one refers to the composition of two displacements

$$\hat{D}(\mathbf{r})\hat{D}(\mathbf{s}) = e^{-\frac{\mathrm{i}}{4}\mathbf{r}^T\Omega\mathbf{s}}\hat{D}(\mathbf{r}+\mathbf{s}), \tag{134}$$

which is easily proven by applying the disentangling Baker-Campbell-Haussdorf lemma (125) with $\hat{A} = \frac{\mathrm{i}}{2}\hat{\mathbf{R}}^T\Omega\mathbf{r}$ and $\hat{B} = \frac{\mathrm{i}}{2}\hat{\mathbf{R}}^T\Omega\mathbf{r}$, noting that

$$[\hat{A},\hat{B}] = \sum_{mnjl=1}^{2}\left(\frac{\mathrm{i}}{2}\right)^2\underbrace{[\hat{R}_m,\hat{R}_j]}_{2\mathrm{i}\Omega_{mj}}\Omega_{mn}r_n\Omega_{jl}s_l = -\frac{\mathrm{i}}{2}\sum_{nl=1}^{2}r_n\underbrace{\left(\sum_{mj=1}^{2}\Omega_{mn}\Omega_{mj}\Omega_{jl}\right)}_{(\Omega^T\Omega\Omega)_{ml}=\Omega_{ml}}s_l = -\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{s}. \tag{135}$$

Using these properties, we then see that expression (110) is correct by applying the displacement operator onto it, and taking the trace

$$\mathrm{tr}\{\hat{D}(\mathbf{s})\hat{\rho}\} = \int_{\mathbb{R}} d^2\mathbf{z}\, \underbrace{\mathrm{tr}\{\hat{D}(\mathbf{s})\underbrace{\hat{D}^\dagger(\mathbf{z})}_{\hat{D}(-\mathbf{z})}\}}_{e^{\frac{i}{4}\mathbf{s}^T\Omega\mathbf{z}}\mathrm{tr}\{\hat{D}(\mathbf{s}-\mathbf{z})\}}\chi_\rho(\mathbf{z}) = \int_{\mathbb{R}} d^2\mathbf{z} e^{\frac{i}{4}\mathbf{s}^T\Omega\mathbf{z}}\delta^{(2)}(\mathbf{s}-\mathbf{z})\chi_\rho(\mathbf{z}) = \chi_\rho(\mathbf{s}),$$

where we have used $\mathbf{s}^T\Omega\mathbf{s} = 0$.

G. Gaussian states

Let us now introduce an important class of states, the so-called *Gaussian states*. As we will argue, these are the type of states that appear most naturally in experiments, and indeed experimentalists need to work very hard to go away of the Gaussian-state manifold.

1. Definition and interpretation

Gaussian states are defined as those states for which all statistics are completely defined by first and second order moments such as $\langle\hat{R}_j\rangle$ and $\langle\hat{R}_j\hat{R}_l\rangle$, respectively. This means that their Wigner function is a Gaussian distribution, which can always be written as[13]

$$W_\rho(\mathbf{r}) = \frac{1}{2\pi\sqrt{\det V}}\exp\left[-\frac{1}{2}(\mathbf{r}-\mathbf{d})^T V^{-1}(\mathbf{r}-\mathbf{d})\right], \tag{137}$$

in terms of the so-called *mean vector* $\mathbf{d}$, and the *covariance matrix* V. It is not difficult to prove (and we do it below, in Section II G 3) that

$$\langle\hat{R}_j\rangle = \int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho(\mathbf{r}) r_j = d_j, \tag{138a}$$

$$\frac{1}{2}\langle\delta\hat{R}_j\delta\hat{R}_l + \delta\hat{R}_l\delta\hat{R}_j\rangle = \int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho(\mathbf{r})\delta r_j\delta r_l = V_{jl}. \tag{138b}$$

where we have defined the fluctuation vector $\delta\mathbf{r} = \mathbf{r} - \mathbf{d}$, which measures how far away the phase-space coordinate is from the mean of the distribution, and we remind that we already defined in Section I A the fluctuation of any operator $\hat{A}$ as $\delta\hat{A} = \hat{A} - \langle\hat{A}\rangle$, which allows us to find its variance as $V(A) = \langle\delta\hat{A}^2\rangle$.

Any higher-order moment can be generated from these ones by using the Gaussian-moment theorem [5]

$$\int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho(\mathbf{r})\delta r_{j_1}\delta r_{j_2}...\delta r_{j_N} = \begin{cases} 0 & \text{if } N \text{ is odd} \\ \sum_{\text{all } (N-1)!! \text{ pairings}}^{\{i_1,i_2,...,i_N\}\in} V_{i_1i_2}V_{i_3i_4}...V_{i_{N-1}i_N} & \text{if } N \text{ is even} \end{cases}, \tag{139}$$

where the sum is restricted to the $(N-1)!!$ different ways in which we can pair the $\{j_1, j_2, ..., j_N\}$ indices. For example, for $N = 4$ this expression explicitly reads as

$$\int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho(\mathbf{r}) \underbrace{\delta x\delta p\delta x\delta p}_{j_1j_2j_3j_4=1,2,1,2} = V_{12}V_{12} + V_{11}V_{22} + V_{12}V_{21} = V_{11}V_{22} + 2V_{12}^2, \tag{140}$$

where in the last step we used the symmetry of the covariance matrix. Using (139) we can then evaluate any higher-order moment of a Gaussian state in a simple fashion. For example,

$$\langle\hat{X}^3\rangle = \langle(\delta\hat{X} + \langle\hat{X}\rangle)^3\rangle = \underbrace{\langle\delta\hat{X}^3\rangle}_{0} + 3\langle\hat{X}\rangle\langle\delta\hat{X}^2\rangle + 3\langle\hat{X}\rangle^2\underbrace{\langle\delta\hat{X}\rangle}_{0} + \langle\hat{X}\rangle^3 = \left[\langle\hat{X}\rangle^2 + 3V(X)\right]\langle\hat{X}\rangle = \left[d_1^2 + 3V_{11}\right]d_1. \tag{141}$$

---

[13] When dealing with Gaussian states, the following integral is quite useful:

$$\int_{\mathbb{R}^N} d^N\mathbf{r}\exp\left(-\frac{1}{2}\mathbf{r}^T A\mathbf{r} + \mathbf{x}^T\mathbf{r}\right) = \sqrt{\frac{(2\pi)^N}{\det A}}\exp\left(\frac{1}{2}\mathbf{x}^T A^{-1}\mathbf{x}\right) \tag{136}$$

where $\mathbf{x} \in \mathbb{R}^N$ and A is a non-singular $N \times N$ matrix. For example, check with it that the Gaussian Wigner function in (137) is indeed normalized.

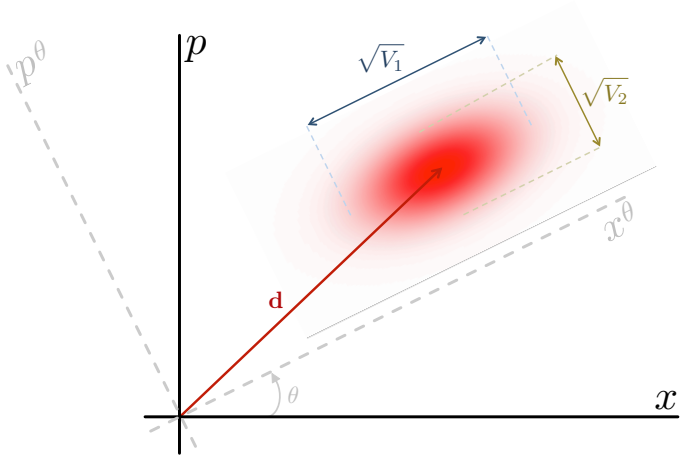

Figure 4. Wigner function of a generic Gaussian state (137). It consists of a single lob with the shape of an ellipse, centered at the position given by the mean vector $\mathbf{d}$. The covariance matrix V can be diagonalized through a rotation of angle θ. Its eigenvalues provide the uncertainty of the quadratures along the principal axes of the ellipse.

Let us now discuss about the interpretation of Gaussian states. As we mentioned above, the mean vector and covariance matrix are related to quantum expectation values by

$$\mathbf{d} = \langle \hat{\mathbf{R}} \rangle = \begin{pmatrix} \langle \hat{X} \rangle \\ \langle \hat{P} \rangle \end{pmatrix}, \tag{142a}$$

$$V = \frac{1}{2}\left[\langle \delta\hat{\mathbf{R}} \delta\hat{\mathbf{R}}^T \rangle + \left(\langle \delta\hat{\mathbf{R}} \delta\hat{\mathbf{R}}^T \rangle \right)^T \right] = \begin{pmatrix} \langle \delta\hat{X}^2 \rangle & \langle (\delta\hat{X}\delta\hat{P})^{(s)} \rangle \\ \langle (\delta\hat{X}\delta\hat{P})^{(s)} \rangle & \langle \delta\hat{P}^2 \rangle \end{pmatrix}. \tag{142b}$$

Now, since Gaussian Wigner functions are positive everywhere, they can be interpreted as probability density functions for quadrature measurements. The mean vector encodes the expectation values describing the measurements, while the covariance matrix encodes the distribution of the measurements around the mean. It is then interesting to plot a typical Gaussian Wigner function, which is what can be seen in Fig. 4. It has the shape of an ellipse centered at the mean vector. The widths along the principal axes of the ellipse inform us about the quadrature variances along those directions. Being symmetric and real, the covariance matrix can always be diagonalized via a proper phase-space rotation, say

$$V = R^T(\theta) V^\theta R(\theta), \quad \text{with } R(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \text{ and } V^\theta = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}. \tag{143}$$

The eigenvalues then inform us about the variance of the quadratures along the two principal axes of the ellipse, the angle of the rotation providing the orientation of the ellipse. In particular, defining the rotated coordinate system $\mathbf{r}^\theta = R(\theta)\mathbf{r} \equiv (x^\theta, p^\theta)$, the Gaussian Wigner function (137) takes the separable form

$$W_\rho(\mathbf{r}^\theta) = e^{-(x^\theta - d_1^\theta)^2/2V_1} e^{-(p^\theta - d_2^\theta)^2/2V_2}, \tag{144}$$

where we have defined the rotated mean vector $\mathbf{d}^\theta = R(\theta)\mathbf{d}$. This expression indeed shows that $\sqrt{V_j}$ corresponds to the standard deviation of the distribution along the corresponding direction r_j^θ. On the other hand, defining the rotated quadratures $\hat{\mathbf{R}}^\theta = R(\theta)\hat{\mathbf{R}} \equiv (\hat{X}^\theta, \hat{P}^\theta)$, such that $\mathbf{d}^\theta = \langle \hat{\mathbf{R}}^\theta \rangle$, the eigenvalues of the covariance matrix correspond to the variances of the quadratures: $V(X^\theta) = \langle (\delta\hat{X}^\theta)^2 \rangle = V_1$ and $V(P^\theta) = \langle (\delta\hat{P}^\theta)^2 \rangle = V_2$.

It is also interesting to note that, in a classical world, Gaussian states are physical for any choice of the mean vector and covariance matrix as long as they are real, and the covariance matrix is symmetric and positive semidefinite (the variances along the principal axes cannot be negative). However, quantum mechanics imposes the extra constrain $\det\{V\} \geq 1$, what comes from the uncertainty principle between quadratures (note that the determinant is invariant under rotations, so this proof is completely general):

$$\det\{V\} = V(X^\theta)V(P^\theta) \geq \frac{1}{4} |\underbrace{\langle [\delta\hat{X}^\theta, \delta\hat{P}^\theta] \rangle}_{2\mathrm{i}}|^2 = 1. \tag{145}$$

A Gaussian state corresponding to any real, symmetric, positive definite covariance matrix satisfying this condition is physically achievable, as we will see during the course.

Let us finally remark that, according to (115), number states are not Gaussian, except for the vacuum state $|0\rangle$, whose mean vector and covariance matrix are given by

$$\mathbf{d} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \qquad V = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

2. *Generation and characterization*

So far we have introduced Gaussian states, but we still haven't provided a criterion to characterize whether a given state $\hat{\rho}$ is indeed Gaussian. Of course, we can always compute its Wigner function and check if it has the Gaussian form of (137). But this is not a very practical method, and it would be nice to have simpler criteria. In the next section, after we have introduced the so-called coherent states, we will provide a simple criterion based on them. Here, however, we will discuss a weaker criterion, which is not of general practical applicability, but it's very useful in many cases. Moreover, it is a criterion with interesting experimental implications.

The criterion says that the state $\hat{\rho}$ is Gaussian, if and only if it can be generated from another Gaussian state $\hat{\rho}_0$ by evolving it with a Hamiltonian that is, at most, quadratic in quadrature operators. More precisely,

$$\hat{\rho} \text{ is Gaussian } \Leftrightarrow \ \hat{\rho} = \hat{U}\hat{\rho}_0\hat{U}^\dagger, \quad \text{with } \hat{U} = e^{\mathrm{i}(\sum_j b_j \hat{R}_j + \sum_{jl} h_{jl}\hat{R}_j\hat{R}_l)} \text{ and } \hat{\rho}_0 \text{ Gaussian.} \tag{146}$$

Note that the unitary $\hat{U}$ can be seen as the time-evolution operator associated to a quadratic Hamiltonian $\hat{H} = -\hbar(\sum_j b_j\hat{R}_j + \sum_{jl} h_{jl}\hat{R}_j\hat{R}_l)/T$ acting during a time T. Note that self-adjointness of the Hamiltonian implies that $b_j \in \mathbb{R}$ and $h_{jl} = h_{lj}^*$. We sometimes refer to $\hat{U}$ and $\hat{H}$ as *Gaussian unitaries* and *Gaussian Hamiltonians*, respectively.

We will prove (146) shortly, but first, let us discuss something concerning its meaning for experiments. As we will see during the course, the most natural states of the electromagnetic field are Gaussian. For example, at zero temperature, a free harmonic oscillator freezes into its ground state, which we have shown to be Gaussian, and even at any other temperature, we will show at the end of this chapter that the corresponding thermal state is Gaussian as well. On the other hand, in optics it is not easy to induce Hamiltonians with terms beyond quadratic in quadrature operators, which requires materials that have a strong nonlinear reaction to the applied fields. Hence, (146) tells us that we have to work very hard in the lab in order to generate non-Gaussian states of light, coming up with clever strategies beyond what's naturally available in optical labs.

Let us now proceed with the proof of (146). Let's start by denoting the mean vector and covariance matrix of the Gaussian state $\hat{\rho}_0$ by $\mathbf{d}_0$ and V_0, respectively, such that the corresponding Wigner function reads

$$W_{\rho_0}(\mathbf{r}) = \frac{1}{2\pi\sqrt{\det V_0}} e^{-\frac{1}{2}(\mathbf{r}-\mathbf{d}_0)^T V_0^{-1}(\mathbf{r}-\mathbf{d}_0)}. \tag{147}$$

On the other hand, if the state $\hat{\rho} = \hat{U}\hat{\rho}_0\hat{U}^\dagger$ is Gaussian, then its Wigner function can also be expressed in the Gaussian form (137). Hence, both $W_{\rho_0}(\mathbf{r})$ and $W_{U\rho_0U^\dagger}(\mathbf{r})$ are represented by the (normalized) exponential of some quadratic form. But we know that two different quadratic forms can always be related by a linear transformation. Hence, it is clear that

$$\sqrt{\det V_0} W_{\rho_0}(\mathbf{r}) = \sqrt{\det V} W_{U\rho_0U^\dagger}(S\mathbf{r}+\mathbf{a}), \tag{148a}$$

$$\Downarrow$$

$$e^{-\frac{1}{2}(\mathbf{r}-\mathbf{d}_0)^T V_0^{-1}(\mathbf{r}-\mathbf{d}_0)} = e^{-\frac{1}{2}(S\mathbf{r}+\mathbf{a}-\mathbf{d})^T V^{-1}(S\mathbf{r}+\mathbf{a}-\mathbf{d})} = e^{-\frac{1}{2}\left[\mathbf{r}+S^{-1}(\mathbf{a}-\mathbf{d})\right]^T S^T V^{-1} S\left[\mathbf{r}+S^{-1}(\mathbf{a}-\mathbf{d})\right]}, \tag{148b}$$

for some $\mathbf{a} \in \mathbb{R}^2$ and some 2×2 matrix S, whose properties will naturally unveil shortly. Comparing the leftmost and rightmost sides of the last equation, we then conclude that

$$\mathbf{d} = S\mathbf{d}_0 + \mathbf{a}, \qquad V = SV_0S^T, \tag{149}$$

and hence, the effect of the unitary transformation is simplified in phase space to this simple transformation of the mean vector and covariance matrix. Using (149), we show below that, seen in the Heisenberg picture, the unitary induces a linear transformation on the quadrature operators, given by

$$\hat{U}^\dagger\hat{\mathbf{R}}\hat{U} = S\hat{\mathbf{R}} + \mathbf{a}. \tag{150}$$

On the other hand, given that the commutator of the quadratures is proportional to the identity, according to the Baker-Campbell-Haussdorf lemma (84), the only way that the unitary $\hat{U} = \exp(\mathrm{i}\hat{B})$ can induce a linear transformation (150) is if the operator $\hat{B}$ is at most quadratic in quadrature operators. Moreover, while the vector $\mathbf{a}$ is arbitrary, the matrix S is easily shown to be constrained by the relation

$$S\Omega S^T = \Omega, \tag{151}$$

easily proven as

$$\hat{U}^\dagger \underbrace{[\hat{R}_m, \hat{R}_n]}_{2\mathrm{i}\Omega_{mn}} \hat{U} = \left[\sum_{j=1}^{2} S_{mj}\hat{R}_j + a_m, \sum_{l=1}^{2} S_{nl}\hat{R}_l + a_n\right] = \sum_{jl=1}^{2} S_{mj}S_{nl}\underbrace{[\hat{R}_j, \hat{R}_l]}_{2\mathrm{i}\Omega_{jl}}, \tag{152}$$

which is equal to (151) when written in matrix form. The set of all matrices satisfying condition (151) forms a group structure with many interesting properties that are heavily exploited both in classical and quantum mechanics. We call it the *symplectic group*, and then say that S is a *symplectic matrix*. Note that the symplectic condition implies that $\det^2 S = 1$, and therefore, $\det V = \det V_0$ from (149).

It is also very useful and interesting to note that Gaussian unitaries induce a very simple transformation of the Wigner function even for non-Gaussian states. In particular, the following expression is true for any state $\hat{\rho}$ as long as $\hat{U}$ is a Gaussian unitary:

$$W_{U\rho U^\dagger}(\mathbf{r}) = W_\rho\left(S^{-1}(\mathbf{r}-\mathbf{a})\right). \tag{153}$$

This is easily proven as follows

$$\begin{aligned}
W_{U\rho U^\dagger}(\mathbf{r}) &= \int_{\mathbb{R}^2} \frac{d^2\mathbf{s}}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{s}} \mathrm{tr}\{\hat{U}\hat{\rho}\hat{U}^\dagger\hat{D}(\mathbf{s})\} = \int_{\mathbb{R}^2} \frac{d^2\mathbf{s}}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{s}} \mathrm{tr}\{\hat{\rho}\hat{U}^\dagger\hat{D}(\mathbf{s})\hat{U}\} \\
&= \int_{\mathbb{R}^2} \frac{d^2\mathbf{s}}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{s}} \mathrm{tr}\{\hat{\rho}e^{\frac{\mathrm{i}}{2}(\hat{U}^\dagger\hat{\mathbf{R}}\hat{U})^T\Omega\mathbf{s}}\} \overset{(150)}{=} \int_{\mathbb{R}^2} \frac{d^2\mathbf{s}}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{s}} \mathrm{tr}\{\hat{\rho}e^{\frac{\mathrm{i}}{2}(S\hat{\mathbf{R}}+\mathbf{a})^T\Omega\mathbf{s}}\} \\
&= \int_{\mathbb{R}^2} \frac{d^2\mathbf{s}}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}(\mathbf{r}-\mathbf{a})^T\Omega\mathbf{s}} \mathrm{tr}\{\hat{\rho}e^{\frac{\mathrm{i}}{2}\hat{\mathbf{R}}^T S^T\Omega\mathbf{s}}\} \overset{(151)}{=} \int_{\mathbb{R}^2} \frac{d^2\mathbf{s}}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}(\mathbf{r}-\mathbf{a})^T\Omega\mathbf{s}} \mathrm{tr}\{\hat{\rho}e^{\frac{\mathrm{i}}{2}\hat{\mathbf{R}}^T\Omega S^{-1}\mathbf{s}}\} \\
&= \int_{\mathbb{R}^2} \frac{d^2\mathbf{s}}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}(\mathbf{r}-\mathbf{a})^T\Omega\mathbf{s}} \chi_\rho(S^{-1}\mathbf{s}) \overset{\mathbf{s}=S\mathbf{z}}{=} \int_{\mathbb{R}^2} \frac{d^2\mathbf{z}}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}(\mathbf{r}-\mathbf{a})^T\Omega S\mathbf{z}} \chi_\rho(\mathbf{z}) \overset{(151)}{=} \int_{\mathbb{R}^2} \frac{d^2\mathbf{z}}{(4\pi)^2} e^{-\frac{\mathrm{i}}{2}(\mathbf{r}-\mathbf{a})^T S^{-1T}\Omega\mathbf{z}} \chi_\rho(\mathbf{z}),
\end{aligned} \tag{154}$$

which from (103) we identify as the expression (153) we wanted to prove.

To conclude, we still need to prove (150) from (149). In order to do this, consider first the expression

$$\mathrm{tr}\{\hat{\rho}_0\hat{U}^\dagger\hat{\mathbf{R}}\hat{U}\} \overset{(\mathrm{cyclic})}{=} \mathrm{tr}\{\underbrace{\hat{U}\hat{\rho}_0\hat{U}^\dagger}_{\hat{\rho}}\hat{\mathbf{R}}\} = \mathbf{d} \overset{(149)}{=} S\mathbf{d}_0 + \mathbf{a} = S\mathrm{tr}\{\hat{\rho}_0\hat{\mathbf{R}}\} + \mathbf{a} = \mathrm{tr}\{\hat{\rho}_0(S\hat{\mathbf{R}} + \mathbf{a})\}. \tag{155}$$

Comparing the left-most and right-most expressions, this relation seems to suggest that (150) is right. However, such a strong conclusion cannot be reached from just this relation, since many different Gaussian states have the same mean. But since Gaussian states are completely characterized by first and second order moments, we simply need to prove a similar expression for the covariance matrix, which we do next. In particular, let us first note that, using the commutation relations of the quadrature operators, we can rewrite the elements of the covariance matrix as $V_{mn} = \langle\delta\hat{R}_m\delta\hat{R}_n\rangle - \mathrm{i}\Omega_{mn}$, and therefore

$$\begin{aligned}
&\mathrm{tr}\{\hat{\rho}_0(\hat{U}^\dagger\hat{\mathbf{R}}\hat{U} - \mathbf{d})(\hat{U}^\dagger\hat{\mathbf{R}}\hat{U} - \mathbf{d})^T\} - \mathrm{i}\Omega \overset{(\mathrm{cyclic})}{=} \mathrm{tr}\{\overbrace{\hat{U}\hat{\rho}_0\hat{U}^\dagger}^{\hat{\rho}}(\hat{\mathbf{R}} - \mathbf{d})(\hat{\mathbf{R}} - \mathbf{d})^T\} - \mathrm{i}\Omega = V \\
&\overset{(149)}{=} SV_0S^T = \mathrm{tr}\{\hat{\rho}_0 S(\hat{\mathbf{R}} - \mathbf{d}_0)(\hat{\mathbf{R}} - \mathbf{d}_0)^T S^T\} - \mathrm{i}S\Omega S^T \overset{(151)}{=} \mathrm{tr}\{\hat{\rho}_0(S\hat{\mathbf{R}} - \underbrace{S\mathbf{d}_0}_{\mathbf{d}-\mathbf{a}})(S\hat{\mathbf{R}} - \underbrace{S\mathbf{d}_0}_{\mathbf{d}-\mathbf{a}})^T\} - \mathrm{i}\Omega.
\end{aligned} \tag{156}$$

Comparing again the left-most and out-most expressions, together with the previous calculation with the mean vector, we are now in conditions to conclude that (150) is correct.

3. *Proof of (138)*

In this final section, let us prove that Eqs. (138), which connect first and second order moments of the quadrature operators to the mean vector and covariance matrix appearing in the Gaussian Wigner function. The first equality in these equations, connecting quantum expectation values with phase-space integrals, is just a consequence of the general relation (105) that we proved for arbitrary Wigner functions, not only Gaussian ones. Then, all that is left to prove is the second equality, specifically

$$\int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho(\mathbf{r}) r_j = d_j, \tag{157a}$$

$$\int_{\mathbb{R}^2} d^2\mathbf{r} W_\rho(\mathbf{r}) \delta r_j \delta r_l = V_{jl}. \tag{157b}$$

In order to do this, it is useful to determine first the characteristic function $\chi_\rho(\mathbf{s})$ associated to the Gaussian Wigner function (137). Note that the we can easily invert the Fourier transform in (103) to write the characteristic function in terms of the Wigner function as[14]

$$\chi_\rho(\mathbf{s}) = \int_{\mathbb{R}^2} d^2\mathbf{r} e^{\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{s}} W_\rho(\mathbf{r}). \tag{158}$$

Then, the characteristic function of a general Gaussian Wigner function is found as

$$\chi_\rho(\mathbf{s}) = \frac{1}{2\pi\sqrt{\det V}} \int_{\mathbb{R}^2} d^2\mathbf{r} e^{-\frac{1}{2}(\mathbf{r}-\mathbf{d})^T V^{-1}(\mathbf{r}-\mathbf{d})+\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{s}} = \frac{e^{\frac{\mathrm{i}}{2}\mathbf{d}^T\Omega\mathbf{s}}}{2\pi\sqrt{\det V}} \int_{\mathbb{R}^2} d^2\mathbf{z} e^{-\frac{1}{2}\mathbf{z}^T V^{-1}\mathbf{z}+\frac{\mathrm{i}}{2}\mathbf{z}^T\Omega\mathbf{s}} = e^{-\frac{1}{8}\mathbf{s}^T\Omega^T V\Omega\mathbf{s}+\frac{\mathrm{i}}{2}\mathbf{d}^T\Omega\mathbf{s}}, \tag{159}$$

where we made the variable change $\mathbf{r} = \mathbf{z} + \mathbf{d}$, and used the Gaussian integral formula (136) in the last step. Hence, we see that the characteristic function is also a Gaussian function. It is convenient for the upcoming derivations to write it in terms of a new variable $\mathbf{t} = \Omega\mathbf{s}$, so that

$$\chi_\rho(\mathbf{t}) = \int_{\mathbb{R}^2} d^2\mathbf{r} e^{\frac{\mathrm{i}}{2}\mathbf{r}^T\mathbf{t}} W_\rho(\mathbf{r}) = e^{-\frac{1}{8}\mathbf{t}^T V\mathbf{t}+\frac{\mathrm{i}}{2}\mathbf{d}^T\mathbf{t}}. \tag{160}$$

We can prove what we seek for by taking derivatives of this expression with respect to $\mathbf{t}$, and then particularizing to $\mathbf{t} = 0$. In particular, from the first equality we see

$$\partial_{t_j}\chi_\rho(\mathbf{t})\big|_{\mathbf{t}=0} = \frac{\mathrm{i}}{2}\int_{\mathbb{R}^2} d^2\mathbf{r}\, r_j e^{\frac{\mathrm{i}}{2}\mathbf{r}^T\mathbf{t}} W(\mathbf{r})\Big|_{\mathbf{t}=0} = \frac{\mathrm{i}}{2}\int_{\mathbb{R}^2} d^2\mathbf{r}\, r_j W(\mathbf{r}), \tag{161a}$$

$$\partial_{t_l}\partial_{t_j}\chi_\rho(\mathbf{t})\big|_{\mathbf{t}=0} = \left(\frac{\mathrm{i}}{2}\right)^2\int_{\mathbb{R}^2} d^2\mathbf{r}\, r_l r_j e^{\frac{\mathrm{i}}{2}\mathbf{r}^T\mathbf{t}} W(\mathbf{r})\Big|_{\mathbf{t}=0} = \left(\frac{\mathrm{i}}{2}\right)^2\int_{\mathbb{R}^2} d^2\mathbf{r}\, r_l r_j W(\mathbf{r}). \tag{161b}$$

On the other hand, taking derivatives of the right-hand-side of (160) instead, we get

$$\partial_{t_j}\chi_\rho(\mathbf{t})\big|_{\mathbf{t}=0} = \left(-\frac{1}{4}\sum_{n=1}^{2} t_n V_{jn} + \frac{\mathrm{i}}{2}d_j\right) e^{-\frac{1}{8}\mathbf{t}^T V\mathbf{t}+\frac{\mathrm{i}}{2}\mathbf{d}^T\mathbf{t}}\Big|_{\mathbf{t}=0} = \frac{\mathrm{i}}{2}d_j, \tag{162a}$$

$$\partial_{t_l}\partial_{t_j}\chi_\rho(\mathbf{t})\big|_{\mathbf{t}=0} = \left[-\frac{1}{4}V_{jl} + \left(-\frac{1}{4}\sum_{n=1}^{2} t_n V_{jn} + \frac{\mathrm{i}}{2}d_j\right)\left(-\frac{1}{4}\sum_{n=1}^{2} t_m V_{lm} + \frac{\mathrm{i}}{2}d_l\right)\right] e^{-\frac{1}{8}\mathbf{t}^T V\mathbf{t}+\frac{\mathrm{i}}{2}\mathbf{d}^T\mathbf{t}}\Big|_{\mathbf{t}=0} = -\frac{1}{4}(V_{jl} + d_j d_l). \tag{162b}$$

Comparing these equations and the previous ones, we then prove expression (138).

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[14] Note that the following representation of the two-dimensional Dirac delta is easily proven

$$\delta^{(2)}(\mathbf{z}) = \int_{\mathbb{R}^2} \frac{d^2\mathbf{r}}{(4\pi)^2} e^{\frac{\mathrm{i}}{2}\mathbf{r}^T\Omega\mathbf{z}},$$

with $\mathbf{r}, \mathbf{z} \in \mathbb{R}^2$.

H. Coherent states

Let us now discuss a very important class of states of the harmonic oscillator, the so-called *coherent states*. These are the most simple type of Gaussian states, and yet, they were introduced by Roy J. Glauber [63–65] in order to explain quantum-mechanically the outstanding coherence properties of the laser, in a series of works which marked the birth of modern theoretical quantum optics for many people (including the Nobel committee, who awarded him with the Nobel prize in 2005 [66]). Moreover, as we discuss below, these states will allow us to reconcile the quantum and classical descriptions of the harmonic oscillator.

1. *Definition and phase-space description*

In the previous section we saw that Gaussian states are mapped into other Gaussian states through the evolution induced by Hamiltonians which are at most quadratic in the quadrature operators. As a first example of a relevant Gaussian state, we then study here the transformation of the simplest Gaussian state, vacuum, by the simplest type of Hamiltonian, one that is linear in the quadratures. In fact, the time-evolution induced by such Hamiltonian is described by a unitary operator which we have already introduced: the *displacement operator* of Eq. (101). Let us here write it in the alternative (so-called *complex*) form

$$\hat{D}(\alpha) = \exp\left(\alpha \hat{a}^\dagger - \alpha^* \hat{a}\right), \tag{163}$$

which is exactly the same as (101), but written in terms of creation and annihilation operators, and a complex parameter $\alpha = (x + \mathrm{i}p)/2$. We define then *coherent states* as 'displaced' vacuum states

$$|\alpha\rangle = \hat{D}(\alpha)\,|0\rangle. \tag{164}$$

Note that when a displacement is applied to the annihilation and creation operators, we get[15]

$$\hat{D}^\dagger(\alpha)\,\hat{a}\hat{D}(\alpha) = \hat{a} + \alpha \quad \text{and} \quad \hat{D}^\dagger(\alpha)\,\hat{a}^\dagger\hat{D}(\alpha) = \hat{a}^\dagger + \alpha^*, \tag{165}$$

which shows where the name 'displacement' comes from. Applying the first of these equations to the vacuum state, and noting that the displacement operator is unitary, we obtain $\hat{a}\hat{D}(\alpha)\,|0\rangle = \alpha\hat{D}(\alpha)\,|0\rangle$, and hence coherent states are (right) eigenvectors of the annihilation operator, which has therefore complex eigenvalues, that is, $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$ with $\alpha \in \mathbb{C}$ (remember that $\hat{a}$ is not Hermitian). Note that this immediately implies that coherent states are left eigenstates of the creation operator, that is, $\langle\alpha|\hat{a}^\dagger = \alpha^*\langle\alpha|$.

In terms of the quadratures, the displacement transformation reads

$$\hat{D}^\dagger(\alpha)\,\hat{X}\hat{D}(\alpha) = \hat{X} + 2\mathrm{Re}\{\alpha\} \quad \text{and} \quad \hat{D}^\dagger(\alpha)\,\hat{P}\hat{D}(\alpha) = \hat{P} + 2\mathrm{Im}\{\alpha\}. \tag{166}$$

This transformation changes the expectation value of the quadratures but not their variance. More specifically, in the notation of the previous section, see Eq. (150), the linear transformation has $\mathbf{a}(\alpha) = 2(\mathrm{Re}\{\alpha\}, \mathrm{Im}\{\alpha\})^T$ and $S = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$, so that for a Gaussian state, it shifts ('displaces') its mean vector, but has no effect on the covariance matrix. Hence, the Wigner function of a coherent state has the same form as that of vacuum, but centered in a different point of phase space,

$$W_{|\alpha\rangle}(\mathbf{r}) = W_{|0\rangle}[\mathbf{r} - \mathbf{a}(\alpha)], \quad \text{with } \mathbf{a}(\alpha) = 2\begin{pmatrix} \mathrm{Re}[\alpha] \\ \mathrm{Im}[\alpha] \end{pmatrix}.$$

We sketch this in Fig. 5a. In other words, $W_{|\alpha\rangle}(\mathbf{r})$ is a Gaussian function of the type (137) with mean vector $\mathbf{d}_{|\alpha\rangle} = 2(\mathrm{Re}\{\alpha\}, \mathrm{Im}\{\alpha\})^T$ and the covariance matrix of vacuum $V_{|\alpha\rangle} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$.

Let us now move to the interpretation of this specific type of Gaussian Wigner function. As we already did in the previous section, let us first define a *general quadrature* defined along an arbitrary direction ϕ of phase space as

$$\hat{X}^\phi = \hat{X}\cos\phi + \hat{P}\sin\phi = e^{-\mathrm{i}\phi}\hat{a} + e^{\mathrm{i}\phi}\hat{a}^\dagger. \tag{167}$$

We will denote the quadrature defined along its orthogonal direction by $\hat{P}^\phi = \hat{X}^{\phi+\pi/2}$. These orthogonal quadratures define a new phase-space coordinate system (x^ϕ, p^ϕ) rotated by an angle ϕ respect to the original (x, p) system (see

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[15] This is trivially proved by using again the Baker–Campbell–Haussdorf lemma (84).

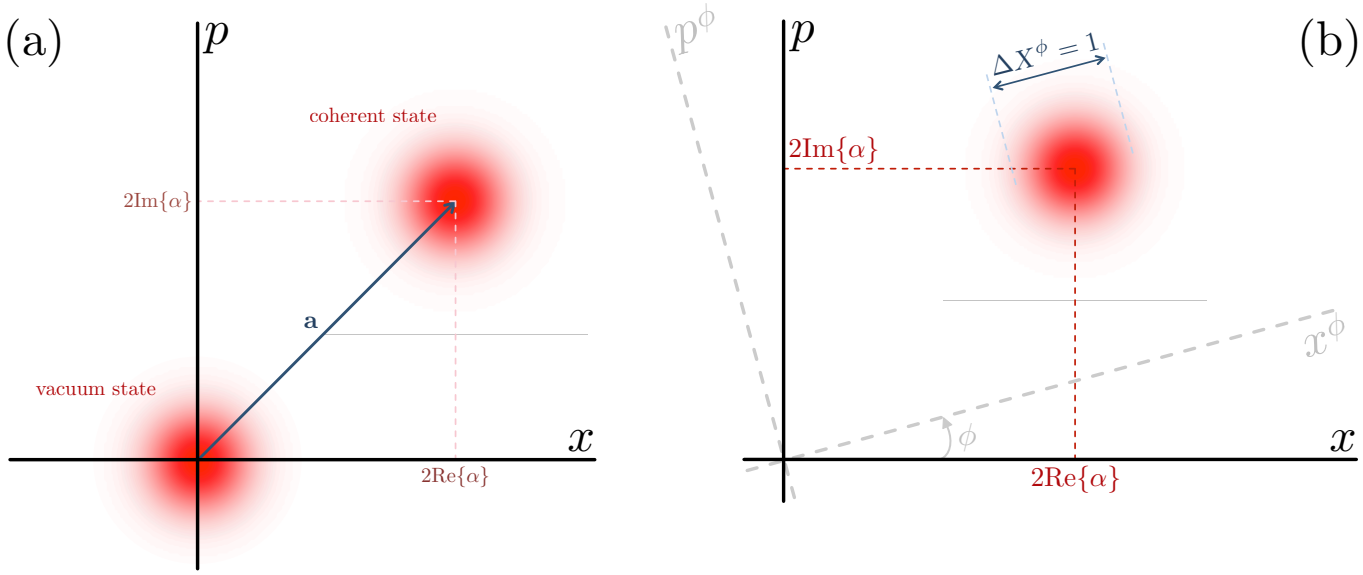

Figure 5. (a) A coherent state of arbitrary amplitude can be generated by applying a displacement to the vacuum state. (b) Wigner function of a coherent state. The function is rotationally symmetric around its center, reflecting the fact that quadratures are affected by vacuum fluctuations in all directions.

Fig. 5b). They also satisfy the commutation relation $[\hat{X}^\phi, \hat{P}^\phi] = 2\mathrm{i}$, and hence must satisfy the uncertainty relation $\Delta X^\phi \Delta P^\phi \geq 1$. The statistics of a measurement of one of such general quadratures $\hat{X}^\phi$ will be described by a Gaussian distribution with mean $\langle \hat{X}^\phi \rangle = 2|\alpha| \cos(\phi - \varphi)$, where φ is the phase of α, and uncertainty $\Delta X^\phi = 1$, irrespective of ϕ (note that V is invariant under rotations for a coherent state). Hence, the statistics of a measurement of the quadratures will be spread around their mean equally in any direction of phase space, as can be appreciated from the fact that the Wigner function is invariant under rotations around its mean (it has a circular shape).

The phase-space representation of coherent states allows us to understand its amplitude and phase properties (Fig. 6). This is not trivial for general states, since these are two observables which still lack a satisfactory description in terms of self-adjoint operators [5, 11]; but for coherent states of sufficiently large amplitude, we now show that it is possible to find a proper description. For general states, the expectation values of the quadratures $\langle \hat{\mathbf{R}} \rangle$ define a phase $\varphi = \arctan\langle \hat{P} \rangle / \langle \hat{X} \rangle$ and an amplitude $\mu = \sqrt{\langle \hat{P} \rangle^2 + \langle \hat{X} \rangle^2}$, which in the case of a coherent state $|\alpha\rangle$, are directly related to the coherent-state amplitude by $\alpha = \mu e^{\mathrm{i}\varphi}/\sqrt{2}$. In the classical limit, neglecting quantum noise, these are exactly the phase and amplitude that would be measured for the oscillator. When quantum uncertainties in the quadratures cannot be neglected, it is reasonable to think that φ and μ will still be the mean values measured for the phase and amplitude of the oscillator, but now they will also be affected by some uncertainties, say $\Delta\varphi$ and $\Delta\mu$. It seems obvious from Fig. 6 that these amplitude and phase uncertainties are related to the uncertainties of the quadratures $\hat{X}^\varphi$ and $\hat{P}^\varphi$ in the direction of the state's phase φ. In particular, we have $\Delta\mu = \Delta X^\varphi$ and $\Delta\varphi = \Delta P^\varphi / \mu$. Consequently, we call *amplitude* and *phase* quadratures, to the quadratures in this direction of phase space. Hence, even if at the quantum level we still don't know how assign assign self-adjoint operators to the (absolute) phase and amplitude observables [5, 11], we can somehow relate their properties to those of the amplitude and phase quadratures, at least for Gaussian states with a well defined amplitude, that is, whenever $\mu > \Delta X^\varphi$.

2. *Properties and general Gaussianity criterion*

In the previous subsection we have introduced coherent states as displaced vacuum states, discussing their Wigner function, as well as showing that they are eigenstates of the annihilation operators. Here we provide several interesting properties of these states, and introduce a general criterion to determine whether a given state $\hat{\rho}$ is gaussian.

It is simple to find an explicit representation of the coherent states in terms of the basis of number states. For that,

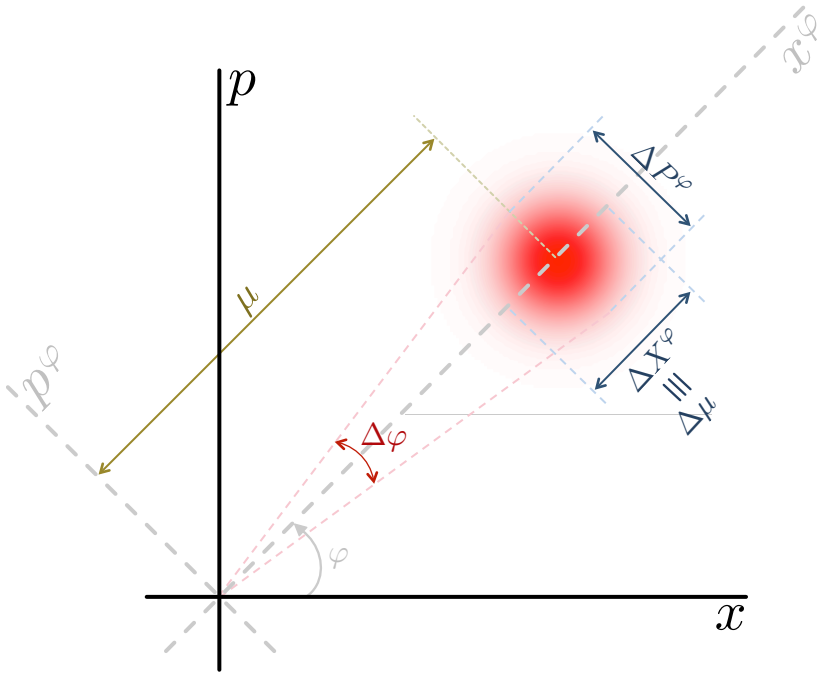

Figure 6. Quantum amplitude–phase properties of a coherent state. $\Delta\mu$ and $\Delta\varphi$ represent the uncertainties in the amplitude and phase, μ and φ, of the oscillator, which are clearly related to the uncertainties of the amplitude and phase quadratures, $\hat{X}^{\varphi}$ and $\hat{P}^{\varphi}$, respectively.

we simply write the displacement operator as[16]

$$\hat{D}\left(\alpha\right)=\exp\left(-|\alpha|^{2}/2\right)\exp\left(\alpha\hat{a}^{\dagger}\right)\exp\left(-\alpha^{*}\hat{a}\right), \tag{168}$$

and Taylor-expand the exponentials to obtain

$$|\alpha\rangle=e^{-|\alpha|^{2}/2}\sum_{n=0}^{\infty}\frac{\alpha^{n}}{n!}\hat{a}^{\dagger n}|0\rangle=\sum_{n=0}^{\infty}e^{-|\alpha|^{2}/2}\frac{\alpha^{n}}{\sqrt{n!}}|n\rangle, \tag{169}$$

where we have used $\hat{a}^{\dagger n}|0\rangle=\sqrt{n!}|n\rangle$ by virtue of (79). Note that for $\alpha=0$, coherent states are nothing but the vacuum state. For any other value of α coherent states do not have a well defined number of excitations; instead, the number of *quanta* is distributed according to a Poisson probability distribution

$$P_{n}\left(\alpha\right)=|\langle n|\alpha\rangle|^{2}=e^{-|\alpha|^{2}}\frac{|\alpha|^{2n}}{n!}, \tag{170}$$

with mean photon number $\langle\hat{N}\rangle=|\alpha|^{2}$ and uncertainty $\Delta N=|\alpha|$. The shape of this distribution is heavily dependent on the value of $|\alpha|^{2}$, as shown in Fig. **ToDo**. When $|\alpha|^{2}\gg1$, the distribution looks quite symmetric and normal, just peaked at the mean $|\alpha|^{2}$ with a relatively thin width $|\alpha|$. In this limit, one can even make a Gaussian approximation for the distribution in many situations, without loosing to much accuracy. However, when $|\alpha|^{2}$ is not so large, the distribution is highly asymmetric, and it's even peaked at 0 when $|\alpha|^{2}\leq1$.

It is easy to show that coherent states form a resolution of the identity. For this, we consider the corresponding sum of projectors and use (169), obtaining

$$\int_{\mathbb{C}}d^{2}\alpha|\alpha\rangle\langle\alpha|\underbrace{=}_{\alpha=re^{\mathrm{i}\phi}}\sum_{m,n=0}^{\infty}\int_{0}^{\infty}drre^{-r^{2}}\frac{r^{m+n}}{\sqrt{m!n!}}\underbrace{\int_{0}^{2\pi}d\phi e^{\mathrm{i}\phi(m-n)}}_{2\pi\delta_{mn}}|m\rangle\langle n|=\pi\sum_{n=0}^{\infty}\frac{1}{n!}\int_{0}^{\infty}dr2r^{2n+1}e^{-r^{2}}|n\rangle\langle n|. \tag{171}$$

[16] This is easy to prove by using the disentangling Baker-Campbell-Haussdorf lemma (125) with $\hat{A}=\alpha\hat{a}^{\dagger}$ and $\hat{B}=-\alpha^{*}\hat{a}$.

The integral is easily carried out[17] as $\int_0^\infty dr 2r^{2n+1}e^{-r^2} = n!$, obtaining then the desired completeness relation

$$\int_{\mathbb{C}} \frac{d^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = \sum_{n=0}^{\infty}|n\rangle\langle n| = \hat{I}. \tag{173}$$

However, coherent states are not orthogonal, and hence, they do not form a standard basis of the Hilbert space. Instead, they form an overcomplete basis, which can still be useful for many calculations, as we shall see later. Let us here prove that coherent states are not orthogonal. To this aim, note that (134) allows us to write the concatenation of two displacements as

$$\hat{D}(\alpha_1)\hat{D}(\alpha_2) = e^{\mathrm{iIm}\{\alpha_1\alpha_2^*\}}\hat{D}(\alpha_1+\alpha_2), \tag{174}$$

and also that $\hat{D}^\dagger(\alpha) = \hat{D}(-\alpha)$. Hence, the overlap between two coherent states can be written as[18]

$$\langle\alpha|\beta\rangle = \langle 0|\hat{D}(-\alpha)\hat{D}(\beta)|0\rangle = e^{-\mathrm{iIm}\{\alpha\beta^*\}}\langle 0|\beta-\alpha\rangle = e^{-\mathrm{iIm}\{\alpha\beta^*\}}e^{-|\alpha-\beta|^2/2}, \tag{176}$$

where we have used the Fock-state representation (169) of coherent states.

Finally, coherent states allow us to find a criterion for a given state $\hat{\rho}$ to be Gaussian. To this aim, just note that, using the completeness of the coherent states and the displacement decomposition[19]

$$\hat{D}(\alpha) = \exp\left(|\alpha|^2/2\right)\exp\left(-\alpha^*\hat{a}\right)\exp\left(\alpha\hat{a}^\dagger\right), \tag{177}$$

the quantum characteristic function can be written as

$$\begin{aligned}\mathrm{tr}\{\hat{\rho}\hat{D}(x,p)\} &\underbrace{=}_{\beta=(x+\mathrm{i}p)/2} e^{|\beta|^2/2}\mathrm{tr}\left\{e^{\beta\hat{a}^\dagger}\hat{\rho}e^{-\beta^*\hat{a}}\right\} = e^{|\beta|^2/2}\mathrm{tr}\left\{\int_{\mathbb{C}}\frac{d^2\nu}{\pi}|\nu\rangle\langle\nu|e^{\beta\hat{a}^\dagger}\hat{\rho}e^{-\beta^*\hat{a}}\right\} \\ &= \int_{\mathbb{C}}\frac{d^2\nu}{\pi}e^{|\beta|^2/2}\langle\nu|e^{\beta\hat{a}^\dagger}\hat{\rho}e^{-\beta^*\hat{a}}|\nu\rangle = \int_{\mathbb{C}}\frac{d^2\nu}{\pi}e^{\beta\nu^*-\beta^*\nu+|\beta|^2/2}\langle\nu|\hat{\rho}|\nu\rangle.\end{aligned} \tag{178}$$

The Wigner function, being a Fourier transform of the characteristic function, will be Gaussian whenever the latter can be written as an exponential of a quadratic form of the phase-space variables. On other hand, it is clear from (178) that this will happen whenever $\langle\nu|\hat{\rho}|\nu\rangle$ also admits such a form in terms of ν. This gives us an easy way of checking whether the state is Gaussian or not: we just need to evaluate its overlap with a coherent state. More precisely:

$$\hat{\rho}\text{ is Gaussian} \Leftrightarrow \langle\nu|\hat{\rho}|\nu\rangle = e^{f(\nu)},\ \text{with } f(\nu)\text{ at most quadratic in } \nu\in\mathbb{C}, \text{and } |\nu\rangle \text{ a coherent state.}$$

Once we are sure that the state is Gaussian, it is typically useful to evaluate the expectation values $\langle\hat{a}\rangle$, $\langle\delta\hat{a}^2\rangle = \langle\hat{a}^2\rangle - \langle\hat{a}\rangle^2$, and $\langle\delta\hat{a}^\dagger\delta\hat{a}\rangle = \langle\hat{a}^\dagger\hat{a}\rangle - |\langle\hat{a}\rangle|^2$, from which we can write down the mean vector and covariance matrix as

$$\mathbf{d} = 2(\mathrm{Re}\{\langle\hat{a}\rangle\}, \mathrm{Im}\{\langle\hat{a}\rangle\})^T, \tag{179a}$$

$$V = (1+2\langle\delta\hat{a}^\dagger\delta\hat{a}\rangle)\begin{pmatrix}1&0\\0&1\end{pmatrix} + 2\begin{pmatrix}\mathrm{Re}\{\langle\delta\hat{a}^2\rangle\} & \mathrm{Im}\{\langle\delta\hat{a}^2\rangle\}\\ \mathrm{Im}\{\langle\delta\hat{a}^2\rangle\} & \mathrm{Re}\{\langle\delta\hat{a}^2\rangle\}\end{pmatrix}. \tag{179b}$$

Of course, coherent states themselves satisfy the criterion established above. In particular, for $\hat{\rho} = |\alpha\rangle\langle\alpha|$ we can write $\langle\nu|\hat{\rho}|\nu\rangle = |\langle\nu|\alpha\rangle|^2 = \exp(|\nu-\alpha|^2)$, which has an exponent quadratic in ν. Moreover, since coherent states are eigenstates of the annihilation operator, in this case the required expectation values are incredibly simple to evaluate, obtaining $\langle\alpha|\hat{a}|\alpha\rangle = \alpha$ and $\langle\alpha|\delta\hat{a}^2|\alpha\rangle = \langle\alpha|\delta\hat{a}^\dagger\delta\hat{a}|\alpha\rangle = 0$, and leading to the mean vector and covariance matrix discussed in the previous section.

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[17] For example, using the variable change $z = x^2$, we can write

$$\begin{aligned}\int_0^\infty dr 2r^{2n+1}e^{-r^2} &= \int_0^\infty dz z^n e^{-z} = \lim_{\kappa\to 1}\int_0^\infty dz(-1)^n\partial_\kappa^n e^{-\kappa z} = (-1)^n\lim_{\kappa\to 1}\partial_\kappa^n\int_0^\infty dz e^{\kappa z} \\ &= (-1)^n\lim_{\kappa\to 1}\partial_\kappa^n\frac{1}{-\kappa}(\underbrace{e^{-\kappa\infty}}_{0}-1) = (-1)^n\lim_{\kappa\to 1}\partial_\kappa^n\frac{1}{\kappa} = (-1)^n n!\lim_{\kappa\to 1}(-1)^n\frac{1}{\kappa^{n+1}} = n!\end{aligned} \tag{172}$$

[18] An alternative proof of this expression can be obtained by using the Fock-state representation (169) as follows:

$$\langle\alpha|\beta\rangle = \sum_{n,m=0}e^{-(|\alpha|^2-|\beta|^2)/2}\frac{\alpha^{*n}\beta^m}{\sqrt{n!m!}}\underbrace{\langle n|m\rangle}_{\delta_{nm}} = e^{-(|\alpha|^2-|\beta|^2)/2}\underbrace{\sum_{n=0}\frac{(\alpha^*\beta)^n}{n!}}_{e^{\alpha^*\beta}} = e^{-\mathrm{iIm}\{\alpha\beta^*\}}e^{-|\alpha-\beta|^2/2}. \tag{175}$$

[19] Again easy to prove by using the (125) with $\hat{A} = -\alpha^*\hat{a}$ and $\hat{B} = \alpha\hat{a}^\dagger$.

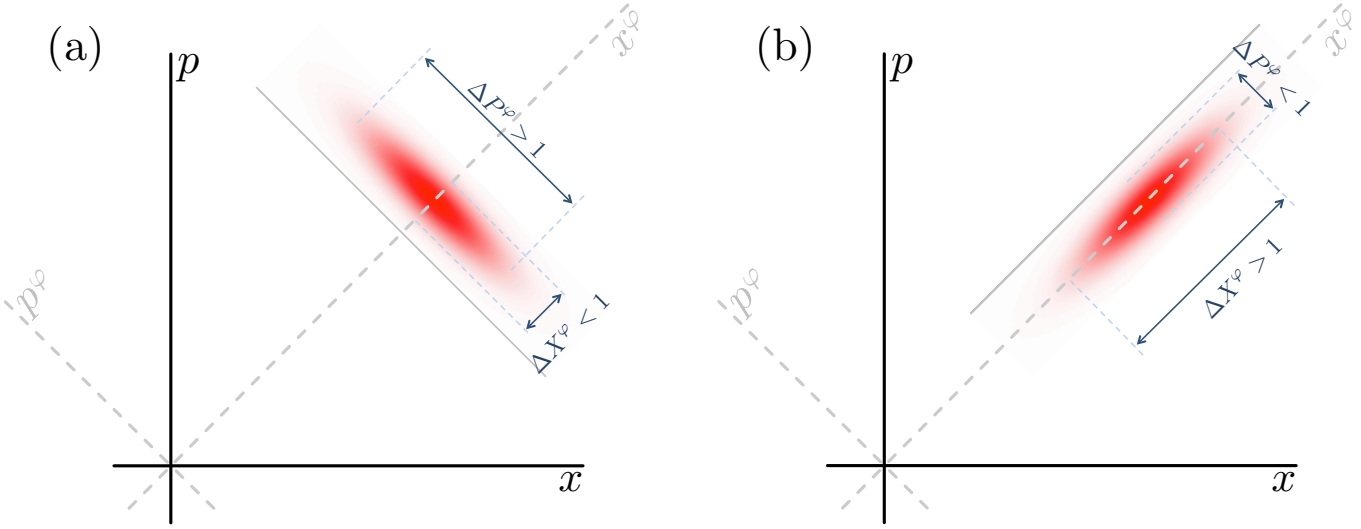

Figure 7. Wigner functions of two squeezed states. In (a) the uncertainty of the amplitude quadrature is reduced below the vacuum level at the expense of increasing the uncertainty of the phase quadrature. In (b), on the other hand, it is the phase quadrature the one which is squeezed, while the amplitude quadrature becomes more noisy.

3. Bridge between quantum and classical physics

We have seen that the classical and quantum formalisms seem dramatically different: While classically the oscillator can have any positive value of the energy and has a definite trajectory in phase space, quantum mechanics allows only for discrete values of the energy and introduces position and momentum uncertainties which prevent the existence of well defined trajectories. In this section we show that coherent states are the easiest way of reconciling these two seemingly contradictory descriptions.

Quantum mechanics is all about predicting the statistics of experiments. Hence, the way of connecting it to classical mechanics is by finding the quantum state that predicts that the statistics obtained in the experiment will coincide with what is classically expected. In the following we show that coherent states with $|\alpha| \gg 1$ satisfy the desired conditions.

Let us start by showing how the classical well-defined trajectories can be recovered. For this, we start from a coherent state $|\psi(0)\rangle = |\alpha\rangle$ at time zero, and let it evolve by the Hamiltonian of the harmonic oscillator (76), that is, by the corresponding time-evolution operator. We obtain

$$|\psi(t)\rangle = e^{-\mathrm{i}\omega t\hat{N}}|\alpha\rangle = \sum_{n=0}^{\infty} e^{-|\alpha|^2/2}\frac{\alpha^n}{\sqrt{n!}}e^{-\mathrm{i}n\omega t}|n\rangle = \left|e^{-\mathrm{i}\omega t}\alpha\right\rangle, \tag{180}$$

that is, another coherent state, with a time-dependent amplitude $\alpha(t) = e^{-\mathrm{i}\omega t}\alpha$, which is equal to the expectation value of the annihilation operator, $\langle\hat{a}(t)\rangle = \alpha(t)$. Reminding that this is precisely the solution for the harmonic oscillator in the complex representation, this means that, on average, the oscillator indeed describes the classical trajectory. Moreover, since the state is coherent at all times, we know that the uncertainty of any quadrature $\hat{X}^\phi$ is independent of is amplitude, specifically $\Delta X^\phi(t) = 1$. Hence, the uncertainty becomes less and less relevant the bigger is the radius of the trajectory, that is, the *signal-to-noise ratio* satisfies $|\alpha|/\Delta X^\phi \overset{|\alpha|\to\infty}{\longrightarrow} \infty$. In other words, *for all practical purposes*, in this limit the oscillator seems to describe the classical trajectory when measured in the laboratory, where other sources of classical noise and imprecision will dominate over the tiny quantum noise.

Let us now move on to the energy-quantization issue. The ratio between the energies of two consecutive number states is $E_{n+1}/E_n = (n+3/2)/(n+1/2)$. Hence, as the number of excitations increases, the discrete character of the energy becomes barely perceptive, that is, $E_{n+1}/E_n \sim 1$ if $n \gg 1$. Thus, *for all practical purposes*, we can recover a seemingly continuous energy spectrum if the state of the oscillator projects only on high-order (approximately contiguous) number states. As we saw in (170), this is precisely the case of coherent states with $|\alpha| \gg 1$, which lead to a narrowly-peaked Poisson number distribution centered at $\langle\hat{N}\rangle = |\alpha|^2$ with width $\Delta N = |\alpha|$.

I. Squeezed states

1. Definition and relevance

Two important applications of harmonic oscillators are *sensing* and *information encoding/trasmission*: The oscillator is put in contact with the system or signal that we want to study or transmit, and it gets codified as phase or amplitude modulations in the oscillator (think, for example, about gravitational waves encoded as amplitude or phase modulations in the light circulating at the LIGO interferometer). We have seen in the previous section that when the oscillator is in a coherent state both its amplitude and phase suffer from uncertainties, and hence the encoded signal cannot be perfectly retrieved from measurements on the oscillator. When any other source of technical noise is removed, that is, when the measurement equipment behaves basically as ideal, this so-called *quantum shot noise* becomes the main limitation. Moreover, when the signal generated by the system that we want to study is tiny (as gravitational waves are), it can even be hidden below the quantum noise, so that it might not be perceived at all.

Squeezed states are the solution to this problem. Suppose that the signal is encoded in the amplitude of the oscillator. In a coherent state the amplitude and phase quadratures are affected by equal uncertainties $\Delta X^{\varphi} = \Delta P^{\varphi} = 1$. However, we can conceive a state of the oscillator in which the uncertainty of the amplitude quadrature is reduced, while that of the phase quadrature is increased, say $\Delta X^{\varphi} \ll 1$ and $\Delta P^{\varphi} \gg 1$, so that the product of uncertainties keeps lower bounded by one, $\Delta X^{\varphi} \Delta P^{\varphi} \geq 1$. The Wigner function of one of such states is depicted in Fig. 7a. In this case the amplitude quadrature is well defined, and one can in principle monitor its modulations with arbitrary accuracy. Of course, this is accomplished at the expense of not being able to retrieve any information from the phase quadrature, but that is not a problem if we only care about the signal encoded in the amplitude quadrature.

We will then define *squeezed states* as those in which some quadrature, say $\hat{X}^{\phi}$, has an uncertainty below the vacuum or coherent level, that is, $\Delta X^{\phi} < 1$. We then say that quadrature $\hat{X}^{\phi}$ is *squeezed*, while its conjugate $\hat{P}^{\phi}$ is *antisqueezed* ($\Delta P^{\phi} > 1$). Together with the *amplitude squeezed state* already introduced (for which $\phi = \varphi$), we show a *phase squeezed state* (for which $\phi = \varphi + \pi/2$) in Fig. 7b. Let us now study one specially relevant type of squeezed states.

2. Minimum uncertainty squeezed states

Minimum uncertainty states are states which satisfy the lower bound of the quadrature uncertainty relation, that is, $\Delta X^{\phi} \Delta P^{\phi} = 1 \ \forall \phi$. The simplest of these states is the vacuum state $|0\rangle$; any other number state $|n \neq 0\rangle$ is not contained in this class, as it is easily checked that it satisfies $\Delta X^{\phi} = 2n + 1$ for any ϕ. Coherent states, on the other hand, are minimum uncertainty states, as they are obtained from vacuum by the displacement transformation, which does not change the quadrature variances.

It is possible to generate squeezed states of this kind by using the *squeezing operator*

$$\hat{S}(z) = \exp\left(\frac{z^*}{2}\hat{a}^2 - \frac{z}{2}\hat{a}^{\dagger 2}\right), \tag{181}$$

where $z \in \mathbb{C}$ is called the *squeezing parameter*. Note that this can be seen as generalization of the displacement operator (163), but with $\hat{a}^2$ instead of $\hat{a}$ in the exponent. Note that since the exponent is still quadratic in the quadratures, the squeezing operator is a Gaussian unitary.

Let us analyze how this transformation acts on the annihilation operators. We will use again the Baker-Campbell-Haussdorf lemma (84), which defining $\hat{B} = \frac{z}{2}\hat{a}^{\dagger 2} - \frac{z^*}{2}\hat{a}^2$, requires the commutators

$$\begin{aligned}
[\hat{B}, \hat{a}] &= -z\hat{a}^{\dagger}, \\
[\hat{B}, [\hat{B}, \hat{a}]] &= |z|^2 \hat{a}, \\
[\hat{B}, [\hat{B}, [\hat{B}, \hat{a}]]] &= -z|z|^2 \hat{a}^{\dagger}, \\
[\hat{B}, [\hat{B}, [\hat{B}, [\hat{B}, \hat{a}]]]] &= |z|^4 \hat{a}, \\
&\vdots
\end{aligned} \tag{182}$$

so that writing z in the polar form $z = r\exp(\mathrm{i}\theta)$, with $r \in [0, \infty]$ and $\theta \in [0, 2\pi[$, and splitting the sum of the lemma

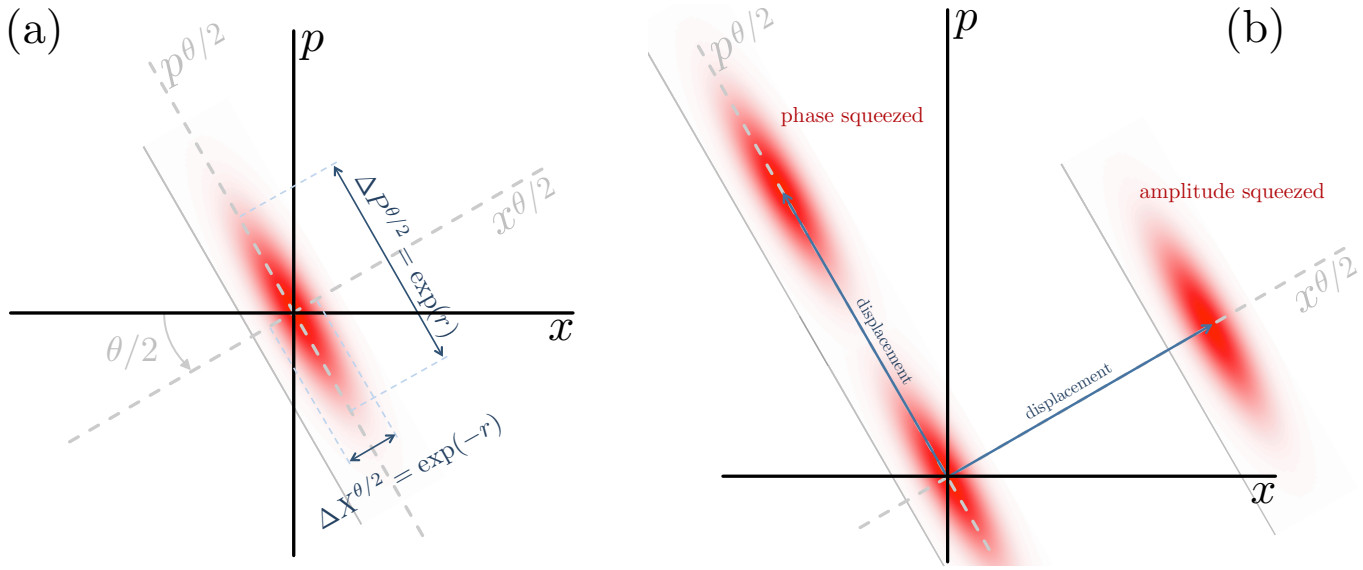

Figure 8. (a) Wigner function of a squeezed vacuum state. (b) Applying displacements in the direction of the squeezed or antisqueezed quadratures, one obtains amplitude or phase squeezed states, respectively.

into even and odd terms, we obtain

$$\begin{aligned}\hat{S}^{\dagger}(z)\,\hat{a}\hat{S}(z) &= \sum_{n=0}^{\infty}\frac{1}{(2n)!}\underbrace{[\hat{B},[\hat{B},...[\hat{B}}_{2n},\underbrace{\hat{a}]...]]}_{2n} + \frac{1}{(2n+1)!}\underbrace{[\hat{B},[\hat{B},...[\hat{B}}_{2n+1},\underbrace{\hat{a}]...]]}_{2n+1} \\ &= \left[\sum_{n=0}^{\infty}\frac{r^{2n}}{(2n)!}\right]\hat{a} - e^{\mathrm{i}\theta}\left[\sum_{n=0}^{\infty}\frac{r^{2n+1}}{(2n+1)!}\right]\hat{a}^{\dagger} \\ &= \hat{a}\cosh r - e^{\mathrm{i}\theta}\hat{a}^{\dagger}\sinh r.\end{aligned} \tag{183}$$

In terms of quadratures, this expression is easily rewritten as

$$\hat{S}^{\dagger}(z)\,\hat{X}^{\theta/2}\hat{S}(z) = e^{-r}\hat{X}^{\theta/2} \qquad \text{and} \qquad \hat{S}^{\dagger}(z)\,\hat{P}^{\theta/2}\hat{S}(z) = e^{r}\hat{P}^{\theta/2}, \tag{184}$$

which shows that the squeezing transformation corresponds to the contraction and dilation of two orthogonal directions of phase space. In the notation of Eq. (150), the linear transformation has $\mathbf{a} = (0,0)^T$ and $S(z) = R^T(\theta/2)Q(r)R(\theta/2)$, where we have defined the matrix $Q(r) = \left(\begin{smallmatrix} e^{-r} & 0 \\ 0 & e^{r} \end{smallmatrix}\right)$, and $R(\theta/2)$ is just a rotation matrix as introduced in Eq. (143).

Suppose now that prior to the transformation the state of the system was vacuum, defined by the statistical properties $\langle\hat{X}^{\phi}\rangle = 0$ and $\Delta X^{\phi} = 1\ \forall\phi$ as already seen. After the transformation (184), the mean of any quadrature is still zero, but the uncertainty of quadrature $\hat{X}^{\theta/2}$ has decreased to $\Delta X^{\theta/2} = \exp(-r)$, while that of quadrature $\hat{P}^{\theta/2}$ has increased to $\Delta P^{\theta/2} = \exp(r)$. Hence, the squeezing operator creates a minimum uncertainty squeezed state, since $\Delta X^{\theta/2}\Delta P^{\theta/2} = 1$. This state $|z\rangle = \hat{S}(z)|0\rangle$ is usually called the *squeezed vacuum state*. It is a Gaussian state centered at the origin of phase space, $\mathbf{d}_{|z\rangle} = (0,0)^T$, and with a covariance matrix

$$V_{|z\rangle}(z) = S(z)V_{|0\rangle}S^T(z) = R^T(\theta/2)Q(2r)R(\theta/2), \tag{185}$$

where we have used (149) and $V_{|0\rangle} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$. We show the corresponding Wigner function in Fig. 8a. The uncertainty circle associated to the vacuum state has turned into an ellipse, with the principal axis oriented along axes rotated by $\theta/2$ in phase space, as shown explicitly by the form we used for the covariance matrix above. An amplitude squeezed state can be then created by applying a subsequent displacement along the $\theta/2$ axis as shown in Fig. 8b. If the displacement is applied along the $(\theta+\pi)/2$ direction, then a phase squeezed state is obtained. As displacements do not change the uncertainty properties of the state, these amplitude or phase squeezed states are still minimum uncertainty states.

It is instructive to show that the squeezed vacuum state is Gaussian by using the criterion that we developed above, based on $\langle\nu|\hat{\rho}|\nu\rangle$, with $|\nu\rangle$ a coherent state. In order to evaluate this, we use the following expansion for the squeezing

operator, which is of general practical use:[20]

$$\hat{S}(z) = e^{-\frac{1}{2}e^{\mathrm{i}\theta}\tanh(r)\hat{a}^{\dagger 2}}(\cosh r)^{-\hat{a}^\dagger\hat{a}-1/2}e^{\frac{1}{2}e^{-\mathrm{i}\theta}\tanh(r)\hat{a}^2}, \tag{187}$$

leading to

$$\langle\nu|\hat{\rho}|\nu\rangle = \left|\langle\nu|\hat{S}(z)|0\rangle\right|^2 = \frac{1}{\cosh r}\left|e^{-\frac{1}{2}\tanh(r)e^{\mathrm{i}\theta}\nu^{*2}}\langle\nu|0\rangle\right|^2 = \frac{1}{\cosh r}e^{-\frac{1}{2}\tanh(r)\left(e^{-\mathrm{i}\theta}\nu^2+e^{\mathrm{i}\theta}\nu^{*2}\right)-|\nu|^2}, \tag{188}$$

which is indeed the exponential of a quadratic form. On the other hand, using (183) it is simple find

$$\langle\hat{a}\rangle = \langle 0|\hat{S}^\dagger(z)\hat{a}\hat{S}(z)|0\rangle = 0, \tag{189a}$$

$$\langle\hat{a}^2\rangle = \langle 0|(\hat{a}\cosh r - e^{\mathrm{i}\theta}\hat{a}^\dagger\sinh r)^2|0\rangle = -e^{\mathrm{i}\theta}\cosh r\sinh r, \tag{189b}$$

$$\langle\hat{a}^\dagger\hat{a}\rangle = \langle 0|(\hat{a}^\dagger\cosh r - e^{-\mathrm{i}\theta}\hat{a}\sinh r)(\hat{a}\cosh r - e^{\mathrm{i}\theta}\hat{a}^\dagger\sinh r)|0\rangle = \sinh^2 r, \tag{189c}$$

which using (179) lead to the mean vector and covariance matrix that we already introduced above.

It is finally interesting to write the squeezed vacuum state in the number state basis. Using (187) and expanding the exponentials in Taylor series, it is immediate to find

$$\hat{S}(z)|0\rangle = \sum_{n=0}^{\infty}\frac{(-1)^n}{2^n n!}\sqrt{\frac{(2n)!}{\cosh r}}e^{\mathrm{i}n\theta}\tanh^n r\,|2n\rangle. \tag{190}$$

The most characteristic feature of this state is that it contains only even Fock states. This comes physically from the fact that the squeezing operator can generate excitations only by pairs, unlike the displacement operator. The mean of the number operator has been provided above, $\langle\hat{N}\rangle = \sinh^2 r$, while we can evaluate its variance from the Gaussian moment theorem (139), which holds as well for annihilation and creation operators (since they are just linear in the quadratures), so that, in this case

$$\langle\hat{N}^2\rangle = \langle\hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}\rangle = \langle\hat{a}^\dagger\hat{a}\rangle\langle\hat{a}^\dagger\hat{a}\rangle + \langle\hat{a}^{\dagger 2}\rangle\langle\hat{a}^2\rangle + \langle\hat{a}^\dagger\hat{a}\rangle\underbrace{\langle\hat{a}\hat{a}^\dagger\rangle}_{\langle\hat{a}^\dagger\hat{a}\rangle+1} = 2\langle\hat{N}\rangle^2 + \langle\hat{N}\rangle + |\langle\hat{a}^2\rangle|^2, \tag{191}$$

leading to a variance

$$V(N) = \langle\hat{N}^2\rangle - \langle\hat{N}\rangle^2 = \sinh^4 r + \sinh^2 r + \frac{1}{4}\sinh^2 2r. \tag{192}$$

Remarkably, the uncertainty of the number of quanta is always of the same order of their mean, specifically,

$$\frac{\langle\hat{N}\rangle}{\Delta N} = \frac{\sinh^2 r}{\sqrt{\sinh^4 r + \sinh^2 r + \frac{1}{4}\sinh^2 2r}} \overset{r\to\infty}{\longrightarrow} \frac{1}{\sqrt{2}}. \tag{193}$$

Hence, unlike for coherent states, the width of the distribution of quanta is large, no matter the number of quanta.

J. Thermal states

So far we have only talked about pure states. However, in general the state of the harmonic oscillator can be mixed. As highlighted in the introduction to quantum mechanics, this will happen whenever the oscillator gets correlated with another system (either classical or quantum) to which we don't have access. This means that information about the oscillator leaks out to this inaccessible system, and we are then forced to use a mixed state for the oscillator that reflects our ignorance.

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[20] The proof of this identity is not entirely trivial, and can be checked in [67]. Regarding this expression, the most important idea to keep is the following. Whenever one has a set of operators $\{\hat{Q}_j\}_{j=1,2,...,J}$ which forms a closed algebra (that is, the commutator of any two operators of the set is proportional to another operator of the set), then, it is possible to *disentangle* any exponential as

$$e^{\sum_{j=1}^J c_j\hat{Q}_j} = \prod_{j=1}^J e^{f_j(\mathbf{c})\hat{Q}_j}, \tag{186}$$

where $\mathbf{c} = (c_1, c_2, ..., c_J)$ collects a set of complex coefficients, and the disentangling coefficients $f_j(\mathbf{c})$ can be found with the procedure explained in [67].

Given a system whose associated Hilbert space has dimension d, we have already seen that its maximally-mixed state is $\hat{\rho}_{\rm MM} = \hat{I}/d$. As it is proportional to the identity, this state is invariant under changes of basis, and hence, the eigenvalues of any observable of the system are equally likely. This agrees with what one expects intuitively from a state which has leaked the maximum amount of information to another system: the joint uncertainty of all observables is maximized. In particular, the von Neumann entropy, which is a measure of the mixedness of the state, reaches its maximum $S[\hat{\rho}_{\rm MM}] = \log d$.

For infinite-dimensional Hilbert spaces ($d \to \infty$) this state is not physical since it has infinite energy, e.g., $\mathrm{tr}\{\hat{\rho}\hat{N}\} = \lim_{d\to\infty} \sum_{n=0}^{d} n/d \to \infty$ for the harmonic oscillator. Hence, finding the maximally-mixed state in infinite dimension makes sense only if one adds an energy constraint such as $\mathrm{tr}\{\hat{\rho}\hat{H}\} = \bar{E}$, where $\bar{E}$ is a positive real. It is easy to prove, and we do so below, that the state that maximizes the von Neumann entropy subject to this constraint is

$$\hat{\rho}_{\rm th}(\bar{E}) = \frac{\exp(-\beta\hat{H})}{\mathrm{tr}\{\exp(-\beta\hat{H})\}}, \tag{194}$$

where β can be found from

$$\bar{E} = \frac{\mathrm{tr}\{\hat{H}\exp(-\beta\hat{H})\}}{\mathrm{tr}\{\exp(-\beta\hat{H})\}} = -\partial_\beta \ln\left[\mathrm{tr}\left\{e^{-\beta\hat{H}}\right\}\right] = -\partial_\beta \ln\left[\sum_n e^{-\beta E_n}\right], \tag{195}$$

where in the last equality we have performed the trace in the basis of eigenstates of the Hamiltonian (assumed countable for simplicity), denoting by E_n the corresponding eigenenergies. The expression between square brackets is known in statistical physics as the *partition function*, $Z = \sum_n e^{-\beta E_n}$, and it's *the* central object in that field. it is remarkable that it appears naturally in this quantum context when maximizing the entropy subject to an energy constraint. But the connection to statistical physics doesn't end there. The probability of obtaining eigenvalue E_n in an energy measurement decreases exponentially with the energy, that is,

$$p(E_n) = \langle E_n|\hat{\rho}_{\rm th}|E_n\rangle = e^{-\beta E_n}/Z, \tag{196}$$

where $|E_n\rangle$ are is the corresponding eigenvector of the Hamiltonian. This is precisely the Boltzman distribution for the energies, as predicted in statistical physics for a system at thermal equilibrium with temperature $T = 1/k_B\beta$, where k_B is the Boltzmann constant. Hence, the state $\hat{\rho}_{\rm th}$ is state is known as *thermal* state, and can be parametrized either by a mean energy $\bar{E}$ or, equivalently, by a temperature T (or its inverse β), related by the constraint equation (195). It is interesting to remark that this result is valid for any dimension d, and we recover the unconstrained maximally-mixed state $\hat{I}/d$ for infinite temperature ($\beta \to 0$).

Let us differ the proof of $\hat{\rho}_{\rm th}(\bar{E})$ as the energy-constrained maximally-mixed state to the end of the section, and focus now on what this means for the harmonic oscillator, whose Hamiltonian is $\hat{H} = \hbar\omega(\hat{N} + 1/2)$. First, taking into account that $\{E_n = \hbar\omega(n + 1/2)\}_{n=0,1,\ldots}$, the sum in (195), that is, the partition function, is easily carried out as[21]

$$Z = \mathrm{tr}\left\{e^{-\beta\hat{H}}\right\} = e^{-\beta\hbar\omega/2}\sum_{n=0}^{\infty}\left(e^{-\beta\hbar\omega}\right)^n = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}}. \tag{197}$$

Hence, equation (195) reads

$$\bar{E} = \partial_\beta\left[\frac{\beta\hbar\omega}{2} + \ln\left(1 - e^{-\beta\hbar\omega}\right)\right] = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}. \tag{198}$$

Writing the mean energy in terms of the mean number of excitations $\bar{n} = \mathrm{tr}\{\hat{\rho}\hat{N}\}$ as $\bar{E} = \hbar\omega(\bar{n} + 1/2)$, we can rewrite the previous expression as

$$\bar{n} = \frac{\bar{E}}{\hbar\omega} - \frac{1}{2} = \frac{1}{e^{\beta\hbar\omega} - 1}, \tag{199}$$

which is the Bose-Einstein distribution for an equilibrium temperature $T = 1/k_B\beta$.

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[21] Note that this is a simple geometric sum $S = \sum_{m=0}^{M} c^n = 1 + c + \ldots + c^M$ with $c \in [0, 1[$. The sum can be performed with a very simple trick. We multiply by it c, obtaining $cS = c + c^2 + \ldots + c^{M+1}$. Hence, we get $S - cS = 1 - c^{M+1}$, leading to $S = (1-c^{M+1})/(1-c) \underset{M\to\infty}{\to} 1/(1-c)$.

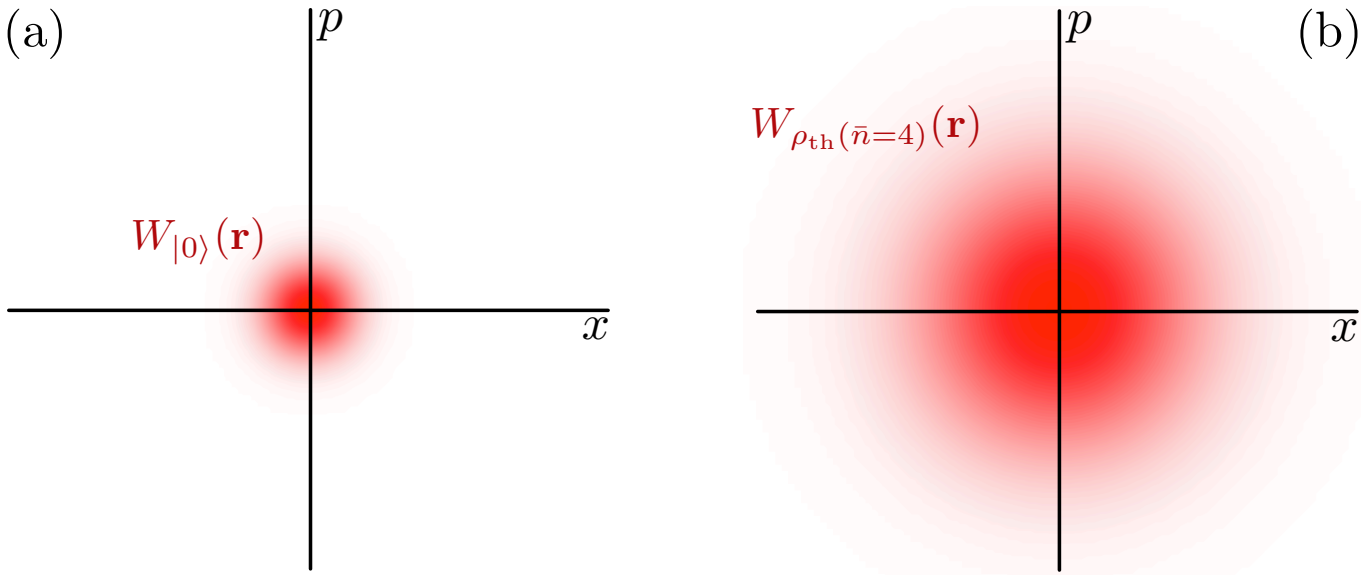

Figure 9. (b) Wigner function of a thermal state with mean excitation number $\bar{n} = 4$. For comparison, we show in (a) the Wigner function of the vacuum state. It can be appreciated that both are rotationally symmetric, but the thermal state has $\sqrt{2\bar{n}+1}$ times more uncertainty than vacuum.

In addition, it is straightforward to show that the thermal state is written in the Fock basis as

$$\hat{\rho}_{\rm th}(\bar{n}) = \sum_{n=0}^{\infty} \underbrace{\frac{\bar{n}^n}{(1+\bar{n})^{1+n}}}_{p_n(\bar{n})} |n\rangle\langle n|, \tag{200}$$

where we parametrize the state in terms of the mean number of quanta $\bar{n}$. As in finite dimension without energy constraints, this state is diagonal, but the distribution is not flat, although it looks flatter the larger is $\bar{n}$, as expected, that is $p_n(\bar{n}) \approx p_{n+1}(\bar{n})$ for $\bar{n} \gg n$.

It is easy to see that the thermal state is Gaussian using the criterion we developed above for the expectation value of the state in a coherent state, $\langle\nu|\hat{\rho}|\nu\rangle$. In this case, we do so by introducing a resolution of the identity $\sum_{n=0}^{\infty} |n\rangle\langle n| = 1$ into this expression, and using the Fock-state representation of coherent states (169). In particular, we get

$$\langle\nu|e^{-\beta\hbar\omega\hat{a}^\dagger\hat{a}}|\nu\rangle = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}\langle\nu|n\rangle\langle n|\nu\rangle = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}|\langle\nu|n\rangle|^2 = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}\frac{|\nu|^{2n}}{n!}e^{-|\nu|^2} = e^{(e^{-\beta\hbar\omega}-1)|\nu|^2}, \tag{201}$$

which is the exponential of a quadratic form in ν. As for the relevant expectation values, we obtain

$$\langle\hat{a}\rangle = \mathrm{tr}\{\hat{a}\hat{\rho}_{\rm th}(\bar{n})\} = \sum_{n=0}^{\infty} \frac{\bar{n}^n}{(1+\bar{n})^{1+n}}\langle n|\hat{a}|n\rangle = 0, \tag{202a}$$

$$\langle\hat{a}^2\rangle = \mathrm{tr}\{\hat{a}^2\hat{\rho}_{\rm th}(\bar{n})\} = \sum_{n=0}^{\infty} \frac{\bar{n}^n}{(1+\bar{n})^{1+n}}\langle n|\hat{a}^2|n\rangle = 0, \tag{202b}$$

$$\langle\hat{a}^\dagger\hat{a}\rangle = \bar{n} \text{ (this is by construction, since it is the energy constrain).} \tag{202c}$$

Hence, using (179), we see that the Wigner function of a thermal state is given by a Gaussian with mean vector $\mathbf{d}_{\rm th} = (0,0)^T$ and a covariance matrix

$$V_{\rm th} = (2\bar{n}+1)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{203}$$

We show it in Fig. 9, where it can be appreciated that thermal states are similar to a vacuum state (rotationally symmetric), but with $\sqrt{2\bar{n}+1}$ times more noise. Consequently, the vacuum state can be seen as a thermal state with zero mean photon number.

Let us conclude this section by proving that the thermal state is the one maximizing the von Neumann entropy of any system when subject to the energy constrain $\mathrm{tr}\{\hat{\rho}\hat{H}\} = \bar{E}$. We do so by Lagrangian optimization, defining the Lagrange function

$$\mathcal{L}[\hat{\rho}] = -\mathrm{tr}\left\{\hat{\rho}\ln\hat{\rho}\right\} + \lambda(1 - \mathrm{tr}\{\hat{\rho}\}) + \beta(\bar{E} - \mathrm{tr}\{\hat{H}\hat{\rho}\}), \tag{204}$$

which includes the energy constraint and the normalization constraint $\mathrm{tr}\{\hat{\rho}\} = 1$ of the state through Lagrange multipliers β and λ, respectively. We use a principle of least action by setting to zero the variation of the Lagrangian function,

$$\delta\mathcal{L}[\hat{\rho}] = \mathcal{L}[\hat{\rho} + \delta\hat{\rho}] - \mathcal{L}[\hat{\rho}] = -\mathrm{tr}\{\delta\hat{\rho}(\ln\hat{\rho} + 1 + \lambda + \beta\hat{H})\} = 0, \tag{205}$$

where we have kept only terms linear in the variation[22] $\delta\hat{\rho}$ and used[23] $\delta(\ln\hat{\rho}) = \delta\hat{\rho}\hat{\rho}^{-1}$. In order to satisfy this condition for arbitrary variations, it must then be satisfied

$$\hat{\rho} = e^{-(\lambda+1)}e^{-\beta\hat{H}}. \tag{206}$$

The Lagrange multipliers are found from the constraints. First, the normalization constraint gives us

$$\mathrm{tr}\{\hat{\rho}\} = e^{-(\lambda+1)}\mathrm{tr}\left\{e^{-\beta\hat{H}}\right\} = 1 \Rightarrow e^{-(\lambda+1)} = 1/\mathrm{tr}\left\{e^{-\beta\hat{H}}\right\}, \tag{207}$$

leading to the form (194) that we wrote for the state. Then, the energy constraint gives us Eq. (195).

K. Final remarks about the quantized expression for the electromagnetic field

Let us conclude this chapter by coming back to the electromagnetic field. It will be convenient to write the fields in terms of annihilation and creation operators, rather than position and momenta as we did in (58). Then for each of the oscillators, we define annihilation and creation operators

$$\hat{a}_n = \sqrt{\frac{\omega_n}{2\hbar}}\left(\hat{q}_n + \frac{\mathrm{i}}{\omega_n}\hat{p}_n\right), \qquad \text{and} \qquad \hat{a}_n^\dagger = \sqrt{\frac{\omega_n}{2\hbar}}\left(\hat{q}_n - \frac{\mathrm{i}}{\omega_n}\hat{p}_n\right), \tag{208a}$$

satisfying canonical commutation relations

$$[\hat{a}_n, \hat{a}_m^\dagger] = \delta_{nm}, \tag{209}$$

leading to following forms of the fields:

$$\hat{\mathbf{A}}(z,t) = \mathbf{e}_x\sum_{n=1}^{\infty}\sqrt{\frac{\hbar}{\varepsilon_0 LS\omega_n}}[\hat{a}_n(t) + \hat{a}_n^\dagger(t)]\sin(k_n z), \tag{210a}$$

$$\hat{\mathbf{E}}(z,t) = \mathrm{i}\mathbf{e}_x\sum_{n=1}^{\infty}\sqrt{\frac{\hbar\omega_n}{\varepsilon_0 LS}}[\hat{a}_n(t) - \hat{a}_n^\dagger(t)]\sin(k_n z), \tag{210b}$$

$$\hat{\mathbf{B}}(z,t) = \mathbf{e}_y\sum_{n=1}^{\infty}\sqrt{\frac{\mu_0\hbar\omega_n}{LS}}[\hat{a}_n(t) + \hat{a}_n^\dagger(t)]\cos(k_n z). \tag{210c}$$

Note that, implicitly, we have adopted the Heisenberg picture in these expressions, since we allow operators to evolve in time.

Along the notes, we will use a notation that is typical in quantum optics: we split the fields in their annihilation and creation parts. For example, for the vector potential we write $\hat{\mathbf{A}}(z,t) = \hat{\mathbf{A}}^{(+)}(z,t) + \hat{\mathbf{A}}^{(-)}(z,t)$, with

$$\hat{\mathbf{A}}^{(+)}(z,t) = \mathbf{e}_x\sum_{n=1}^{\infty}\sqrt{\frac{\hbar}{\varepsilon_0 LS\omega_n}}\hat{a}_n(t)\sin(k_n z) = \left[\hat{\mathbf{A}}^{(-)}(z,t)\right]^\dagger, \tag{211}$$

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[22] Note that we can assume that $[\delta\hat{\rho}, \hat{\rho}] = 0$, in other words, we can restrict variations that only perturb the eigenvalues of the density operator, but not its eigenstates. The reason for this is that, since we are seeking for a time-independent state, the von-Neumann equation implies $[\hat{H}, \hat{\rho}] = 0$, and therefore, we know from the start that the eigenvectors of $\hat{\rho}$ are just the energy eigenstates.

[23] This expression is found as follows. Define $\hat{V} = \ln\hat{\rho}$. Then, taking the variation of this expression, we get $\delta\hat{V} = \ln(\hat{\rho} + \delta\hat{\rho}) - \ln\hat{\rho} = \ln(1 + \delta\hat{\rho}\hat{\rho}^{-1})$, where we have used the fact that $\delta\hat{\rho}$ and $\hat{\rho}$ commute. Now, taking the exponential of this expression and expanding it to first order in $\delta\hat{V}$, we obtain $1 + \delta\hat{\rho}\hat{\rho}^{-1} = e^{\delta\hat{V}} \approx 1 + \delta\hat{V}$, which provides the expression we were looking for.

and we do the same for any other field. This will make some of our derivations more economic in the next chapters.

In terms of annihilation and creation operators, the Hamiltonian for the light field reads then

$$\hat{H}_{\rm L} = \sum_{n=1}^{\infty} \hbar\omega_n \hat{a}_n^\dagger \hat{a}_n, \tag{212}$$

where we have removed the ground-state energy $\hbar\omega_n/2$ of each mode because it will not play any role in future derivations, since the corresponding Hamiltonian term commutes with any other operator. Let us finally remark that the excitations associated to this Hamiltonian are what we call *photons*.

III. QUANTUM THEORY OF ATOMS AND THE TWO-LEVEL APPROXIMATION

The electromagnetic field is composed of degrees of freedom characterized by a uniform energy spectrum, as represented in Fig. **ToDo**. In contrast, with full generality, in quantum optics we call *matter* to any system that interacts with the electromagnetic field, and is composed by degrees of freedom characterized by a non-uniform energy spectrum, which interact with the electromagnetic field. In order to fix ideas, we will focus here on simple atoms, but more complicated systems such as molecules, confined electrons, or even solid-state systems can be approached with similar tools as the ones we will learn here.

A. Atomic energy spectrum

We start by considering the simplest type of matter possible, apart from fundamental particles: the *hydrogen atom*. It consists of a proton and an electron interacting with each other in three dimensions. Let's start first by discussing the degrees of freedom of these system. We first consider the spin 1/2 of the electron and the proton, denoted by the three-component vector operators $\hat{\mathbf{S}}$ and $\hat{\mathbf{I}}$, respectively. These operators commute with each other, and satisfy the angular momentum algebra $[\hat{S}_j, \hat{S}_k] = \mathrm{i}\hbar\sum_{l=1}^{3}\hat{S}_l$, and similarly for the components of $\hat{\mathbf{I}}$. The other degrees of freedom correspond to the relative coordinates between the proton and the electron in 3D, denoted by $\hat{\mathbf{r}}$, which satisfy the canonical commutation relations $[\hat{r}_j, \hat{p}_l] = \mathrm{i}\hbar\delta_{jl}$ and $[\hat{r}_j, \hat{r}_l] = 0 = [\hat{p}_j, \hat{p}_l]$, where $\hat{\mathbf{p}}$ is the proton-electron relative's momentum. The total Hilbert space associated to the system is then $\mathcal{H}_{3\mathrm{D}} \otimes \mathcal{H}_{S=1/2} \otimes \mathcal{H}_{I=1/2}$, where the last two Hilbert spaces are 2-dimensional, while $\mathcal{H}_{3\mathrm{D}}$ is composed of three infinite-dimensional spaces (one for each direction in real space), each the same as the one we used to describe the harmonic oscillator in the previous chapter. We will ignore the center-of-mass motion, which essentially behaves as a free particle, unless we expose the atom to extra external fields or other particles, as we will see towards the end of the notes.

Within the simplest, so-called *Bohr approximation*, the Hamiltonian is the sum of a kinetic term and a Coulomb potential term, that is,

$$\hat{H}_{\mathrm{A}} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{e^2}{4\pi\epsilon_0|\hat{\mathbf{r}}|}, \tag{213}$$

where m is the reduced mass of the system and e the charge of the electron. Of course, since the mass of the proton is much larger than that of the electron, to a good approximation it can be assumed that the proton is sitting motionless at the origin, so that $\hat{\mathbf{r}}$ and m are just the coordinates and mass of the electron. The spectrum of this Hamiltonian is well studied [39–44], and next we briefly review it.

The spectrum of this Hamiltonian has both countable and continuous parts. The continuous part has only positive eigenenergies $\{\hbar|\mathbf{k}|^2/2m\}_{\mathbf{k}\in\mathbb{R}^3}$, corresponding essentially to scattering states in electron-proton collisions, with a wave function that behaves as a plane wave $e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$ at large distances $|\mathbf{k}\cdot\mathbf{r}| \to \infty$. We focus then on the negative eigenvalues, which correspond to bound states that we would characterize as truly atomic states.

The structure of the Hilbert space requires 5 quantum numbers to uniquely identify a basis element, 3 for each direction in $\mathcal{H}_{3\mathrm{D}}$, and 1 for each value of the spins along the chosen quantization axis (see below). In the case of the Hydrogen atom, it is indeed very simple to find four operators that commute with Hamiltonian (213). First, because it is independent of the spin operators, it commutes with any of the components of $\hat{\mathbf{S}}$ and $\hat{\mathbf{I}}$. In addition, because it is invariant under rotations, it commutes with the *orbital angular momentum* operator $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$, as well as with $\hat{\mathbf{L}}^2$, which also commutes with $\hat{\mathbf{L}}$. Of course, the spin operators commute with the orbital angular momentum. Hence, choosing the z direction as the so-called *quantization axis* for any angular momentum operator (that is, we choose to work with eigenstates of $\hat{L}_3$, $\hat{S}_3$, and $\hat{I}_3$), the eigenstates of the Hamiltonian can be labeled by an index containing 5 quantum numbers, $\mathbf{n} = (n, l, m_L, m_S, m_I)$, and satisfy the eigenvalue expressions

$$\hat{H}_{\mathrm{A}}|\mathbf{n}\rangle = E_n|\mathbf{n}\rangle, \qquad \text{with } E_n = -E_0/n^2, \quad n = 1, 2, 3..., \tag{214a}$$

$$\hat{\mathbf{L}}^2|\mathbf{n}\rangle = l(l+1)\hbar^2|\mathbf{n}\rangle, \qquad l = 0, 1, ..., n-1, \tag{214b}$$

$$\hat{L}_3|\mathbf{n}\rangle = m_L\hbar|\mathbf{n}\rangle, \qquad m_L = -l, -l+1, ..., l-1, l, \tag{214c}$$

$$\hat{S}_3|\mathbf{n}\rangle = m_S\hbar|\mathbf{n}\rangle, \qquad m_S = \pm 1/2, \tag{214d}$$

$$\hat{I}_3|\mathbf{n}\rangle = m_I\hbar|\mathbf{n}\rangle, \qquad m_I = \pm 1/2, \tag{214e}$$

where $E_0 = me^4/2(4\pi\epsilon_0)^2\hbar$ the so-called *Rydberg energy* that we need to give to the ground-state Hydrogen in order to free its constituents and reach unbounded states. On the other hand, n, l, m_L, and $m_{S,I}$ are known as

principal, *orbital*, *magnetic*, and *spin* quantum numbers. Note that the eigenenergies depend only on the principal quantum number, and are then $2 \times 2 \times n^2$ degenerate, as represented in Fig. **ToDo**. This is owed to the so-called *accidental degeneracy* in l of the Coulomb potential, since general rotationally-symmetric potentials $V(|\hat{\mathbf{r}}|)$ lead to energy eigenvalues that depend also on l. In contrast, the independence on m_L is characteristic of all $V(|\hat{\mathbf{r}}|)$, and is thus dubbed *essential degeneracy*.

The situation is much more complicated for heavier atoms [43]. However, in quantum optics experiments we usually work with atoms or ions that have all their electrons in closed shells, except for a single one, the so-called *valence electron* (think of alkaline atoms such us Li, Na, K, or Rb, or alkaline-earth ions such as Be^+, Mg^+, Ca^+, or Sr^+). Under such circumstances, one can adopt a hydrogen-like model for the atom, which differs from the one introduced above just by the fact that the closed-shell electrons screen the Coulomb interaction between the valence electron and the nucleus, turning it into a different potential $V(|\hat{\mathbf{r}}|) = -Z_{\text{eff}}(|\hat{\mathbf{r}}|)e^2/4\pi\epsilon_0|\hat{\mathbf{r}}|$, with an effective position-dependent nucleus charge that is fully screened at large distances, $Z_{\text{eff}} \overset{|\mathbf{r}|\to\infty}{\longrightarrow} 1$, and not screened at all at very short ones, $Z_{\text{eff}} \overset{|\mathbf{r}|\to 0}{\longrightarrow} Z$, where Z is the atomic number of the atom. In such case, the accidental degeneracy in l is broken, as represented in Fig. **ToDo**, and the eigenenergies must be labeled with two quantum numbers, that is, E_{nl}. Their explicit expressions are not important for our purposes, and can be checked in [43].

Before proceeding, let us remark a small detail: heavier atoms will no longer have necessarily total nuclear spin $i = 1/2$, where we denote the eigenvalue of $\hat{\mathbf{I}}^2$ by $i(i+1)\hbar^2$. Instead, their nucleons (protons and neutrons) can add up to any of the values of i allowed by the rules of composition of angular momenta, although some make the atoms more stable than others, of course (the lowest ones, intuitively). However, note that quantum optics experiments typically occur at energy scales in which nuclear processes capable of changing i are not possible. Therefore, in the following we don't to include it as a quantum number, since it remains fixed during experiments.

Most of the other degeneracies mentioned above are broken once a more accurate atomic Hamiltonian is considered. In particular, there is a hierarchy of corrections, which can be mainly collected in two sets, the so-called *fine* and *hyperfine* corrections [40, 43]. Let us briefly discuss them now. The fine corrections include relativistic effects, corresponding mainly to corrections of the kinetic energy term and to a new term that couples the orbital angular momentum and the electronic spin as $\hat{\mathbf{S}}\cdot\hat{\mathbf{L}}$, the so-called *spin-orbit coupling*. Let us define $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$, sometimes called *electronic angular momentum*, which is readily shown to commute with $\hat{\mathbf{L}}^2$ and $\hat{\mathbf{S}}^2$. Noting that $\hat{\mathbf{S}}\cdot\hat{\mathbf{L}} \propto \hat{\mathbf{J}}^2 - \hat{\mathbf{S}}^2 - \hat{\mathbf{L}}^2$, we then see that the eigenenergies of the Hamiltonian will require now an additional label j, the quantum number associated to the total electronic angular momentum. Hence, the quantum numbers m_L and m_S are not good ones in the presence of relativistic effects, but instead we can use $\mathbf{n} = (n, l, j, m_J, m_I)$, with

$$\hat{\mathbf{J}}^2|\mathbf{n}\rangle = j(j+1)\hbar^2|\mathbf{n}\rangle, \qquad j = |l \pm 1/2|, \tag{215a}$$

$$\hat{J}_3|\mathbf{n}\rangle = m_J\hbar|\mathbf{n}\rangle, \qquad m_J = -j, -j+1, ..., j-1, j, \tag{215b}$$

added to the previous eigenvalue equations (214) for the other quantum numbers, and keeping in mind that the eigenenergies have three indices now E_{nlj}, whose explicit expressions can be checked in [40, 43]. Hence, only the degeneracy in m_J and m_I remains. The fine correction to the spectrum is sketched in Fig. **ToDo**.

The hyperfine corrections, called that way because they typically produce an even smaller correction than the fine ones, include interactions between the electron and the nucleus that go beyond the Coulomb one. The most important correction is due to interaction between the electronic and nuclear magnetic dipoles, that is, an interaction of the $\hat{\mathbf{J}}\cdot\hat{\mathbf{I}}$ type. It is then convenient to define now the *atomic angular momentum* operator $\hat{\mathbf{F}} = \hat{\mathbf{J}} + \hat{\mathbf{I}}$, which commutes with $\hat{\mathbf{J}}^2$ and $\hat{\mathbf{I}}^2$. Noting again that $\hat{\mathbf{J}}\cdot\hat{\mathbf{I}} \propto \hat{\mathbf{F}}^2 - \hat{\mathbf{J}}^2 - \hat{\mathbf{I}}^2$, now the eigenenergies will require an additional label f, the quantum number associated to $\hat{\mathbf{F}}^2$. Hence, in the presence of hyperfine interactions, the quantum numbers m_J and m_I must be replaced, and instead we can use $\mathbf{n} = (n, l, j, f, m_F)$, with

$$\hat{\mathbf{F}}^2|\mathbf{n}\rangle = f(f+1)\hbar^2|\mathbf{n}\rangle, \qquad f = |j-i|, |j-i|+1, ..., j+i, \tag{216a}$$

$$\hat{F}_3|\mathbf{n}\rangle = m_F\hbar|\mathbf{n}\rangle, \qquad m_F = -f, -f+1, ..., f-1, f, \tag{216b}$$

The hyperfine correction to the spectrum is sketched in Fig. **ToDo**, where we show the lowest values of E_{nljf}. Note that only the degeneracy in m_F remains after all these corrections, but this can be lifted by applying an external magnetic field $\boldsymbol{e}B$, whose direction $\boldsymbol{e}$ defines the quantization axis in experiments, leading to a term proportional to $B\hat{F}_3$ in the Hamiltonian (Zeeman effect). For this reason, m_F is sometimes called *atomic magnetic quantum number*.

From this discussion and the sketches of Fig. **ToDo**, it is clear that atoms have a highly non-uniform energy spectrum. Of course, more complicated matter systems such as molecules or materials have even more intricate spectra.

A final important property that will become very relevant when studying the interaction of atoms with light refers to the parity of the atomic eigenstates. The parity operator $\hat{\Pi}$ is a unitary operator defined by its action on the

coordinate operator $\hat{\Pi}^\dagger\hat{\mathbf{r}}\hat{\Pi} = -\hat{\mathbf{r}}$ (which automatically implies $\hat{\Pi}^\dagger\hat{\mathbf{p}}\hat{\Pi} = -\hat{\mathbf{p}}$, as easily proven[24]). Note that this implies that $\hat{\Pi}^2 = \hat{I}$, which means that $\hat{\Pi}^{-1} = \hat{\Pi}^\dagger = \hat{\Pi}$ and that the parity operator has eigenvalues ± 1. Atomic Hamiltonians are generally invariant under parity transformations (all the interactions and fundamental particles are spherically symmetric), and hence, the parity operator commutes with the Hamiltonian. Therefore, the eigenstates of the Hamiltonian can be chosen with well-defined parity. This has the consequence that the expectation value of the coordinate operator $\hat{\mathbf{r}}$ in any of the eigenstates of the Hamiltonian is zero. In order to prove this, simply consider one of such eigenstates $|a\rangle$, which will also be an eigenstate of the parity operator, $\hat{\Pi}|a\rangle = \pi_a|a\rangle$, with $\pi_a = \pm 1$. Then, it follows that $\langle a|\hat{\mathbf{r}}|a\rangle = \langle a|\hat{\Pi}^2\hat{\mathbf{r}}\hat{\Pi}^2|a\rangle = -\pi_a^2\langle a|\hat{\mathbf{r}}|a\rangle = -\langle a|\hat{\mathbf{r}}|a\rangle$, which can hold only if $\langle a|\hat{\mathbf{r}}|a\rangle = \mathbf{0}$. In general, it is clear from this derivation that the coordinate operator can only connect states with opposite parity, that is, $\langle a|\hat{\mathbf{r}}|b\rangle \neq \mathbf{0}$ only if $\pi_a = -\pi_b$.

B. Two-level approximation: Pauli pseudo-spin operators, atomic states, and Bloch space

The fact that the spectrum of atoms is so complicated seems to suggest that describing their interaction with light will be extremely difficult. However, we argue here that in most situations of interest in quantum optics, all atomic levels but a few can be ignored. The argument proceeds as follows. Light can provide atoms with the energy to perform transitions from some state to another with higher energy, say $|g\rangle \to |e\rangle$, where the labels refer to *ground* and *excited*. In the simplest case, this happens because a photon gives its energy $\hbar\omega$ to the electron[25], which can therefore use that energy to effect the transition (ω is the frequency of the photon). However, energy conservation tells us that the transition will only be possible when the energy of the photon matches (at least approximately) the energy difference between the atomic states, $E_e - E_g$. Now, since the atomic energy spectrum is non-uniform, each transition has essentially a unique energy difference, a unique *spectral fingerprint*. Therefore, if we shine the atom with monochromatic light, we only expect two specific levels to react, the ones whose energy difference matches the frequency of light. Any other level can be simply ignored, as photons cannot generate any dynamics involving them. Below we indeed give explicit mathematical support to this intuitive arguments.

In order to be more precise, let us collect all the atomic quantum numbers into an index $\mathbf{n}$ as we did in the previous section. From the previous discussion, we see that if we shine light matching the energy difference between two atomic states labeled as $|g\rangle$ and $|e\rangle$, we can make the approximation

$$\hat{H}_{\rm A} = \sum_{\mathbf{n}} E_{\mathbf{n}}|\mathbf{n}\rangle\langle\mathbf{n}| \approx E_g|g\rangle\langle g| + E_e|e\rangle\langle e|, \tag{217}$$

which has a considerably simpler form than that of the original atomic Hamiltonian. This is known as the *two-level approximation*.

Once the Hilbert space of the problem has been reduced to a two-dimensional one, we have a lot of mathematical machinery developed for spin-1/2 angular momentum that we can use. In particular, let us rewrite the atomic Hamiltonian as

$$\hat{H}_{\rm A} = \frac{E_e + E_g}{2}(|e\rangle\langle e| + |g\rangle\langle g|) + \frac{E_e - E_g}{2}(|e\rangle\langle e| - |g\rangle\langle g|). \tag{218}$$

Since $|e\rangle\langle e| + |g\rangle\langle g| = \hat{I}$ is the identity of the two-dimensional Hilbert subspace we are working on, the first term is just a constant shift of the energy that plays no role in the dynamics of the system. We thus remove it, or, in other words, we set the energy origin at the center of the transition for convenience. The second term, on the other hand, has a very suggestive form, as we discuss next.

If we identify the excited and ground states with the $\pm 1/2$ states of a fictitious spin-1/2 system (a so-called *pseudo-spin*), it is then natural to define the Pauli operators

$$\hat{\sigma}_x = |g\rangle\langle e| + |e\rangle\langle g|, \quad \hat{\sigma}_y = \mathrm{i}(|g\rangle\langle e| - |e\rangle\langle g|), \quad \hat{\sigma}_z = |e\rangle\langle e| - |g\rangle\langle g|, \tag{219}$$

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[24] A simple proof is based on the canonical commutation relations. Let us do it for one component of the position and momentum, say $\hat{q}$ and $\hat{p}$, with $[\hat{q},\hat{p}] = \mathrm{i}\hbar$. Applying the parity operator from the left and right, we can rewrite this commutator as $-\hat{q}\hat{\Pi}^\dagger\hat{p}\hat{\Pi} + \hat{\Pi}^\dagger\hat{p}\hat{\Pi}\hat{q} = \mathrm{i}\hbar$, or $[\hat{q},\hat{p}] = -[\hat{q},\hat{\Pi}^\dagger\hat{p}\hat{\Pi}]$, which implies $\hat{\Pi}^\dagger\hat{p}\hat{\Pi} = -\hat{p} + c$. In this expression, c is a constant that we can determine by, for example, evaluating the matrix element $\langle q|\hat{\Pi}^\dagger\hat{p}\hat{\Pi}|q'\rangle$, where $|q\rangle$ and $|q'\rangle$ are eigenstates of the coordinate $\hat{q}$. Using the previous expression, we obtain $\langle q|\hat{\Pi}^\dagger\hat{p}\hat{\Pi}|q'\rangle = c\langle q|q'\rangle - \langle q|\hat{p}|q'\rangle = c\delta(q-q') + \mathrm{i}\hbar\partial_x\delta(q-q')$, where we have used (90), which in terms of position and momentum (instead of quadratures) reads $\langle q|\hat{p}|\psi\rangle = -\mathrm{i}\partial_q\langle q|\psi\rangle$. On the other hand, using $\hat{\Pi}|q\rangle = |-q\rangle$, we can also write $\langle q|\hat{\Pi}^\dagger\hat{p}\hat{\Pi}|q\rangle = \langle -q|\hat{p}|-q'\rangle = \mathrm{i}\hbar\partial_{(-q)}\langle -q|-q'\rangle = \mathrm{i}\hbar\partial_q\delta(q-q')$. Finally, comparing both expressions we obtain $c = 0$.

[25] Note that inelastic (Compton) scattering in which the photon cedes only part of its energy to the electron and changes its frequency, is irrelevant at optical frequencies. In particular, the change of wavelength induced by such process is at most on the order of the electron's de Broglie wavelength, which is on the order of 10^{-3}nm, very far away from optical wavelengths, typically on the order of hundreds of nanometres.

which satisfy the commutation and anticommutation relations[26] $[\hat{\sigma}_j,\hat{\sigma}_k]=2\mathrm{i}\sum_{l=x,y,z}\epsilon_{jkl}\hat{\sigma}_l$ and $\hat{\sigma}_j\hat{\sigma}_k+\hat{\sigma}_k\hat{\sigma}_j=2\delta_{jk}\hat{I}$, apart from the useful properties $\mathrm{tr}\{\hat{\sigma}_j\}=0$ and $\det\{\hat{\sigma}_j\}=-1$. The property $\hat{\sigma}_j\hat{\sigma}_k=\delta_{jk}\hat{I}+\mathrm{i}\sum_{l=x,y,z}\epsilon_{jkl}\hat{\sigma}_l$ is also useful.

It is also important to remark that the Pauli operators, together with the identity, form a basis in the space of operators acting on two-dimensional Hilbert spaces (which itself is a four-dimensional Hilbert space with respect the inner product defined by the trace product $\mathrm{tr}\{\hat{A}^\dagger\hat{B}\}$ for any two operators $\hat{A}$ and $\hat{B}$). While this sounds a bit technical, the proof is actually completely trivial by making use of the representation of the Pauli operators in the $\{|e\rangle,|g\rangle\}$ basis, the so-called *Pauli matrices*

$$\sigma_x=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0&-\mathrm{i}\\\mathrm{i}&0\end{pmatrix},\quad \sigma_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

Together with the representation of the identity, it is obvious the linear combination

$$c_0I+c_1\sigma_x+c_2\sigma_y+c_3\sigma_z=\begin{pmatrix}c_0+c_3&c_1-\mathrm{i}c_2\\c_1+\mathrm{i}c_2&c_0-c_3\end{pmatrix},$$

with parameters $c_j\in\mathbb{C}$ allows writing any complex 2×2 matrix.

Using the Pauli operators, the atomic Hamiltonian is then turned into

$$\hat{H}_\mathrm{A}=\frac{\hbar\varepsilon}{2}\hat{\sigma_z},\tag{220}$$

where we have defined $\varepsilon=(E_e-E_g)/\hbar$, the so-called *transition frequency*.

It is also convenient to define *raising* and *lowering* operators that effect transitions in between the atomic levels,

$$\hat{\sigma}=|g\rangle\langle e|=(\hat{\sigma}_x-\mathrm{i}\hat{\sigma}_y)/2,\quad \hat{\sigma}^\dagger=|e\rangle\langle g|=(\hat{\sigma}_x+\mathrm{i}\hat{\sigma}_y)/2,\tag{221}$$

which obey the commutation relations $[\hat{\sigma},\hat{\sigma}^\dagger]=-\hat{\sigma}_z$, $[\hat{\sigma},\hat{\sigma}_z]=2\hat{\sigma}$, and $[\hat{\sigma}^\dagger,\hat{\sigma}_z]=-2\hat{\sigma}^\dagger$.

Let's move on now to the description of atomic states. As mentioned above, Together with the identity, the Pauli operators form a basis for any other operator. Hence, the density operator representing the atomic state can be expanded as $\hat{\rho}=(b_0\hat{I}+\mathbf{b}^T\hat{\boldsymbol{\sigma}})/2$, where we have introduced the Pauli vector $\hat{\boldsymbol{\sigma}}=(\hat{\sigma}_x,\hat{\sigma}_y,\hat{\sigma}_z)^T$, the expansion coefficients b_0 and $\mathbf{b}=(b_x,b_y,b_z)^T$, and we have divided by two for future convenience. The properties that physical density operators must satisfy restrict the values that these coefficients can take. For example, they must be real, since $\hat{\rho}^\dagger=b_0^*\hat{I}+\mathbf{b}^\dagger\hat{\boldsymbol{\sigma}}=\hat{\rho}$ can hold only if that is the case. Next, the normalization of the state fixes $b_0=1$, since $\mathrm{tr}\{\hat{\rho}\}=b_0\mathrm{tr}\{\hat{I}\}/2=b_0$ must be equal to 1. Finally, the eigenvalues of the density operator must be positive, but smaller than or equal to 1. Since the matrix representation of the operator is only 2×2, these are trivial to find. In particular, the characteristic equation reads

$$\det\{\hat{\rho}-\lambda\hat{I}\}=\det\left\{\frac{1}{2}\begin{pmatrix}1-2\lambda+b_z&b_x-\mathrm{i}b_y\\b_x+\mathrm{i}b_y&1-2\lambda-b_z\end{pmatrix}\right\}=\frac{1}{4}\left[(1-2\lambda)^2-|\mathbf{b}|^2\right]=0,\tag{222}$$

leading to eigenvalues $(1\pm|\mathbf{b}|)/2$, and hence to the condition $|\mathbf{b}|\leq1$. Therefore, a general atomic state within the two-level approximation can be written as

$$\hat{\rho}=\frac{1}{2}(\hat{I}+\mathbf{b}^T\hat{\boldsymbol{\sigma}}),\quad \text{with } |\mathbf{b}|\leq1.\tag{223}$$

$\mathbf{b}$ is known as the *Bloch vector*, whose components can be interpreted as the expectation values of the Pauli operators, as readily seen from

$$\langle\hat{\sigma}_j\rangle=\mathrm{tr}\{\hat{\rho}\hat{\sigma}_j\}=\frac{1}{2}\underbrace{\mathrm{tr}\{\hat{\sigma}_j\}}_{0}+\sum_{k=x,y,z}\frac{b_k}{2}\underbrace{\mathrm{tr}\{\hat{\sigma}_k\hat{\sigma}_j\}}_{2\delta_{kj}}=b_j.\tag{224}$$

Of particular relevance is b_z, which provides the probability of being in the excited or ground states as $p_e=\langle e|\hat{\rho}|e\rangle=(1+b_z)/2$ and $p_g=\langle g|\hat{\rho}|g\rangle=(1-b_z)/2$, respectively. These are usually called the excited and ground state *populations*.

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[26] Note that ϵ_{jkl} is the so-called Levi-Civita symbol, defined by being completely antisymmetric under the exchange of any two indices and $\epsilon_{xyz}=1$.

This way of writing density operators naturally leads to a way of visualizing them in the space generated by the expectation values of the Pauli operators, which we call *Bloch space*. State (223) corresponds to a point $\mathbf{b}$ in that space. This is represented in Figure **ToDo**.

Note that, since the eigenvalues of the density matrix depend solely on $\mathbf{b}^2$, states of equal entropy live all in a sphere centered at the origin of Bloch space (see Figure **ToDo**). In particular, note that the maximally mixed state $\hat{\rho} = \hat{I}/2$ corresponds to $\mathbf{b} = \mathbf{0}$, while pure states have $|\mathbf{b}| = 1$, since only then the density operator has eigenvalues 1 and 0, as corresponds to a rank-1 projector (that is, a single state contributing to the mixture). Hence, pure states are specified in the Bloch space by a point in a sphere of radius one centered at the origin, the so-called *Bloch sphere*. In particular, we can use the polar ϕ and azimuthal θ angles of spherical coordinates to pinpoint them, $\mathbf{b} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi[$. In the Hilbert space, this means that any pure state can be written as

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|e\rangle + e^{\mathrm{i}\phi}\sin\left(\frac{\theta}{2}\right)|g\rangle, \tag{225}$$

as can be readily checked. We thus see that the north pole of the Bloch sphere ($\theta = 0$, $\phi = 0$) corresponds to the excited state $|e\rangle$, while the south pole ($\theta = \pi$, $\phi = 0$) corresponds to the ground state $|g\rangle$. The eigenstates of the other Pauli operators are located then in the equator $\theta = \pi/2$.

C. Unsupervised evolution of two-level systems

1. General Hamiltonian and Bloch equations

Using again the fact that the Pauli matrices together with the identity are a basis for any operator acting on a two-dimensional Hilbert space, we can write the most general type of Hamiltonian acting on a two-level system as

$$\hat{H}(t) = \frac{\hbar}{2}\boldsymbol{\alpha}^T(t)\hat{\boldsymbol{\sigma}}, \tag{226}$$

where $\boldsymbol{\alpha}(t)$ is a vector with arbitrary real functions of time as entries and we have dismissed terms proportional to the identity, since they don't play any role in the dynamics of the atom.

One convenient way of analyzing the dynamics of the system is based on the evolution of the Bloch vector in the Bloch space. The evolution equation of the Bloch vector can be easily found in many ways. Since we know that its components are the expectation values of the Pauli operators, possibly the simplest way consists in finding the Heisenberg equations of these operators, and then take their expectation values. Let's proceed this way. We get

$$\frac{d\hat{\sigma}_j}{dt} = \left[\hat{\sigma}_j, \frac{\hat{H}(t)}{\mathrm{i}\hbar}\right] = -\frac{\mathrm{i}}{2}\sum_{k=x,y,z}\alpha_k(t)[\hat{\sigma}_j, \hat{\sigma}_k] = \sum_{k,l=x,y,z}\epsilon_{jkl}\alpha_k(t)\hat{\sigma}_l, \tag{227}$$

and taking the expectation value

$$\frac{db_j}{dt} = \sum_{k,l=x,y,z}\epsilon_{jkl}\alpha_k(t)b_l. \tag{228}$$

These are known as the *Bloch equations* of the two-level system, and can be written in matrix form as

$$\dot{\mathbf{b}} = \mathcal{B}(t)\mathbf{b}, \quad \text{with } \mathcal{B}(t) = \begin{bmatrix} 0 & -\alpha_z(t) & \alpha_y(t) \\ \alpha_z(t) & 0 & -\alpha_x(t) \\ -\alpha_y(t) & \alpha_x(t) & 0 \end{bmatrix}. \tag{229}$$

In principle, being a 3×3 linear system, it is not difficult to solve these equations for any choice of $\boldsymbol{\alpha}(t)$, numerically in the worst case. In the following we will consider a couple of examples of special interest for quantum optics. But before that, let us show that $|\mathbf{b}|$ is a conserved quantity, and therefore, the trajectory $\mathbf{b}(t)$ in Bloch space is restricted to a sphere with radius equal to $|\mathbf{b}(0)|$. We simply evaluate

$$\frac{d|\mathbf{b}|^2}{dt} = \sum_{j=x,y,z}\frac{db_j^2}{dt} = 2\sum_{j=x,y,z}b_j\frac{db_j}{dt} = 2\sum_{j,k,l=x,y,z}\epsilon_{jkl}b_j\alpha_k b_l = 0, \tag{230}$$

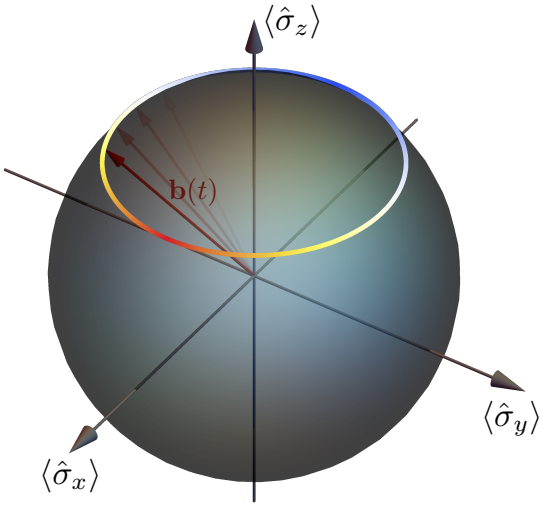

Figure 10. Evolution of the Bloch vector when the atom is subject to its free Hamiltonian (220). The trajectory is shown with a color gradient, where the initial condition is shown in red. The trail of the Bloch vector indicates the direction of its motion. As explained in the main text, the evolution induced by any Hamiltonian is constrained to a sphere of radius $|\mathbf{b}(0)|$, shown in black in the figure. Hence, we see that when allowed to evolve freely, the atom describes right-handed circular rotation around the z axis.

where in the last equality we have used that ϵ_{jkl} is antisymmetric in (jl) while $b_j\alpha_k b_l$ is symmetric. Note that this result is actually quite intuitive once we remember that unitary transformations cannot change the entropy of the state, which in the case of two-level systems depends solely on $|\mathbf{b}|$.

We will see that most of the time it is useful to work with the raising and lowering operators instead of $\hat{\sigma}_x$ and $\hat{\sigma}_y$. We can rewrite the Hamiltonian in terms of these as

$$\hat{H}(t) = \frac{\hbar}{2}[\alpha_z(t)\hat{\sigma}_z + \alpha(t)\hat{\sigma} + \alpha^*(t)\hat{\sigma}^\dagger], \tag{231}$$

with $\alpha(t) = \alpha_x(t) + \mathrm{i}\alpha_y(t)$. Defining then $b = (b_x - \mathrm{i}b_y)/2 = \langle\hat{\sigma}\rangle$, the Bloch equations are rewritten as

$$\dot{b} = -\mathrm{i}\alpha_z(t)b + \frac{\mathrm{i}}{2}\alpha^*(t)b_z, \tag{232a}$$

$$\dot{b}_z = \mathrm{i}\alpha(t)b - \mathrm{i}\alpha^*(t)b^*, \tag{232b}$$

which we will call *complex Bloch equations*.

2. *Free evolution*

Let us consider as a first, trivial example the free evolution of the two-level system. This corresponds to the choice $\boldsymbol{\alpha} = (0, 0, \varepsilon)^T$, leading to complex Bloch equations

$$\dot{b} = -\mathrm{i}\varepsilon b, \quad \dot{b}_z = 0 \quad \Longrightarrow \quad b(t) = b(0)e^{-\mathrm{i}\varepsilon t},\ b_z(t) = b_z(0). \tag{233}$$

Note how simple the solution looks in terms of the complex representation of the Bloch vector. In terms of the cartesian components of the Bloch vector, we then get

$$b_x(t) = b_x(0)\cos(\varepsilon t) - b_y(0)\sin(\varepsilon t), \tag{234a}$$

$$b_y(t) = b_y(0)\cos(\varepsilon t) + b_x(0)\sin(\varepsilon t), \tag{234b}$$

$$b_z(t) = b_z(0). \tag{234c}$$

As expected, the populations of the excited and ground states, $[1 \pm b_z(t)]/2$, do not change in time ($\hat{\sigma}_z$ commutes with $\hat{H}$). The Bloch vector evolves along a circular trajectory parallel to the $x - y$ plane, undergoing right-handed harmonic rotation around the z axis, as shown in Figure 10. This effect is known as (*pseudo-*)*spin precession*.

3. Rabi oscillations and the rotating-wave approximation

Let us now take one step forward, and consider a Hamiltonian

$$\hat{H}(t) = \frac{\hbar\varepsilon}{2}\hat{\sigma}_z + \hbar\Omega\cos(\omega t)\hat{\sigma}_x, \tag{235}$$

described by $\boldsymbol{\alpha}(t) = (2\Omega\cos\omega t, 0, \varepsilon)$. As we will see in the next chapter, this Hamiltonian, known as the *semiclassical Rabi Hamiltonian*, describes an atom subject to a (classical) monochromatic light field of frequency ω. Hence, we expect the atom to react to this field only when ω is close to ε, as discussed in the first section of this chapter. Among other things, this example will actually allow us to specify what "close" means. We will also assume that $\Omega \ll \omega$, a natural assumption for optical frequencies ($\omega \sim 10^{15}$Hz), which are quite large, and would require unconceivable large field intensities, as we shall see in the next chapter.

The complex Bloch equations (232) read in this case as

$$\dot{b} = -\mathrm{i}\varepsilon b + \mathrm{i}\Omega\cos(\omega t)b_z, \tag{236a}$$

$$\dot{b}_z = 2\mathrm{i}\Omega\cos(\omega t)(b - b^*). \tag{236b}$$

It is convenient to define a *slowly-varying* variable $\tilde{b}(t) = e^{\mathrm{i}\omega t}b(t)$. Since ω must be close to ε for the arguments exposed above, this transformation removes a large part of the spin precession around the z axis induced by the free term of the Hamiltonian, so that we expect the new variable to vary slowly compared to ε. We will later check that this is indeed the case. In terms of this new variable, and expanding $2\cos\omega t = e^{\mathrm{i}\omega t} + e^{-\mathrm{i}\omega t}$, the previous equations read

$$\dot{\tilde{b}} = \mathrm{i}(\omega - \varepsilon)\tilde{b} + \mathrm{i}\frac{\Omega}{2}\left(1 + e^{2\mathrm{i}\omega t}\right)b_z, \tag{237a}$$

$$\dot{b}_z = \mathrm{i}\Omega\left(1 + e^{-2\mathrm{i}\omega t}\right)\tilde{b} - \text{c.c.} \quad . \tag{237b}$$

These equations are exact, but not easy to analyze analytically because of the time-dependent coefficients $e^{2\mathrm{i}\omega t}$. However, next we argue that this coefficients are negligible. This is known as the *rotating-wave approximation*, and is of paramount importance in quantum optics, as we shall see through many examples over the next chapters. An easy way of understanding the conditions under which such an approximation works consists in integrating the equations above over one optical cycle, obtaining

$$\int_{t-\pi/\omega}^{t+\pi/\omega} d\tau\dot{\tilde{b}}(\tau) = \mathrm{i}(\omega - \varepsilon)\int_{t-\pi/\omega}^{t+\pi/\omega} d\tau\tilde{b}(\tau) + \mathrm{i}\frac{\Omega}{2}\left(\int_{t-\pi/\omega}^{t+\pi/\omega} d\tau b_z(\tau) + \int_{t-\pi/\omega}^{t+\pi/\omega} d\tau b_z(\tau)e^{2\mathrm{i}\omega\tau}\right), \tag{238a}$$

$$\int_{t-\pi/\omega}^{t+\pi/\omega} d\tau\dot{b}_z(\tau) = \mathrm{i}\Omega\left(\int_{t-\pi/\omega}^{t+\pi/\omega} d\tau\tilde{b}(\tau) + \int_{t-\pi/\omega}^{t+\pi/\omega} d\tau\tilde{b}(\tau)e^{-2\mathrm{i}\omega\tau}\right) - \text{c.c.} \quad . \tag{238b}$$

The key idea now is that once we perform the rotating-wave approximation, the evolution of $\tilde{b}(t)$ and $b_z(t)$ will depend only on $|\omega - \varepsilon|$ and Ω, which are assumed to be much smaller than ω. In other words, these variables are approximately constant over one optical cycle. Hence, approximating these variables by their value at the center of the integration domain, so that, for example,

$$\int_{t-\pi/\omega}^{t+\pi/\omega} d\tau\tilde{b}(\tau) \approx \frac{2\pi}{\omega}\tilde{b}(t), \tag{239a}$$

$$\int_{t-\pi/\omega}^{t+\pi/\omega} d\tau\tilde{b}(\tau)e^{2\mathrm{i}\omega\tau} \approx \tilde{b}(t)\int_{t-\pi/\omega}^{t+\pi/\omega} d\tau e^{2\mathrm{i}\omega\tau} = 0, \tag{239b}$$

we obtain

$$\dot{\tilde{b}} = \mathrm{i}\Delta\tilde{b} + \mathrm{i}\frac{\Omega}{2}b_z, \tag{240a}$$

$$\dot{b}_z = \mathrm{i}\Omega(\tilde{b} - \tilde{b}^*), \tag{240b}$$

where we have defined the *detuning* $\Delta = \omega - \varepsilon$. These are precisely the equations (237) but without the time-dependent terms, and will be a good approximation to these as long as $|\omega - \varepsilon| \ll \omega$ and $\Omega \ll \omega$. The arguments leading to this

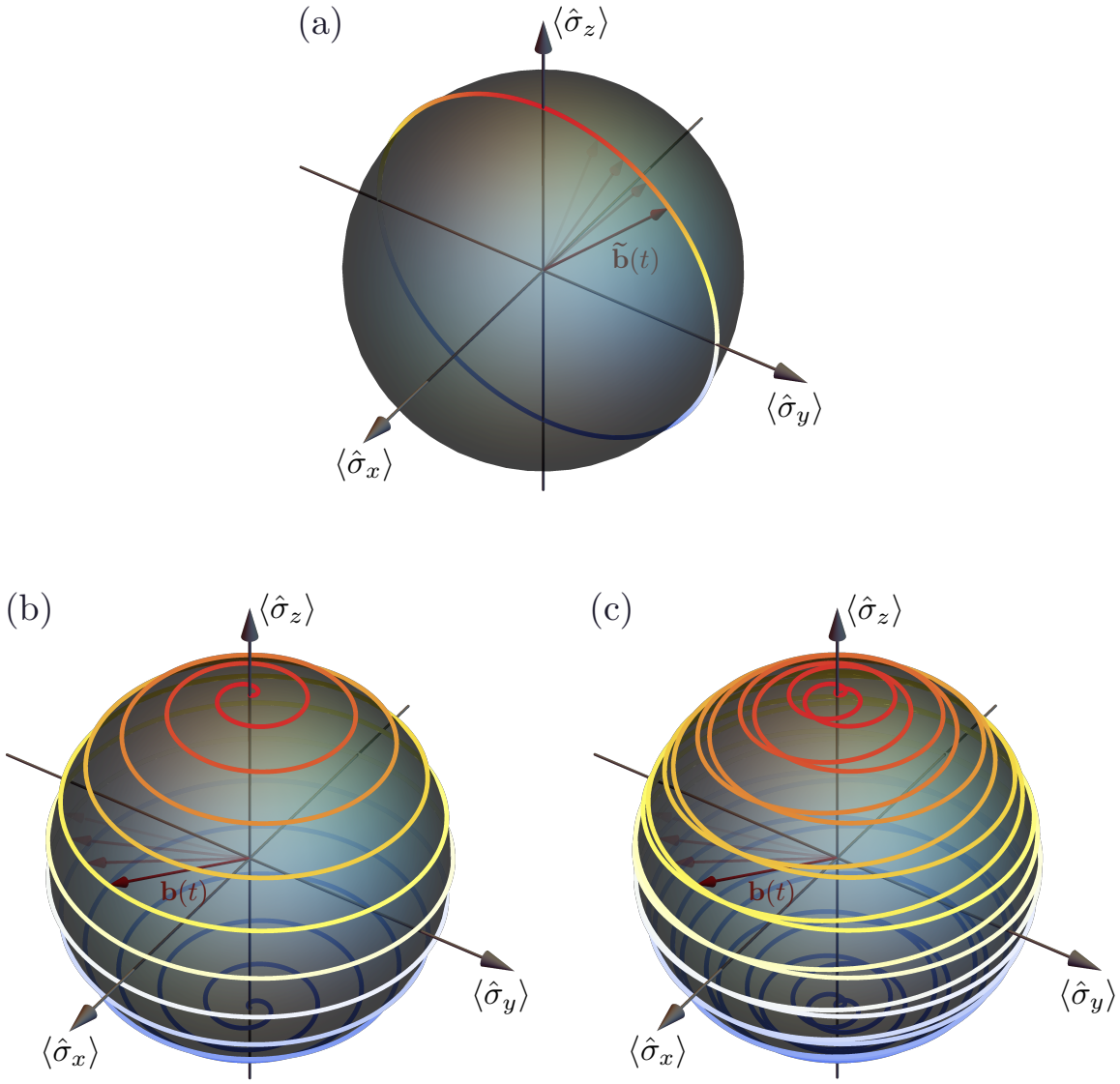

Figure 11. Evolution of the Bloch vector when the atom is subject to the semiclassical Rabi Hamiltonian (235). As in the previous figure, the trajectory is shown with a color gradient, where the initial condition is marked in red, here chosen to be the excited state $|e\rangle$ (north pole). In (a) we show the evolution of the slowly-varying Bloch vector $\tilde{\mathbf{b}} = (\tilde{b}_x, \tilde{b}_y, b_z)^T$, which undergoes right-handed precession around the x axis. In contrast, the trajectory of the original Bloch vector, which includes the precession around the z axis, describes a spiral trajectory as shown in (b) and (c), for half a period and a full period, respectively (note that on the second half of the evolution the trajectory is also spiral, but not the same as the spiral described by the first half, as that would require the precession along the z axis to change from right-handed to left-handed after half a period). We have chosen $\varepsilon = 25\Omega$ in order to be able to see the spiral trajectory to the naked eye, but keep in mind that in common quantum optics experiments atomic transitions can get much larger than that.

rotating-wave approximation can be put in more rigorous mathematical terms by using time-dependent perturbation theory, which we shall do later as an exercise for completeness.

Now that we have removed explicit time dependences, these equations can be solved analytically. For the sake of keeping the discussion going, we will do this at the end of the section, and here we just discuss the solution, which reads

$$b_z(t) = \frac{\delta^2 b_z(0) - \delta b_x(0) + [b_z(0) + \delta b_x(0)]\cos(\Omega_R t) + \sqrt{1+\delta^2}\, b_y(0)\sin(\Omega_R t)}{1+\delta^2}, \tag{241a}$$

$$\tilde{b}(t) = \frac{b_x(0) - \delta b_z(0) + [\delta b_z(0) + 2\delta^2 b(0) - \mathrm{i} b_y(0)]\cos(\Omega_R t) + \mathrm{i}\sqrt{1+\delta^2}[b_z(0) + 2\delta b(0)]\sin(\Omega_R t)}{2(1+\delta^2)}, \tag{241b}$$

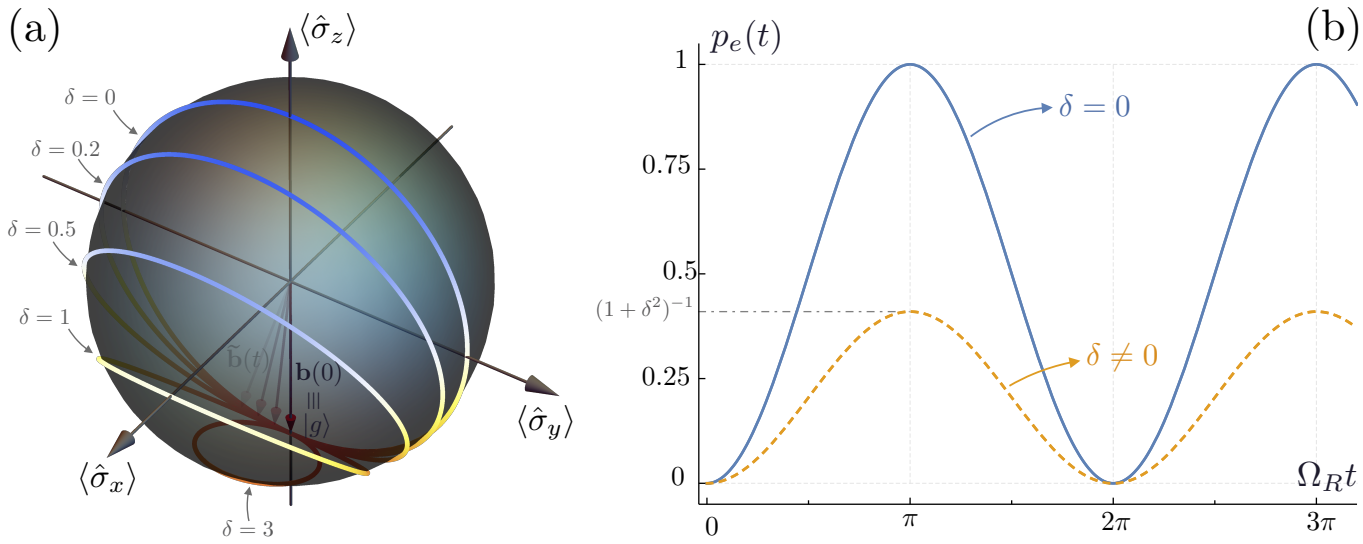

Figure 12. (a) Evolution of the slowly-varying Bloch vector when the atom is initialized in the ground state $|g\rangle$ (south pole) and then subject to the semiclassical Rabi Hamiltonian (235), for different values of the normalized detuning δ. Conventions are as in the previous figures. All the trajectories are circular and touch the south pole, but their radius is smaller the larger δ is. We show in (b) the excited state population as a function of time for $\delta = 0$ and a generic $\delta \neq 0$. It displays clear Rabi oscillations that periodically transfer population from the ground to the excited state, but with an efficiency that decreases as the detuning increases.

where we have introduced the normalized detuning $\delta = \Delta/\Omega$, the *Rabi frequency* $\Omega_R = \sqrt{\Omega^2 + \Delta^2}$, and used the relation $2b(0) = b_x(0) - \mathrm{i}b_y(0)$ to shorten a bit the expressions. Note that, importantly, both $b_z(t)$ and $\tilde{b}(t)$ oscillate at frequency Ω_R, and are therefore slowly varying variables as compared to ω, which proves the consistency of the rotating-wave approximation performed above[27]. Note as well that the populations $[1 \pm b_z(t)]$ oscillate in time, which is a phenomenon known as *Rabi oscillations*.

We consider now some specific limits of this solution. First, let us consider the $|\delta| \gg 1$ limit (remember that $|\mathbf{b}| \leq 1$), which leads to $b_z(t) = b_z(0)$ and $\tilde{b}(t) = b(0)e^{\mathrm{i}\Delta t}$, or $b(t) = b(0)e^{-\mathrm{i}\varepsilon t}$ in terms of the original variable. This is precisely the solution (233) that we found for an atom evolving freely. Hence, as expected, the atom won't feel the light field if $|\Delta| \gg \Omega$. Most importantly, this also justifies the two-level approximation, that is, neglecting all transitions which are far from resonance with respect to the light frequency.

The opposite limit, $\delta = 0$, is also interesting. This corresponds to a light field resonant with the atomic transition, where, writing $2\tilde{b}(t) = \tilde{b}_x(t) + \mathrm{i}\tilde{b}_y(t)$, the solution for the original variables reads

$$\tilde{b}_x(t) = b_x(0), \tag{242a}$$

$$\tilde{b}_y(t) = b_y(0)\cos(\Omega t) - b_z(0)\sin(\Omega t), \tag{242b}$$

$$b_z(t) = b_z(0)\cos(\Omega t) + b_y(0)\sin(\Omega t), \tag{242c}$$

which corresponds to a (slowly-varying) Bloch vector precessing left-handedly around the x axis, as shown in Fig. 11a. Of course, the true Bloch vector $\mathbf{b}(t)$ combines this precession with a faster optical precession around the z axis at frequency ω, adding up to a double-spiraled trajectory in Bloch space, as shown in Figures 11b and c.

A final interesting limit corresponds to the situation where the atom starts in the ground state, that is, $\mathbf{b}(0) = (0, 0, -1)^T$. In this case, equations (241) are simplified to

$$\tilde{b}_x(t) = \frac{\delta}{1+\delta^2}\left[1 - \cos\left(\frac{\Omega_R t}{2}\right)\right], \quad \tilde{b}_y(t) = \frac{1}{\sqrt{1+\delta^2}}\sin(\Omega_R t), \quad b_z(t) = -\frac{\cos(\Omega_R t) + \delta^2}{1+\delta^2}. \tag{243}$$

The corresponding trajectory in the Bloch sphere is shown in Fig. 12a for different values of the detuning δ. Note that trajectory starts at the south pole, and describes a circle of smaller radius the larger is δ. This is to be expected,

[27] As a general lesson, never forget how important it is to check that the solution obtained at the end of a calculation is consistent with any approximations performed on the way to finding it.

since for $\delta = 0$ we should recover the precession around the x axis that we analyzed in the previous figure, while in the limit $|\delta| \to \infty$ we already saw that the free-atom limit is recovered, so that starting from an eigenstate of the bare atomic Hamiltonian (220) we should not move at all.

It is interesting to track the population of the excited state in time for different values of $|\delta|$, which is given by

$$p_e(t) = \frac{1 - \cos(\Omega_R t)}{2(1+\delta^2)}, \tag{244}$$

and shown in Fig. 12b. For $\delta = 0$ the population is completely transferred from the ground to the excited state in the middle of the Rabi cycle. The effect of a finite detuning $\delta \neq 0$ is to induce an incomplete population transfer, as now the maximum population available in the excited state is $(1+\delta^2)^{-1}$, which is negligible when $|\delta| \gg 1$.

Let us finish this section by explaining in detail how to obtain the solution (241) of the complex Bloch equations (240). We will do it with a method that is useful for general linear problems, certainly for many different problems in quantum optics. Let us consider the system of N coupled linear equations

$$\dot{\mathbf{x}} = \mathcal{B}\mathbf{x} + \mathbf{y}(t), \tag{245}$$

where $\mathbf{x} \in \mathbb{C}^N$ is a vector of complex variables, $\mathbf{y}(t) \in \mathbb{C}^N$ a vector of complex functions of time which we assume to be given, and $\mathcal{B}$ is an $N \times N$ complex matrix. In the particular case of (240), we have $N = 3$, $\mathbf{x} = (\tilde{b}, \tilde{b}^*, b_z)^T$, $\mathbf{y} = (0,0,0)^T$, and

$$\mathbf{x} = \begin{pmatrix} \tilde{b} \\ \tilde{b}^* \\ b_z \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \text{and } \mathcal{B} = \mathrm{i}\begin{pmatrix} \Delta & 0 & \Omega/2 \\ 0 & -\Delta & -\Omega/2 \\ \Omega & -\Omega & 0 \end{pmatrix}. \tag{246}$$

The whole method relies on our ability to find a matrix $\mathcal{S}$ that diagonalizes $\mathcal{B}$ through a similarity transformation

$$\mathcal{S}^{-1}\mathcal{B}\mathcal{S} = \mathcal{D}, \tag{247}$$

where $\mathcal{D}$ is a diagonal matrix containing the eigenvalues $\{\lambda_j\}_{j=1,\ldots,N}$ of $\mathcal{B}$. Note that for all practical purposes, in finite dimension we can assume that all matrices are diagonalizable[28]. In the case of our linear system, we have

$$\mathcal{D} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\mathrm{i}\Omega_R & 0 \\ 0 & 0 & \mathrm{i}\Omega_R \end{pmatrix}, \qquad \mathcal{S} = \frac{1}{2}\begin{pmatrix} 1 & \delta - \sqrt{1+\delta^2} & \delta + \sqrt{1+\delta^2} \\ 1 & \delta + \sqrt{1+\delta^2} & \delta - \sqrt{1+\delta^2} \\ -\delta & 1 & 1 \end{pmatrix} \tag{248}$$

which is easily checked or found with the help of some symbolic mathematics software. Defining then the projected vectors $\mathbf{c}(t) = \mathcal{S}^{-1}\mathbf{x}(t)$ and $\mathbf{d}(t) = \mathcal{S}^{-1}\mathbf{y}(t)$, the coupled linear system turns into a decoupled one,

$$\dot{\mathbf{c}} = \mathcal{D}\mathbf{c} + \mathbf{d}(t) \quad \Longrightarrow \quad \dot{c}_j = \lambda_j c_j + d_j(t), \tag{249}$$

with generic solutions

$$c_j(t) = c_j(0)e^{\lambda_j t} + \int_0^t dt' e^{\lambda_j(t-t')} d_j(t'), \tag{250}$$

as shown below. Finally, we can retrieve the original variables from these projections as $\mathbf{x}(t) = \mathcal{S}\mathbf{c}(t)$. In our simple case, in which $\mathbf{y} = \mathbf{0}$, this can be rewritten as $\mathbf{x}(t) = \mathcal{S}e^{\mathcal{D}t}\mathcal{S}^{-1}\mathbf{x}(0)$, which using (248) directly leads to the solutions (241) after some algebra.

As a final detail, and since the type of linear equations (249) with forcing will appear many times, let us show how to deal with them in general. Consider the equation $\dot{c} = \lambda c + d(t)$. In order to solve it, we make the variable change $z(t) = c(t)e^{-\lambda t}$, and proceed as $\dot{z} = (\dot{c} - \lambda c)e^{-\lambda t} = d(t)e^{-\lambda t} \Rightarrow z(t) = z(t_0) + \int_{t_0}^t dt' e^{-\lambda t'} d(t')$. Undoing the variable change lead us to the final solution

$$c(t) = c(t_0)e^{\lambda(t-t_0)} + \int_{t_0}^t dt' e^{\lambda(t-t')} d(t'). \tag{251}$$

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[28] More precisely, the set of non-diagonalizable matrices of finite dimension has zero measure. This means that the probability of drawing a non-diagonalizable matrix at random is zero. It also means that all non-diagonalizable matrices have diagonalizable matrices infinitely close to them. These properties are actually obvious once we remember that the condition for a matrix to be non-diagonalizable is that its eigenvectors must not be linearly independent. This means that matrix $\mathcal{S}$ satisfying $\mathcal{B}\mathcal{S} = \mathcal{S}\mathcal{D}$ is not invertible, that is, $\det \mathcal{S} = 0$. For finite dimension, there are a finite number of terms adding up to match this condition, which therefore requires a lot of fine tuning. In practical terms, this means that by slightly perturbing some of the elements of matrix $\mathcal{B}$, we move away from this condition, and obtain a diagonalizable matrix. Now, since an infinitesimal change of $\mathcal{B}$ should only change the physical results infinitesimally as well (otherwise it means that we are in some exotic physical regime that is probably not well described by our model, such as a phase transition that cannot be perfectly described by a linear model), we can confidently state that finite-dimensional linear problems such as the one presented here can always be solved with this method.

IV. LIGHT-MATTER INTERACTION

A. Interacting Hamiltonians and the dipole approximation

In the previous chapters we have quantized light and matter (through the example of atoms) under the assumption that they are isolated, non-interacting systems. We introduced interesting quantum states and dynamics though, but without explaining how these can be obtained in the laboratory. As we will see, state preparation and the generation of dynamics require using the interaction between light and matter. In this chapter we introduce the basic theory that describes light-matter interaction. We do it through two especially relevant examples that contain already many generic properties of more complex systems: the interaction of light with a single atom and with a nonlinear dielectric material.

Let us start by introducing some general ideas behind the description of light-matter interactions. When the frequency of the electromagnetic field is above 10^{20}Hz, electron-positron pair production can start occurring, and interactions must be necessarily described by relativistic quantum electrodynamics, considering an interacting (local $U(1)$ gauge) quantum field theory of vector and fermionic fields [71–73]. Fortunately, optical frequencies sit around 10^{15}Hz, safely away from such high-energy scenarios. Hence, quantization of the light-matter interaction can be done in a non-relativistic way. The most rigorous non-relativistic quantization scheme consists in a procedure similar to what we did in the previous chapters, but where now the charged particles forming matter enter the Maxwell equations as sources, while the electromagnetic field is added through minimal coupling to the multi-particle Schrödinger equation describing matter [2]. It is easy to understand that such a procedure is still incredibly complex in most situations.

Therefore, it is interesting to consider simpler approximate approaches, even if they work only under restricted, but well-specified conditions. We will use one of such approaches, usually referred to as light-matter interaction within the *dipole approximation*. This approach works quite well whenever the interactions can be treated as perturbations, that is, when they are much smaller than the characteristic energy of the interacting degrees of freedom. It is also incredibly intuitive, because it builds on how light-matter interaction is treated classically in most situations. The approach relies on the following ideas. With a lot of generality, we assume that matter consists of a collection of massive charged particles (e.g., electrons and nuclei) in some equilibrium configuration, possibly charge neutral. To the lowest order, the effect of an external electromagnetic field consists in pulling apart positive and negative charges, without ripping them off from the material. In essence, this means that matter is described as a collection of electric dipoles that we introduce based on reasonable and general assumptions. The interaction is then brought about by the coupling between these dipoles and the electric field of light. Except for the fact that we will quantize the interaction, this is actually how the classical description works as well, in particular, through the so-called Lorentz model [74, 75], which provides the macroscopic optical properties of matter starting from a microscopic model for the electric dipoles.

Being more concrete, let us denote by $\hat{H}_{\rm L}$ and $\hat{H}_{\rm M}$ the free Hamiltonians of light and matter in the absence of interaction. With full generality, consider a continuous model of matter characterized by an electric polarization density $\mathbf{P}(\mathbf{r},t)$ at every point $\mathbf{r}$ (electric dipole moment per unit volume). Note that the discrete case of matter formed by N dipoles $\{\mathbf{d}_n(t)\}_{n=1,2,\dots,N}$ localized at positions $\{\mathbf{r}_n\}_{n=1,2,\dots,N}$, can be recovered by taking $\mathbf{P}(\mathbf{r},t)=\sum_{n=1}^{N}\delta^{(3)}(\mathbf{r}-\mathbf{r}_n)\mathbf{d}_n$. Within the dipole approximation, the light-matter system is then described by a Hamiltonian $\hat{H}=\hat{H}_{\rm L}+\hat{H}_{\rm M}+\hat{H}_{\rm LM}$, with interaction Hamiltonian

$$\hat{H}_{\rm LM}=-\int_{\mathbb{R}^3}d^3\mathbf{r}\hat{\mathbf{E}}(\mathbf{r})\cdot\hat{\mathbf{P}}(\mathbf{r}). \tag{252}$$

This Hamiltonian comes from the classical expression of the electromagnetic energy of a collection of dipoles [59, 61]. The operator associated to the electric field is the one we built in Chapter II, see (210b). As for the operator associated to the polarization density, it is found simply by quantizing the degrees of freedom that are used in the description of matter. We will see this through specific examples next.

As a final note, let us point out that we could try a description where matter is quantized, but not the electromagnetic field, which is known as the *semiclassical limit* of quantum optics. In this case, we would proceed in the same way, just removing the light's Hamiltonian $\hat{H}_{\rm L}$ and substituting the operator $\hat{\mathbf{E}}(\mathbf{r})$ by its classical version $\mathbf{E}(\mathbf{r},t)$ governed by Maxwell equations (which might incorporate the matter dipoles as sources if we intend to model the backaction of matter onto the classical field as well). In this limit, the Hamiltonian simply reads

$$\hat{H}_{\rm semiclass}=\hat{H}_{\rm M}-\int_{\mathbb{R}^3}d^3\mathbf{r}\mathbf{E}(\mathbf{r},t)\cdot\hat{\mathbf{P}}(\mathbf{r}). \tag{253}$$

B. Interaction between light and a single atom

1. *Single-mode, two-level, and rotating-wave approximations: the Jaynes-Cummings Hamiltonian*

Let us put the previous discussion to practice with the specific example of a single atom (the simplest example of a matter system) interacting with the light of an optical cavity. We know the free Hamiltonians for both the light field and the atom, see (212) and (217)—or (220) within the two-level approximation. Hence, all that is left is introducing a dipole model for the atom. In the case of atoms with a single valence electron such as the ones we discussed in the previous chapter, this is fairly simple: the core (nucleus plus the closed-shell electrons) and the valence electron gives us, respectively, a positive and negative charge separated by their relative coordinate, which we called just $\mathbf{r}$ in the previous chapter. Here, however, we will denote this relative coordinate by $\mathbf{r}_{\rm A}$ to avoid confusion with the coordinate vector $\mathbf{r}$ appearing in the fields $\hat{\mathbf{E}}(\mathbf{r})$ and $\hat{\mathbf{P}}(\mathbf{r})$. This type of atoms are then the paradigm of an electric dipole, which is given by $\mathbf{d} = -e\mathbf{r}_{\rm A}$, where we have taken into account that electric dipoles are defined from negative to positive charges [59, 61], while the relative coordinate $\mathbf{r}_{\rm A}$ points from the atomic core to the valence electron. The quantized dipole is obtained by quantizing the relative coordinate, that is, $\hat{\mathbf{d}} = -e\hat{\mathbf{r}}_{\rm A}$. Assuming without loss of generality that the center of mass of the atom is located in some position $\mathbf{r}_0 = (0, 0, z_0)$ within the cavity, so that $\hat{\mathbf{P}}(\mathbf{r}) = \hat{\mathbf{d}}\delta^{(3)}(\mathbf{r}-\mathbf{r}_0)$, the interaction Hamiltonian (252) is then given by

$$\hat{H}_{\rm LM} = e\hat{\mathbf{E}}(z_0)\cdot\hat{\mathbf{r}}_{\rm A}, \tag{254}$$

where we remind that we only specify the z coordinate in the electric field because we are using a quasi-1D approximation, as explained in detailed in Chapter II. Note that we have also made the implicit assumption that the electric field does not vary within the size of the atom, which is very reasonable since optical variations (wavelengths) occur on the 100nm scale while atomic sizes are typically three order of magnitude below, on the 100pm scale.

We can now use the expression of the electric field (210b), together with the generic expansion of the atomic relative coordinate in the atomic basis $\hat{\mathbf{r}}_{\rm A} = \sum_{\mathbf{n},\mathbf{n}'}\langle\mathbf{n}|\hat{\mathbf{r}}_{\rm A}|\mathbf{n}'\rangle|\mathbf{n}\rangle\langle\mathbf{n}'|$, to write

$$\hat{H}_{\rm LM} = \sum_{m=1}^{\infty}\sum_{\mathbf{n}\mathbf{n}'} {\rm i}e\sqrt{\frac{\hbar\omega_m}{\varepsilon_0 LS}}\sin(k_m z_0)\langle\mathbf{n}|\hat{x}_A|\mathbf{n}'\rangle(\hat{a}_m - \hat{a}_m^\dagger)|\mathbf{n}\rangle\langle\mathbf{n}'|, \tag{255}$$

where $\hat{x}_A = \mathbf{e}_x\cdot\hat{\mathbf{r}}_{\rm A}$. Finally, we assume that all the cavity frequencies are far off-resonant with all the atomic transitions except for one, denoted by ω, which is close to resonance with a single atomic transition, for which we use the two-level notation of the previous chapter. Moreover, for the sake of simplicity we take the matrix element $\langle g|\hat{x}_A|e\rangle$ real[29] (remember that $\langle g|\hat{x}_A|g\rangle = 0 = \langle e|\hat{x}_A|e\rangle$ from parity arguments), arriving to the the Hamiltonian

$$\hat{H} = \hbar\omega\hat{a}^\dagger\hat{a} + \frac{\hbar\varepsilon}{2}\hat{\sigma}_z + {\rm i}\hbar g(\hat{a} - \hat{a}^\dagger)\hat{\sigma}_x, \tag{256}$$

where we have defined the coupling frequency $g = e\sqrt{\frac{\omega}{\hbar\varepsilon_0 LS}}\langle g|\hat{x}_A|e\rangle\sin(\omega z_0/c)$, assumed to be much smaller than ε as happens in most quantum optics experiments and for consistency with the dipole approximation. This is known as the *quantum Rabi Hamiltonian*. Despite being one of the simplest Hamiltonians in quantum physics, since it describes a single optical mode interacting with a single atomic transition, it wasn't found to be analytically solvable until recently [76, 77], with techniques that definitely go beyond the scope of these notes.

Fortunately, the condition $g \ll \varepsilon$ allows us to make one further rotating-wave approximation similar to the one introduced in the previous chapter. In order to see this, we just move to the interaction picture, defined by the transformation operator $\hat{U}_{\rm c}(t) = e^{\hat{H}_{\rm c}t/{\rm i}\hbar}$, with $\hat{H}_{\rm c} = \hbar\omega\hat{a}^\dagger\hat{a} + \hbar\varepsilon\hat{\sigma}_z/2$ (see Section 40a, where it is summarized how to move in between pictures). Using the Baker-Campbell-Haussdorf lemma (84), we obtain the transformation properties

$$\hat{U}_{\rm c}^\dagger(t)\hat{a}\hat{U}_{\rm c}(t) = e^{-{\rm i}\omega t}\hat{a} \quad\text{and}\quad \hat{U}_{\rm c}^\dagger(t)\hat{\sigma}\hat{U}_{\rm c}(t) = e^{-{\rm i}\varepsilon t}\hat{\sigma}, \tag{257}$$

leading to the interaction-picture Hamiltonian

$$\hat{H}_{\rm I}(t) = \hat{U}_{\rm c}^\dagger(t)\hat{H}\hat{U}_{\rm c}(t) - \hat{H}_{\rm c} = \underbrace{{\rm i}\hbar g\left(e^{-{\rm i}(\omega-\varepsilon)t}\hat{a}\hat{\sigma}^\dagger - e^{{\rm i}(\omega-\varepsilon)t}\hat{a}^\dagger\hat{\sigma}\right)}_{\hat{H}_{\rm R}} + \underbrace{{\rm i}\hbar g\left(e^{-{\rm i}(\omega+\varepsilon)t}\hat{a}\hat{\sigma} - e^{{\rm i}(\omega+\varepsilon)t}\hat{a}^\dagger\hat{\sigma}^\dagger\right)}_{\hat{H}_{\rm NR}}, \tag{258}$$

[29] This choice reflects in the appearance of $\hat{\sigma}_x$ in the interaction Hamiltonian. Taking a different phase of the matrix element would simply introduce a linear combination of $\hat{\sigma}_x$ and $\hat{\sigma}_y$ instead, that would complicate the analysis mathematically, but would not introduce any new physics.

where we have used the expansion $\hat{\sigma}_x = \hat{\sigma} + \hat{\sigma}^\dagger$. The $\hat{H}_{\rm R}$ term oscillates slowly, since the atom and the cavity mode are assumed to be nearly resonant. On the other hand, the $\hat{H}_{\rm NR}$ term oscillates very fast compared with the coupling g. Hence, according to what we saw in the previous chapter, we can neglect the latter within the rotating-wave approximation. Note that since $\hat{H}_{\rm LM}$ is just a perturbation onto $\hat{H}_{\rm L} + \hat{H}_{\rm M}$, we have an alternative way of looking at the rotating-wave approximation based on energy-conservation arguments. In particular, note that $\hat{H}_{\rm L} + \hat{H}_{\rm M}$ sets the energy scales of the problem and available transitions, which are only slightly perturbed by the interaction of order g. The terms in $\hat{H}_{\rm R}$ induce processes in which the atom is excited by absorbing a photon (or de-excited by emitting one), so they preserve the energy as long as the frequency mismatch $\omega - \varepsilon$ is at most on the order of the perturbation g. On the contrary, the terms in $\hat{H}_{\rm NR}$ induce processes where the atomic excitation (de-excitation) is accompanied by the creation (annihilation) of a photon, and will be highly suppressed by energy conservation requirements as long as g is small compared with $\omega + \varepsilon$, the energy required to ignite the process.

Coming back to the original picture, we can then write the Hamiltonian within the rotating-wave approximation as

$$\hat{H}_{\rm JC} = \hbar\omega \hat{a}^\dagger \hat{a} + \frac{\hbar\varepsilon}{2}\hat{\sigma}_z + \mathrm{i}\hbar g(\hat{a}\hat{\sigma}^\dagger - \hat{a}^\dagger\hat{\sigma}), \tag{259}$$

which is known as the *Jaynes-Cummings Hamiltonian*. As we are about to see, this Hamiltonian is easily diagonalizable and predicts some interesting quantum phenomena.

2. *Dressed states*

Before diagonalizing this Hamiltonian, let us remark that the Hilbert space of the system is the tensor product of the one for a harmonic oscillator with Fock basis $\{|n\rangle\}_{n=0,1,\ldots}$ and a two-level system with basis $\{|g\rangle, |e\rangle\}$. We then find a basis of the composite Hilbert space as $\{|n, g\rangle, |n, e\rangle\}_{n=0,1,\ldots}$, where we use the notation $|n\rangle \otimes |a\rangle = |n, a\rangle$. The reason why the Jaynes-Cummings Hamiltonian is so easy to diagonalized is that it connects the basis states by pairs $|n, g\rangle \leftrightharpoons |n-1, e\rangle$, and hence, the Hamiltonian is a direct sum of two-dimensional problems.

More rigorously, let us define the operator $\hat{E} = \hat{a}^\dagger\hat{a} + \hat{\sigma}^\dagger\hat{\sigma}$. This operator "counts" the total number of excitations. In particular, we have $\hat{E}|n, g\rangle = n|n, g\rangle$ and $\hat{E}|n, e\rangle = (n+1)|n, e\rangle$. Hence, except for the 0 eigenvalue, corresponding to the ground state $|0, g\rangle$, all the rest of eigenvalues $n \in \mathbb{N}$ are doubly degenerate, with subspaces spanned by the vectors $\{|n, g\rangle, |n-1, e\rangle\}$. It is straightforward to check that this operator commutes with the Hamiltonian, $[\hat{E}, \hat{H}_{\rm JC}] = 0$. Hence, they have common eigenstates. This means that $|0, g\rangle$ is necessarily an eigenstate of the Hamiltonian (indeed, with $E_0 = -\hbar\varepsilon/2$ eigenvalue, remember that the energy origin is in the center of the atomic transition). On the other hand, the rest of energy eigenstates must be superpositions of the eigenstates of $\hat{E}$ living in the same degenerate subspace (otherwise, $\hat{H}_{\rm JC}$ and $\hat{E}$ would not have common eigenstates). In order to find these states, we simply represent $\hat{H}_{\rm JC}$ in the basis $\{|0, g\rangle, |1, g\rangle, |0, e\rangle, |2, g\rangle, |1, e\rangle, ...\}$, obtaining a matrix that can be written as a direct sum of low-dimensional matrices (we say it has 'box structure')

$$H_{\rm JC} = \bigoplus_{n=0}^{\infty} H^{(n)} = \begin{pmatrix} H^{(0)} & & & \\ & H^{(1)} & & \\ & & H^{(2)} & \\ & & & \ddots \end{pmatrix}, \tag{260}$$

where $H^{(0)} = \langle 0, g|\hat{H}_{\rm JC}|0, g\rangle = -\hbar\varepsilon/2$, while for $n \geq 1$

$$H^{(n)} = \begin{pmatrix} \langle n, g|\hat{H}_{\rm JC}|n, g\rangle & \langle n, g|\hat{H}_{\rm JC}|n-1, e\rangle \\ \langle n-1, e|\hat{H}_{\rm JC}|n, g\rangle & \langle n-1, e|\hat{H}_{\rm JC}|n-1, e\rangle \end{pmatrix} = \hbar \begin{pmatrix} n\omega - \varepsilon/2 & \mathrm{i}\sqrt{n}g \\ -\mathrm{i}\sqrt{n}g & (n-1)\omega + \varepsilon/2 \end{pmatrix}. \tag{261}$$

These are Hermitian 2×2 matrices, and we show how to diagonalize them easily at the end of the section. Applied to our current case, we find the eigenenergies

$$E_\pm^{(n)} = (n - 1/2)\hbar\omega \pm \hbar\Omega_n/2, \tag{262}$$

where we have defined the *quantum Rabi frequency* $\Omega_n = \sqrt{\Delta^2 + 4ng^2}$, whose name will get meaning soon, and the *detuning* $\Delta = \omega - \varepsilon$. The corresponding eigenvectors can be written as

$$|\psi_+^{(n)}\rangle = \cos(\theta_n)|n, g\rangle - \mathrm{i}\sin(\theta_n)|n-1, e\rangle, \tag{263a}$$

$$|\psi_-^{(n)}\rangle = \sin(\theta_n)|n, g\rangle + \mathrm{i}\cos(\theta_n)|n-1, e\rangle, \tag{263b}$$

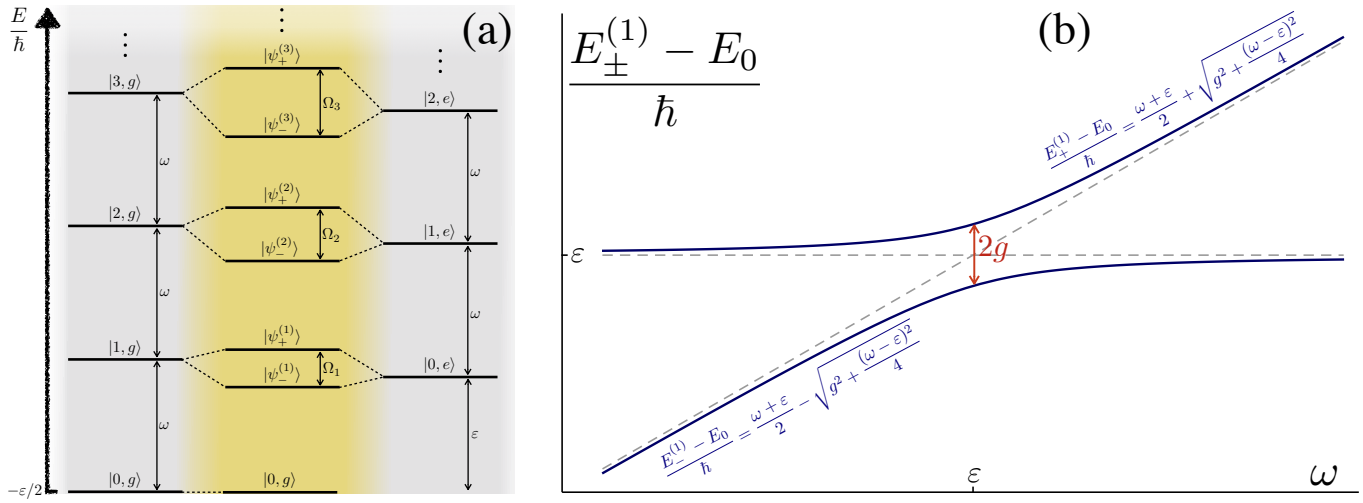

Figure 13. (a) Representation of the energy spectrum of the Jaynes-Cummings model. In the absence of coupling, it contains two harmonic ladders shifted by the atomic transition ε, corresponding to the states $|n,g\rangle$ and $|n,e\rangle$ (grey levels at both sides in the figure). Except for the ground state $|0,g\rangle$, the coupling hybridizes states $|n,g\rangle$ and $|n-1,e\rangle$, generating the states $|\psi_\pm^{(n)}\rangle$, whose energies show a splitting $\hbar\Omega_n$ (yellow levels in the middle). (b) First two transitions of the Jaynes-Cummings model as a function of the cavity frequency. For large detunings, the transitions tend to the free ones, ε and ω, shown as dashed grey lines. The effect of the coupling is to create an avoided crossing with $2g$ splitting.

where $\theta_n = \frac{1}{2}\arg\{\Delta + \mathrm{i}2\sqrt{n}g\} \in [0,\pi/2]$. Together with the $|0,g\rangle$ state, these so-called *dressed states* are the energy eigenstates associated to the (rotating-wave) interaction between a single optical mode and a single atomic transition, and form a basis of their combined Hilbert space. The expressions $\cos(2\theta_n) = \Delta/\sqrt{\Delta^2+4ng^2}$ and $\sin(2\theta_n) = 2\sqrt{n}g/\sqrt{\Delta^2+4ng^2}$ will also be useful for some calculations, and are obvious from the definition of θ_n.

In Fig. 13a we represent the energy spectrum. In the absence of coupling ($g=0$) we find two harmonic ladders with uniform level separation $\hbar\omega$, shifted by $\hbar\varepsilon$ (grey regions at the right and left sides of the figure). The effect of the coupling is to hybridize the states with the same number of excitations, $|n,g\rangle$ and $|n-1,e\rangle$, which in the absence of interaction have a splitting $\hbar|\Delta|$, but after switching on the interaction acquire a splitting $\hbar\Omega_n$ (yellow region in the center of the figure).

It is also interesting to analyze the level splitting as a function of the detuning. In order to do this, we make the following thought experiment: for a fixed atomic frequency ε we vary the cavity frequency ω and measure the first two energy transitions $E_\pm^{(1)} - E_0 = (\omega+\varepsilon)/2 \pm \sqrt{g^2+(\omega-\varepsilon)^2/4}$. The result is shown in Fig. 13b. In the absence of coupling, these transitions are simply given by ω and ε, and hence, they cross at $\omega=\varepsilon$. The coupling turns this crossing into an *avoided crossing* with splitting $2g$. The observation of such an avoided crossing is quite general for many types of interactions, and is one of the usual experimental methods by which couplings are measured in quantum optics.

Let us now, for completeness, show how to find the eigensystem of a general Hermitian matrix

$$H = \begin{pmatrix} a & e^{\mathrm{i}\psi}c \\ e^{-\mathrm{i}\psi}c & b \end{pmatrix}, \tag{264}$$

where all the parameters are real, and we take $c>0$. We denote the eigenvectors and eigenvalues by $\mathbf{v}_\pm$ and $E_\pm$, respectively, so that $H\mathbf{v}_\pm = E_\pm\mathbf{v}_\pm$. Let us start by noting that the matrix can be decomposed as $H = FSF^\dagger$, where F is diagonal and S a real symmetric matrix, specifically

$$F = \begin{pmatrix} 1 & 0 \\ 0 & e^{-\mathrm{i}\psi} \end{pmatrix}, \quad \text{and} \quad S = \begin{pmatrix} a & c \\ c & b \end{pmatrix}. \tag{265}$$

On the other hand, any real symmetric matrix can be diagonalized with a rotation, and then, $S = R(\theta)DR^T(\theta)$, withcan be diagonalized with a rotation $R(\theta) = \left(\begin{smallmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{smallmatrix}\right)$

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \quad \text{and} \quad D = \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}, \tag{266}$$

where the eigenvalues $E_\pm$ are easily found from the characteristic polynomial of S,

$$\det\left\{\begin{pmatrix} a-E_\pm & c \\ c & b-E_\pm \end{pmatrix}\right\}=0 \quad\Rightarrow\quad E_\pm=\frac{a+b\pm\sqrt{(a-b)^2+4c^2}}{2}, \tag{267}$$

while the angle θ is found from the condition

$$R^T(\theta)SR(\theta)=D \quad\Rightarrow\quad \begin{pmatrix} a\cos^2\theta+b\sin^2\theta+c\sin 2\theta & \frac{1}{2}(b-a)\sin 2\theta+c\cos 2\theta \\ \frac{1}{2}(b-a)\sin 2\theta+c\cos 2\theta & a\sin^2\theta+b\cos^2\theta-c\sin 2\theta \end{pmatrix}=\begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}, \tag{268}$$

whose anti-diagonal terms imply $2c=(a-b)\tan 2\theta$, while from the diagonal ones we get $E_+-E_-=(a-b)\cos 2\theta+2c\sin 2\theta=(a-b)/\cos 2\theta$, leading to

$$\cos 2\theta=\frac{a-b}{\sqrt{(a-b)^2+4c^2}}, \quad\text{and}\quad \sin 2\theta=\frac{2c}{\sqrt{(a-b)^2+4c^2}}. \tag{269}$$

These imply that $2\theta\in[0,\pi]$, which allows us to write $2\theta=\arg\{a-b+2\mathrm{i}c\}$.

Combining the diagonalization of S and the initial decomposition of H, we then see that $HU=UD$, where $U=FR(\theta)$ is unitary. Hence, up to an arbitrary phase, the columns of U are the eigenvectors of H, that is,

$$U=\begin{pmatrix} \cos\theta & -\sin\theta \\ e^{-\mathrm{i}\psi}\sin\theta & e^{-\mathrm{i}\psi}\cos\theta \end{pmatrix}=(e^{\mathrm{i}\phi_+}\mathbf{v}_+ \quad e^{\mathrm{i}\phi_-}\mathbf{v}_-), \tag{270}$$

where $\phi_\pm$ are arbitrary. For example, by choosing $e^{\mathrm{i}\phi_\pm}=\pm 1$, we obtain the eigenvectors

$$\mathbf{v}_+=\begin{pmatrix} \cos\theta \\ e^{-\mathrm{i}\psi}\sin\theta \end{pmatrix}, \quad\text{and}\quad \mathbf{v}_-=\begin{pmatrix} \sin\theta \\ -e^{-\mathrm{i}\psi}\cos\theta \end{pmatrix}. \tag{271}$$

Particularizing (261), (269), and (271) to $a=n\omega-\varepsilon/2$, $b=(n-1)\omega+\varepsilon/2$, $c=\sqrt{n}g$, and $\psi=\pi/2$, we obtain the eigensystem of $H^{(n)}$ as we presented it after (261).

3. *Quantum Rabi oscillations*

As an example of the use of the dressed-state basis, let's consider the evolution of the system when starting from the atom in the ground state with the field in an arbitrary pure state, that is,

$$|\psi(0)\rangle=\sum_{n=0}^{\infty}c_n|n,g\rangle=c_0|0,g\rangle+\sum_{n=1}^{\infty}c_n\left[\cos(\theta_n)|\psi_+^{(n)}\rangle+\sin(\theta_n)|\psi_-^{(n)}\rangle\right], \tag{272}$$

where in the second equality we have used $(n>0)$

$$|n,g\rangle=\cos(\theta_n)|\psi_+^{(n)}\rangle+\sin(\theta_n)|\psi_-^{(n)}\rangle, \tag{273a}$$

$$|n-1,e\rangle=\mathrm{i}\sin(\theta_n)|\psi_+^{(n)}\rangle-\mathrm{i}\cos(\theta_n)|\psi_-^{(n)}\rangle, \tag{273b}$$

found by inverting (263). Since we have written the initial state in terms of eigenstates of the Hamiltonian, it is straightforward to find the state at any other time,

$$|\psi(t)\rangle=e^{\hat{H}_{\mathrm{JC}}t/\mathrm{i}\hbar}|\psi(0)\rangle=c_0e^{\mathrm{i}\varepsilon t/2}|0,g\rangle+\sum_{n=1}^{\infty}c_ne^{-\mathrm{i}(n-1/2)\omega t}[\cos(\theta_n)e^{-\mathrm{i}\Omega_nt/2}|\psi_+^{(n)}\rangle+\sin(\theta_n)e^{\mathrm{i}\Omega_nt/2}|\psi_-^{(n)}\rangle]. \tag{274}$$

Using this state, we can make predictions for measurements of any observable at time t. For example, consider the probability of finding the atom in the excited state (irrespective of the optical state), which can be evaluated as the expectation value of the projector $\hat{I}\otimes|e\rangle\langle e|$, that is,

$$p_e(t)=\langle\psi(t)|\left(\hat{I}\otimes|e\rangle\langle e|\right)|\psi(t)\rangle=\langle\psi(t)|\left(\sum_{n=0}^{\infty}|n,e\rangle\langle n,e|\right)|\psi(t)\rangle=\sum_{n=0}^{\infty}|\langle n,e|\psi(t)\rangle|^2, \tag{275}$$

which is the sum of the probabilities of finding the atom in the excited state for all the possible photon numbers. Noting that $\langle n,e|\psi_+^{(m)}\rangle = -\mathrm{i}\sin(\theta_m)\delta_{n+1,m}$ and $\langle n,e|\psi_-^{(m)}\rangle = \mathrm{i}\cos(\theta_m)\delta_{n+1,m}$, so that

$$\langle n,e|\psi(t)\rangle = c_{n+1}e^{\mathrm{i}(n+1/2)\omega t}\sin(2\theta_{n+1})\sin(\Omega_{n+1}t/2),$$

we easily obtain

$$p_e(t) = \sum_{n=1}^{\infty}|c_n|^2\sin^2(2\theta_n)\sin^2(\Omega_n t/2) = \sum_{n=1}^{\infty}|c_n|^2\frac{1-\cos(\Omega_n t)}{2(1+\Delta^2/4ng^2)}, \tag{276}$$

where we have used $\sin^2\phi = (1-\cos 2\phi)/2$ and the expression $\sin(2\theta_n) = 2\sqrt{n}g/\Omega_n$ that we found in the previous section.

As a simple example, consider first that the initial state is the absolute ground state $|0,g\rangle$, so that $c_n = \delta_{n0}$. In such case, we obtain $p_e(t) = 0$ as expected. On the other hand, consider an initial Fock state $|N\rangle$ for the field, so that $c_n = \delta_{nN}$, obtaining the excited-state population

$$p_e(t) = \frac{1-\cos(\Omega_N t)}{2(1+\Delta^2/4Ng^2)}. \tag{277}$$

Starting from the ground state, when interacting with a field with N photons the atom then oscillates between the ground and excited states at frequency $\Omega_N = \sqrt{\Delta^2+4Ng^2}$, with a maximum population $p_e^{\max} = (1+\Delta^2/4Ng^2)^{-1}$ which is equal to 1 on resonance ($\Delta = 0$) but tends to 0 for large detuning ($|\Delta| \gg 4ng^2$). This is exactly the same as the Rabi oscillations that we studied in the previous chapter. In fact, the expression above is the same as (244), just with the identification $\Omega = 2\sqrt{N}g$.

4. Coherent light: Rabi oscillations (revisited), collapses, and revivals

We find ourselves now in a very peculiar situation. In the previous chapter, we argue that Rabi oscillations occur when the atom interacts with classical light. Indeed, let us consider the interaction (254), but with a classical monochromatic field

$$\mathbf{E}(z_0,t) = \mathbf{e}_x\sqrt{\frac{4\hbar\omega\bar{n}}{\varepsilon_0 LS}}\cos(\omega t)\sin(kz_0), \tag{278}$$

instead of a quantized one, where we have chosen $\cos(\omega t)$ for convenience, and we parametrize the electric field amplitude by a real number $\sqrt{\bar{n}}$. In the quantum description, this is equivalent to assuming that the field is in the coherent state $|-\mathrm{i}\sqrt{\bar{n}}e^{-\mathrm{i}\omega t}\rangle$ with average photon number $\bar{n}$, that is, $\langle -\mathrm{i}\sqrt{\bar{n}}e^{-\mathrm{i}\omega t}|\hat{\mathbf{E}}(z_0)|-\mathrm{i}\sqrt{\bar{n}}e^{-\mathrm{i}\omega t}\rangle$. Note that we are neglecting any back-action of the atom onto this field, whose amplitude remains unaffected over time. Proceeding in the same way as we did, we would obtain the semiclassical Rabi Hamiltonian (235) introduced in the previous chapter with the identification $\Omega = 2\sqrt{\bar{n}}g$. Since coherent states are the states that link quantum and classical physics, we would then expect equation (276) to predict Rabi oscillations when the field starts in a large-amplitude coherent state. However, it seems highly unlikely that when introducing in that equation the Poisson distribution $|c_n|^2 = e^{-\bar{n}}\bar{n}^n/n!$ corresponding to the coherent state, we will find the simple Rabi oscillations that we introduced at the end of the previous chapter in (244). Moreover, in the previous section we have seen that a fully quantum mechanical model predicts Rabi oscillations when the field is in a Fock state, which is actually one of the most quantum states one can think of. Therefore, it seems that we found a bit of a puzzle that needs to be understood.

In order to do so, let us work in resonance ($\Delta = 0$) for simplicity, so that, with the field in the initial coherent state considered above, the atomic population reads

$$p_e(t) = \sum_{n=0}^{\infty}|c_n|^2\frac{1-\cos(2\sqrt{n}gt)}{2} = \frac{1}{2} - \frac{1}{2}\sum_{n=0}^{\infty}e^{-\bar{n}}\frac{\bar{n}^n}{n!}\cos(2\sqrt{n}gt), \tag{279}$$

where we have extended the sum to zero from below for convenience, since the $n = 0$ term does not contribute when $\Delta = 0$. In Figure 14 we plot the population as a function of time with the help of a computer to perform the sum. We certainly observe oscillations, but contrary to the ones found in the previous chapter, they are damped towards $p_e = 1/2$ and reamplified cyclically. In order to understand the puzzle exposed above, we need to figure out where these *collapses* and *revivals* come from.

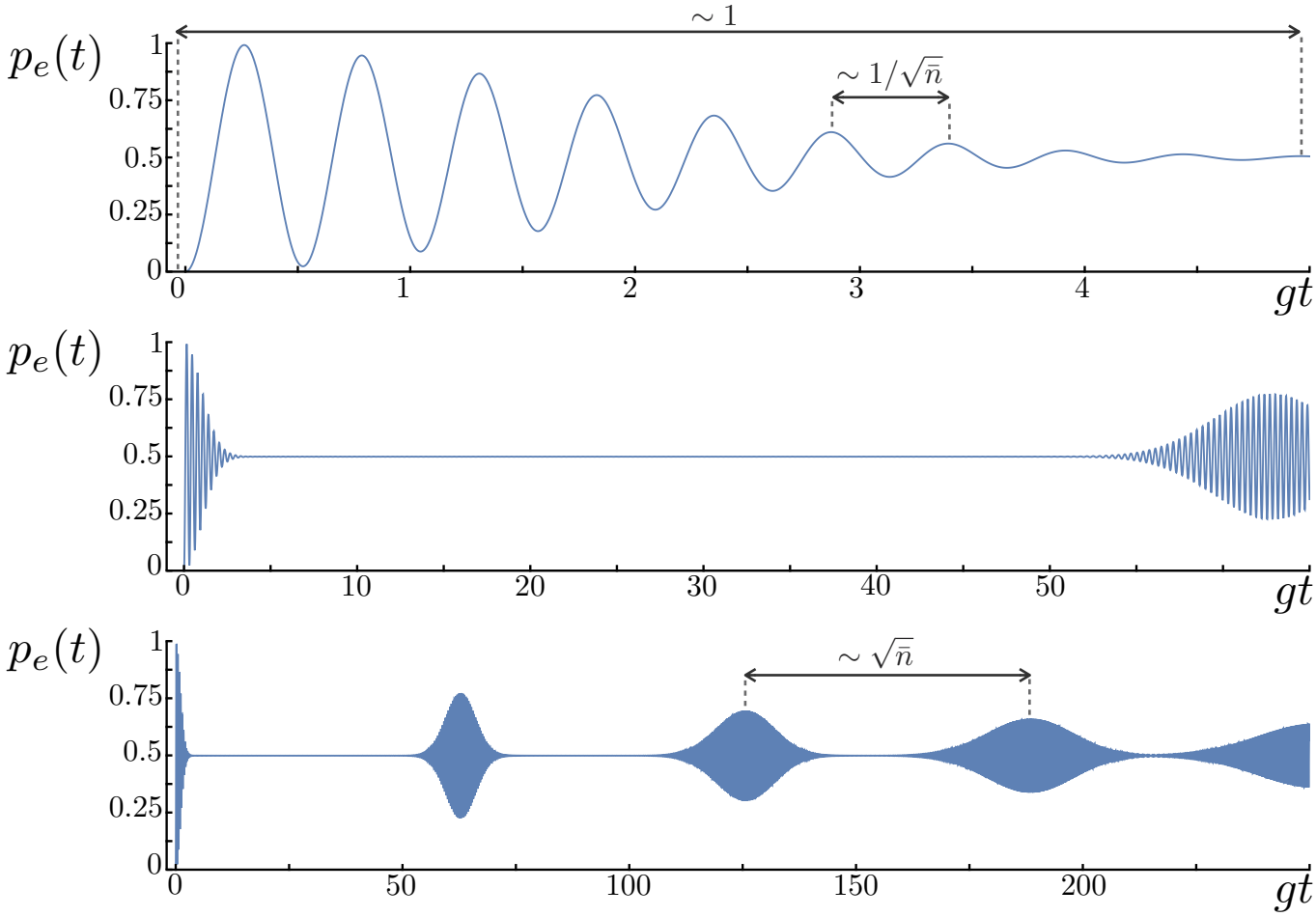

Figure 14. Excited-state population $p_e(t)$ as a function of time for an initial state $|-\mathrm{i}\sqrt{\bar{n}}\rangle \otimes |g\rangle$ with the field in a coherent state and the atom in the ground state. We take $\bar{n} = 100$ and show the evolution for three different time domains: $gt \in [0, 3]$ (upper figure), $gt \in [0, 65]$ (middle figure), and $gt \in [0, 250]$ (lower figure). We also show how the different relevant time scales scale with the parameters: Rabi oscillations ($gt \sim 1/\sqrt{\bar{n}}$), collapses ($gt \sim 1$), and revivals ($gt \sim \sqrt{\bar{n}}$).

In order to look for initial clues, let us find some approximate expression for the sum (279) that will give us the collapse rate. We are interested in the large-photon-number limit $\bar{n} \gg 1$, which is when coherent states link quantum and classical physics. In such case we can take the continuous limit and approximate the Poisson distribution by a Gaussian of width $\sqrt{\bar{n}}$. Specifically, we have

$$e^{-\bar{n}}\frac{\bar{n}^n}{n!} \approx \frac{1}{\sqrt{2\pi\bar{n}}}e^{-(n-\bar{n})^2/2\bar{n}}. \tag{280}$$

We can then replace the sum by an integral and even extend the lower integration limit to $-\infty$, since the Gaussian ensures that the negative values will not contribute effectively. On the other hand, writing $\cos(2\sqrt{n}gt) = [\exp(2\mathrm{i}\sqrt{n}gt) + \text{c.c.}]/2$ and expanding $\sqrt{n}$ around the mean photon number $\bar{n}$ as $\sqrt{n} \approx \sqrt{\bar{n}} + (n-\bar{n})/2\sqrt{\bar{n}} = \sqrt{\bar{n}}/2 + n/2\sqrt{\bar{n}}$, we get a simple Gaussian integral that can be analytically carried out[30]. In particular, we obtain

$$p_e(t) \approx \frac{1}{2} - \frac{1}{4}\left[\int_{-\infty}^{+\infty} dn \frac{1}{\sqrt{2\pi\bar{n}}}e^{-(n-\bar{n})^2/2\bar{n}}e^{\mathrm{i}\left(\sqrt{\bar{n}}+n/\sqrt{\bar{n}}\right)gt} + \text{c.c.}\right] = \frac{1}{2} - \frac{1}{2}e^{-g^2t^2/2}\cos(2g\sqrt{\bar{n}}t). \tag{281}$$

This expression contains two interesting features. First, we see that it provides the expected Rabi frequency and an expression for the population that matches the one we obtained in the previous chapter for short times $t \ll \sqrt{2}/g$,

[30] In general:

$$\int_{\mathbb{R}} dz e^{Bz - z^2/2A} = \sqrt{2\pi A}e^{AB^2/2},$$

for any $B > 0$ and $A \in \mathbb{C}$.

see (244). However, we find that the oscillations are damped at a rate $\gamma_c = g/\sqrt{2}$, which provides the collapse rate. Interestingly, this rate depends solely on the coupling g and not on the coherent photon number $\bar{n}$. Now, note that in the classical limit $\bar{n} \gg 1$ and therefore the frequency of the Rabi oscillations $\Omega = 2\sqrt{\bar{n}}g$ is much larger than the collapse rate $\gamma_c = g/\sqrt{2}$. Hence, the classical picture studied in the previous chapter is indeed correct during many Rabi cycles, and quantum effects can only be appreciated on longer time scales.

Now that we have managed to reconcile our previous semiclassical result (244) with the fully quantum expression (279), let us now discuss the origin of the collapses and revivals. In fact, they are relatively simple to understand based on expression (279). First, note that the Poisson distribution in the sum cuts off essentially all Fock numbers n outside the interval $\left[\bar{n} - \sqrt{\bar{n}}, \bar{n} + \sqrt{\bar{n}}\right]$. On the other hand, as $\bar{n}$ becomes larger and larger, the quantum Rabi frequencies $\Omega_n = 2\sqrt{n}g$ in that interval become closer and closer. Hence, initially it will look as if all the terms in the sum oscillate in phase at a similar rate $\Omega_{\bar{n}} = 2\sqrt{\bar{n}}g$. However, as time goes by, the terms will start dephasing more and more, eventually getting completely out of phase and averaging to zero. If this intuition is true, then the rate of collapse should be proportional to the difference between the Rabi frequencies at the edge of the interval, that is,

$$\gamma_c \sim \Omega_{\bar{n}+\sqrt{\bar{n}}} - \Omega_{\bar{n}-\sqrt{\bar{n}}} = 2g\left(\sqrt{\bar{n}+\sqrt{\bar{n}}} - \sqrt{\bar{n}-\sqrt{\bar{n}}}\right) = 2g\sqrt{\bar{n}}\Bigg(\underbrace{\sqrt{1+\frac{1}{\sqrt{\bar{n}}}}}_{\approx 1+\frac{1}{2\sqrt{\bar{n}}}} - \underbrace{\sqrt{1-\frac{1}{\sqrt{\bar{n}}}}}_{\approx 1-\frac{1}{2\sqrt{\bar{n}}}}\Bigg) \approx 2g. \tag{282}$$

Indeed, apart from a numerical prefactor, this is in agreement with the collapse rate $\gamma_c = g/\sqrt{2}$ found above.

According to this picture, the revivals can then be interpreted as the re-phasing of the elements of the sum. We can estimate the times when the revivals appear by evaluating the times t_r for which neighboring terms re-phase, which in turn can be estimated as

$$\left(\Omega_{\bar{n}+1} - \Omega_{\bar{n}-1}\right) t_r = 2\pi m, \quad \text{with } m \in \mathbb{N}. \tag{283}$$

Using the approximation $\sqrt{\bar{n} \pm 1} = \sqrt{\bar{n}} \pm 1/2\sqrt{\bar{n}}$, we then obtain

$$t_r \approx \frac{\pi\sqrt{\bar{n}}}{g} m, \quad \text{with } m \in \mathbb{N}. \tag{284}$$

This predicts that the revivals are uniformly spaced in time, which is exactly what we observe in Fig. 14. On the other hand, it predicts that the spacing will increase as the square root of the coherent photon number, which is easily checked to be true.

C. Light in a nonlinear dielectric

1. *Dielectric media in the dipole approximation and the refractive index*

After studying the interaction of light with a single atom, now we analyze another paradigmatic example of light-matter interaction in a completely different regime. In particular, we consider now dielectric media, which are insulating materials with all their charges bound (with no free charges they cannot support electrical currents), but where light can still propagate by polarizing those bound charges (that is, pulling apart positive and negative charges). Most optical elements including, for example, beam splitters and mirrors, are made out of this type of materials. When the coupling between light and the dielectric is not very strong, we can assume that the electric polarization density acquired by the medium depends on the applied electric field as a low-order polynomial,

$$P_j(\mathbf{r},t) = \underbrace{\sum_{k=x,y,z} \varepsilon_0 \chi^{(1)}_{jk} E_k(\mathbf{r},t)}_{P^{(1)}_j(\mathbf{r},t)} + \underbrace{\sum_{k,l=x,y,z} \varepsilon_0 \chi^{(2)}_{jkl} E_k(\mathbf{r},t) E_l(\mathbf{r},t)}_{P^{(2)}_j(\mathbf{r},t)} + ..., \tag{285}$$

so that the medium is treated as a passive system whose information is all contained in the $\chi^{(n)}_{j_1 j_2 \ldots j_n}$ coefficients (assumed larger than zero for all orders for simplicity), called n^{th}-order susceptibilities. Note that we are further assuming an instantaneous and homogeneous response of the medium, as the electric polarization at time t depends only on the electric fields at that time and the susceptibilities are independent of $\mathbf{r}$.

Let us now discuss how Maxwell equations are modified inside the dielectric medium. It is a well-known result in electrodynamics [61] that an electric polarization density $\mathbf{P}(\mathbf{r},t)$ creates a charge density given by $\rho(\mathbf{r},t) = -\boldsymbol{\nabla}\cdot\mathbf{P}(\mathbf{r},t)$.

On the other hand, the continuity equation $\partial_t \rho(\mathbf{r},t) = -\boldsymbol{\nabla}\cdot\mathbf{j}(\mathbf{r},t)$ tells us that an effective current $\mathbf{j}(\mathbf{r},t) = \partial_t \mathbf{P}(\mathbf{r},t)$ is also induced in the material. These induced charge and current densities, which are responsible for allowing the electromagnetic field to propagate in the otherwise isolating medium, must be included in the inhomogeneous Maxwell equations (51). We obtain then the so-called *macroscopic Maxwell equations*

$$\begin{aligned} \boldsymbol{\nabla}\cdot\mathbf{D}(\mathbf{r},t) &= 0, \qquad & \boldsymbol{\nabla}\times\mathbf{B}(\mathbf{r},t) &= \mu_0\partial_t\mathbf{D}(\mathbf{r},t), \\ \boldsymbol{\nabla}\cdot\mathbf{B}(\mathbf{r},t) &= 0, & \boldsymbol{\nabla}\times\mathbf{E}(\mathbf{r},t) &= -\partial_t\mathbf{B}(\mathbf{r},t), \end{aligned} \tag{286}$$

where we have defined the *displacement field*

$$\mathbf{D}(\mathbf{r},t) = \varepsilon_0\mathbf{E}(\mathbf{r},t) + \mathbf{P}(\mathbf{r},t). \tag{287}$$

This expression, together with (285), is known as the *constitutive relation* of the dielectric medium.

Let us now neglect higher order terms, and discuss the effect that the linear term $\mathbf{P}^{(1)}(\mathbf{r},t)$ has on a field propagating in the dielectric medium. For simplicity, we assume a diagonal susceptibility that doesn't couple different components of the electric field, that is

$$\chi^{(1)}_{jk} = \chi^{(1)}_j \delta_{jk}. \tag{288}$$

Note that this can always be obtained in the experiment by properly orienting the nonlinear medium, so that its principal axes (the ones that diagonalize their linear susceptibility matrix, which for crystalline materials with a cubic lattice simply follow the crystal axes) follow the directions that we define as x, y, and z. The displacement field can then be written as

$$D_j(\mathbf{r},t) = \underbrace{\varepsilon_0(1+\chi^{(1)}_j)}_{\varepsilon_j} E_j(\mathbf{r},t), \tag{289}$$

leading to a set of Maxwell equations with the same form as those in the absence of charges and currents, but with modified electric permeabilities ε_j along the corresponding coordinate axis instead of ε_0. We discuss now the three most dramatic effects that this modified electric permeability has: wavelength and amplitude reduction, as well as the possibility of phase shifts, see Fig. **ToDo**. In order to illustrate these, we consider a monochromatic plane wave with vector potential $\mathbf{A}(z,t) = \mathbf{e}_j A e^{\mathrm{i}(kz-\omega t)} + \text{c.c.}$ and $A \in \mathbb{R}$ for simplicity, propagating from vacuum into the dielectric, and analyze the changes that it suffers when entering the medium:

- Defining the refractive index $n_j = \sqrt{1+\chi^{(2)}_j}$ along $\mathbf{e}_j$, and defining the Coulomb gauge by the condition $\sum_{j=x,y,z}\varepsilon_j\partial_j A_j = 0$ (which turns into the usual $\boldsymbol{\nabla}\cdot\mathbf{A} = 0$ when $\varepsilon_x = \varepsilon_y = \varepsilon_z$), the wave equation for the vector potential is now written as

$$\left(\frac{c^2}{n_j^2}\boldsymbol{\nabla}^2 - \partial_t^2\right) A_j(\mathbf{r},t) = 0, \tag{290}$$

  which shows that the speed of light is reduced in the medium, following intuition (now the field has to go through the dipoles in order to advance). Note that this means that when using plane waves to expand the fields we must be careful to modify accordingly the wave vector[31] by a factor n_j, so that the monochromatic plane wave is modified as

$$\mathbf{e}_j e^{\mathrm{i}(kz-\omega t)} \quad \to \quad \mathbf{e}_j e^{\mathrm{i}(n_j kz-\omega t)}, \tag{291}$$

  where we still define $k = \omega/c$, writing the refractive index explicitly in the equation.

- The next effect is more subtle, and has to do with how the amplitude A is modified when crossing the dielectric interface. In general, part of the amplitude will be transmitted and part will be reflected, as specified by the well-known Fresnel relations [74]. Therefore, adding a dielectric inside an optical cavity leads in general to nontrivial interference effects between the various waves being transmitted and reflected at the dielectric and the

[31] An important side note is in order. Sometimes there is a bit of confusion regarding the relation between wavelength and frequency. The frequency of a generated monochromatic wave, that is, the speed of oscillations in time, is an intrinsic property of the wave that doesn't change no matter where it propagates. On the other hand, the wavelength refers to the periodicity of the wave in space. Clearly, for a fixed temporal oscillation (with frequency $\nu = \omega/2\pi$), this will depend on the speed of the wave, say v. The wavelength will then be $\lambda = v/\nu$, and hence, for the monochromatic wave it is larger in vacuum ($v = c$) than in the dielectric ($v = c/n$).

mirror surfaces. For this reason, in experiments one usually uses some anti-reflecting coating on the surface of the dielectric, so that all the incoming power enters the dielectric, and interference effects between the incoming wave and the wave reflected at the dielectric are minimized. Fortunately, in such case the effect of the dielectric on the amplitude A can be understood very easily, just by conservation of power arguments.
Let us set the position of the input plane of the dielectric material at $z = 0$ for simplicity, and denote by $z = 0^-$ and $z = 0^+$ its left and right sides, where we have vacuum and the dielectric material, respectively (see Fig. **ToDo**). The vector potential, electric and magnetic fields at either side are then

$$\mathbf{A}(0^\pm, t) = \mathbf{e}_x A_\pm e^{\varphi_\pm - \mathrm{i}\omega t} + \text{c.c.}, \tag{292a}$$

$$\mathbf{E}(0^\pm, t) = -\,\partial_t \mathbf{A}(z,t)|_{z=0^\pm} = 2\mathbf{e}_x \omega A_\pm \sin(\omega t - \varphi_\pm), \tag{292b}$$

$$\mathbf{B}(0^\pm, t) = \boldsymbol{\nabla} \times \mathbf{A}(z,t)|_{z=0^\pm} = 2\mathbf{e}_y n_\pm k A_\pm \sin(\omega t - \varphi_\pm), \tag{292c}$$

where $A_- = A$, $\varphi_+ = 0$, $n_- = 1$, and $n_+ = n_x$, while A_+ and φ_+ (amplitude and phase of the transmitted wave) are the only parameters left to determine. In order to do this, we evaluate the instantaneous power by integrating the absolute value of the Poynting vector $[\mathbf{E}(z,t) \times \mathbf{B}(z,t)]/\mu_0$ in the transverse plane. At the either side of the input plane of the dielectric we then obtain the power

$$P_\pm(t) = \int_{\mathbb{R}^2} dxdy \frac{|\mathbf{E}(0^\pm, t) \times \mathbf{B}(0^\pm, t)|}{\mu_0} = \frac{4S\omega^2 n_\pm}{c\mu_0} A_\pm^2 \sin^2(\omega t - \varphi_\pm). \tag{293}$$

Then, imposing that power is conserved upon transmission through the dielectric interface, so that $P_-(t) = P_+(t)$, we obtain

$$A_+ = A/\sqrt{n_x}, \quad \text{and} \quad \varphi_- = 0 \text{ or } \pi. \tag{294}$$

Hence, we have been able to determine the amplitude of the transmitted wave, which is reduced by a factor $\sqrt{n_x}$ as anticipated above. As for the phase, the conservation of power argument fully determines it up to a π indeterminacy, which will not play any relevant role in our future derivations.

Finally, we need to consider how the quantization of the electromagnetic field that we introduced in Chapter II gets affected when a dielectric medium is introduced in the optical cavity.

- In principle, with a dielectric medium inside the cavity, we would also need to modify the cavity modes and the quantization procedure. In order to see this, consider for definiteness the situation depicted in Figure **ToDo**. The phase picked up during a round trip is not $2kL$ but $2k(L - l + n_j l)$ for a wave polarized along $\mathbf{e}_j$, and hence, the resonant frequencies obtained when asking this phase to be an integer multiple of 2π are modified in the presence of the dielectric. Moreover, the electric contribution to the electromagnetic energy contained inside the dielectric is given by the volume integral of $\mathbf{D}(\mathbf{r},t) \cdot \mathbf{E}(\mathbf{r},t)$ not $\varepsilon_0 \mathbf{E}^2(\mathbf{r},t)$ as in (62). However, in order to keep things as simple as possible, we will assume that the dielectric is much smaller than the cavity length ($l \ll L$), so we can neglect these contributions to the cavity modes and frequencies, as well as to the electromagnetic energy.

With these considerations in mind, in the following we will write the cavity electric field inside the dielectric as $\hat{\mathbf{E}}(z,t) = \hat{\mathbf{E}}^{(+)}(z,t) + \hat{\mathbf{E}}^{(-)}(z,t)$, with

$$\hat{\mathbf{E}}^{(+)}(z,t) = \mathrm{i} \sum_{j=x,y} \mathbf{e}_j \sum_{m=1}^{\infty} \sqrt{\frac{\hbar\omega_m}{\varepsilon_0 n_j LS}} \hat{a}_{m,j}(t) \sin\left(n_j k_m z + \varphi_{m,j}\right), \tag{295}$$

where for future purposes we allow the electric field to be polarized either along the $\mathbf{e}_x$ or $\mathbf{e}_y$ directions, which see different refractive indices in general. Moreover, we allow different modes to have different phases φ_m within the dielectric, which is what naturally happens in an optical cavity owed to many other elements that conform it (lenses, phase plates, polarizers, etc...). In general, different cavity geometries would lead to different mode profiles inside the crystal, and this is our way to include in a simple manner such effects. Indeed, we'll see that optimizing the geometry is crucial in order to obtain the desired effects.

2. Basic second-order processes: frequency conversion

Before proceeding with the quantum description of nonlinear dielectrics, it is convenient to understand at least conceptually, the classical phenomena they lead to. We will now discuss this on the basis of a wave equation for the

electric field that we can easily find from the macroscopic Maxwell equations (working with potentials in nonlinear dielectrics is now more complicated, and an equation for the electric field will suffice for our purposes). In order to find such equation, we take the curl of the homogeneous Maxwell equation $\boldsymbol{\nabla}\times\mathbf{E}(\mathbf{r},t)=-\partial_t\mathbf{B}(\mathbf{r},t)$, and use the identity $\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{E}=\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{E})-\boldsymbol{\nabla}^2\mathbf{E}$, together with the macroscopic Maxwell equations (286) and the form $D_j(\mathbf{r},t)=\varepsilon_j E_j(\mathbf{r},t)+P_j^{(2)}(\mathbf{r},t)$ of the displacement field (we will consider only second order effects for now). Using a quasi-1D approximation where the fields propagate along the z axis with transverse polarization and no dependence on the transverse variables, we finally arrive to

$$\partial_z^2 E_j(z,t)-\mu_0\varepsilon_j\partial_t^2 E_j(z,t)=\mu_0\partial_t^2 P_j^{(2)}(z,t). \tag{296}$$

This is just a wave equation for the electric field, in which the nonlinear polarization acts as a source for electromagnetic waves. As we are about to see, this gives rise to the phenomenon of frequency conversion, that is, the possibility of generating light at frequencies different than the one we feed the dielectric with.

We can see this with a simple example. Consider a monochromatic light wave at some frequency ω_0 entering the dielectric material. Right at the input plane inside the dielectric material, which here we take as $z=0$ for convenience (see Fig. **ToDo**), we write the corresponding electric field as $\mathbf{E}(0,t)=\mathbf{e}_x E_{\omega_0}\cos(\omega_0 t)$. The quadratic polarization density (285) takes then the form

$$P_j^{(2)}(0,t)=\varepsilon_0\chi_{jxx}^{(2)}E_{\omega_0}^2\cos^2(\omega_0 t)=\frac{1}{2}\varepsilon_0\chi_{jxx}^{(2)}E_{\omega_0}^2[1+\cos(2\omega_0 t)], \tag{297}$$

which, apart from an irrelevant constant term, oscillates at frequency $2\omega_0$. When introduced in the wave equation (296), this polarization will then act as a source for waves at frequency $2\omega_0$, that is, the medium will generate the *second harmonic* of the original light wave (Figure **ToDo**).

Consider now an input light wave with two frequencies with different polarization, say $\mathbf{E}(0,t)=\mathbf{e}_x E_{\omega_1}\cos(\omega_1 t)+\mathbf{e}_y E_{\omega_2}\cos(\omega_2 t)$ with $\omega_1>\omega_2$ for definiteness. Furthermore, in order to simplify things, let us assume $\chi_{jxx}^{(2)}=0=\chi_{jyy}^{(2)}$, so that $\chi_{jxy}^{(2)}=\chi_{jyx}^{(2)}$ are the only susceptibilities different than zero. In such case, the quadratic polarization density reads

$$P_j^{(2)}(0,t)=2\varepsilon_0\chi_{jxy}^{(2)}E_{\omega_1}E_{\omega_2}\cos(\omega_1 t)\cos(\omega_2 t)=\varepsilon_0\chi_{jxy}^{(2)}E_{\omega_1}E_{\omega_2}[\cos(\omega_+ t)+\cos(\omega_- t)], \tag{298}$$

where we have defined the sum and difference frequencies $\omega_\pm=\omega_1\pm\omega_2$. These terms will then act as sources of new waves at those frequencies, leading to the processes known as *sum-frequency* and *difference-frequency* generation. Obviously, second-harmonic generation can be understood as a particular case of sum-frequency generation with $\omega_1=\omega_2=\omega_0$. In general, these frequency-conversion processes generated by $\mathbf{P}^{(2)}(\mathbf{r},t)$ are known as *three-wave mixing*, because two waves combine to generate a third one.

For our quantum purposes, the most interesting three-wave mixing process is that in which we feed both a frequency and its second harmonic, that is, $\omega_1=2\omega_0$ and $\omega_2=\omega_0$. Let us focus in particular on the frequency difference term, which reads

$$P_j^{(2)}(0,t)=\varepsilon_0\chi_{jxy}^{(2)}E_{2\omega_0}E_{\omega_0}\cos(\omega_0 t), \tag{299}$$

and acts then a source for waves at frequency ω_0. The most interesting regime in this case is $E_{\omega_0}\ll E_{2\omega_0}$. In such situation, the process induced by this term can be understood as the transfer of energy from the $2\omega_0$ wave to the ω_0 wave, which will gain intensity as the field propagates in the medium (Figure **ToDo**). Such a process is known as *down-conversion*[32], which can be understood as the dual of second-harmonic generation. In this context, it is common to called *pump* to the $2\omega_0$ wave. Note that down-conversion cannot start without some light at the down-converted frequency ω_0 already present in the medium, as for $E_{\omega_0}=0$ the relevant term (299) of the polarization density vanishes. However, this trigger need not be a monochromatic field that we feed, but could simply be light generated by random fluctuations of thermal or even quantum origin. In such situation, we talk then about *spontaneous* down-conversion (Figure **ToDo**).

In the remaining of the chapter we focus on this type of process, which leads to very interesting quantum properties of the down-converted light, and squeezing in particular.

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[32] Or *parametric down-conversion*, though the term "parametric" has an obscure origin, and we will not use it here (especially because later we will introduce what we will call the "parametric approximation", and we don't want to confuse these terms).

3. Down-conversion Hamiltonian

We turn now our attention to the quantum mechanical description of nonlinear optics by means of the light-matter interaction model within the dipole approximation introduced in Section IV A. As explained above, dielectric media admit an effective description in terms of an electric polarization density that can be expanded in powers of the electric field, so that matter does not have dynamical degrees of freedom. The linear term can be included in the free description of the electric field as explained in Section IV C 1, see Eq. (295). Hence, for the interaction terms we only consider the nonlinear terms of the polarization density, focusing here on the quadratic one. The Hamiltonian is then written as $\hat{H} = \hat{H}_{\mathrm{L}} + \hat{H}_{\mathrm{LM}}$, with

$$\hat{H}_{\mathrm{LM}} = -\int_{\mathrm{medium}} d^3\mathbf{r}\hat{\mathbf{E}}(\mathbf{r}) \cdot \hat{\mathbf{P}}^{(2)}(\mathbf{r}), \tag{300}$$

where we have implicitly chosen the Schrödinger picture to write the expression, as operators do not evolve. In order to favor down-conversion, we assume that the medium is inside a cavity where all three-wave mixing processes are far off resonant except for the one involving two cavity modes at frequencies ω_0 and ω_2 (close to $2\omega_0$), with orthogonal polarizations and annihilation operators $\hat{a}$ and $\hat{b}$, respectively. Considering only these relevant modes, the electric field inside the dielectric medium can be written within our usual quasi-1D approximation as $\hat{\mathbf{E}}(z) = \hat{\mathbf{E}}_0(z) + \hat{\mathbf{E}}_2(z)$, with

$$\hat{\mathbf{E}}_0(z) = \mathrm{i}\mathbf{e}_y \sqrt{\frac{\hbar\omega_0}{\varepsilon_0 n_y L S}} (\hat{a} - \hat{a}^\dagger) \sin\left(n_y k_0 z + \varphi_0\right), \tag{301a}$$

$$\hat{\mathbf{E}}_2(z) = \mathrm{i}\mathbf{e}_x \sqrt{\frac{\hbar\omega_2}{\varepsilon_0 n_x L S}} (\hat{b} - \hat{b}^\dagger) \sin\left(n_x k_2 z + \varphi_2\right). \tag{301b}$$

The free Hamiltonian reads in this case as

$$\hat{H}_{\mathrm{L}} = \hbar\omega_0 \hat{a}^\dagger \hat{a} + \hbar\omega_2 \hat{b}^\dagger \hat{b}. \tag{302}$$

Let us now find an expression of the interaction Hamiltonian in terms of annihilation and creation operators. In order to simplify the calculation, we assume that the only non-vanishing second-order susceptibility coefficient is $\chi^{(2)}_{xyy}$ (you can convince yourself easily that a more general case would lead to the same final form of the Hamiltonian, just with more effort), so that the quadratic polarization density is written as

$$\hat{\mathbf{P}}^{(2)}(z) = \mathbf{e}_x \varepsilon_0 \chi^{(2)}_{xyy} \hat{\mathbf{E}}_0^2(z) = -\mathbf{e}_x \chi^{(2)}_{xyy} \frac{\hbar\omega_0}{n_y L S} \sin^2\left(n_y k_0 z + \varphi_0\right) \left(\hat{a} - \hat{a}^\dagger\right)^2. \tag{303}$$

Introducing this expression into (300) we obtain

$$\begin{aligned} \hat{H}_{\mathrm{LM}} &= -S \int_{z_0 - l/2}^{z_0 + l/2} \hat{\mathbf{E}}_2(z) \cdot \hat{\mathbf{P}}^{(2)}(z) \\ &= \mathrm{i}\chi^{(2)}_{xyy} \sqrt{\frac{\hbar^3 \omega_2 \omega_0^2}{\varepsilon_0 n_x n_y^2 L^3 S}} \underbrace{(\hat{b} - \hat{b}^\dagger)\left(\hat{a} - \hat{a}^\dagger\right)^2}_{\hat{h}} \underbrace{\int_{z_0 - l/2}^{z_0 + l/2} dz \sin^2\left(n_y k_0 z + \varphi_0\right) \sin\left(n_x k_2 z + \varphi_2\right)}_{J}, \end{aligned} \tag{304}$$

where z_0 is the position of the medium's center in the cavity, see Figure **ToDo**, and we have assumed that the medium is as large as the cavity along the transverse direction, so that $\int_{\mathrm{medium}} dxdy = S$. This Hamiltonian can be greatly simplified by using energy and momentum conservation. Let's see how these come about.

First we bring our attention to the operator part of the expression, which we can write as $\hat{h} = \hat{b}\hat{a}^{\dagger 2} - \hat{b}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger) + \hat{b}\hat{a}^2 - \mathrm{H.c.}$. Keeping in mind that $\hat{H}_{\mathrm{LM}}$ is supposed to be just a perturbation onto $\hat{H}_{\mathrm{L}}$, the energies associated with creation or annihilation of down-converted and pump photons are $\hbar\omega_0$ and $\hbar\omega_2 \approx 2\hbar\omega_0$, respectively. Hence, while the first term in $\hat{h}$ is consistent with energy conservation (two down-converted photons appear from the annihilation of a pump photon), the other two are not, since we annihilate energies $\hbar(\omega_2 + \omega_0)$ and $\hbar(\omega_2 + 2\omega_0)$, but create only energies $\hbar\omega_0$ and 0, respectively. Hence, within the rotating-wave approximation we can approximate the operator part of this interaction Hamiltonian by $\hat{h} \approx \hat{b}\hat{a}^{\dagger 2} - \hat{b}^\dagger \hat{a}^2$.

Let us now consider the integral along z, which is easily found to be[33]

$$\frac{4}{l}J = -\sin\left[\varphi_2 - 2\varphi_0 + (n_x k_2 - 2n_y k_0)z_0\right]\operatorname{sinc}\left[(n_x k_2 - 2n_y k_0)l/2\right] \\ -\sin\left[\varphi_2 + 2\varphi_0 + (n_x k_2 + 2n_y k_0)z_0\right]\operatorname{sinc}\left[(n_x k_2 + 2n_y k_0)l/2\right] + 2\sin\left(\varphi_2 + n_x k_2 z_0\right)\operatorname{sinc}\left(n_x k_2 l/2\right) \tag{305}$$

where $\operatorname{sinc} x = \frac{\sin x}{x}$ is a symmetric function that starts at 1 for $x = 0$ and decays as $1/|x|$ with oscillations. Hence, we see that the interaction will be non-negligible only as long as at least one among $(2n_y k_0 \pm n_x k_2)l/2$ or $n_x k_2 l/2$ is small. Reminding that typical optical wave vectors are on the order of $(100\text{nm})^{-1}$ and the refractive index for dielectric materials is order 1, while dielectric media in nonlinear experiments is usually never as small as 100nm, we see that the terms in the second line of (305) will always be negligible. Only the term in the first line can provide a non-negligible contribution, but it requires the so-called *phase-matching condition*

$$\phi = (2n_y k_0 - n_x k_2)l/2 \ll 1, \tag{306}$$

where ϕ is known as the *phase mismatch*. Note that this condition can be understood as momentum conservation of the photons involved in the three-wave mixing process: one pump photon with momentum $n_x \hbar k_2$ generates two down-converted photons with momenta $n_y \hbar k_0$. Note also that this condition is not only achieved by adjusting the mode frequencies, but also by a proper tuning of the refractive indices along the different axes, which can be done experimentally in many ways (e.g., changing the temperature of the dielectric medium or applying a static electric field on it). Since this term is rooted in momentum conservation, it will always appear no matter the cavity geometry or the optical elements we put around the dielectric. In contrast, the sine term multiplying it is dependent on the cavity geometry, as evidenced by the fact that it depends on the phase factor $\varphi_2 - 2\varphi_0$. Hence, this term will take different forms for different configurations, and one has to be careful to optimize it. For example, in our case, we simply let the phases φ_0 and φ_2 be zero, we obtain a negligible interaction. In the following we will assume that the geometry is optimized (e.g., $\varphi_2 - 2\varphi_0 = -\pi/2$ in our setting) and that perfect phase matching has been obtained ($\phi = 0$), so that the integral can be approximated by $J \approx l/4$.

Taking into account all these considerations, we write the final Hamiltonian as

$$\hat{H}_{\text{DC}} = \hbar\omega_0 \hat{a}^\dagger \hat{a} + \hbar\omega_2 \hat{b}^\dagger \hat{b} + \mathrm{i}\hbar\frac{g_0}{2}(\hat{b}\hat{a}^{\dagger 2} - \hat{b}^\dagger \hat{a}^2), \tag{307}$$

where we have defined the *down-conversion rate*

$$g_0 = \chi^{(2)}_{xyy}\frac{l}{2}\sqrt{\frac{\hbar\omega_2\omega_0^2}{\varepsilon_0 n_x n_y^2 L^3 S}}, \tag{308}$$

which is typically several orders of magnitude below optical frequencies.

Despite its seemingly simple form, this Hamiltonian cannot be diagonalized analytically. This is indeed a common feature of bosonic Hamiltonians with terms beyond quadratic in the annihilation and creation operators, except in very specific cases. However, in the following we perform a simple approximation that will turn the Hamiltonian into a quadratic one that we can treat analytically.

4. Parametric approximation: Bogoliubov physics, squeezing generation, and bosonic instabilities.

When we are interested in the situation depicted in Figure **ToDo**, in which the down-converted field is generated from a pump field of very large amplitude, we can make one more approximation: the so-called *parametric approximation*, in which the pump is treated as a classical source field that doesn't get depleted. Let us perform now such an approximation, and analyze the Hamiltonian we are left with.

Similarly to the semiclassical approximation for the light-atom interaction discussed in Section IV B 4, specifically Eq. (278), we can perform the parametric approximation by replacing the operator $\hat{\mathbf{E}}_2(z)$ in (304) by the classical field

$$\mathbf{E}_2(z,t) = -\mathbf{e}_x\sqrt{\frac{4\hbar\omega_2\bar{N}_2}{\varepsilon_0 n_x L S}}\cos(\omega_2 t)\sin\left(n_x k_2 z + \varphi_2\right), \tag{309}$$

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[33] Just write all the sine functions as complex exponentials, perform the integrals, and simplify.

where we again parametrize the field amplitude by the square of the mean photon number $\bar{N}_2$, and we choose the $-\cos(\omega_2 t)$ oscillations for furutre convenience. Equivalently, we are just assuming that the pump field is in a coherent state $|\mathrm{i}\sqrt{\bar{N}_2}e^{-\mathrm{i}\omega_2 t}\rangle$, so that $\mathbf{E}_2(z,t) = \langle \mathrm{i}\sqrt{\bar{N}_2}e^{-\mathrm{i}\omega_2 t}|\hat{\mathbf{E}}_2(z)|\mathrm{i}\sqrt{\bar{N}_2}e^{-\mathrm{i}\omega_2 t}\rangle$. The Hamiltonian can be written in this case as

$$\hat{H}_{\mathrm{PDC}} = \hbar\omega_0 \hat{a}^\dagger \hat{a} + \hbar g_0 \sqrt{\bar{N}_2}\sin(\omega_2 t)\left(\hat{a} - \hat{a}^\dagger\right)^2 \approx \hbar\omega_0 \hat{a}^\dagger\hat{a} - \frac{\hbar g}{2}(e^{-\mathrm{i}\omega_2 t}\hat{a}^{\dagger 2} + e^{\mathrm{i}\omega_2 t}\hat{a}^2), \tag{310}$$

where in the last step we have performed the rotating-wave approximation and defined a *dressed down-conversion rate*

$$g = \sqrt{\bar{N}_2}g_0, \tag{311}$$

which can be many orders of magnitude above the bare rate g_0, but still well below ω_0 for typical quantum optics experiments. Note that the final Hamiltonian (310) within the parametric approximation is equivalent to taking the expectation value of the full Hamiltonian (307) in the pump's coherent state $|\mathrm{i}\sqrt{\bar{N}_2}e^{-\mathrm{i}\omega_2 t}\rangle$ (and removing the free energy contribution of the pump, which is just a constant shift).

In contrast to (307), this Hamiltonian is quadratic in annihilation and creation operators, and can be treated analytically. In order to do so, first we move to a picture where it becomes time independent, which can be accomplished by using the unitary transformation $\hat{U}_{\mathrm{c}}(t) = e^{\hat{H}_{\mathrm{c}}t/\mathrm{i}\hbar}$, with $\hat{H}_{\mathrm{c}} = \hbar\omega_2\hat{a}^\dagger\hat{a}/2$ (see Section I C). Using the Baker-Campbell-Haussdorf lemma (84), it's easy to show that the annihilation operator is transformed as $\hat{U}_{\mathrm{c}}^\dagger\hat{a}\hat{U}_{\mathrm{c}} = e^{-\mathrm{i}\omega_2 t/2}\hat{a}$, leading to a so-called *rotating picture*, where the Hamiltonian reads

$$\hat{H}_{\mathrm{I}} = \hat{U}_{\mathrm{c}}^\dagger\hat{H}_{\mathrm{PDC}}\hat{U}_{\mathrm{c}} - \hat{H}_{\mathrm{c}} = \hbar\Delta\hat{a}^\dagger\hat{a} - \frac{\hbar g}{2}(\hat{a}^{\dagger 2} + \hat{a}^2), \tag{312}$$

where we define the *detuning* as $\Delta = \omega_0 - \omega_2/2$. This Hamiltonian is the simplest non-trivial one that allows us to introduce the so-called *Bogoliubov-deGennes theory*, which appears in any branch of physics involving bosons or fermions (e.g., condensed matter and high-energy physics).

We can understand this Hamiltonian analytically by rewriting it in terms of a new bosonic operator $\hat{c} = \hat{S}^\dagger(r)\hat{a}\hat{S}(r)$, where $\hat{S}(r) = e^{r(\hat{a}^2 - \hat{a}^{\dagger 2})/2}$ is a squeezing unitary operator, as defined in Section II I. We will choose the parameter r such that the Hamiltonian takes a simple form that we are familiar with in terms of the new annihilation and creation operators, which obviously satisfy canonical commutation relations, $[\hat{c}, \hat{c}^\dagger] = 1$. We will call *Bogoliubov mode* to the one associated to these bosonic operators. Using (183), we obtain the following relations between the original and Bogoliubov operators

$$\hat{c} = \hat{a}\cosh r - \hat{a}^\dagger \sinh r \qquad \Leftrightarrow \qquad \hat{a} = \hat{c}\cosh r + \hat{c}^\dagger \sinh r. \tag{313}$$

This is known as a *Bogoliubov transformation*, although for our single-mode case, it is nothing but the simple squeezing transformation that we saw in Section II I. The real power of Bogoliubov transformations is evidenced in multi-mode situations, and in particular, it generalizes to particle non-conserving situations the *normal mode theory* that is usually studied in the context of coupled oscillators.

Inserting (313) into (312), we can rewrite the Hamiltonian into the form

$$\hat{H}_{\mathrm{I}} = E_0(r) + \hbar\Omega(r)\hat{c}^\dagger\hat{c} - \frac{\hbar\kappa(r)}{2}(\hat{c}^2 + \hat{c}^{\dagger 2}), \tag{314}$$

with parameters

$$\Omega(r) = \Delta\cosh 2r - g\sinh 2r, \tag{315a}$$
$$\kappa(r) = g\cosh 2r - \Delta\sinh 2r, \tag{315b}$$
$$E_0(r) = \hbar[\Omega(r) - \Delta]/2. \tag{315c}$$

This calls for the choice $\tanh 2r = g/\Delta$ for the parameter r, such that, in terms of the Bogoliubov mode, the Hamiltonian takes the simple free-harmonic oscillator form[34] $\hat{H}_{\mathrm{I}} = E_0 + \hbar\Omega\hat{c}^\dagger\hat{c}$, with $\Omega = \mathrm{sign}(\Delta)\sqrt{\Delta^2 - g^2}$. We

[34] Note that $\tanh 2r = g/\Delta$ implies that (keep in mind that, by definition, $\cosh x > 0\ \forall x$, so the sign of $\tanh x$ is always encoded in $\sinh x$)

$$\sinh 2r = \mathrm{sign}(\Delta)\frac{g}{\sqrt{\Delta^2 - g^2}} \qquad \text{and} \qquad \cosh 2r = \frac{|\Delta|}{\sqrt{\Delta^2 - g^2}}. \tag{316}$$

From these, we can also relate $\sinh^2 r = [\cosh(2r) - 1]/2$ and $\cosh^2 r = [\cosh(2r) + 1]/2$ with Δ and g.

know the spectrum of this Hamiltonian very well from previous chapters: $\{E_0+\hbar\Omega n\}_{n=0,1,...}$. An interesting property of the spectrum is that it is lower or upper bounded depending on the sign of Δ, since that's also the sign of the energy step $\hbar\Omega$. As for the eigenvectors, they are the Fock states associated to the annihilation operator $\hat{c}$. It is interesting to understand the meaning of these eigenstates in relation to the original mode $\hat{a}$, which is the one that describes the down-converted field $\hat{\mathbf{E}}_0(z)$. Let us denote by $|n\rangle_c$ the eigenstates of $\hat{c}^\dagger\hat{c}$, and by $|n\rangle_a$ the eigenstates of $\hat{a}^\dagger\hat{a}$. It is then easy to prove that $|n\rangle_c = \hat{S}(-r)|n\rangle_a$, so that the eigenstates of the Hamiltonian are squeezed Fock states of the down-converted field. In order to prove this, we first proceed by proving the relation for the vacuum state:

$$0 = \hat{c}|0\rangle_c = \hat{S}^\dagger(r)\hat{a}\hat{S}(r)|0\rangle_c \quad \Rightarrow \quad \hat{a}\hat{S}(r)|0\rangle_c = 0 \quad \Rightarrow \quad |0\rangle_a = \hat{S}(r)|0\rangle_c, \tag{317}$$

which proves the relation for $n=0$. On the other hand,

$$|n\rangle_c = \frac{1}{\sqrt{n!}}\hat{c}^{\dagger n}|0\rangle_c = \frac{1}{\sqrt{n!}}\left[\hat{S}^\dagger(r)\hat{a}^{\dagger n}\hat{S}(r)\right]\hat{S}(-r)|0\rangle_a = \hat{S}^\dagger(r)\frac{1}{\sqrt{n!}}\hat{a}^{\dagger n}|0\rangle_a = \hat{S}(-r)|n\rangle_a,$$

as we wanted to prove. Hence, this shows the strong connection that exists between down-conversion and the generation of squeezing, as we shall see in more detail later in this section, and along the next chapters.

The theory above is neat, but we have omitted a huge implicit assumption: because $|\tanh x| < 1$ for any finite x, the theory we developed above works only when $|\Delta| > g$. In the limit $|\Delta| = g$ the squeezing parameter tends to infinity, $|r| \to \infty$. In fact, writing the annihilation operator as $\hat{a} = (\hat{X}+\mathrm{i}\hat{P})/2$ in terms of the position and momentum quadratures ($[\hat{X},\hat{P}] = 2\mathrm{i}$), in this case the Hamiltonian (312) reads

$$\hat{H}_\mathrm{I} = \frac{\hbar g}{4}\left[\mathrm{sign}(\Delta)+1\right]\hat{P}^2 + \frac{\hbar g}{4}\left[\mathrm{sign}(\Delta)-1\right]\hat{X}^2 = \begin{cases} \hbar g\hat{P}^2/2, & \text{for } \Delta > 0 \\ -\hbar g\hat{X}^2/2, & \text{for } \Delta < 0 \end{cases}, \tag{318}$$

showing that the energy eigenstates are position or momentum eigenstates depending on the sign of the detuning Δ, with the spectrum becoming continuous (and lower or upper bounded for $\Delta > 0$ or $\Delta < 0$, respectively).

Past this point, that is, for $|\Delta| < g$, there is no choice of r in Eq. (314) that leads to a diagonalizable Hamiltonian. In contrast, the best we can do to simplify the Hamiltonian is setting $\Omega = 0$ by choosing $\tanh 2r = \Delta/g$, implying[35] $\kappa = \sqrt{g^2-\Delta^2}$. In this case, the Hamiltonian reads $\hat{H}_\mathrm{I} = E_0 - \hbar\kappa(\hat{c}^2 - \hat{c}^{\dagger 2})/2$. This Hamiltonian is very special, and, in particular, it cannot be diagonalized, since it is completely unbounded. In order to see this, just note that writing $\hat{c} = (\hat{x}+\mathrm{i}\hat{p})/2$, in terms of the position and momentum quadratures of the Bogoliubov mode ($[\hat{x},\hat{p}] = 2\mathrm{i}$), we obtain the Hamiltonian $\hat{H}_\mathrm{I} = E_0 + \hbar\kappa(\hat{p}^2 - \hat{x}^2)/4$. This corresponds to a particle moving in an inverted parabolic potential, which is obviously an unbounded problem, lacking normalizable stationary eigenstates (not even in the Dirac continuous sense) and real eigenvalues. In particular, the time evolution induced by this Hamiltonian will simply exponentially push any initial state towards states with larger and larger number of excitations, as we are about to see now through an example.

It is then common to denote the $|\Delta| > g$ regime as the *stable phase,* and the $|\Delta| < g$ regime as the *unstable phase.* Hence, the simple down-conversion Hamiltonian (312) leads to a wide variety of behaviors or phases depending on the ratio Δ/g, see Figure **ToDo**: standard harmonic spectrum (uniformly-spaced, lower-bounded) for $\Delta > g$, standard free-particle spectrum (continuous, lower-bounded) for $\Delta = g$, instability for $g > \Delta > -g$, continuous upper-bounded spectrum for $\Delta = -g$, and upper-bounded uniformly-spaced spectrum for $\Delta < -g$.

In order to get a grip of the meaning and interpretation of the instability, let us consider now the evolution of the number of excitations $\bar{N} = \langle\hat{a}^\dagger\hat{a}\rangle$ when we start from the vacuum state $|0\rangle_a$. Note that the number operator is invariant under the change of picture, that is, $\hat{U}_\mathrm{c}^\dagger(t)\hat{a}^\dagger\hat{a}\hat{U}_\mathrm{c}(t) = \hat{a}^\dagger\hat{a}$, while in the rotating picture the state evolves as $|\psi(t)\rangle_\mathrm{I} = \hat{U}_\mathrm{I}(t)|0\rangle_a$, being $\hat{U}_\mathrm{I}(t) = \exp(\hat{H}_\mathrm{I}t/\mathrm{i}\hbar)$ the time-evolution operator in the rotating picture, and where we have also used $|\psi(0)\rangle_\mathrm{I} = |\psi(0)\rangle$. Hence, we can evaluate the evolution of the number of excitations as

$$\bar{N}(t) = {}_a\langle 0|\hat{U}_\mathrm{I}^\dagger(t)\hat{a}^\dagger\hat{a}\hat{U}_\mathrm{I}(t)|0\rangle_a = \left|\hat{U}_\mathrm{I}^\dagger(t)\hat{a}\hat{U}_\mathrm{I}(t)|0\rangle_a\right|^2. \tag{320}$$

In other words, we just need to time-evolve the annihilation operator, apply it to vacuum, and evaluate the norm of the resulting state. Let's do this for the stable and unstable phases. In both cases the trick to evaluate the quantity

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[35] Note that in this case $\tanh 2r = \Delta/g$ implies that

$$\sinh 2r = \frac{\Delta}{\sqrt{g^2-\Delta^2}} \qquad \text{and} \qquad \cosh 2r = \frac{g}{\sqrt{g^2-\Delta^2}}. \tag{319}$$

above is the same: since the Hamiltonian takes a simple form in terms of $\hat{c}$, we use (313) to write $\hat{a}$ in terms of $\hat{c}$ and $\hat{c}^\dagger$, time-evolve these, and then use (313) to bring the expression back to the original bosonic operators (and we only need to keep the $\hat{a}^\dagger$ term, since $\hat{a}$ annihilates $|0\rangle_a$). In the stable case, $|\Delta| > g$, and taking into account that $\hat{U}_{\rm I}(t) = \exp(E_0 t/{\rm i}\hbar)\exp(-{\rm i}\Omega t\hat{c}^\dagger\hat{c})$, such that $\hat{U}_{\rm I}^\dagger(t)\hat{c}\hat{U}_{\rm I}(t) = e^{-{\rm i}\Omega t}\hat{c}$, we easily get

$$\hat{U}_{\rm I}^\dagger(t)\hat{a}\hat{U}_{\rm I}(t) = \left(e^{-{\rm i}\Omega t}\hat{c}\cosh r + e^{{\rm i}\Omega t}\hat{c}^\dagger\sinh r\right) = \left(e^{{\rm i}\Omega t} - e^{-{\rm i}\Omega t}\right)\hat{a}^\dagger\cosh r\sinh r + \hat{a}\text{-terms}, \tag{321}$$

$$= {\rm i}\sinh(2r)\sin(\Omega t)\hat{a}^\dagger + \hat{a}\text{-terms} \tag{322}$$

leading to

$$\bar{N}(t) = |{\rm i}\sinh(2r)\sin(\Omega t)|1\rangle_a|^2 = \frac{g^2}{\Delta^2 - g^2}\sin^2(\Omega t). \tag{323}$$

We plot this in Fig. **ToDo**. Note that the number of excitations starts at zero, and proceeds with bounded periodic oscillations reaching maxima at $g^2/(\Delta^2 - g^2)$.

On the other hand, in the unstable phase $|\Delta| < g$ the time evolution operator $\hat{U}_{\rm I}(t) = \exp(E_0 t/{\rm i}\hbar)\exp[{\rm i}\kappa t(\hat{c}^{\dagger 2} + \hat{c}^2)/2]$ is equivalent to a squeezing operator, such that $\hat{U}_{\rm I}^\dagger(t)\hat{c}\hat{U}_{\rm I}(t) = \hat{c}\cosh(\kappa t) + {\rm i}\hat{c}^\dagger\sinh(\kappa t)$ according to (183), leading to

$$\hat{U}_{\rm I}^\dagger(t)\hat{a}\hat{U}_{\rm I}(t) = \hat{U}_{\rm I}^\dagger(t)\hat{c}\hat{U}_{\rm I}(t)\cosh r + \hat{U}_{\rm I}^\dagger(t)\hat{c}^\dagger\hat{U}_{\rm I}(t)\sinh r \tag{324}$$

$$= [\cosh(\kappa t)\cosh r - {\rm i}\sinh(\kappa t)\sinh r]\,\hat{c} + [\cosh(\kappa t)\sinh r + {\rm i}\sinh(\kappa t)\cosh r]\,\hat{c}^\dagger \tag{325}$$

$$= {\rm i}\cosh(2r)\sinh(\kappa t)\hat{a}^\dagger + \hat{a}\text{-terms}, \tag{326}$$

so that

$$\bar{N}(t) = |{\rm i}\cosh(2r)\sinh(\kappa t)|1\rangle_a|^2 = \frac{g^2}{g^2 - \Delta^2}\sinh^2(\kappa t). \tag{327}$$

As shown in Fig. **ToDo**, in this case the number of excitations is not bounded, and simply increases exponentially with time, following the hyperbolic sine of the expression. This is indeed generic for any initial state, since the time evolution operator is a squeezing transformation with a squeezing parameter κt that increases with time. Hence, we see that in this case there are no stationary eigenstates.

At the physical level, the most interesting message that we can get from these results is that down-conversion can extract energy from the pump mode to amplify the quantum vacuum fluctuations of the signal mode, populating it in the form of a squeezed state.

V. QUANTUM OPTICS IN OPEN SYSTEMS

In the previous chapters we have dealt with *closed* quantum systems, that is, systems that are fully described by a Hamiltonian. However, most physical systems are *open*, in the sense that they interact with other systems to which experimentalists do not have access to. The paradigmatic example is *dissipation*, by which the system under study leaks energy to a substrate or *environment* which is too complex to be monitored in experiments. In this section we will learn how to model quantum systems subject to such type of situation. In particular, we will learn that there exists a description of the system's dynamics involving only system operators and states, with the environmental degrees of freedom effectively integrated out. We will introduce this description through two paradigmatic examples of outmost quantum-optical relevance: an optical cavity with a partially-transmitting mirror and an atom in free space. We start with the former, introducing a model for the system (cavity), the environment (external electromagnetic modes), and their interaction (photons tunneling in and out of the cavity through the mirror). Then we proceed to integrate out the environmental degrees of freedom either in the Heisenberg or the Schrödinger pictures. We will see that the system's dynamics will no longer be ruled by the Heisenberg or von Neumann equations, but by some generalization of these called, respectively, *quantum Langevin* and *master equations.*

A. Open optical cavities

In Chapter II we study the quantum description of the electromagnetic field inside an optical cavity with perfectly reflecting mirrors. However, in reality optical cavities must have at least one partially transmitting mirror allowing us to both inject light inside it and observe or use the light that comes out of it. In this section we explain how to deal with such an open cavity within the quantum formalism.

1. *The open cavity model*

For simplicity, we consider only one cavity mode with frequency $\omega_{\rm c}$, whose annihilation operator we denote by $\hat{a}$. In addition, we assume that there are no intracavity processes, just free evolution (e.g., no atoms or nonlinear dielectric media in the cavity). We will discuss the generalization to many modes and nontrivial intracavity dynamics later.

We propose a model in which the cavity mode is coupled through the partially transmitting mirror to the external modes. These external modes can be modeled as the modes of a second cavity which shares the partially transmitting mirror with the main cavity, but has the second mirror placed at infinity. According to the previous chapter, the field corresponding to such cavity can be written as (note that we still take the origin of the z axis in the perfectly reflecting mirror of the main cavity)

$$\hat{\mathbf{A}}_{\rm ext}(z) = \lim_{L_{\rm ext}\to\infty} \mathbf{e}_x \sum_{m=1}^{\infty} \sqrt{\frac{\hbar}{\varepsilon_0 L_{\rm ext} S \omega_m}} (\hat{b}_m + \hat{b}_m^\dagger) \sin\left[\omega_m (z-L)/c\right], \qquad \text{with } z \in [L, L+L_{\rm ext}] \tag{328}$$

where the boson operators satisfy the commutation relations $[\hat{b}_m, \hat{b}_{m'}^\dagger] = \delta_{mm'}$, and $\omega_m = (\pi c/L_{\rm ext})m$. Now, as the length of this auxiliary cavity goes to infinity, the set of longitudinal modes becomes infinitely dense in frequency space (the distance between them, $\pi c/L_{\rm ext}$, goes to zero), so that the sum over m can be replaced by an integral over continuous frequencies[36]:

$$\lim_{L_{\rm ext}\to\infty} \sum_{m=1}^{\infty} = \frac{L_{\rm ext}}{\pi c} \int_0^\infty d\omega. \tag{329}$$

Accordingly, the Kronecker delta, which must preserve the property $\lim_{L_{\rm ext}\to\infty} \sum_{m=1}^{\infty} \delta_{mm'} = 1$, converges to a Dirac delta as

$$\lim_{L_{\rm ext}\to\infty} \delta_{mm'} = \frac{\pi c}{L_{\rm ext}} \delta(\omega - \omega'). \tag{330}$$

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[36] Note that going as low in frequency as $\omega = 0$ or as high as $\omega \to \infty$ makes no physical sense. However, these fine details are irrelevant within our level of description, since we will see that only frequencies around the transitions of the cavity Hamiltonian play a non-negligible role effectively.

It is then convenient to define a continuous set of annihilation operators

$$\hat{b}(\omega) = \sqrt{\frac{L_{\rm ext}}{\pi c}} \lim_{L_{\rm ext}\to\infty} \hat{b}_m, \tag{331}$$

which satisfy continuous canonical commutation relations

$$[\hat{b}(\omega), \hat{b}(\omega')] = 0, \qquad [\hat{b}(\omega), \hat{b}^\dagger(\omega')] = \delta(\omega - \omega'). \tag{332}$$

Then, we can finally write the vector potential of the field outside the cavity as

$$\hat{\mathbf{A}}_{\rm ext}(z) = \mathbf{e}_x \int_0^\infty d\omega \sqrt{\frac{\hbar}{\pi c \varepsilon_0 S \omega}} [\hat{b}(\omega) + \hat{b}^\dagger(\omega)] \sin[\omega(z-L)/c]\,. \tag{333}$$

At this point, it is important to remark that the frequency dependence of the continuous annihilation operators is by no means a Fourier of the time-dependent operators. It is merely a label for the external available electromagnetic modes, just like the discrete index m is for the cavity with finite length. In fact, note that we have implicitly written the above expressions in the Schrödinger picture, since operators are time independent.

Now that we have a description of the field outside the cavity, we can proceed to model the evolution of the whole system through a suitable Hamiltonian. From Chapter II, we know that the free evolution of the cavity mode and the external modes is ruled by the Hamiltonian $\hat{H}_{\rm cav} + \hat{H}_{\rm ext}$ with

$$\hat{H}_{\rm cav} = \hbar\omega_{\rm c} \hat{a}^\dagger \hat{a} \qquad \text{and} \qquad \hat{H}_{\rm ext} = \int_0^\infty d\omega \hbar\omega \hat{b}^\dagger(\omega)\hat{b}(\omega). \tag{334}$$

The coupling between the cavity and the external modes can also be modeled via a simple Hamiltonian, namely

$$\hat{H}_{\rm int} = \mathrm{i}\hbar \int_0^\infty d\omega g(\omega)[\hat{b}^\dagger(\omega)\hat{a} - \hat{b}(\omega)\hat{a}^\dagger], \tag{335}$$

corresponding to the tunneling of photons between the cavities via the partially transiting mirror, at a rate determined by the parameter $g(\omega)$, which is allowed to depend on the frequency of the external modes. This form for interaction Hamiltonian is supported by many arguments[37]. Perhaps the most general one consists in noting that mirrors are judiciously chosen to be absent of nonlinear optical effects (e.g., they are typically built of dielectrics on the linear regime), as otherwise they would not only transmit/reflect light, but also change its fundamental properties (e.g., through the frequency conversion effects that we saw in the previous chapter). We then expect the contribution of the mirror to the Hamiltonian to be quadratic in annihilation and creation operators. In addition, since the mirror is a passive element and we will take the interaction as perturbative, so that the energy scales are approximately set by $\hat{H}_0$, terms such as $\hat{b}^\dagger(\omega)\hat{a}^\dagger$ are not allowed, which would require an energy $\hbar(\omega_{\rm c} + \omega)$ coming from some kind of source. A more pragmatic argument is that we know how mirrors and linear dielectric plates (beam splitters) act on classical laser beams, in particular splitting them into reflected and transmitted beams with the same spatiotemporal properties as the original beam (except for the propagation direction), and whose intensities add up to the intensity of the original beam. Now, since at the quantum level these classical beams are described by coherent states, the only Hamiltonian that provides an evolution consistent with that classical picture has the properties mentioned above.

We can simplify the the model even further. Note that the coupling $g(\omega)$ depends essentially on the transmissivity of the mirror at the corresponding frequency, and we are assuming that $g^2(\omega) \ll \omega_{\rm c}$ for optical frequencies, as the mirror is still assumed to have large reflectivity (otherwise, we cannot even consider a model with two separate cavities, but need to quantize the electromagnetic field of the full space with appropriate boundary conditions as a whole). On the other hand, from previous chapters we expect energy conservation to imply that only frequencies close to the cavity frequency will contribute to the interaction (*resonant interaction*), what allows us to rewrite $g(\omega) = \sqrt{\gamma/\pi}$ in terms of a frequency-independent constant γ, as the transmissivity of typical mirrors is pretty flat[38] as a function of the frequency at least within the interval $[\omega_{\rm c} - \gamma, \omega_{\rm c} + \gamma]$. In addition, it allows us to extend the integration limits to $[-\infty, +\infty]$ to simplify the upcoming integrals, because any fictitious unphysical negative frequency mode $\hat{b}(-|\omega|)$ will

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[37] Actually, any form of the type $\hbar\int_0^\infty d\omega g(\omega)[e^{\mathrm{i}\varphi}\hat{b}^\dagger(\omega)\hat{a} + e^{-\mathrm{i}\varphi}\hat{a}^\dagger\hat{b}(\omega)]$ is perfectly acceptable. The phase φ of the interaction is actually irrelevant for the final results, and it has been conveniently chosen here as $\pi/2$ for notational simplicity in upcoming derivations.

[38] A comment on a typical misconception is in order: $g(\omega)$ does not refer to the transmissivity of the whole cavity, but just to the coupling induced by the mirror between the field to its right and the field to its left, irrespective of what it has around it. As we will see, the transmission coefficient of the whole cavity has a Lorentzian shape as a function of the external probe's frequency. However, this will come naturally from the model we are developing, and in particular from a model with a flat $g(\omega)$. Giving a Lorentzian shape to $g(\omega)$ is a totally wrong move.

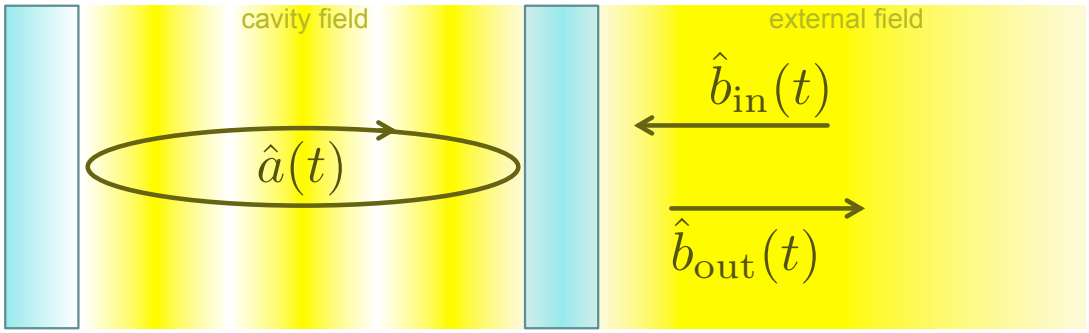

Figure 15. Schematic view of the open cavity model. Each cavity mode (we show only the third one) interacts with the external modes through a partially transmitting mirror. The external modes form a continuum that can be modeled as a second cavity sharing the partially transmitting mirror with the main cavity, but with the other mirror placed at infinity (hence not shown in the figure). As explained in this and the next chapter, the external modes can be described by an input field driving the cavity and an output field coming out of the cavity.

not contribute to the physics, as they are very off resonant. These approximations are one version of the more general *Markov approximation* that we will comment on later, at the end of the chapter. Hence, this allows us to finally write the interaction as

$$\hat{H}_{\rm int} = {\rm i}\hbar\sqrt{\frac{\gamma}{\pi}}\int_{-\infty}^{+\infty} d\omega[\hat{b}^\dagger(\omega)\hat{a} - \hat{b}(\omega)\hat{a}^\dagger]. \tag{336}$$

In Section V A 8, we show that the explicit relation between γ and the cavity parameters is

$$\gamma = \frac{c\mathcal{T}}{4L}, \tag{337}$$

where $\mathcal{T}$ is the (intensity) transmissivity of the mirror, and we remind that L is the cavity length.

This is the basic model that we will use to 'open the cavity'. In the following we show how to derive reduced evolution equations for the intracavity mode alone both at the level of operators (Heisenberg picture) and states (Schrödinger picture), leading, respectively, to the so-called *quantum Langevin* and *master equations*.

2. *Heisenberg picture approach: The quantum Langevin equation*

Given the Hamiltonian written above, $\hat{H}_0 + \hat{H}_{\rm int}$, the Heisenberg equations of motion of the annihilation operators are

$$\partial_t\hat{a} = -{\rm i}\omega_{\rm c}\hat{a} - \sqrt{\frac{\gamma}{\pi}}\int_{-\infty}^{+\infty} d\omega\hat{b}(\omega), \tag{338a}$$

$$\partial_t\hat{b}(\omega) = -{\rm i}\omega\hat{b}(\omega) + \sqrt{\frac{\gamma}{\pi}}\hat{a}. \tag{338b}$$

We now proceed to reduce these equations to an evolution equation solely for $\hat{a}$. For this, reminding the general solution (251) of a linear differential equation, we can formally integrate the second equation as

$$b(\omega;t) = b_0(\omega)e^{-{\rm i}\omega t} + \sqrt{\frac{\gamma}{\pi}}\int_0^t dt' e^{{\rm i}\omega(t'-t)}\hat{a}(t'), \tag{339}$$

where $b_0(\omega) \equiv b(\omega;0)$ is a shorter notation for the external annihilation operators at the initial time, which we take as $t = 0$. Introducing this solution into the evolution equation for $\hat{a}$, we get

$$\partial_t\hat{a} = -{\rm i}\omega_{\rm c}\hat{a} - \sqrt{\frac{\gamma}{\pi}}\int_{-\infty}^{+\infty} d\omega b_0(\omega)e^{-{\rm i}\omega t} - \frac{\gamma}{\pi}\int_0^t dt' \underbrace{\int_{-\infty}^{+\infty} d\omega e^{{\rm i}\omega(t'-t)}}_{2\pi\delta(t-t')}\hat{a}(t'). \tag{340}$$

Next we use the property

$$\int_{\tau_-}^{\tau_+} d\tau f(\tau)\delta(\tau-\tau_\pm) = f(\tau_\pm)/2, \tag{341}$$

valid for any function $f(\tau)$ that is continuous in all the integration domain[39], and define the *input operator*

$$\hat{b}_{\rm in}(t) = -\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} d\omega e^{-{\rm i}\omega t}\hat{b}_0(\omega), \tag{342}$$

which is easily shown to satisfy the commutation relations

$$[\hat{b}_{\rm in}(t),\hat{b}_{\rm in}(t')] = 0, \qquad [\hat{b}_{\rm in}(t),\hat{b}^\dagger_{\rm in}(t')] = \delta(t-t'), \tag{343}$$

which correspond to (continuous) canonical commutation relations *in time*. We then turn the previous equation into

$$\partial_t\hat{a} = -\left(\gamma+{\rm i}\omega_{\rm c}\right)\hat{a} + \sqrt{2\gamma}\hat{b}_{\rm in}(t), \tag{344}$$

which is an evolution equation for the intracavity mode. This equation is known as the *quantum Langevin equation* for its similarity with stochastic Langevin equations [8] (first order differential equations forced by noise), the operator $\hat{b}_{\rm in}(t)$ playing the role of the external noisy force. $\hat{b}_{\rm in}(t)$ is interpreted as an operator accounting for the input field driving the cavity at each instant (see Fig. 15). It is important to remark that $\hat{b}_{\rm in}(t)$ is not a dynamical variable, it is just the Fourier transform of the external annihilation operators at the origin of time. Hence, it is completely determined by the initial quantum state of the external modes, as we will see next through some examples. Additionally, we obtain a damping term $-\gamma\hat{a}$, much expected since energy is leaking out of the cavity.

In practical terms, the solution for the intracavity operator $\hat{a}(t)$ is found in terms of integrals of $\hat{b}_{\rm in}(t)$, and since we know the statistics of this operator (assuming that we know the initial state of the external modes), this allows us to calculate the statistics of the intracavity field. We will see this in action with several examples along the next sections.

It is then interesting to understand the properties of $\hat{b}_{\rm in}(t)$ for different initial states for the external modes, which we will denote by $|\psi_{\rm ext}\rangle$ and $\hat{\rho}_{\rm ext}$, for pure and mixed states, respectively:

- **Vacuum.** Consider first that they are in the vacuum state initially, that is $|\psi_{\rm ext}\rangle = \bigotimes_\omega |0\rangle$, where $\bigotimes_\omega$ must be understood as a symbolic notation, since ω is a continuous index. We then have[40] $\langle\hat{b}_0(\omega)\rangle = \langle\hat{b}_0(\omega)\hat{b}_0(\omega')\rangle = \langle\hat{b}_0^\dagger(\omega)\hat{b}_0(\omega')\rangle = 0$, leading to the following statistical properties of the input operator:

$$\langle\hat{b}_{\rm in}(t)\rangle = \langle\hat{b}^\dagger_{\rm in}(t)\hat{b}_{\rm in}(t')\rangle = 0, \qquad \text{and} \qquad \langle\hat{b}_{\rm in}(t)\hat{b}^\dagger_{\rm in}(t')\rangle = \delta(t-t'), \tag{345}$$

  which are actually quite reminiscent of the statistical properties of complex white Gaussian noises in stochastic Langevin equations [8].

- **Coherent (laser driving).** Let us next consider the injection of a classical (laser) beam, which means that the external field is in a coherent state

$$|\psi_{\rm ext}\rangle = e^{\int_{-\infty}^{+\infty} d\omega[\alpha(\omega)\hat{b}^\dagger(\omega)-\alpha^*(\omega)\hat{b}(\omega)]}\bigotimes_\omega|0\rangle \equiv \bigotimes_\omega|\alpha(\omega)\rangle,$$

  that is, each external mode of frequency ω is in a coherent state $|\alpha(\omega)\rangle$. In this case, we obtain

$$\langle\hat{b}_0(\omega)\rangle = \alpha(\omega), \quad \langle\hat{b}_0(\omega)\hat{b}_0(\omega')\rangle = \alpha(\omega)\alpha(\omega'), \quad \text{and} \quad \langle\hat{b}_0^\dagger(\omega)\hat{b}_0(\omega')\rangle = \alpha^*(\omega)\alpha(\omega'), \tag{346}$$

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[39] A convincing argument in pro of this property comes from considering the integral $\int_{\tau_0}^{\tau_2} d\tau f(\tau)\delta(\tau-\tau_1) = f(\tau_1)$ for $\tau_0<\tau_1<\tau_2$. Now, we also require the natural property of integrals $\int_{\tau_0}^{\tau_2} d\tau f(\tau)\delta(\tau-\tau_1) = \int_{\tau_0}^{\tau_1} d\tau f(\tau)\delta(\tau-\tau_1) + \int_{\tau_1}^{\tau_2} d\tau f(\tau)\delta(\tau-\tau_1)$. On the other hand, if we want this expression to be independent of the function to be integrated and the integration limits, we must choose $\int_{\tau_0}^{\tau_1} d\tau f(\tau)\delta(\tau-\tau_1) = \int_{\tau_1}^{\tau_2} d\tau f(\tau)\delta(\tau-\tau_1) = f(\tau_1)/2$. For example, it is enough to consider the particular case $\tau_0=-\tau_2$ (hence $\tau_2>0$), $\tau_1=0$, and a symmetric function $f(\tau)=f(-\tau)$; we then have $\int_{-\tau_2}^{0} d\tau f(\tau)\delta(\tau) = \int_0^{\tau_2} d\tau' f(-\tau')\delta(-\tau') = \int_0^{\tau_2} d\tau f(\tau)\delta(\tau)$, in agreement with the choice we made.

[40] Note that for Gaussian states, we only need to evaluate first and second order moments, since higher order moments are completely determined by these.

so that the input operator satisfies the properties

$$\langle \hat{b}_{\rm in}(t)\rangle = -\frac{1}{\sqrt{2\pi}} \underbrace{\int_{-\infty}^{+\infty} d\omega e^{-{\rm i}\omega t}\alpha(\omega)}_{\tilde{\alpha}(t)} = -\frac{\tilde{\alpha}(t)}{\sqrt{2\pi}}, \tag{347a}$$

$$\langle \hat{b}_{\rm in}(t)\hat{b}_{\rm in}(t')\rangle = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega e^{-{\rm i}\omega t}\int_{-\infty}^{+\infty} d\omega' e^{-{\rm i}\omega' t')} \underbrace{\langle \hat{b}_0(\omega)\hat{b}_0(\omega')\rangle}_{\alpha(\omega)\alpha(\omega')} = \frac{\tilde{\alpha}(t)\tilde{\alpha}(t')}{2\pi} = \langle \hat{b}_{\rm in}(t)\rangle\langle \hat{b}_{\rm in}(t')\rangle, \tag{347b}$$

$$\langle \hat{b}^\dagger_{\rm in}(t)\hat{b}_{\rm in}(t')\rangle = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega e^{{\rm i}\omega t}\int_{-\infty}^{+\infty} d\omega' e^{-{\rm i}\omega' t'} \underbrace{\langle \hat{b}^\dagger_0(\omega)\hat{b}_0(\omega')\rangle}_{\alpha^*(\omega)\alpha(\omega')} = \frac{\tilde{\alpha}^*(t)\tilde{\alpha}(t')}{2\pi} = \langle \hat{b}_{\rm in}(t)\rangle^*\langle \hat{b}_{\rm in}(t')\rangle. \tag{347c}$$

In other words, each of the input modes (which form a continuous set of harmonic oscillators obeying canonical commutation relations), is in a coherent state $|\alpha_{\rm in}(t)\rangle$ with an amplitude $\alpha_{\rm in}(t) = -\tilde{\alpha}(t)/\sqrt{2\pi}$, which is just proportional to the Fourier transform of the spectral components $\alpha(\omega)$ of the laser. Hence, the external state admits an alternative description in the time domain as $|\psi_{\rm ext}\rangle = \bigotimes_t |\alpha_{\rm in}(t)\rangle$, with $\hat{b}_{\rm in}(t)|\alpha_{\rm in}(t)\rangle = \alpha_{\rm in}(t)|\alpha_{\rm in}(t)\rangle$, and where $\bigotimes_t$ is again a symbolic notation, since t is a continuous index.
In this case, it is recommendable to define a new input operator

$$\hat{a}_{\rm in}(t) = \hat{b}_{\rm in}(t) - \langle \hat{b}_{\rm in}(t)\rangle, \tag{348}$$

which using the previous equations is easily shown to satisfy the vacuum correlators (345). In terms of this operator the quantum Langevin equation for the intracavity mode reads

$$\partial_t \hat{a} = \mathcal{A}(t) - (\gamma + {\rm i}\omega_{\rm c})\,\hat{a} + \sqrt{2\gamma}\hat{a}_{\rm in}(t), \tag{349}$$

with $\mathcal{A} = -\sqrt{\gamma/\pi}\tilde{\alpha}(t)$. Hence, the injection of laser field is equivalent to the addition of the following time-dependent term in the Hamiltonian

$$\hat{H}_{\rm inj}(t) = {\rm i}\hbar\left(\mathcal{A}(t)a^\dagger - \mathcal{A}^*(t)a\right), \tag{350}$$

while considering the external modes in vacuum.
As a common example, consider a laser containing L frequency components $\{\omega_\ell\}_{\ell=1,2,\ldots,L}$, so that $\alpha(\omega) = \sum_{\ell=1}^{L}\alpha_\ell\delta(\omega-\omega_\ell)$. This leads to a driving term in the quantum Langevin equation with

$$\mathcal{A}(t) = \sum_{\ell=1}^{L}\mathcal{E}_\ell e^{-{\rm i}\omega_\ell t}, \quad \text{with } \mathcal{E}_\ell = -\sqrt{\frac{\gamma}{\pi}}\alpha_\ell. \tag{351}$$

The most relevant case is that in which each spectral component is resolved by the cavity, that is, their spectral separation is larger than γ, but still small enough compared with the free spectral range $\pi c/L$ such that they address the same cavity mode of frequency $\omega_{\rm c}$. In such case, we show in Section V A 8 the explicit relation of the rates $\mathcal{E}_\ell$ and the physical or experimental parameters is

$$\mathcal{E}_\ell = \sqrt{\frac{2\gamma}{\hbar\omega_{\rm c}}P_{{\rm inj},\ell}}e^{{\rm i}\phi_\ell}, \tag{352}$$

where $P_{{\rm inj},\ell}$ and ϕ_ℓ are, respectively, the power (averaged over an optical cycle) and phase of the ℓ'th spectral component.

- **Thermal.** Consider now also the case in which the external field is at thermal equilibrium at temperature T, corresponding, as we saw in Section II J, to the state

$$\hat{\rho}_{\rm ext} = \frac{e^{-\hat{H}_{\rm ext}/k_BT}}{{\rm tr}\left\{e^{-\hat{H}_{\rm ext}/k_BT}\right\}} \equiv \bigotimes_\omega \hat{\rho}_{\rm th}[\bar{n}(\omega)], \tag{353}$$

where $\hat{\rho}_{\rm th}(\bar{n})$ is a thermal Gaussian state for each mode, with an average number of excitations (photons) given by the Bose-Einstein distribution

$$\bar{n}(\omega) = \frac{1}{\exp(\hbar\omega/k_BT)-1}. \tag{354}$$

Again, note that the right-hand-side of (353) is a symbolic notation. The first and second moments of the external field are then

$$\langle \hat{b}_0(\omega)\rangle = 0 = \langle \hat{b}_0(\omega)\hat{b}_0(\omega')\rangle, \qquad \text{and} \qquad \langle \hat{b}_0^\dagger(\omega)\hat{b}_0(\omega')\rangle = \bar{n}(\omega)\delta(\omega-\omega') \approx \bar{n}(\omega_c)\delta(\omega-\omega'). \tag{355}$$

In the last step we have made the approximation $\bar{n}(\omega) \approx \bar{n}(\omega_c) \equiv \bar{n}$, since only a narrow band of frequencies in the interval $[\omega_c - \gamma, \omega_c + \gamma]$ contribute to the problem as argued above, where the Bose-Einstein distribution can be considered flat to a good approximation. The statistical properties of the input operators are then enormously simplified, obtaining

$$\langle \hat{a}_{\rm in}(t)\rangle = 0 = \langle \hat{a}_{\rm in}(t)\hat{a}_{\rm in}(t')\rangle, \quad \langle \hat{a}_{\rm in}^\dagger(t)\hat{a}_{\rm in}(t')\rangle = \bar{n}\delta(t-t'), \quad \text{and} \quad \langle \hat{a}_{\rm in}(t)\hat{a}_{\rm in}^\dagger(t')\rangle = (\bar{n}+1)\delta(t-t'), \tag{356}$$

where, by using the modified input operator $\hat{a}_{\rm in}(t)$ of Eq. (348), we are implicitly allowing for the injection of a laser field on top of the thermal excitations.

As a final remark, let us extend the model a bit, in particular by considering the possibility of having nontrivial intracavity processes given by a Hamiltonian $\hat{H}_{\rm intra}(t)$. As we saw in the previous chapter, these might account for the down-conversion in a nonlinear dielectric or the interaction with a single atom, for example. Taking a look at the derivation of the quantum Langevin equation, the only place where the intracavity process could make a difference is in the assumption that only external modes around the cavity resonance ω_c will contribute, since now the energy needed to annihilate or create an intracavity photon is not $\hbar\omega_c$ but the energy transitions associated to the total intracavity Hamiltonian $\hat{H}_{\rm cav} + \hat{H}_{\rm intra}(t)$, that is, differences between its eigenvalues. Hence, as long as $\hat{H}_{\rm intra}(t)$ can be treated as a perturbation with respect to optical energies $\hbar\omega_c$, we can still simply introduce it in the quantum Langevin equation without further modifications to a very good approximation. We will assume that this is the case, so that the final form of the quantum Langevin equation of a mode in an open cavity reads

$$\partial_t \hat{a} = \mathcal{A}(t) - (\gamma + {\rm i}\omega_c)\,\hat{a} + \left[\hat{a}, \frac{\hat{H}_{\rm intra}(t)}{{\rm i}\hbar}\right] + \sqrt{2\gamma}\hat{a}_{\rm in}(t), \tag{357}$$

where, we further assume an external electromagnetic field at thermal equilibrium, so the input operator satisfies the statistical properties (356).

It is important to note that, in general, the interplay between damping, driving, and interactions makes the state settle into a well-defined *asymptotic state* at long times, irrespective of the initial state. This state is commonly denoted in the literature by *steady* or *stationary state*, although it's important to keep in mind that it is time dependent in general.

We will discuss the extension of this description to a multi-mode cavity coupled to more than one environment in Section V A 7. Now, let us consider one example to fix ideas.

3. *Example in the Heisenberg picture: asymptotic states of an driven empty cavity*

In order to learn how to use the quantum Langevin equation, let us consider now the simplest example possible: that of an empty cavity with no intracavity processes other than free evolution and driven by a monochromatic laser, that is, $\hat{H}_{\rm intra} = 0$ and $\mathcal{A}(t) = \mathcal{E}e^{-{\rm i}\omega_L t}$. Note that in this case the evolution equations of the whole "cavity + external field" (338) are linear, and hence, if initially all the fields are in a Gaussian state, the state will remain Gaussian at all times (a linear combination of Gaussian variables is Gaussian). This is also clear from the quantum Langevin equation itself, since a linear equation, with a Gaussian input field, will lead to Gaussian variables at all times, provided that these are Gaussian initially. Otherwise, the variables will be Gaussian only asymptotically (since the asymptotic state is independent of the initial conditions).

The solution of the resulting linear quantum Langevin equation (357) is, according to Eq. (251),

$$\hat{a}(t) = e^{-(\gamma+{\rm i}\omega_c)t}\hat{a}(0) + \int_0^t dt' \left[\mathcal{E}e^{-{\rm i}\omega_L t'} + \sqrt{2\gamma}\hat{a}_{\rm in}(t')\right] e^{-(\gamma+{\rm i}\omega_c)(t-t')}. \tag{358}$$

Making the variable change $t' = t - \tau$ in the integral we obtain

$$\hat{a}(t) = e^{-(\gamma+{\rm i}\omega_c)t}\hat{a}(0) + \mathcal{E}e^{-{\rm i}\omega_L t}\underbrace{\int_0^t d\tau e^{-(\gamma+{\rm i}\omega_c-{\rm i}\omega_L)\tau}}_{\frac{1-e^{-(\gamma-{\rm i}\Delta)t}}{(\gamma-{\rm i}\Delta)}} + \sqrt{2\gamma}\int_0^t d\tau e^{-(\gamma+{\rm i}\omega_c)\tau}\hat{a}_{\rm in}(t-\tau), \tag{359}$$

where $\Delta = \omega_L - \omega_c$ is the cavity detuning. For $\gamma t \to \infty$, two terms vanish, the one containing the initial condition and the second term of the definite integral in the middle, obtaining

$$\lim_{\gamma t\to\infty} \hat{a}(t) = \frac{\mathcal{E}}{\gamma - i\Delta} e^{-i\omega_L t} + \sqrt{2\gamma} \lim_{t\to\infty} \int_0^t d\tau e^{-(\gamma+i\omega_c)\tau} \hat{a}_{in}(t-\tau). \tag{360}$$

Note that all the information about the initial state of the cavity mode has disappeared, as mentioned above. In order to understand the type of asymptotic state that the cavity reaches, we consider now the first and second order moments of the intracavity mode. In the case of the first order moment, we get

$$\lim_{\gamma t\to\infty} \langle \hat{a}(t)\rangle = \frac{\mathcal{E}}{\gamma - i\Delta} e^{-i\omega_L t}. \tag{361}$$

Defining the fluctuation operator $\delta\hat{a}(t) = \hat{a}(t) - \langle \hat{a}(t)\rangle$, the second order moments then read

$$\lim_{\gamma t\to\infty} \langle \delta\hat{a}^2(t)\rangle = 2\gamma \lim_{\gamma t\to\infty} \int_0^t d\tau \int_0^t d\tau' e^{-(\gamma+i\omega_c)(\tau+\tau')} \underbrace{\langle \hat{a}_{in}(t-\tau)\hat{a}_{in}(t-\tau')\rangle}_{0} = 0, \tag{362a}$$

$$\lim_{\gamma t\to\infty} \langle \delta\hat{a}^\dagger(t)\delta\hat{a}(t)\rangle = 2\gamma \lim_{\gamma t\to\infty} \int_0^t d\tau \int_0^t d\tau' e^{-\gamma(\tau+\tau')+i\omega_c(\tau-\tau')} \underbrace{\langle \hat{a}^\dagger_{in}(t-\tau)\hat{a}_{in}(t-\tau')\rangle}_{\bar{n}\delta(\tau-\tau')} = 2\gamma\bar{n} \lim_{\gamma t\to\infty} \underbrace{\int_0^t d\tau e^{-2\gamma\tau}}_{\frac{1-e^{-2\gamma t}}{2\gamma}} = \bar{n}. \tag{362b}$$

Using then expression (179), these moments lead to a Gaussian state with a mean vector with components given by the real and imaginary parts of $[2\mathcal{E}/(\gamma - i\Delta)]e^{-i\omega_L t}$, and a thermal covariance matrix $V = (2\bar{n}+1)I$, see Figure **ToDo**. In other words, we obtain a displaced thermal state, rotating at frequency ω_L in phase space.

It is interesting to analyze total photon number, which is given by

$$\lim_{\gamma t\to\infty} \langle \hat{a}^\dagger(t)\hat{a}(t)\rangle = \lim_{\gamma t\to\infty} \left[\langle \delta\hat{a}^\dagger(t)\delta\hat{a}(t)\rangle + \langle \hat{a}(t)\rangle^*\langle \hat{a}(t)\rangle\right] = \frac{|\mathcal{E}|^2}{\gamma^2+\Delta^2} + \bar{n}, \tag{363}$$

which has a classical (or coherent) contribution coming from the laser field, and a thermal background coming from an equilibration with the environment at temperature T. It is interesting to plot this quantity as a function of the laser frequency ω_L, see Figure **ToDo**. We obtain the characteristic Lorentzian shape of a cavity, where it can be appreciated that only laser frequencies close to the cavity resonance (within a bandwidth of order γ) can excite the cavity. This proves that only the external frequencies around the cavity resonance are relevant, and hence the approximations that we made in the model are consistent, see Section V A 1. It is interesting to note that using the relation of the amplitude $|\mathcal{E}|$ with the power of the injected laser P_{inj}, $|\mathcal{E}|^2 = 2\gamma P_{inj}/\hbar\omega_c$ (we prove this in a later section), we can interpret the maximum coherent contribution as

$$\frac{|\mathcal{E}|^2}{\gamma^2} = \frac{P_{inj}}{\hbar\omega_c} \times \frac{2}{\gamma} \sim \left(\frac{\text{energy/time}}{\text{energy/photon}}\right) \times (\sim \text{damping time}) \equiv \begin{array}{c}\text{photons accumulated}\\ \text{in a damping cycle}\end{array}. \tag{364}$$

It is also interesting to consider the expression for the coherent amplitude, which writing the injection parameter as $\mathcal{E} = |\mathcal{E}|e^{i\phi}$, can be written as

$$\lim_{t\to\infty} \langle \hat{a}(t)\rangle = \frac{|\mathcal{E}|}{\sqrt{\gamma^2+\Delta^2}} e^{i[\phi+\delta\phi_\Delta]} e^{-i\omega_L t}, \tag{365}$$

with $\delta\phi_\Delta = \arg(\gamma + i\Delta) \in [-\pi/2, \pi/2]$. There are two interesting features here. First, note that the field oscillates at the laser frequency, not the cavity frequency. Second, note that the intracavity field is in phase with the laser only when injecting on resonance ($\Delta = 0$), otherwise, they have a phase difference of $\delta\phi_\Delta$. This provides a way to measure the cavity resonance (and hence, its length), simply by analyzing the relative phase between the injected laser and the output light. This has many applications in the world of high precision measurements.

4. *Schrödinger picture approach: The master equation*

In the previous sections we have treated the open cavity within a Heisenberg-picture formalism. Now we will do it in the Schrödinger picture. Hence, we consider now the density operator $\hat{\rho}(t)$ corresponding to the state of the whole system "cavity mode + external modes", which evolves according to the von Neumann equation

$$i\hbar\partial_t\hat{\rho} = [\hat{H}_{cav} + \hat{H}_{ext} + \hat{H}_{int}, \hat{\rho}], \tag{366}$$

where the Hamiltonian terms are provided in (334) and (336). Our goal now is finding an evolution equation for the reduced state of the cavity mode $\hat{\rho}_{\rm cav}(t) = {\rm tr}_{\rm ext}\{\hat{\rho}(t)\}$, by tracing out the external degrees of freedom. As we are about to see, this goal is relatively easy to achieve if we keep effects only up to second order on the weak interaction.

The derivation is easier to handle by moving to a more convenient picture. Specifically, it is a picture composed of a sequence of two picture changes, both of which appear very naturally from the following arguments. First, as we did in the Heisenberg picture, we are going to assume that the external field is initially at thermal equilibrium, except for the possibility of a coherent laser contribution of amplitude $\alpha(\omega)$ for the external modes of frequency ω. Specifically, we assume that

$$\hat{\rho}_{\rm ext}(0) = \hat{D}(0)\frac{e^{-\hat{H}_{\rm ext}/k_BT}}{{\rm tr}_{\rm ext}\left\{e^{-\hat{H}_{\rm ext}/k_BT}\right\}}\hat{D}^\dagger(0), \qquad \text{with } \hat{D}(0) = e^{\int_{-\infty}^{+\infty} d\omega[\alpha(\omega)\hat{b}^\dagger(\omega) - \alpha^*(\omega)\hat{b}(\omega)]}, \tag{367}$$

where we denote by $\hat{\rho}_{\rm ext}(t)$ the state of the external field. As it will be clear shortly, it is then convenient to move to a picture that discounts the displacement, which will simplify the statistical properties of the environment (similarly to what we saw in the Heisenberg picture) and will remove the part of $\hat{H}_{\rm int}$ that could be non-perturbative for large $\alpha(\omega)$. This is accomplished by using a time-dependent displacement operator

$$\hat{D}(t) = e^{\int_{-\infty}^{+\infty} d\omega[\beta(\omega,t)\hat{b}^\dagger(\omega) - \beta^*(\omega,t)\hat{b}(\omega)]}, \tag{368}$$

as the unitary transformation to the new picture, where we show at the end of the section that $\beta(\omega,t) = \alpha(\omega)e^{-{\rm i}\omega t}$ is the most appropriate choice, which corresponds precisely to the evolution of $\langle\hat{b}(\omega)\rangle$ in the absence of interaction. In particular, we show at the end of the section that the Hamiltonian in the new picture is given by

$$\hat{H}_D(t) = \underbrace{\hat{H}_{\rm cav} + \hat{H}_{\rm inj}(t) + \hat{H}_{\rm ext}}_{\hat{H}_0(t)} + \hat{H}_{\rm int}, \tag{369}$$

where $\hat{H}_{\rm inj}(t) = {\rm i}\hbar[\mathcal{A}(t)\hat{a}^\dagger - \mathcal{A}^*(t)\hat{a}]$, with $\mathcal{A}(t) = -\sqrt{\gamma/\pi}\int_{-\infty}^{+\infty} d\omega e^{-{\rm i}\omega t}\alpha(\omega)$, is the same Hamiltonian that appeared naturally in the Heisenberg picture when we discounted the laser contribution from the input operator, see Eq. (350). Next, in order to set the stage for a proper perturbation theory, the second change of picture will discount the evolution induced by $\hat{H}_0(t)$, which defines the interaction picture. This is accomplished by the unitary operator satisfying the equation ${\rm i}\hbar\partial_t\hat{U}_{\rm c} = \hat{H}_0(t)\hat{U}_{\rm c}$ with $\hat{U}_{\rm c}(0) = \hat{I}$. As we saw in Section I C, Eq. (49), using the Dyson series and the time-ordering symbol, this operator is written explicitly as

$$\hat{U}_{\rm c}(t) = \mathcal{T}\left\{e^{\int_0^t dt'\hat{H}_0(t')/{\rm i}\hbar}\right\} = e^{-{\rm i}\omega_c t\hat{a}^\dagger\hat{a} + B(t)\hat{a}^\dagger - B^*(t)\hat{a}}e^{-{\rm i}\int_{-\infty}^{+\infty} d\omega\,\omega\hat{b}^\dagger(\omega)\hat{b}(\omega)}, \tag{370}$$

with $B(t) = \int_0^t dt'\mathcal{A}(t)$. The interaction-picture Hamiltonian takes then the form

$$\begin{aligned}\hat{H}_{\rm I}(t) &= \hat{U}_{\rm c}^\dagger(t)\hat{H}_D(t)\hat{U}_{\rm c}(t) - {\rm i}\hbar\hat{U}_{\rm c}^\dagger(t)\partial_t\hat{U}_{\rm c}(t) = \hat{U}_{\rm c}^\dagger(t)\hat{H}_{\rm int}\hat{U}_{\rm c}(t) \\ &= {\rm i}\hbar\sqrt{\frac{\gamma}{\pi}}\int_{-\infty}^{+\infty} d\omega\left[e^{{\rm i}\omega t}\hat{b}^\dagger(\omega)\hat{a}_{\rm I}(t) - e^{-{\rm i}\omega t}\hat{b}(\omega)\hat{a}_{\rm I}^\dagger(t)\right],\end{aligned} \tag{371}$$

where we have used $\hat{U}_{\rm c}^\dagger(t)\hat{b}(\omega)\hat{U}_{\rm c}(t) = e^{-{\rm i}\omega t}\hat{b}(\omega)$, easily found from the Baker-Campbell-Haussdorf lemma (84) as usual, and we have defined the interaction-picture operators $\hat{a}_{\rm I}(t) = \hat{U}_{\rm c}^\dagger(t)\hat{a}\hat{U}_{\rm c}(t)$, whose explicit form in terms of the Schrödinger-picture operators $\hat{a}$ is easy to find, but we won't need it. In this final interaction picture, the state $\hat{\rho}_{\rm I}(t) = \hat{U}_{\rm c}^\dagger(t)\hat{D}^\dagger(t)\hat{\rho}(t)\hat{D}(t)\hat{U}_{\rm c}(t)$ evolves then according to the von Neumann equation

$${\rm i}\hbar\partial_t\hat{\rho}_{\rm I} = [\hat{H}_{\rm I}(t), \hat{\rho}_{\rm I}], \qquad \text{with } \hat{\rho}_{\rm I}(0) = \hat{\rho}_{\rm c}(0)\bigotimes_{\omega}\hat{\rho}_{\rm th}(\bar{n}), \tag{372}$$

where we have already made the approximation that the number of thermal excitations is independent of the frequency and given by the Bose-Einstein distribution at the cavity frequency, $\bar{n} = [\exp(\hbar\omega_{\rm c}/k_BT) - 1]^{-1}$, just as we did in the Heisenberg picture, see the discussion around Eq. (353).

We are now in conditions to find an equation for the reduced state of the intracavity field. Since, as already mentioned, we will be doing so in the style of a perturbation theory up to second order on the interaction, it is first convenient to manipulate the von Neumann equation such that terms quadratic in the interaction Hamiltonian $\hat{H}_{\rm I}(t)$ appear explicitly. This is easily accomplished by formally integrating the von Neumann equation (372) as

$$\hat{\rho}_{\rm I}(t) = \hat{\rho}_{\rm I}(0) + \frac{1}{{\rm i}\hbar}\int_0^t dt'[\hat{H}_{\rm I}(t'), \hat{\rho}_{\rm I}(t')], \tag{373}$$

and reinserting this expression back into the von Neumann equation (372), obtaining

$$\partial_t \hat{\rho}_{\rm I}(t) = \frac{1}{{\rm i}\hbar}[\hat{H}_{\rm I}(t), \hat{\rho}_{\rm I}(0)] - \frac{1}{\hbar^2}\int_0^t dt'[\hat{H}_{\rm I}(t), [\hat{H}_{\rm I}(t'), \hat{\rho}_{\rm I}(t')]]. \tag{374}$$

Since we are interested in the reduced state of the cavity, we can now make the partial trace over the external modes, leading to

$$\partial_t \hat{\rho}_{\rm cav,I}(t) = \frac{1}{{\rm i}\hbar}{\rm tr}_{\rm ext}\{[\hat{H}_{\rm I}(t), \hat{\rho}_{\rm I}(0)]\} - \frac{1}{\hbar^2}\int_0^t dt'{\rm tr}_{\rm ext}\{[\hat{H}_{\rm I}(t), [\hat{H}_{\rm I}(t'), \hat{\rho}_{\rm I}(t')]]\}, \tag{375}$$

where[41] $\hat{\rho}_{\rm cav,I}(t) = \hat{U}_{\rm c}^\dagger(t)\hat{\rho}_{\rm cav}(t)\hat{U}_{\rm c}(t)$ is the state of the cavity in the interaction picture. Finally, taking into account that the initial condition term ${\rm tr}_{\rm ext}\{[\hat{H}_{\rm I}(t), \hat{\rho}_{\rm I}(0)]\}$ is proportional to ${\rm tr}_{\rm ext}\{\hat{b}(\omega)\bigotimes_\omega \hat{\rho}_{\rm th}(\bar{n})\} = 0$, and making the variable change $t' = t - \tau$ in the time integral, we get the following integro-differential equation for the reduced density operator:

$$\partial_t \hat{\rho}_{\rm cav,I}(t) = -\frac{1}{\hbar^2}\int_0^t d\tau{\rm tr}_{\rm ext}\{[\hat{H}_{\rm I}(t), [\hat{H}_{\rm I}(t-\tau), \hat{\rho}_{\rm I}(t-\tau)]]\}. \tag{376}$$

This equation is exact, but now we are going to introduce two important approximations that will lead to huge simplifications, in particular by keeping terms only up to quadratic order in the interaction Hamiltonian $\hat{H}_{\rm I}$. At a first sight, since (376) is explicitly quadratic in $\hat{H}_{\rm I}$ already, it might not seem obvious where the higher-order $\hat{H}_{\rm I}$-dependence comes from. In fact, it is not explicit, but implicit in $\hat{\rho}_{\rm I}(t-\tau)$. To see this, note that starting from the uncorrelated state $\hat{\rho}_{\rm I}(0) = \hat{\rho}_{\rm cav,I}(0)\bigotimes_\omega \hat{\rho}_{\rm th}(\bar{n})$, the interaction $\hat{H}_{\rm I}$ creates correlations between the intracavity and external fields. Hence, any deviations from an uncorrelated state $\hat{\rho}_{\rm I}(t) = \hat{\rho}_{\rm cav,I}(t)\otimes\hat{\rho}_{\rm ext,I}(t)$ will contribute as beyond-second order in the equation above. Neglecting these correlations is known as the *Born approximation*. In addition, note that the external field is formed by an infinite number of modes that form a huge system compared to the "tiny" intracavity mode. Therefore, we expect the back-action of the cavity onto the external field to occur only at a much larger order in the interaction $\hat{H}_{\rm I}$, so that we can make the approximation $\hat{\rho}_{\rm I}(t) = \hat{\rho}_{\rm cav,I}(t)\bigotimes_\omega \hat{\rho}_{\rm th}(\bar{n})$ in (376). A note on nomenclature: in the literature, you will sometimes see that this absence of back-action is also included in the definition of the Born approximation.

It is important to remark that we are not saying that $\hat{\rho}_{\rm I}(t) = \hat{\rho}_{\rm cav,I}(t)\bigotimes_\omega \hat{\rho}_{\rm th}(\bar{n})$ is the state of the system, but only that deviations from this state appear as higher-order effects in the dynamics of $\hat{\rho}_{\rm cav,I}(t)$. In fact, we will see that $\hat{\rho}_{\rm cav,I}(t)$ is mixed in general, even when we start from a pure cavity state, and this is only possible if it gets correlated with the environment during the evolution. Also, we will see in the next chapter that the field coming out of the cavity has properties such as anti-bunching and squeezing (when an atom or a nonlinear dielectric are placed inside the cavity), which means that the external modes are no longer in the original displaced thermal state, but indeed receive corrections.

Using these approximations, Eq. (376) is turned into

$$\partial_t \hat{\rho}_{\rm cav,I}(t) = -\frac{1}{\hbar^2}\int_0^t d\tau{\rm tr}_{\rm ext}\{[\hat{H}_{\rm I}(t), [\hat{H}_{\rm I}(t-\tau), \hat{\rho}_{\rm cav,I}(t-\tau)\bigotimes_\omega \hat{\rho}_{\rm th}(\bar{n})]]\}. \tag{377}$$

Note that the cavity state inside the integral is not evaluated at time t, but all along its past. On the other hand, since the evolution is produced by the interaction $\hat{H}_{\rm I}$, this means that, in principle, we are still keeping terms beyond second order on $\hat{H}_{\rm I}$. However, as we will see next, the Born and absence of backaction approximations, together with the frequency-independent coupling $g(\omega) = \sqrt{\gamma/\pi}$, are enough to remove all those higher-order terms. In contrast, we will see later in this chapter that when the coupling is allowed to depend on the frequency, an extra assumption known as *Markov approximation* is required to eliminate these higher-order terms.

Inserting the specific form of the Hamiltonian (371) into (377), we obtain an expression that is proportional to second-order moments of the external operators, which in the picture we are working on take the simple thermal form

$$\begin{aligned} {\rm tr}_{\rm ext}\left\{\hat{b}(\omega)\bigotimes_\omega \hat{\rho}_{\rm th}(\bar{n})\right\} &= {\rm tr}_{\rm ext}\left\{\hat{b}(\omega)\hat{b}(\omega')\bigotimes_\omega \hat{\rho}_{\rm th}(\bar{n})\right\} = 0, \\ {\rm tr}_{\rm ext}\left\{\hat{b}^\dagger(\omega)\hat{b}(\omega')\bigotimes_\omega \hat{\rho}_{\rm th}(\bar{n})\right\} &= \bar{n}\delta(\omega-\omega'), \quad {\rm tr}_{\rm ext}\left\{\hat{b}(\omega')\hat{b}^\dagger(\omega)\bigotimes_\omega \hat{\rho}_{\rm th}(\bar{n})\right\} = (\bar{n}+1)\delta(\omega-\omega'). \end{aligned} \tag{378}$$

[41] Beware of the loose notation: $\hat{U}_{\rm c}(t)$ acts on the total Hilbert space, while $\hat{\rho}_{\rm cav,I}(t)$ acts only on the cavity's Hilbert space. It is then understood that the part of $\hat{U}_{\rm c}(t)$ acting on the Hilbert space of the external modes has no effect in these type of expressions.

Now, after expanding the double commutator in Eq. (376), we obtain 16 terms. 8 of these terms are proportional to $\mathrm{tr}_{\mathrm{ext}}\{\hat{b}(\omega)\hat{b}(\omega')\bigotimes_\omega \hat{\rho}_{\mathrm{th}}\}=0$ or $\mathrm{tr}_{\mathrm{ext}}\{\hat{b}^\dagger(\omega)\hat{b}^\dagger(\omega')\bigotimes_\omega \hat{\rho}_{\mathrm{th}}\}=0$, and do not contribute. For example, one of such terms is

$$\frac{\gamma}{\pi}\int_0^t d\tau\int_{-\infty}^{+\infty}d\omega\int_{-\infty}^{+\infty}d\omega'\hat{a}_{\mathrm{I}}(t)\hat{a}_{\mathrm{I}}(t-\tau)\hat{\rho}_{\mathrm{cav,I}}(t-\tau)e^{\mathrm{i}\omega t}e^{\mathrm{i}\omega'(t-\tau)}\mathrm{tr}_{\mathrm{ext}}\{\hat{b}^\dagger(\omega)\hat{b}^\dagger(\omega')\bigotimes_{\omega}\hat{\rho}_{\mathrm{th}}\}=0. \tag{379}$$

The other 8 terms are either proportional to $\mathrm{tr}_{\mathrm{ext}}\{\hat{b}^\dagger(\omega)\hat{b}(\omega')\bigotimes_\omega \hat{\rho}_{\mathrm{th}}\}=\bar{n}\delta(\omega-\omega')$ or $\mathrm{tr}_{\mathrm{ext}}\{\hat{b}(\omega)\hat{b}^\dagger(\omega')\bigotimes_\omega \hat{\rho}_{\mathrm{th}}\}=(\bar{n}+1)\delta(\omega-\omega')$, and hence provide a non-zero contribution. For example, one of such terms is

$$\begin{aligned}\frac{\gamma}{\pi}\int_0^t d\tau\int_{-\infty}^{+\infty}d\omega\int_{-\infty}^{+\infty}d\omega'\hat{a}_{\mathrm{I}}(t)\hat{a}_{\mathrm{I}}^\dagger(t-\tau)\hat{\rho}_{\mathrm{cav,I}}(t-\tau)e^{\mathrm{i}\omega t}e^{-\mathrm{i}\omega'(t-\tau)}\mathrm{tr}_{\mathrm{ext}}\{\hat{b}(\omega)\hat{b}^\dagger(\omega')\bigotimes_{\forall\omega}\hat{\rho}_{\mathrm{th}}\}\\ =\frac{\gamma\bar{n}}{\pi}\int_0^t d\tau\hat{a}_{\mathrm{I}}(t)\hat{a}_{\mathrm{I}}^\dagger(t-\tau)\hat{\rho}_{\mathrm{cav,I}}(t-\tau)\underbrace{\int_{-\infty}^{+\infty}d\omega e^{\mathrm{i}\omega\tau}}_{2\pi\delta(\tau)}=\gamma\bar{n}\hat{a}_{\mathrm{I}}(t)\hat{a}_{\mathrm{I}}^\dagger(t)\hat{\rho}_{\mathrm{cav,I}}(t),\end{aligned} \tag{380}$$

where we have made use of the property (341) of the Dirac delta. After taking care of all this 16 terms, we end up with the equation

$$\partial_t\hat{\rho}_{\mathrm{cav,I}}=(\bar{n}+1)\gamma\left(2\hat{a}_{\mathrm{I}}\hat{\rho}_{\mathrm{cav,I}}\hat{a}_{\mathrm{I}}^\dagger-\hat{a}_{\mathrm{I}}^\dagger\hat{a}_{\mathrm{I}}\hat{\rho}_{\mathrm{cav,I}}-\hat{\rho}_{\mathrm{cav,I}}\hat{a}_{\mathrm{I}}^\dagger\hat{a}_{\mathrm{I}}\right)+\bar{n}\gamma\left(2\hat{a}_{\mathrm{I}}^\dagger\hat{\rho}_{\mathrm{cav,I}}\hat{a}_{\mathrm{I}}-\hat{a}_{\mathrm{I}}\hat{a}_{\mathrm{I}}^\dagger\hat{\rho}_{\mathrm{cav,I}}-\hat{\rho}_{\mathrm{cav,I}}\hat{a}_{\mathrm{I}}\hat{a}_{\mathrm{I}}^\dagger\right), \tag{381}$$

where all the operators are evaluated at the same time. Finally, coming back to the Schrödinger picture, and including a Hamiltonian $\hat{H}_{\mathrm{intra}}(t)$ that describes any additional intracavity processes (allowed within the formalism as long as they are just a perturbation onto $\hat{H}_{\mathrm{cav}}$), we obtain

$$\begin{aligned}\partial_t\hat{\rho}_{\mathrm{cav}}=&\left[\frac{\hat{H}_{\mathrm{cav}}+\hat{H}_{\mathrm{intra}}(t)+\hat{H}_{\mathrm{inj}}(t)}{\mathrm{i}\hbar},\hat{\rho}_{\mathrm{cav}}\right]\\ &+(\bar{n}+1)\gamma\left(2\hat{a}\hat{\rho}_{\mathrm{cav}}\hat{a}^\dagger-\hat{a}^\dagger\hat{a}\hat{\rho}_{\mathrm{cav}}-\hat{\rho}_{\mathrm{cav}}\hat{a}^\dagger\hat{a}\right)+\bar{n}\gamma\left(2\hat{a}^\dagger\hat{\rho}_{\mathrm{cav}}\hat{a}-\hat{a}\hat{a}^\dagger\hat{\rho}_{\mathrm{cav}}-\hat{\rho}_{\mathrm{cav}}\hat{a}\hat{a}^\dagger\right)\end{aligned} \tag{382}$$

This equation is known as the *master equation* of the intracavity mode. It contains two very different types of terms. First, a commutator of the state with a Hamiltonian accounting for all the coherent processes occurring within the cavity (which might get corrections from the interaction with the external field, e.g., the one coming from the injection of lasers). On the other hand, we have terms that cannot be written as a commutator of the state with an operator, and account for any incoherent processes occurring in the system mediated by the external field (in this case, photons leaking out of the cavity irreversibly or entering the cavity incoherently from the thermal external field). In general, similarly to what we saw in the Heisenberg picture, the coherent and incoherent processes reach a dynamical balance, leading to an asymptotic state in the long term $t\to\infty$, which does not depend on the initial state.

To finish this section, let us prove that the Hamiltonian after the first change of picture

$$\hat{H}_D(t)=\hat{D}^\dagger(t)(\hat{H}_{\mathrm{cav}}+\hat{H}_{\mathrm{ext}}+\hat{H}_{\mathrm{int}})\hat{D}(t)-\mathrm{i}\hbar\hat{D}^\dagger(t)\partial_t\hat{D}(t), \tag{383}$$

takes the form (369). In order to find $\partial_t\hat{D}(t)$, we first use the disentangling Baker-Cambell-Haussdorf lemma (125) with $\hat{A}=\int_{-\infty}^{+\infty}d\omega\beta(\omega,t)\hat{b}^\dagger(\omega)$ and $\hat{B}=-\int_{-\infty}^{+\infty}d\omega\beta^*(\omega,t)\hat{b}(\omega)$, so that using the commutation relations (332) of the external operators, we write

$$\hat{D}(t)=e^{-\int_{-\infty}^{+\infty}d\omega|\beta(\omega,t)|^2/2}e^{\int_{-\infty}^{+\infty}d\omega\beta(\omega,t)\hat{b}^\dagger(\omega)}e^{-\int_{-\infty}^{+\infty}d\omega\beta^*(\omega,t)\hat{b}(\omega)}. \tag{384}$$

Applying the chain rule, we then obtain

$$\begin{aligned}\partial_t\hat{D}(t)&=\int_{-\infty}^{+\infty}d\omega\left[\dot{\beta}(\omega,t)\partial_{\beta(\omega,t)}+\dot{\beta}^*(\omega,t)\partial_{\beta^*(\omega,t)}\right]\hat{D}(t)\\ &=\int_{-\infty}^{+\infty}d\omega\left\{\dot{\beta}(\omega,t)\left[\hat{b}^\dagger(\omega)-\frac{\beta^*(\omega,t)}{2}\right]\hat{D}(t)-\hat{D}(t)\dot{\beta}^*(\omega,t)\left[\hat{b}(\omega)+\frac{\beta(\omega,t)}{2}\right]\right\}\\ &=\hat{D}(t)\int_{-\infty}^{+\infty}d\omega\dot{\beta}(\omega,t)\left[\hat{b}^\dagger(\omega)+\frac{\beta^*(\omega,t)}{2}\right]-\mathrm{H.c.},\end{aligned} \tag{385}$$

here in the last step we have used $\hat{b}^\dagger(\omega)\hat{D}(t) = \hat{D}(t)[\hat{b}^\dagger(\omega) + \beta^*(\omega,t)]$, which is just an alternative form of the displacement formula $\hat{D}^\dagger(t)\hat{b}(\omega)\hat{D}(t) = \hat{b}(\omega) + \beta(\omega,t)$, trivially found by using the Baker-Cambell-Haussdorf lemma (84). Applying this formula and (125) to (383), we then obtain

$$\hat{H}_D(t) = \hat{H}_{\rm cav} + \hat{H}_{\rm ext} + \hat{H}_{\rm int} + \hat{H}_{\rm inj}(t) + \int_{-\infty}^{+\infty} d\omega \left\{ \hbar[\omega\beta(\omega,t) - \mathrm{i}\dot{\beta}(\omega,t)] \left[\hat{b}^\dagger(\omega) + \frac{\beta^*(\omega,t)}{2}\right] + \text{H.c.} \right\}. \tag{386}$$

The largest simplification of this Hamiltonian is then obtained by asking the last term of this expression to vanish, obtaining the differential equation $\dot{\beta}(\omega,t) = -\mathrm{i}\omega\beta(\omega,t)$. Choosing the initial condition $\beta(\omega,0) = \alpha(\omega)$ as the initial condition, in order to remove the initial displacement of the environmental state (367), we then obtain $\beta(\omega,t) = \alpha(\omega)e^{-\mathrm{i}\omega t}$, and the form (369) for $\hat{H}_D(t)$, as we wanted to prove.

5. *Master equations and their interpretation*

The form of the master equation above is not accidental, and indeed, within the level of approximation that we are working with (Born-Markov), it is possible (but beyond the scope of this introductory course, although we'll get a glimpse of it at the end of the chapter) to show that the most general evolution equation for the state $\hat{\rho}$ of the system, after tracing out the environment, takes the so-called *Lindblad* form

$$\partial_t\hat{\rho}(t) = \left[\frac{\hat{V}(t)}{\mathrm{i}\hbar}, \hat{\rho}(t)\right] + \sum_j \kappa_j \left(2\hat{J}_j\hat{\rho}\hat{J}_j^\dagger - \hat{J}_j^\dagger\hat{J}_j\hat{\rho} - \hat{\rho}\hat{J}_j^\dagger\hat{J}_j\right). \tag{387}$$

Here, $\hat{V}(t)$ is a Hermitian operator that can be interpreted as the Hamiltonian of the system (modified by interactions with the environment). On the other hand, $\hat{J}_j$ are some operators with related rates $\kappa_j > 0$, all of which (including how many we get) depend on the specific form of the interaction between the system and its environments, as well as the properties of the latter. This form is so common, that we typically define the so-called *dissipative superoperator* or *dissipator* $\mathcal{D}_J$, which acts on operators as

$$\mathcal{D}_J[\hat{\rho}] = 2\hat{J}\hat{\rho}\hat{J}^\dagger - \hat{J}^\dagger\hat{J}\hat{\rho} - \hat{\rho}\hat{J}^\dagger\hat{J}. \tag{388}$$

The word 'superoperator' refers to the fact that $\mathcal{D}_J$ can be seen as a linear map from operators to operators, similarly to how an operator is a map from kets to kets. In fact, the whole master equation can be seen as the evolution equation generated by the so-called *Lindblad superoperator* or *Lindbladian* $\mathcal{L}$, so that $\partial_t\hat{\rho} = \mathcal{L}[\hat{\rho}]$. While all this seems rather anecdotical at this point, we will see that it directly inspires methods for the efficient numerical coding and simulation of master equations, see [78].

Note that the master equation (382) for the open cavity has exactly this Lindblad form with $\hat{V}(t) = \hat{H}_{\rm cav} + \hat{H}_{\rm intra}(t) + \hat{H}_{\rm inj}(t)$, $\{\kappa_1 = (\bar{n}+1)\gamma, \hat{J}_1 = \hat{a}\}$ and $\{\kappa_2 = \bar{n}\gamma, \hat{J}_2 = \hat{a}^\dagger\}$.

Let us now provide a more explicit interpretation of the terms of the master equation, and in particular of the so-called *jump operators* $\hat{J}_j$. For this, consider a simple master equation with only one of such operators and a time-independent Hamiltonian (the generalization is trivial). Defining an effective non-Hermitian Hamiltonian

$$\hat{H}_{\rm eff} = \hat{V} - \mathrm{i}\kappa\hat{J}^\dagger\hat{J}, \tag{389}$$

the master equation can be rewritten as

$$\partial_t\hat{\rho} = \frac{1}{\mathrm{i}\hbar}\left(\hat{H}_{\rm eff}\hat{\rho} - \hat{H}_{\rm eff}^\dagger\hat{\rho}\right) + 2\kappa\hat{J}\hat{\rho}\hat{J}^\dagger. \tag{390}$$

This form offers a very suggestive interpretation. The dynamics is generated by two types of terms: the first one similar to a commutator, $\hat{H}_{\rm eff}\hat{\rho} - \hat{H}_{\rm eff}^\dagger\hat{\rho}$; the second one just the direct action of the jump operator on the state, $\hat{J}\hat{\rho}\hat{J}^\dagger$. We now show that these two terms are of extremely different nature. In particular, the first one induces *reversible* dynamics, while the second generates *irreversible* dynamics. In order to show this, consider the following probabilistic protocol for the generation of $\hat{\rho}(t+dt)$ from $\hat{\rho}(t)$, which is shown at the end to be equivalent to the master equation. With probability $p(t) = 2\kappa dt\langle\hat{J}^\dagger\hat{J}\rangle$, we apply a quantum jump to the state, so the state is transformed as

$$\hat{\rho}(t) \longrightarrow \frac{\hat{J}\hat{\rho}(t)\hat{J}^\dagger}{\mathrm{tr}\{\hat{J}\hat{\rho}(t)\hat{J}^\dagger\}} \equiv \hat{\rho}_{\rm irrev}(t). \tag{391}$$

On the other hand, with the complementary probability $1-p(t)$, we apply the effective time-evolution operator $\hat{U}_{\rm eff}(t)=e^{\hat{H}_{\rm eff}t/{\rm i}\hbar}$, so that now the state is transformed as

$$\hat{\rho}(t)\longrightarrow\frac{\hat{U}_{\rm eff}(dt)\hat{\rho}(t)\hat{U}_{\rm eff}^{\dagger}(dt)}{{\rm tr}\{\hat{U}_{\rm eff}(dt)\hat{\rho}(t)\hat{U}_{\rm eff}^{\dagger}(dt)\}}\equiv\hat{\rho}_{\rm rev}(t). \tag{392}$$

The point now is that while the inverse of the effective time-evolution operator exists (we just need to change the sign of the Hamiltonian), $\hat{U}_{\rm eff}^{-1}(t)=\hat{U}_{\rm eff}(-t)$, that's not the general case for jump operators $\hat{J}$ (think of the annihilation or creation operators, which are not invertible). Therefore, $\hat{\rho}_{\rm rev}(t)$ can always be reversed into $\hat{\rho}(t)$, but once a jump happens, and we have $\hat{\rho}_{\rm irrev}(t)$, there is nothing trivial we can do to come back to the original state[42]. If we add to this that quantum jumps are random (they occur only probabilistically), we conclude that the second term in the master equation (390) is the one responsible for irreversible dynamics. Note, in addition, that the evolution induced by $\hat{U}_{\rm eff}(t)$ is continuous, while the one induced by quantum jumps is discontinuous (hence the word 'jump').

Let us now prove that, in the $dt\to 0$ limit, this probabilistic protocol is equivalent to the master equation (390). According to the definition and interpretation of mixed state that we saw in Section I B, the quantum state right after applying the protocol to $\hat{\rho}(t)$ can be written as

$$\hat{\rho}(t+dt)=p(t)\hat{\rho}_{\rm irrev}+[1-p(t)]\hat{\rho}_{\rm rev}. \tag{393}$$

On the other hand, using the order-dt expansions

$$\hat{U}_{\rm eff}(dt)\approx 1+\frac{dt}{{\rm i}\hbar}\hat{H}_{\rm eff}, \tag{394a}$$

$$\hat{U}_{\rm eff}^{\dagger}(dt)\hat{U}_{\rm eff}(dt)\approx 1-2\kappa dt\hat{J}^{\dagger}\hat{J}, \tag{394b}$$

and noting that the cyclic property of the trace allows us to write

$${\rm tr}\{\hat{J}\hat{\rho}(t)\hat{J}^{\dagger}\}=\langle\hat{J}^{\dagger}\hat{J}\rangle(t)=p(t)/2\kappa dt, \tag{395a}$$

$${\rm tr}\{\hat{U}_{\rm eff}(dt)\hat{\rho}(t)\hat{U}_{\rm eff}^{\dagger}(dt)\}=\langle\hat{U}_{\rm eff}^{\dagger}(dt)\hat{U}_{\rm eff}(dt)\rangle(t)\approx 1-2\kappa dt\langle\hat{J}^{\dagger}\hat{J}\rangle(t)=1-p(t), \tag{395b}$$

we can rewrite (393) to first order in dt as

$$\hat{\rho}(t+dt)=\hat{\rho}(t)+\frac{dt}{{\rm i}\hbar}\left(\hat{H}_{\rm eff}\hat{\rho}-\hat{H}_{\rm eff}^{\dagger}\hat{\rho}\right)+2\kappa dt\hat{J}\hat{\rho}\hat{J}^{\dagger}, \tag{396}$$

which is the finite-differences version of the master equation (390), and hence coincides with it in the $dt\to 0$ limit, as we wanted to prove.

6. *General dynamics of expectation values and example in the Schrödinger picture: driven empty cavity*

In order to learn how to use the master equation, we study again the simplest example possible: that of an empty cavity ($\hat{H}_{\rm intra}=0$), driven by a single monochromatic laser, so that $\mathcal{A}(t)=\mathcal{E}e^{-{\rm i}\omega_{\rm L}t}$. For this case, we already argued that the state of the cavity remains Gaussian if it is Gaussian initially (otherwise, only the asymptotic state will be Gaussian). With more generality, this happens whenever the master equation is quadratic in annihilation and creation operators, as we will prove next.

In order to find the evolution equations of the first and second order moments required to determine the Gaussian state, we first consider the time evolution of the expectation value of a generic operator $\hat{A}$, that is, $\langle\hat{A}\rangle(t)={\rm tr}\{\hat{A}\hat{\rho}(t)\}$, where we allow $\hat{\rho}$ to satisfy a generic master equation (387). We then have

$$\partial_t\langle\hat{A}\rangle={\rm tr}\left\{\hat{A}\partial_t\hat{\rho}\right\}={\rm tr}\left\{\hat{A}\left[\frac{\hat{V}}{{\rm i}\hbar},\hat{\rho}\right]\right\}+\sum_j\kappa_j{\rm tr}\left\{2\hat{A}\hat{J}_j\hat{\rho}\hat{J}_j^{\dagger}-\hat{A}\hat{J}_j^{\dagger}\hat{J}_j\hat{\rho}-\hat{A}\hat{\rho}\hat{J}_j^{\dagger}\hat{J}_j\right\}. \tag{397}$$

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[42] See however reference [79] for an impressive example of the advances that modern experimental platforms, together with a very mature theoretical understanding of quantum-jump processes, are allowing in this field: even though the jumps are random, under proper conditions they are preceded by a warning signal that allows catching and reversing them.

Using the cyclic property of the trace, we can rewrite this expression in terms of commutators of $\hat{A}$ with the Hamiltonian and the jump operators:

$$\mathrm{tr}\left\{\hat{A}\left[\frac{\hat{V}}{\mathrm{i}\hbar},\hat{\rho}\right]\right\}=\mathrm{tr}\left\{\hat{A}\frac{\hat{V}}{\mathrm{i}\hbar}\hat{\rho}-\hat{A}\hat{\rho}\frac{\hat{V}}{\mathrm{i}\hbar}\right\}=\mathrm{tr}\left\{\left(\hat{A}\frac{\hat{V}}{\mathrm{i}\hbar}-\frac{\hat{V}}{\mathrm{i}\hbar}\hat{A}\right)\hat{\rho}\right\}=\left\langle\left[\hat{A},\frac{\hat{V}}{\mathrm{i}\hbar}\right]\right\rangle, \tag{398a}$$

$$\mathrm{tr}\left\{\hat{A}\hat{J}_j\hat{\rho}\hat{J}_j^\dagger-\hat{A}\hat{J}_j^\dagger\hat{J}_j\hat{\rho}\right\}=\mathrm{tr}\left\{\left(\hat{J}_j^\dagger\hat{A}-\hat{A}\hat{J}_j^\dagger\right)\hat{J}_j\hat{\rho}\right\}=\left\langle\left[\hat{J}_j^\dagger,\hat{A}\right]\hat{J}_j\right\rangle, \tag{398b}$$

$$\mathrm{tr}\left\{\hat{A}\hat{J}_j\hat{\rho}\hat{J}_j^\dagger-\hat{A}\hat{\rho}\hat{J}_j^\dagger\hat{J}_j\right\}=\mathrm{tr}\left\{\hat{J}_j^\dagger\left(\hat{A}\hat{J}_j-\hat{J}_j\hat{A}\right)\hat{\rho}\right\}=\left\langle\hat{J}_j^\dagger\left[\hat{A},\hat{J}_j\right]\right\rangle, \tag{398c}$$

leading to a final simple form of the evolution equation

$$\partial_t\langle\hat{A}\rangle=\left\langle\left[\hat{A},\frac{\hat{V}}{\mathrm{i}\hbar}\right]\right\rangle+\sum_j\kappa_j\left(\left\langle\left[\hat{J}_j^\dagger,\hat{A}\right]\hat{J}_j\right\rangle+\left\langle\hat{J}_j^\dagger\left[\hat{A},\hat{J}_j\right]\right\rangle\right). \tag{399}$$

Since for bosonic problems the commutator always reduces the order in annihilation and creation operators by a factor 2, this expression evidences that the equations of motion of first and second order moments will form a closed set, only if the Hamiltonian is quadratic in annihilation and creation operators and the jump operators are linear. In any other case, information about higher-order moments will enter in the dynamical equations of the mean vector and covariance matrix, and the state will not remain Gaussian.

Considering the example at hand (driven empty cavity), we can particularize the equation above to the first and second order moments of the cavity mode. However, before diving into such calculations, it is always advisable to move to a picture where the master equation becomes time independent. Hence, we need to learn how a general master equation (387) is transformed under a change of picture with associated unitary operator $\hat{U}_\mathrm{c}(t)$. It is very easy to see, just by taking the time derivative of the transformed state $\hat{\rho}_\mathrm{I}(t)=\hat{U}_\mathrm{c}^\dagger(t)\hat{\rho}(t)\hat{U}_\mathrm{c}(t)$, that it still satisfies a Lindblad-form master equation

$$\partial_t\hat{\rho}_\mathrm{I}(t)=\left[\frac{\hat{H}_\mathrm{I}(t)}{\mathrm{i}\hbar},\hat{\rho}_\mathrm{I}(t)\right]+\sum_j\kappa_j\left(2\hat{J}_{j,\mathrm{I}}(t)\hat{\rho}\hat{J}_{j,\mathrm{I}}^\dagger(t)-\hat{J}_{j,\mathrm{I}}^\dagger(t)\hat{J}_{j,\mathrm{I}}(t)\hat{\rho}-\hat{\rho}\hat{J}_{j,\mathrm{I}}^\dagger(t)\hat{J}_{j,\mathrm{I}}(t)\right), \tag{400}$$

with the same intermediate-picture Hamiltonian $\hat{H}_\mathrm{I}(t)=\hat{U}_\mathrm{c}^\dagger(t)\hat{V}(t)\hat{U}_\mathrm{c}(t)-\mathrm{i}\hbar\hat{U}_\mathrm{c}^\dagger(t)\partial_t\hat{U}_\mathrm{c}(t)$ as we found for closed systems (see Section I C), and transformed jump operators $\hat{J}_{j,\mathrm{I}}(t)=\hat{U}_\mathrm{c}^\dagger(t)\hat{J}_j\hat{U}_\mathrm{c}(t)$.

In our master equation at hand, that of an empty open cavity (382), the only explicit time dependence comes from the injection Hamiltonian. This can be easily removed by changing to a picture that rotates at the laser frequency, with corresponding transformation operator $\hat{U}_\mathrm{c}(t)=e^{-\mathrm{i}\omega_\mathrm{L}t\hat{a}^\dagger\hat{a}}$. This transforms the annihilation operator as $\hat{U}_\mathrm{c}^\dagger(t)\hat{a}\hat{U}_\mathrm{c}(t)=e^{-\mathrm{i}\omega_\mathrm{L}t}\hat{a}$, as we have seen several times. The transformed state $\hat{\rho}_\mathrm{I}(t)=\hat{U}_\mathrm{c}^\dagger(t)\hat{\rho}_\mathrm{cav}(t)\hat{U}_\mathrm{c}(t)$, evolves then according to the master equation

$$\partial_t\hat{\rho}_\mathrm{I}=\left[\mathrm{i}\Delta\hat{a}^\dagger\hat{a}+\mathcal{E}\hat{a}^\dagger-\mathcal{E}^*\hat{a},\hat{\rho}_\mathrm{I}\right]+(\bar{n}+1)\gamma\mathcal{D}_a[\hat{\rho}_\mathrm{I}]+\bar{n}\gamma\mathcal{D}_{a^\dagger}[\hat{\rho}_\mathrm{I}], \tag{401}$$

where we remind that $\Delta=\omega_\mathrm{L}-\omega_\mathrm{c}$ is the detuning between the cavity and the driving laser. Note that the incoherent terms didn't change, because the jump operators, annihilation and creation operators in this case, transform with simple $e^{\mp\mathrm{i}\omega_\mathrm{L}t}$ phases, which cancel in every term.

Let us further note one subtle issue. The relation between the expression for the expectation of an operator $\hat{A}$ can be written either either as $\mathrm{tr}\{\hat{A}\hat{\rho}_\mathrm{cav}(t)\}$ in the Schrödinger picture or as $\mathrm{tr}\{\hat{U}_\mathrm{c}^\dagger(t)\hat{A}\hat{U}_\mathrm{c}(t)\hat{\rho}_\mathrm{I}(t)\}$ in the rotating picture. However, given the master equation (401) in the rotating picture, the natural object that can be evaluated is what we will define as the *intermediate-picture expectation value* $\langle\hat{A}\rangle_\mathrm{I}(t)=\mathrm{tr}\{\hat{A}\hat{\rho}_\mathrm{I}(t)\}=\mathrm{tr}\{\hat{U}_\mathrm{c}(t)\hat{A}\hat{U}_\mathrm{c}^\dagger(t)\hat{\rho}_\mathrm{cav}(t)\}$, whose relation with the true expectation value $\mathrm{tr}\{\hat{A}\hat{\rho}_\mathrm{cav}(t)\}$ can only be found by working out the transformation $\hat{U}_\mathrm{c}(t)\hat{A}\hat{U}_\mathrm{c}^\dagger(t)$, as we will see in the example.

We are now in conditions to proceed with the evaluation of the first and second order moments. In particular, we now particularize (399) to the master equation (401) and the operators needed for these moments: $\hat{a}$, $\hat{a}^2$, and $\hat{a}^\dagger\hat{a}$. Using the canonical commutation relations, we easily find

$$\partial_t\langle\hat{a}\rangle_\mathrm{I}=\mathcal{E}-(\gamma-\mathrm{i}\Delta)\langle\hat{a}\rangle_\mathrm{I}, \tag{402a}$$

$$\partial_t\langle\hat{a}^2\rangle_\mathrm{I}=-2(\gamma-\mathrm{i}\Delta)\langle\hat{a}^2\rangle_\mathrm{I}+2\mathcal{E}\langle\hat{a}\rangle_\mathrm{I}, \tag{402b}$$

$$\partial_t\langle\hat{a}^\dagger\hat{a}\rangle_\mathrm{I}=2\mathrm{Re}\left\{\mathcal{E}^*\langle\hat{a}\rangle_\mathrm{I}\right\}-2\gamma\langle\hat{a}^\dagger\hat{a}\rangle_\mathrm{I}+2\bar{n}\gamma, \tag{402c}$$

Note that in terms of the fluctuation operator $\delta\hat{a} = \hat{a} - \langle\hat{a}\rangle_{\rm I}$, the equations for the second order moments are written as

$$\partial_t\langle\delta\hat{a}^2\rangle_{\rm I} = \partial_t\left(\langle\hat{a}^2\rangle_{\rm I} - \langle\hat{a}\rangle_{\rm I}^2\right) = \left(\partial_t\langle\hat{a}^2\rangle_{\rm I} - 2\langle\hat{a}\rangle_{\rm I}\partial_t\langle\hat{a}\rangle_{\rm I}\right) = -2(\gamma - {\rm i}\Delta)\langle\delta\hat{a}^2\rangle_{\rm I}, \tag{403a}$$

$$\partial_t\langle\delta\hat{a}^\dagger\delta\hat{a}\rangle_{\rm I} = \partial_t\left(\langle\hat{a}^\dagger\hat{a}\rangle_{\rm I} - \langle\hat{a}\rangle_{\rm I}^*\langle\hat{a}\rangle_{\rm I}\right) = \left(\partial_t\langle\hat{a}^\dagger\hat{a}\rangle_{\rm I} - 2{\rm Re}\left\{\langle\hat{a}\rangle_{\rm I}^*\partial_t\langle\hat{a}\rangle_{\rm I}\right\}\right) = -2\gamma\langle\delta\hat{a}^\dagger\delta\hat{a}\rangle_{\rm I} + 2\bar{n}\gamma. \tag{403b}$$

Hence, we find a set of decoupled linear equations for all the required moments, with solutions

$$\langle\hat{a}\rangle_{\rm I}(t) = e^{-(\gamma-{\rm i}\Delta)t}\langle\hat{a}\rangle_{\rm I}(0) + \mathcal{E}\int_0^t dt' e^{-(\gamma-{\rm i}\Delta)(t-t')} = e^{-(\gamma-{\rm i}\Delta)t}\langle\hat{a}\rangle_{\rm I}(0) + \mathcal{E}\left(\frac{1-e^{-(\gamma-{\rm i}\Delta)t}}{\gamma-{\rm i}\Delta}\right), \tag{404a}$$

$$\langle\delta\hat{a}^2\rangle_{\rm I}(t) = e^{-2(\gamma-{\rm i}\Delta)t}\langle\delta\hat{a}^2\rangle_{\rm I}(0), \tag{404b}$$

$$\langle\delta\hat{a}^\dagger\delta\hat{a}\rangle_{\rm I}(t) = e^{-2\gamma t}\langle\delta\hat{a}^\dagger\delta\hat{a}\rangle_{\rm I}(0) + 2\bar{n}\gamma\int_0^t dt' e^{-2\gamma(t-t')} = e^{-2\gamma t}\langle\delta\hat{a}^\dagger\delta\hat{a}\rangle_{\rm I}(0) + \bar{n}\left(1-e^{-2\gamma t}\right), \tag{404c}$$

leading to the asymptotic solutions

$$\lim_{t\to\infty}\langle\hat{a}\rangle_{\rm I}(t) = \frac{\mathcal{E}}{\gamma+{\rm i}\Delta}, \quad \lim_{t\to\infty}\langle\delta\hat{a}^2\rangle_{\rm I}(t) = 0, \quad \lim_{t\to\infty}\langle\delta\hat{a}^\dagger\delta\hat{a}\rangle_{\rm I}(t) = \bar{n}. \tag{405}$$

Finally, note that in our case $\hat{U}_{\rm c}^\dagger(t)\hat{a}\hat{U}_{\rm c}(t) = e^{-{\rm i}\omega_{\rm L}t}\hat{a}$, and hence, the relations between the true expectation values and the interaction-picture expectation values are very simple in this case

$$\langle\hat{a}\rangle(t) = e^{-{\rm i}\omega_{\rm L}t}\langle\hat{a}\rangle_{\rm I}(t), \quad \langle\delta\hat{a}^2\rangle(t) = e^{-2{\rm i}\omega_{\rm L}t}\langle\delta\hat{a}^2\rangle_{\rm I}(t), \quad \langle\delta\hat{a}^\dagger\delta\hat{a}\rangle(t) = \langle\delta\hat{a}^\dagger\delta\hat{a}\rangle_{\rm I}(t), \tag{406}$$

leading to the asymptotic moments

$$\lim_{t\to\infty}\langle\hat{a}(t)\rangle = \frac{\mathcal{E}}{\gamma+{\rm i}\Delta}e^{-{\rm i}\omega_{\rm L}t}, \quad \lim_{t\to\infty}\left\langle\delta\hat{a}^2(t)\right\rangle = 0, \quad \lim_{t\to\infty}\left\langle\delta\hat{a}^\dagger(t)\delta\hat{a}(t)\right\rangle = \bar{n}. \tag{407}$$

These are exactly the same expressions that we found with the quantum Langevin equation in Section V A 3.

7. *Extension to many modes and several environments*

Soon...

8. *Relation of the model parameters to physical parameters*

Apart from the thermal number of excitations and intracavity parameters such as the cavity frequency, the quantum Langevin and master equations of an open cavity turned out to have only two more basic parameters, $\mathcal{A}(t)$ and γ, describing the rates at which coherent light is injected into the cavity and intracavity light is lost through the partially transmitting mirror, respectively. In this section we prove that these model parameters are connected to relevant physical parameters like the transmissivity of the mirror $\mathcal{T}$ and the power of the injected laser beam $P_{\rm inj}$ through the expressions (337) and (352) provided above.

Loss rate. To determine the relation between γ and $\mathcal{T}$ it is enough to consider the undriven case ($\mathcal{A} = 0$) and follow classical arguments. We then neglect quantum fluctuations and focus on the classical part of the intracavity field. Using (210a) and (359), the classical vector potential of the cavity field of the mode of interest can then be written as

$$\mathbf{A}(z,t) = \left\langle\hat{\mathbf{A}}(z,t)\right\rangle = \mathbf{e}_x\sqrt{\frac{\hbar}{\varepsilon_0 LS\omega_{\rm c}}}e^{-(\gamma+{\rm i}\omega_{\rm c})t}\alpha(0)\sin(k_{\rm c}z) + {\rm c.c.}, \tag{408}$$

where $\alpha(0) = \langle\hat{a}(0)\rangle$ is the initial classical amplitude of the cavity field. On the other hand, note that every roundtrip a fraction $\mathcal{R}^{1/2}$ is lost through the cavity mirror, with reflectivity $\mathcal{R} = 1-\mathcal{T}$. Hence, after $n \in \mathbb{N}$ roundtrips, we have the relation

$$\mathbf{A}(z,t_n) = \mathcal{R}^{n/2}\mathbf{A}(z,0) \quad \Rightarrow \quad e^{-(\gamma+{\rm i}\omega_{\rm c})t_n} = \mathcal{R}^{n/2}\alpha(0), \tag{409}$$

where $t_n = 2nL/c$ is the time lapsed after n roundtrips. Taking into account that $\exp(\mathrm{i}\omega_c t_n) = 1$ by definition of the resonance frequencies ($\omega_c = m\pi c/L$ for some $m \in \mathbb{N}$), and assuming $\mathcal{T} \ll 1$ so that $\ln \mathcal{R} = \log(1-\mathcal{T}) \approx -\mathcal{T}$, we obtain

$$\gamma = -\frac{c}{4L}\ln \mathcal{R} \simeq \frac{c\mathcal{T}}{4L}, \tag{410}$$

as we wanted to prove.

Injection parameter. We follow again classical arguments, but considering this time the injection of a resonant monochromatic field (later we extend it to more spectral components), for which $\langle \hat{b}_0(\omega)\rangle = \alpha(\omega_c)\delta(\omega-\omega_c)$, so that $\mathcal{A}(t) = \mathcal{E}e^{-\mathrm{i}\omega_c t}$ with $\mathcal{E} = -\sqrt{\gamma/\pi}\alpha(\omega_c)$, see Eq. (351). We remind that $\hat{b}_0(\omega)$ are the external annihilation operators the origin of time. We proceed then by relating the coherent amplitude $\alpha(\omega_c)$ to the power and phase of the injected beam. Since these are all quantities that do not relate in any way to the cavity, it is enough to consider the limit in which there is no interaction between the intracavity and external fields, and hence the external field operators evolve as $\hat{b}(\omega;t) = \hat{b}_0(\omega)e^{-\mathrm{i}\omega t}$. Hence, according to (333), the part of the classical vector potential of the external field propagating towards the cavity, say $\mathbf{A}_{\leftarrow}(z,t)$, reads

$$\mathbf{A}_{\leftarrow}(z,t) = \frac{\mathrm{i}}{2}\mathbf{e}_x\int_0^\infty d\omega\sqrt{\frac{\hbar}{\pi c\varepsilon_0 S\omega}}\langle\hat{b}(\omega;t)\rangle e^{-\mathrm{i}k(z-L)} + \text{c.c.} = -\mathbf{e}_x\sqrt{\frac{\hbar}{\pi c\varepsilon_0 S\omega_c}}|\alpha(\omega_c)|\sin[\omega_c t + k_c(z-L) - \phi], \tag{411}$$

where ϕ is the phase of $-\alpha(\omega_c)$, which we show next to be the phase of the laser's electric field. Indeed, the electric and magnetic fields corresponding to this vector potential read

$$\mathbf{E}_{\leftarrow}(z,t) = -\partial_t\mathbf{A}_{\leftarrow}(z,t) = \mathbf{e}_x\sqrt{\frac{\hbar\omega_c}{\pi c\varepsilon_0 S}}|\alpha(\omega_c)|\cos[\omega_c t + k_c(z-L) - \phi], \tag{412a}$$

$$\mathbf{B}_{\leftarrow}(z,t) = \boldsymbol{\nabla}\times\mathbf{A}_{\leftarrow}(z,t) = -\mathbf{e}_y\sqrt{\frac{\hbar\omega_c}{\pi c^3\varepsilon_0 S}}|\alpha(\omega_c)|\cos[\omega_c t + k_c(z-L) - \phi], \tag{412b}$$

. Consider now the instantaneous power impinging the mirror, which we obtain by integrating the absolute value of the Poynting vector $[\mathbf{E}_{\leftarrow}(z,t)\times\mathbf{B}_{\leftarrow}(z,t)]/\mu_0$ at $z = L$, obtaining

$$P_{\leftarrow}(t) = \int_{\mathbb{R}^2} dxdy\frac{|\mathbf{E}_{\leftarrow}(z,t)\times\mathbf{B}_{\leftarrow}(z,t)|}{\mu_0} = \frac{\hbar\omega_c}{\pi}|\alpha(\omega_c)|^2\cos^2[\omega_c t - \phi]. \tag{413}$$

Instead of the instantaneous power, it is common to use the power averaged over an optical cycle, since resolving optical oscillations is not possible in standard power measurements. Let us denote this by $P_{\mathrm{inj}} = \frac{\omega}{2\pi}\int_{-\omega/\pi}^{+\omega/\pi} dtP_{\leftarrow}(t) = \hbar\omega_c|\alpha(\omega_c)|^2/2\pi$, from which we obtain the relation

$$\mathcal{E} = \sqrt{\frac{\gamma}{\pi}}|\alpha(\omega_c)|e^{\mathrm{i}\phi} = \sqrt{\frac{2\gamma}{\hbar\omega_c}P_{\mathrm{inj}}}e^{\mathrm{i}\phi}, \tag{414}$$

which coincides with the relation that we wanted to prove, Eq. (352), particularized to a single frequency component.

Consider now the effect of having several frequency components in the injected light. We are interested in the case in which each component can be resolved by the cavity, that is, their spectral separation is larger than γ (but still below the free spectral range $\pi c/L$, so that different components address the same cavity resonance). It feels natural that, under such circumstances, the total power will just be the direct sum of the power of each spectral component, which can also have their own independent phase (for example, each spectral component may come from a different laser). This brings us directly to the expression provided in Eq. (352).

B. Incoherent atomic processes

Having studied the model for an open cavity, let us now analyze another equally paradigmatic and important open quantum optical system: an atom interacting with the electromagnetic field in free space. As we will see, this will allow us to introduce master equations following a different route to the Markov approximation of even more general use, and discuss some very relevant physics such as spontaneous emission and the Lamb shift.

1. Revisiting field quantization in free space

In the previous section we made a continuous model for the field outside the cavity. In principle, we could consider the interaction of an atom with an electromagnetic continuum by following a similar route in which we place the atom in a cavity and make the length go to infinity. However, the way that we have quantized the cavity, with a mirror place at $z = 0$ would naturally lead to the interaction of an atom with a field in half the real line, not the whole (1D) space. Moreover, without reflective boundaries, modes with opposite wave vector should be independent, while quantization in a cavity always assumes that they cannot be excited independently. Hence, it is instructive and timely to introduce here the quantization of the electromagnetic field in free space starting from scratch. In addition, this will allow us to learn a slightly different route towards quantization, based on the normal variable of the harmonic oscillator instead of the position and momentum.

Let us recall that the normal variable of an oscillator of frequency ω, mass m, position $q(t)$, and momentum $p(t)$, is defined as $\nu(t) = q(t) + \mathrm{i}p(t)/m\omega$. Using the canonical equations of motion (66) of position and momentum, it is easily proven to satisfy the evolution equation $\dot{\nu} = -\mathrm{i}\omega\nu$. In addition, the Hamiltonian of the oscillator is written in terms of this variable as $H_\mathrm{o} = m\omega^2\nu^*\nu/2$. On the other hand, in terms of true position and momentum operators instead of quadratures, the annihilation operator reads $\hat{a} = \sqrt{m\omega/2\hbar}(\hat{q} + \mathrm{i}\hat{p}/m\omega)$, which means that quantization can be carried away by symmetrizing the Hamiltonian with respect ν and ν^* as $H_\mathrm{o} = m\omega^2(\nu^*\nu + \nu\nu^*)/4$, making then the correspondence $\{\nu, \nu^*\} \to \sqrt{2\hbar/m\omega}\{\hat{a}, \hat{a}^\dagger\}$. Note that the symmetrization of the Hamiltonian can be overlooked if we don't need to keep the constant $\hbar\omega/2$ contribution of vacuum to the oscillator's energy. We will use these formulation in what follows.

Within our usual quasi-1D approximation, let us start by expanding the vector potential in plane waves with all the possible wave vectors, that is,

$$\mathbf{A}(z,t) = \mathbf{e}_x \int_{\mathbb{R}} dk \mathcal{A}(k,t) e^{\mathrm{i}kz}, \tag{415}$$

where $\mathcal{A}(k,t)$ are complex expansion coefficients. Note that we are not doubling the number of degrees of freedom of the electromagnetic field by taking complex coefficients, since the amplitudes are related by $\mathcal{A}(-k,t) = \mathcal{A}^*(k,t)$. This is easily proven by using the reality of the vector potential, $\mathbf{A} = \mathbf{A}^*$, which implies[43]

$$\int_{-\infty}^{+\infty} dk \mathcal{A}(k,t) e^{\mathrm{i}kz} = \int_{-\infty}^{+\infty} dk \mathcal{A}^*(k,t) e^{-\mathrm{i}kz} = \int_{-\infty}^{+\infty} dk \mathcal{A}^*(-k,t) e^{\mathrm{i}kz}. \tag{416}$$

Operating with $\int_{-\infty}^{+\infty} dz e^{\mathrm{i}k'z}$ and using the definition of the Dirac delta function, $\int_{-\infty}^{+\infty} dz e^{\mathrm{i}(k+k')z} = 2\pi\delta(k+k')$, we obtain the desired result. Plugging (415) into the wave equation for the vector potential, $(\partial_t^2 - c^2\partial_z^2)\mathbf{A}(z,t) = 0$, and applying $\int_{-\infty}^{+\infty} dz e^{\mathrm{i}k'z}$ on the expression, we obtain

$$\ddot{\mathcal{A}}(k,t) + c^2k^2\mathcal{A}(k,t) = 0. \tag{417}$$

While this is the equation of motion of a harmonic oscillator, the amplitude $\mathcal{A}(k,t)$ cannot be interpreted as the position of the oscillator because it can be complex. However, we next show that a simple manipulation allows us to relate it to the normal variable of a harmonic oscillator, which is complex. To this aim, we rewrite the previous expression as

$$(\partial_t + \mathrm{i}c|k|)(\partial_t - \mathrm{i}c|k|)\mathcal{A}(k,t) = 0, \tag{418}$$

so we can easily define a variable that evolves just like the normal variable of a harmonic oscillator of frequency $c|k|$ as follows

$$\nu(k,t) = N_k^{-1}\left[\dot{\mathcal{A}}(k,t) - \mathrm{i}c|k|\mathcal{A}(k,t)\right] \quad \Rightarrow \quad \dot{\nu}(k,t) = -\mathrm{i}c|k|\nu(k,t). \tag{419}$$

Next we find the normalization factor N_k by imposing that the electromagnetic energy must be equal to the sum of the Hamiltonians of each of the harmonic oscillators associated to the wave vectors k. In particular, we use the expression

$$E_\mathrm{em}(t) = \frac{\varepsilon_0}{2}\int_{\mathbb{R}^3} d^3\mathbf{r}\left[\mathbf{E}^2(z,t) + c^2\mathbf{B}^2(z,t)\right], \tag{420}$$

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[43] In the following, like in the last equality of this equation, we will be continuously inverting the sign of the wave vector as a variable change in integrals, leading to $\int_{-\infty}^{+\infty} dk f(k) = \int_{-\infty}^{+\infty} dk f(-k)$.

for the electromagnetic energy. Taking into account that

$$\mathbf{E}(z,t) = -\partial_t \mathbf{A} = -\mathbf{e}_x \int_{\mathbb{R}} dk \dot{\mathcal{A}}(k,t) e^{\mathrm{i}kz} \quad \text{and} \quad \mathbf{B}(z,t) = \boldsymbol{\nabla} \times \mathbf{A} = -\mathrm{i}\mathbf{e}_x \int_{\mathbb{R}} dk k \mathcal{A}(k,t) e^{\mathrm{i}kz}, \tag{421}$$

the electric and magnetic contributions to the energy can be written as

$$\int_{-\infty}^{+\infty} dz \mathbf{E}^2(z,t) = \int_{\mathbb{R}} dk \int_{\mathbb{R}} dk' \dot{\mathcal{A}}(k,t)\dot{\mathcal{A}}(k',t) \int_{-\infty}^{+\infty} dz e^{\mathrm{i}(k+k')z} = 2\pi \int_{\mathbb{R}} dk \dot{\mathcal{A}}(k,t)\dot{\mathcal{A}}(-k,t) = 2\pi \int_{\mathbb{R}} dk |\dot{\mathcal{A}}(k,t)|^2, \tag{422a}$$

$$\int_{-\infty}^{+\infty} dz \mathbf{B}^2(z,t) = -\int_{\mathbb{R}} dk \int_{\mathbb{R}} dk' \mathcal{A}(k,t)\mathcal{A}(k',t) k k' \int_{-\infty}^{+\infty} dz e^{\mathrm{i}(k+k')z} = 2\pi \int_{\mathbb{R}} dk k^2 \mathcal{A}(k,t)\mathcal{A}(-k,t) = 2\pi \int_{\mathbb{R}} dk k^2 |\mathcal{A}(k,t)|^2, \tag{422b}$$

leading to

$$E_{\mathrm{em}}(t) = \varepsilon_0 S\pi \int_{\mathbb{R}} dk \left[|\dot{\mathcal{A}}(k,t)|^2 + c^2 k^2 |\mathcal{A}(k,t)|^2 \right]. \tag{423}$$

In order to write this expression as a function of the normal variable $\nu(k,t)$, we first invert (419) as

$$\dot{\mathcal{A}}(k,t) = \frac{1}{2}\left[N_k \nu(k,t) + N_{-k}^* \nu^*(-k,t) \right], \quad \mathcal{A}(k,t) = \frac{\mathrm{i}}{2c|k|}\left[N_k \nu(k,t) - N_{-k}^* \nu^*(-k,t) \right], \tag{424}$$

leading to

$$|\dot{\mathcal{A}}(k,t)|^2 = \frac{1}{4}\left[|N_k|^2 |\nu(k,t)|^2 + |N_{-k}|^2 |\nu(-k,t)|^2 + N_k N_{-k}^* \nu(k,t)\nu^*(-k,t) + N_k^* N_{-k} \nu^*(k,t)\nu(-k,t) \right], \tag{425a}$$

$$c^2 k^2 |\mathcal{A}(k,t)|^2 = \frac{1}{4}\left[|N_k|^2 |\nu(k,t)|^2 + |N_{-k}|^2 |\nu(-k,t)|^2 - N_k N_{-k}^* \nu(k,t)\nu^*(-k,t) - N_k^* N_{-k} \nu^*(k,t)\nu(-k,t) \right], \tag{425b}$$

which implies

$$E_{\mathrm{em}}(t) = \frac{\varepsilon_0 S\pi}{2} \int_{\mathbb{R}} dk \left[|N_k|^2 |\nu(k,t)|^2 + |N_{-k}|^2 |\nu(-k,t)|^2 \right] = \varepsilon_0 S\pi \int_{\mathbb{R}} dk |N_k|^2 \nu^*(k,t)\nu(k,t). \tag{426}$$

Choosing the normalization factor $N_k = -\mathrm{i}c|k|/\sqrt{2\pi\varepsilon_0 S}$ (note that we can choose the phase at will, and this one will turn out to be convenient for future purposes), we then find the electromagnetic energy

$$E_{\mathrm{em}}(t) = \int_{\mathbb{R}} dk \frac{c^2 k^2}{2} \nu^*(k,t)\nu(k,t), \tag{427}$$

which is the correct classical Hamiltonian for a collection of independent harmonic oscillators labeled by a continuous index $k \in \mathbb{R}$ and with frequency $c|k|$.

Quantization is then performed through the correspondence $\{\nu(k,t), \nu^*(k,t)\} \to \sqrt{2\hbar/c|k|}\{\hat{a}(k,t), \hat{a}^\dagger(k,t)\}_{k\in\mathbb{R}}$, with annihilation and creation operators satisfying canonical commutation relations

$$[\hat{a}(k,t), \hat{a}(k',t)] = 0, \quad [\hat{a}(k,t), \hat{a}^\dagger(k',t)] = \delta(k-k') \tag{428}$$

, which in the previous section were proven to be the right commutation relations for a set of independent oscillators labeled by a continuous index (wave vector in our case). The Hamiltonian for light in free (1D) space takes then the form

$$\hat{H}_{\mathrm{L}} = \int_{-\infty}^{+\infty} dk \hbar c|k| \hat{a}^\dagger(k)\hat{a}(k) = \int_0^{+\infty} dk \hbar c k \left[\hat{a}^\dagger(k)\hat{a}(k) + \hat{a}^\dagger(-k)\hat{a}(-k) \right], \tag{429}$$

with quantized electric field

$$\hat{\mathbf{E}}(z) = \mathrm{i}\mathbf{e}_x \int_{-\infty}^{+\infty} dk \sqrt{\frac{\hbar c|k|}{4\pi\varepsilon_0 S}} \left[\hat{a}(k) e^{\mathrm{i}kz} - \hat{a}^\dagger(k) e^{-\mathrm{i}kz} \right] = \mathrm{i}\mathbf{e}_x \int_0^{+\infty} dk \sqrt{\frac{\hbar c k}{4\pi\varepsilon_0 S}} \left[\hat{a}(k) e^{\mathrm{i}kz} + \hat{a}(-k) e^{-\mathrm{i}kz} - \mathrm{H.c.} \right], \tag{430}$$

where the right hand sides stress the fact that for a given frequency $c|k|$ there are two contributions from modes with wave vector $\pm|k|$. It is important to keep this in mind, so we don't confuse the integration over negative wave vectors with the integration over fictitious negative frequencies that we introduced in (336) as a convenient approximation.

2. Atomic master equation in free space and spontaneous emission

We can now consider the interaction of an atom with the electromagnetic continuum in free space. As we explained in Section IV B, within the dipole approximation, we can write the interaction Hamiltonian as $\hat{H}_{\rm LM} = e\hat{\mathbf{E}}(z_0)\cdot\hat{\mathbf{r}}_{\rm A}$, where z_0 is the position of the atom's center of mass (assumed fixed) and $\hat{\mathbf{r}}_{\rm A}$ is the atomic relative coordinate. Using the expression for the electric field given above, focusing on two atomic levels $\{|e\rangle, |g\rangle\}$ as usual for simplicity (everything is easily generalized to more atomic levels under reasonable approximations, similarly to the generalization of the single-mode cavity to the multi-mode one), we then find

$$\hat{H}_{\rm LM} = \mathrm{i}\int_{\mathbb{R}} dk e\sqrt{\frac{\hbar c|k|}{4\pi\varepsilon_0 S}}\left[\hat{a}(k)e^{\mathrm{i}kz_0} - \hat{a}^\dagger(k)e^{-\mathrm{i}kz_0}\right]\left[\langle g|\hat{x}_A|e\rangle\hat{\sigma} + \langle g|\hat{x}_A|e\rangle^*\hat{\sigma}^\dagger\right]. \tag{431}$$

Performing the rotating-wave approximation to neglect terms such as $\hat{a}(k)\hat{\sigma}$, and defining the couplings

$$g(k) = -e\sqrt{\frac{c|k|}{4\pi\hbar\varepsilon_0 S}}\langle g|\hat{x}_A|e\rangle e^{-\mathrm{i}kz_0}, \tag{432}$$

which we assume to be real for simplicity, in particular setting $z_0 = 0$ and taking $\langle g|\hat{x}_A|e\rangle \in \mathbb{R}$, we obtain

$$\hat{H}_{\rm LM} = \mathrm{i}\hbar\int_{\mathbb{R}} dk g(k)\left[\hat{a}^\dagger(k)\hat{\sigma} - \hat{a}(k)\hat{\sigma}^\dagger\right]. \tag{433}$$

The final Hamiltonian is then given by $\hat{H} = \hat{H}_{\rm A} + \hat{H}_{\rm L} + \hat{H}_{\rm LM}$, where $\hat{H}_{\rm L}$ is given in Eq. (429) and $\hat{H}_{\rm A} = \hbar\varepsilon\hat{\sigma}_z/2$ is the atomic Hamiltonian within the two-level approximation.

Note that this simple model leads to an unphysical situation in which the coupling $g(k)$ increases arbitrarily with the light frequency, diverging for $|k| \to \infty$. Of course, in reality this is not the case: the coupling remains close to $g(\varepsilon/c)$ in all the relevant frequency interval around the atomic transition ε, and includes a natural cut off for large and small frequencies that is not captured with the simple dipole Hamiltonian $e\hat{\mathbf{E}}(z_0)\cdot\hat{\mathbf{r}}_{\rm A}$ (e.g., for really large frequencies such as X rays the wavelength enters atomic scales, so the point-like approximation for the atom breaks down). In any case, let us proceed with the expressions we have but keeping this issue in mind.

In the following we will find a master equation for the reduced atomic state $\hat{\rho}_{\rm A}$. If we perform a frequency-independent approximation $g(k) = g(\varepsilon/c) \equiv \sqrt{\gamma c/2\pi}$ for the coupling (the factor 2 in the denominator comes from the fact that now for each frequency $\hbar c|k|$ we have two modes with opposite wave vectors $\pm|k|$ that contribute to the decay, while the factor c appears because we are labeling the modes by the wave vector instead of the frequency), we can proceed just like we did with the open cavity, finding exactly the same results at each step with the obvious replacements ($\omega_{\rm c} \to \varepsilon$, $\hat{a} \to \hat{\sigma}$,...), obtaining the master equation

$$\partial_t\hat{\rho}_{\rm A} = \left[\frac{\hat{H}_{\rm A} + \hat{H}_{\rm inj}(t)}{\mathrm{i}\hbar}, \hat{\rho}_{\rm A}\right] + (\bar{n}+1)\gamma\left(2\hat{\sigma}\hat{\rho}_{\rm A}\hat{\sigma}^\dagger - \hat{\sigma}^\dagger\hat{\sigma}\hat{\rho}_{\rm A} - \hat{\rho}_{\rm A}\hat{\sigma}^\dagger\hat{\sigma}\right) + \bar{n}\gamma\left(2\hat{\sigma}^\dagger\hat{\rho}_{\rm A}\hat{\sigma} - \hat{\sigma}\hat{\sigma}^\dagger\hat{\rho}_{\rm A} - \hat{\rho}_{\rm A}\hat{\sigma}\hat{\sigma}^\dagger\right), \tag{434}$$

where in this case

$$\hat{H}_{\rm inj}(t) = \mathrm{i}\hbar\left(\mathcal{A}(t)\hat{\sigma}^\dagger e^{-\mathrm{i}\omega_{\rm L}t} - \mathcal{A}^*(t)\hat{\sigma}e^{\mathrm{i}\omega_{\rm L}t}\right), \tag{435}$$

is the Hamiltonian related to the coherent contribution (laser) of the external fields. Just as in the case of the cavity, if the injection is composed of multiple monochromatic components with wave vectors $\{k_\ell\}_{\ell=1,2,\ldots,L}$ and corresponding frequencies $\omega_\ell = c|k_\ell|$, we have

$$\mathcal{A}(t) = \sum_{\ell=1}^{L}\mathcal{E}_\ell e^{-\mathrm{i}\omega_\ell t}, \tag{436}$$

where in this case the injection rates $\mathcal{E}_\ell$ can be easily related the power $P_{{\rm inj},\ell}$ (averaged over an optical cycle) of each wave vector component by

$$\mathcal{E}_\ell = -\mathrm{i}\frac{e}{\hbar}\langle e|\hat{x}_A|g\rangle\sqrt{\frac{P_{{\rm inj},\ell}}{2\varepsilon_0 cS}}e^{\mathrm{i}(k_\ell z_0 + \phi_\ell)}, \tag{437}$$

where ϕ_ℓ is the electric field's phase of the corresponding component, and we assume that the spectral separation between the different components is larger than γ, but are still close enough to drive the same atomic transition.

This expression is easily proven by noting that the injection Hamiltonian simply corresponds to the interaction of the atomic dipole with the classical part of the electric field, that is, the semiclassical Rabi Hamiltoinan $\hat{H}_{\rm inj}(t) = e\mathbf{E}(z_0)\cdot\hat{\mathbf{r}}_{\rm A}$. On the other hand, for each wave vector component, the electric field was shown in (412a) to be written as $\mathbf{E}\,(z_0,t) = \sum_{\ell=1}^{L}\mathbf{e}_x\sqrt{P_{{\rm inj},\ell}/c\varepsilon_0 S}\cos(\omega_\ell t - k_\ell z_0 - \phi_\ell)$, which substituted in the previous expression for $\hat{H}_{\rm inj}(t)$, and after performing the rotating-wave approximation, leads to (435) and (437).

In order to interpret this master equation and its effect on the dynamics of the atom, let us next focus on the specific situation of an atom in the electromagnetic vacuum, that is, at zero temperature ($\bar{n} = 0$) and with no laser light shinned on it ($\mathcal{A} = 0$). Following what we saw in Section III B, we write the atomic state in terms of its (complex) Bloch vector components $b_z(t) = \langle\hat{\sigma}_z\rangle(t)$ and $b(t) = \langle\hat{\sigma}\rangle(t)$ as

$$\hat{\rho}_{\rm A}(t) = \frac{1}{2}\left(\hat{I} + b_z(t)\hat{\sigma}_z + 2b^*(t)\hat{\sigma} + 2b(t)\hat{\sigma}^\dagger\right).$$

The complex Bloch equations are easily found from (399) and (434) as

$$\partial_t b = \partial_t\langle\hat{\sigma}\rangle = -{\rm i}\frac{\varepsilon}{2}\langle[\hat{\sigma},\hat{\sigma}_z]\rangle + \gamma\left\langle\left[\hat{\sigma}^\dagger,\hat{\sigma}\right]\hat{\sigma}\right\rangle = -{\rm i}\varepsilon\langle\hat{\sigma}\rangle + \gamma\langle\hat{\sigma}_z\hat{\sigma}\rangle = -(\gamma+{\rm i}\varepsilon)\langle\hat{\sigma}\rangle = -(\gamma+{\rm i}\varepsilon)b, \tag{438a}$$

$$\partial_t b_z = \partial_t\langle\hat{\sigma}_z\rangle = \gamma\left(\left\langle\left[\hat{\sigma}^\dagger,\hat{\sigma}_z\right]\hat{\sigma}\right\rangle + \left\langle\hat{\sigma}^\dagger\left[\hat{\sigma}_z,\hat{\sigma}\right]\right\rangle\right) = -4\gamma\left\langle\hat{\sigma}^\dagger\hat{\sigma}\right\rangle = -2\gamma\left(b_z+1\right), \tag{438b}$$

where we have used $\hat{\sigma}_z\hat{\sigma} = -\hat{\sigma}$ and $\hat{\sigma}_z = 2\hat{\sigma}^\dagger\hat{\sigma} - 1$, leading to the solutions

$$b(t) = b(0)e^{-(\gamma+{\rm i}\varepsilon)t} \underset{\gamma t\to\infty}{\longrightarrow} 0, \tag{439a}$$

$$b_z(t) = [b_z(0)+1]\,e^{-2\gamma t} - 1 \underset{\gamma t\to\infty}{\longrightarrow} -1, \tag{439b}$$

corresponding to the ground state. Hence, no matter the initial state of the atom, it eventually emits a photon and ends up in the ground state. We call this effect *spontaneous emission*: the electromagnetic vacuum fluctuations trigger emission of the atomic excitation as a photon, which gets lost in the continuum of modes and never comes back to the atom (shortly we will see this even more explicitly). It's interesting to consider the case in which the atom is initially in the excited state, $b_z(0) = 1$ and $b(0) = 0$. In this case the state can be written as

$$\hat{\rho}_{\rm A}(t) = e^{-2\gamma t}|e\rangle\langle e| + \left(1 - e^{-2\gamma t}\right)|g\rangle\langle g|, \tag{440}$$

showing that starting in the excited state it decays to the ground state by going through all possible mixed states of them (e.g., reaching the maximally mixed state at time $t_{\rm MM} = \ln(2)/2\gamma$). This shows that except at the initial and final states of the evolution, the atom becomes correlated with the electromagnetic field. This is a direct evidence of something that we mentioned right before performing the Born approximation in Eq. (377): even though we assume that the state can be approximately factorized as $\hat{\rho}_{\rm A}(t)\otimes_k|0\rangle\langle 0|$ in the dynamical equation of the reduced atomic state, the resulting equation still keeps track (to some degree) of the effect that correlations have on the dynamics of the system.

In order to get a deeper understanding of how the correlation comes into this scenario, we proceed now to solve analytically the full dynamical problem including both the atom and the field. This is possible because, just as in the Jaynes-Cummings model, the interaction Hamiltonian (433) conserves the total number of excitations, as first identified by Wigner and Weisskopf, from whom the upcoming derivation takes the name. Starting with the field in vacuum and the atom in the excited state, we can only reach states with one photon and the atom in the ground state, that is, we are bound to the single-excitation subspace spanned by $\{|0,e\rangle, \hat{a}^\dagger(k)|0,g\rangle\}_{k\in\mathbb{R}}$. Let us then expand the state at any as

$$|\psi(t)\rangle = \alpha(t)e^{-{\rm i}\varepsilon t/2}|0,e\rangle + \int_{-\infty}^{+\infty}dk\beta(k;t)e^{-{\rm i}(c|k|-\varepsilon/2)t}\hat{a}^\dagger(k)|0,g\rangle, \tag{441}$$

where $\alpha(t)$ and $\beta(k;t)$ are complex expansion coefficients. Let us next consider the Schrödinger equation ${\rm i}\hbar\partial_t|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$, where we remind that the Hamiltonian is given by , where the first term is the atomic Hamiltonian ... while the other two are provided in Eqs. (429) and (433). Projecting the Schrödinger equation onto[44] $|e,0\rangle$ or $\hat{a}^\dagger(k)|g,0\rangle$,

[44] In order to evaluate the action of the Hamiltonian onto the state, simply use the commutation relations (428) to bring annihilation operators to the right when needed, and use the property $\hat{a}(k)|0\rangle = 0$. The projections are then found from $\langle 0,a|0,a'\rangle = \delta_{aa'}$, $\langle 0,a|\hat{a}^\dagger(k)|0,a'\rangle = 0 = \langle 0,a|\hat{a}(k)|0,a'\rangle$, and $\langle 0,a|\hat{a}(k)\hat{a}^\dagger(k')|0,a'\rangle = \delta_{aa'}\delta(k-k')$.

we obtain

$$\dot{\alpha} = -\int_{-\infty}^{+\infty} dk g(k) e^{-\mathrm{i}(c|k|-\varepsilon)t}\beta(k), \tag{442a}$$

$$\dot{\beta}(k) = g(k)e^{\mathrm{i}(c|k|-\varepsilon)t}\alpha. \tag{442b}$$

We proceed by formally integrating the second equation as

$$\beta(k;t) = \int_0^t dt' g(k) e^{\mathrm{i}(c|k|-\varepsilon)t'}\alpha(t'), \tag{443}$$

where we already took $\beta(k;0) = 0$ as the initial condition. Inserted in the first equation, and performing the integration-variable change $t' = t - \tau$, leads to

$$\dot{\alpha} = -\int_0^t d\tau \alpha(t-\tau) \underbrace{\int_{-\infty}^{+\infty} dk g^2(k) e^{-\mathrm{i}(c|k|-\varepsilon)\tau}}_{C^*(\tau)e^{\mathrm{i}\varepsilon\tau}}. \tag{444}$$

The function $C(\tau)$ will be shown in the next section to play a fundamental role in the Markovian properties of the dynamics. For now, however, let's simply evaluate it under the same approximations that we used to derive the master equation above: the flat form of the coupling, $g(k) = \sqrt{\gamma c/2\pi}$, and extending the lower integration limit of the frequency integrals to $-\infty$. We then obtain

$$C^*(\tau) \approx \frac{\gamma c}{2\pi}\int_{-\infty}^{+\infty} dk e^{-\mathrm{i}c|k|\tau} = \frac{\gamma c}{\pi}\int_0^{+\infty} dk e^{-\mathrm{i}ck\tau} \approx \frac{\gamma}{\pi}\int_{-\infty}^{+\infty} d\omega e^{-\mathrm{i}ck\tau} = 2\gamma\delta(\tau), \tag{445}$$

where we have made the variable change $\omega = ck$ in the second to last step, and extended the lower integration limit. Inserting this expression into (444) and using the property (341) of the Dirac delta function, we then get

$$\dot{\alpha} = -\gamma\alpha \quad \Rightarrow \quad \alpha(t) = e^{-\gamma t}, \tag{446}$$

where we have used the initial condition $\alpha(0) = 1$. We can now come back to (443) and find

$$\beta(k;t) = \sqrt{\frac{\gamma c}{2\pi}}\int_0^t dt' e^{-[\gamma - \mathrm{i}(c|k|-\varepsilon)]t'} = \sqrt{\frac{\gamma c}{2\pi}}\frac{1-e^{-[\gamma-\mathrm{i}(c|k|-\varepsilon)]t}}{\gamma - \mathrm{i}(c|k|-\varepsilon)}. \tag{447}$$

Hence, the probability of finding a photon with wave vector k at time t is given by

$$|\beta(k;t)|^2 = \frac{\gamma c}{2\pi}\frac{1+e^{-2\gamma t} - 2e^{-\gamma t}\cos[(c|k|-\varepsilon)t]}{\gamma^2 + (c|k|-\varepsilon)^2}, \tag{448}$$

which depends only on the frequency $c|k|$ and not the propagation direction, as expected (there are no preferred directions in free space). Moreover, it is interesting to remark that asymptotically, this probability has a Lorentzian shape centered around the atomic resonance as a function of the frequency,

$$\lim_{\gamma t\to\infty} |\beta(k;t)|^2 = \frac{\gamma c/2\pi}{\gamma^2 + (c|k|-\varepsilon)^2}. \tag{449}$$

Hence, the atom can only emit photons with frequencies close to its resonance, similarly to how we saw that the cavity can only be excited by lasers close to one of its resonances. Finally, note that

$$\int_{-\infty}^{+\infty} dk|\beta(k;t)|^2 = \frac{2}{c}\int_0^{+\infty} d\omega|\beta(\omega/c;t)|^2 \approx \frac{\gamma}{\pi}\int_{-\infty}^{+\infty} d\omega \frac{1+e^{-2\gamma t} - 2e^{-\gamma t}\cos[(\omega-\varepsilon)t]}{\gamma^2+(\omega-\varepsilon)^2} = 1 - e^{-2\gamma t} = 1 - |\alpha(t)|^2, \tag{450}$$

which is further prove of the consistency of the various approximations we have used, since this relation must be satisfied at all times (unitary evolution must keep the state normalized).

Hence, we see that starting from the excited state with no photons, we end up with the atom in the ground state and a single photon distributed among the electromagnetic frequencies following a Lorentzian distribution. In order for the photon to not be able to be reabsorbed by the atom, it is crucial to have a continuum of modes. If instead we would have a discrete set, the dynamics would reveal revivals of the atomic population. The extreme example is

be that in which all modes can be ignored but one, obtaining then a Jaynes-Cummings model with perfectly periodic quantum Rabi oscillations. A (sufficiently) larger number of modes would make the population collapse, and then revive in some fashion that would depend on the specific relation between the frequencies of the mode.

Interestingly, at intermediate times, we have a superposition between the excitation being in the atom or the field, leading to an entangled state of these. Moreover, using the relations

$$\langle 0|\psi(t)\rangle = \alpha(t)e^{-\mathrm{i}\varepsilon t}|e\rangle, \quad \langle 0|\hat{a}(k)|\psi(t)\rangle = \beta(k;t)e^{-\mathrm{i}(c|k|-\varepsilon)t}|g\rangle, \tag{451}$$

we obtain the following reduced atomic state

$$\begin{aligned}\hat{\rho}_{\mathrm{A}}(t) &= \mathrm{tr}_{\mathrm{L}}\left\{|\psi(t)\rangle\langle\psi(t)|\right\} = \langle 0|\psi(t)\rangle\langle\psi(t)|0\rangle + \int_{-\infty}^{\infty} dk \langle 0|\hat{a}(k)|\psi(t)\rangle\langle\psi(t)|\hat{a}^{\dagger}(k)|0\rangle \\ &= |\alpha(t)|^2|e\rangle\langle e| + \left[\int_{-\infty}^{+\infty} dk|\beta(k;t)|^2\right]|g\rangle\langle g|,\end{aligned} \tag{452}$$

which leads precisely to the state (440) obtained with the master equation. Hence, we see that the origin of the mixed atomic state is in quantum correlations (entanglement) of the system (atom) with the environment (field).

3. *Frequency-dependent coupling: Markov approximation and the Lamb shift*

While the frequency-independent approximation for the coupling simplifies things immensely, there are systems in which it is not possible to do it. Hence, it is interesting to consider how to proceed when the frequency dependence of the coupling cannot be ignored. Moreover, as we are about to see, a very important effect is found when going beyond such a raw approximation: the Lamb shift, whose experimental observation in 1947 played a major role in the theoretical development quantum electrodynamics (and renormalization in particular).

Let us, for simplicity, consider zero temperature for the electromagnetic field (hence all the modes are in vacuum initially), and laser ignore the injection, which we know we can add at the end as Hamiltonian (435) in any case. All the way up to the Born and non-backaction approximations, we proceed in the same way as before. In particular, we obtain

$$\partial_t\hat{\rho}_{\mathrm{A,I}}(t) = -\frac{1}{\hbar^2}\int_0^t d\tau \mathrm{tr}_{\mathrm{L}}\{[\hat{H}_{\mathrm{I}}(t),[\hat{H}_{\mathrm{I}}(t-\tau),\hat{\rho}_{\mathrm{A,I}}(t-\tau)\bigotimes_{\forall k}|0\rangle\langle 0|]]\}, \tag{453}$$

where $\hat{\rho}_{\mathrm{A,I}}(t) = \mathrm{tr}_{\mathrm{L}}\{\hat{\rho}_{\mathrm{I}}(t)\}$ is the reduced atomic state in the interaction picture, $\hat{\rho}_{\mathrm{I}}(t) = \hat{U}_{\mathrm{c}}^{\dagger}(t)\hat{\rho}(t)\hat{U}_{\mathrm{c}}(t)$ is the transformed state of the whole system, and we define the change of picture through the unitary transformation is $\hat{U}_{\mathrm{c}}(t) = e^{\hat{H}_0/\mathrm{i}\hbar}$, with $\hat{H}_0 = \hat{H}_{\mathrm{A}} + \hat{H}_{\mathrm{L}}$, leading to the interaction picture Hamiltonian

$$\hat{H}_{\mathrm{I}}(t) = \hat{U}_{\mathrm{c}}^{\dagger}(t)\left[\hat{H}_0 + \hat{H}_{\mathrm{LM}}\right]\hat{U}_{\mathrm{c}}(t) - \hat{H}_0 = \mathrm{i}\hbar\int_{-\infty}^{+\infty} dk g(|k|)\left[\hat{a}^{\dagger}(k)\hat{\sigma}e^{\mathrm{i}(c|k|-\varepsilon)t} - \hat{a}(k)\hat{\sigma}^{\dagger}e^{-\mathrm{i}(c|k|-\varepsilon)t}\right], \tag{454}$$

where we remark that the coupling depends solely on the magnitude of the wave vector and not on its sign, since the atom doesn't have a preferred orientation.

Out of the 16 terms appearing in this expression when expanding the commutators and the products, only the terms proportional to $\mathrm{tr}_{\mathrm{L}}\{\hat{a}(k)\hat{a}^{\dagger}(k')\bigotimes_{\forall k}|0\rangle\langle 0|\} = \delta(k-k')$ are nonzero. This leaves us with

$$\begin{aligned}\partial_t\hat{\rho}_{\mathrm{A,I}}(t) &= \int_0^t d\tau\int_{-\infty}^{+\infty} dk g^2(|k|)\left[\hat{\sigma}\hat{\rho}_{\mathrm{A,I}}(t-\tau)\hat{\sigma}^{\dagger}e^{\mathrm{i}(c|k|-\varepsilon)\tau} - \hat{\rho}_{\mathrm{A,I}}(t-\tau)\hat{\sigma}^{\dagger}\hat{\sigma}e^{\mathrm{i}(c|k|-\varepsilon)\tau} + \mathrm{H.c.}\right] \\ &= \int_0^t d\tau e^{-\mathrm{i}\varepsilon\tau}C(\tau)\left[\hat{\sigma}\hat{\rho}_{\mathrm{A,I}}(t-\tau)\hat{\sigma}^{\dagger} - \hat{\rho}_{\mathrm{A,I}}(t-\tau)\hat{\sigma}^{\dagger}\hat{\sigma} + \mathrm{H.c.}\right],\end{aligned} \tag{455}$$

where we have combined all the terms under the wave-vector integral into the so-called *environmental correlation function* (note the usual change of variable in the integral, $\omega = c|k|$)

$$C(\tau) = \int_0^{+\infty} d\omega \underbrace{\frac{2}{c}g^2(\omega/c)}_{G(\omega)} e^{\mathrm{i}\omega\tau}. \tag{456}$$

This function contains all the information about the environment, and its decay determines how far into the past the dynamics of the atom can see. While we have found this expression for our particular problem, it can be shown that even for completely general problems, such a correlation function appears and can be written as half the Fourier transform of the so-called *environmental spectral density*, $G(\omega)$, which in our case takes the specific form written above. When the spectral density is taken as constant $G(\omega) = \gamma/\pi$, we are left with integrals of the type $C(\tau) \propto \int_0^\infty d\omega e^{\mathrm{i}\omega\tau}$, which are proportional to $\delta(\tau)$ when we extend the lower integration limit to $-\infty$. This would set $\tau = 0$ in Eq. (455), and lead to the master equation (434) that we analyzed in the previous section. However, when we cannot make this approximation, we need to proceed in a different way.

In situations where $C(\tau)$ is known and tractable analytically, one can try using Laplace transform techniques to solve the remaining time non-local equation. However, in most situations this is not the case, and we are forced to perform approximations. The most common one is the so-called *Markov approximation*, in which we assume that the evolution of the state is independent of its history, that is, we set $\hat{\rho}_{\mathrm{A,I}}(t-\tau)$ to $\hat{\rho}_{\mathrm{A,I}}(t)$ in the integral. Let us understand the conditions under which this approximation holds. First, note that since we are working in the interaction picture, changes in the state are fully due to the interaction, that is, they are expected to occur at a rate of order $\pi G(\varepsilon)$. On the other hand, while the correlation function $C(\tau)$ will not be a delta function, we still expect it to decay with τ, quite fast if $G(\omega)$ varies slowly with ω. Hence, if the decay rate of $C(\tau)$ is larger than $\pi G(\varepsilon)$, one can assume[45] that $\hat{\rho}_{\mathrm{A,I}}(t-\tau)$ is approximately equal to $\hat{\rho}_{\mathrm{A,I}}(t)$ in (455).

Let us assume that the required conditions are met, and perform the Markov approximation on (**??**), obtaining

$$\partial_t \hat{\rho}_{\mathrm{A,I}} = \Gamma(t)\left(\hat{\sigma}\hat{\rho}_{\mathrm{A,I}}\hat{\sigma}^\dagger - \hat{\rho}_{\mathrm{A,I}}\hat{\sigma}^\dagger\hat{\sigma}\right) + \mathrm{H.c.}, \tag{457}$$

with

$$\Gamma(t) = \int_0^t d\tau \int_0^{+\infty} d\omega G(\omega) e^{\mathrm{i}(\omega-\varepsilon)\tau}. \tag{458}$$

If $\Gamma(t)$ was real, this would be exactly the same master equation as (434), just with a modified time-dependent rate $\Gamma(t)$ instead of γ. However, as we will see shortly, this parameter is complex in general. Actually, for short times, there is no way of evaluating the integrals without the specific form of the coupling. However, for long times we prove at the end of the section that

$$\lim_{t\to\infty} \Gamma(t) = \underbrace{\pi G(\varepsilon)}_{\gamma} + \mathrm{i}\mathcal{P}\int_0^{+\infty} d\omega \frac{G(\omega)}{\omega - \varepsilon}, \tag{459}$$

where $\mathcal{P}\int$ refers to the integral's Cauchy principal value[46]. Hence, in the long time limit the real part provides the same result as we found with the frequency-independent approximation, but an imaginary part also appears. Plugging this result (459) into (457), we get the asymptotic master equation

$$\partial_t \hat{\rho}_{\mathrm{A,I}}(t) = -\mathrm{i}\frac{\Delta\varepsilon}{2}\left[\hat{\sigma}_z, \hat{\rho}_{\mathrm{A,I}}\right] + \gamma\left(2\hat{\sigma}\hat{\rho}_{\mathrm{A,I}}\hat{\sigma}^\dagger - \hat{\rho}_{\mathrm{A,I}}\hat{\sigma}^\dagger\hat{\sigma} + \hat{\sigma}\hat{\rho}_{\mathrm{A,I}}\hat{\sigma}^\dagger - \hat{\sigma}^\dagger\hat{\sigma}\hat{\rho}_{\mathrm{A,I}}\right), \tag{460}$$

where we have used $\hat{\sigma}_z = 2\hat{\sigma}^\dagger\hat{\sigma} - 1$ in the commutator term, and we have defined

$$\Delta\varepsilon = -\mathcal{P}\int_0^{+\infty} d\omega \frac{G(\omega)}{\omega - \varepsilon}, \tag{461}$$

which provides a contribution to the atomic transition frequency known as the *Lamb shift*.

It's interesting to try to calculate this shift, or at least understand its order of magnitude relative to the decay rate γ. The problem is that the unphysical coupling (432) leads to a spectral density $G(\omega) \propto \omega$, which makes the integral diverge (and this is even worse in 2D and 3D, where $G(\omega) \sim \omega^2$ and ω^3). A serious calculation of the Lamb shift would require the use of relativistic quantum electrodynamics and renormalization. However, in our weakly (logarithmically) divergent 1D case we can make a rough estimation of $\Delta\varepsilon$ by perform a frequency-independent approximation for the

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[45] Interestingly, note that when for long times we expect $\hat{\rho}_{\mathrm{A,I}}(t)$ to reach a stationary state, this approximation becomes exact for any finite decay rate of $C(\tau)$. Hence, even in situations where the Markov approximation is not valid for the dynamics, one can still use it to derive a reduced steady-state equation for stationary state of the system.

[46] Given a function $f(x)$ that diverges at some point x_0 (trivially extensible to multiple poles), the Cauchy principal value of the integral $\int_a^b dx f(x)$ with $a < x_0 < b$ is defined as $\mathcal{P}\int_{\mathbb{R}} dx f(x) = \lim_{\epsilon\to 0}\left[\int_a^{x_0-\epsilon} dx f(x) + \int_{x_0+\epsilon}^b dx f(x)\right]$. In other words, we perform the integral, but skipping the poles.

coupling, $G(\omega) = \gamma/\pi$, and introducing a cutoff in the integral up to some frequency $\varepsilon + \Lambda$ that we will choose later. We then obtain

$$\Delta\varepsilon = -\frac{\gamma}{\pi}\lim_{\epsilon\to 0}\left[\int_0^{\varepsilon-\epsilon}\frac{d\omega}{\omega-\varepsilon}+\int_{\varepsilon+\epsilon}^{\varepsilon+\Lambda}\frac{d\omega}{\omega-\varepsilon}\right] = -\frac{\gamma}{\pi}\lim_{\epsilon\to 0}\underbrace{[\log(-\epsilon)-\log(-\varepsilon)+\log(\Lambda)-\log(\epsilon)]}_{\log(\Lambda/\varepsilon)} = -\frac{\gamma}{\pi}\log\frac{\Lambda}{\varepsilon}. \tag{462}$$

Hence, we find a logarithmic divergence, which suggests that the Lamb shift is of the same order as the decay rate γ. Indeed, let us consider physical cutoffs. Of course, $\Lambda \gg \varepsilon$. However, it feels that taking a cutoff beyond the energies where electron-positron pair production makes little sense, which is on the order of 1MeV. On the other hand, we can estimate the transition frequency of the atom by considering, for example, the one between the two lowest lying energy eigenstates of Hydrogen that we discussed in Chapter III A. We obtain a transition on the order of the Rydberg energy, which means 13eV. Hence, in this situation we obtain $\pi^{-1}\log(\Lambda/\varepsilon) \sim 3.5$. Even for transitions between hyperfine levels (usually on the order of 10^{-6} times that of between states with different principal atomic quantum number), the logarithmic dependence would still keep this number on a similar order of magnitude. Hence, our rough estimation tells us that the Lamb shift and the decay rate are on the same order, which is indeed in agreement with experimental observations. Note, however, that while the decay rate is easy to spot (just wait for the atom to decay!), the Lamb shift is a tiny correction to the transition frequency ε, and requires very well designed and sensitive experiments to measure it.

Let us finally prove (459)... **soon**.

VI. ANALYZING THE EMISSION FROM OPEN SYSTEMS

In the previous chapter we have introduced the model for two prototypical open quantum optical systems: open cavities and radiating atoms. The tools develop there allowed us to evaluate the state (mixed, in general) of the cavity modes and the atoms. However, usually one is more interested in the properties of the light radiated by these systems, since this is the one that we can measure easily and use for applications. This chapter is devoted to this issue. We will first learn how to easily relate the field coming out of the system (cavity or atom) with system operators that we know how to characterize via the master or quantum Langevin equations. Next we will comment on the usual way in which this output field is measured and characterized through specific observables and correlation functions with strong physical meaning.

A. Output fields

1. *The output field from a cavity*

Let us start by discussing the output field associated with one mode of an open cavity. It is convenient to work in the Heisenberg picture for the upcoming calculations. Using the expression of the vector potential outside the resonator (333), we see that the part of the field coming out from the cavity (hence propagating along the positive z direction) can be written as

$$\hat{\mathbf{A}}^{(+)}_{\rm out}(z,t) = -\mathrm{i}\mathbf{e}_x \int_0^\infty d\omega \sqrt{\frac{\hbar}{4\pi c\varepsilon_0 S\omega}}\hat{b}(\omega;t)e^{\mathrm{i}\omega(z-L)/c}, \tag{463}$$

where the operator $\hat{b}(\omega;t)$ is given by (339) in terms of the initial operators $\hat{b}_0(\omega)$ and the intracavity mode $\hat{a}$. Now, given that only the frequencies around the cavity resonance contribute to the dynamics as we argued all along the notes, we can replace the slowly varying function of the frequency $1/\sqrt{\omega}$ by its value at $\omega_{\rm c}$, as well as extending the lower integration limit to $-\infty$, arriving to

$$\hat{\mathbf{A}}^{(+)}_{\rm out}(z,t) = -\mathrm{i}\mathbf{e}_x \sqrt{\frac{\hbar}{4\pi c\varepsilon_0 S\omega_{\rm c}}} \int_{-\infty}^\infty d\omega \hat{b}(\omega;t)e^{\mathrm{i}\omega(z-L)/c}. \tag{464}$$

Introducing the solution (339) for $\hat{b}(\omega;t)$ in this equation and defining the *retarded time* $t_R = t-(z-L)/c$, we can write the output field as

$$\hat{\mathbf{A}}^{(+)}_{\rm out}(z,t) = -\mathrm{i}\mathbf{e}_x \sqrt{\frac{\hbar}{4\pi c\varepsilon_0 S\omega_{\rm c}}} \left[\underbrace{\int_{-\infty}^\infty d\omega \hat{b}_0(\omega)e^{-\mathrm{i}\omega t_R}}_{-\sqrt{2\pi}\hat{a}_{\rm in}(t_R)} + \sqrt{\frac{\gamma}{\pi}}\int_0^t dt'\hat{a}(t') \underbrace{\int_{-\infty}^\infty d\omega e^{\mathrm{i}\omega(t'-t_R)}}_{2\pi\delta(t'-t_R)} \right] = -\mathrm{i}\mathbf{e}_x \sqrt{\frac{\hbar}{2c\varepsilon_0 S\omega_{\rm c}}}\hat{b}_{\rm out}(t_R), \tag{465}$$

where we have defined the *output operator*

$$\hat{b}_{\rm out}(t) = \sqrt{2\gamma}\hat{a}(t) - \hat{b}_{\rm in}(t). \tag{466}$$

The field coming out from the cavity is therefore a superposition of the intracavity field leaking through the partially transmitting mirror and the part of the input field which is reflected, just as expected by the classical boundary conditions at the mirror (Fresnel relations), see Fig. 15. In this context, we denote (466) by the *input-output relation*.

A note on the interpretation of $\hat{n}_{\rm out}(t) = \hat{b}^\dagger_{\rm out}(t)\hat{b}_{\rm out}(t)$. It is not difficult to show that the power coming out of the cavity is essentially given by $\hbar\omega_{\rm c}\langle\hat{n}_{\rm out}(t)\rangle$. Hence, we can interpret $\hat{n}_{\rm out}(t)$ as the operator associated to the number of photons per unit time that come out of the cavity. Indeed, we will show in the next section that the output annihilation and creation operators satisfy canonical commutation relations in time, that is,

$$[\hat{b}_{\rm out}(t),\hat{b}^\dagger_{\rm out}(t')] = \delta(t-t'), \qquad [\hat{b}_{\rm out}(t),\hat{b}_{\rm out}(t')] = 0, \tag{467}$$

reinforcing the interpretation of $\hat{n}_{\rm out}(t)$ as a number operator per unit time. Note that, similarly, we could interpret $\hat{n}_{\rm in}(t) = \hat{b}^\dagger_{\rm in}(t)\hat{b}_{\rm in}(t)$ as the operator associated to the number of photons per unit time impinging the cavity.

2. Alternative form of the output operator and causality

Let us now find an alternative form for the output operator, one that will allow us to prove that the output operators satisfy the canonical commutation relations in time of Eq. (484), as well as proving that this theory of inputs and outputs satisfies the expected causality

$$[\hat{c}(t), \hat{b}_{\rm in}(t')] = 0 \quad \text{if } t' > t, \tag{468a}$$

$$[\hat{c}(t), \hat{b}_{\rm out}(t')] = 0 \quad \text{if } t' < t, \tag{468b}$$

where $\hat{c}(t)$ is any intracavity operator. These simply state that the physics inside the cavity cannot depend on a future input that hasn't yet arrived, while the output cannot depend on intracavity processes yet to come. This will turn out to be very relevant when discussing the detection and characterization of the output field later.

We start by solving again formally the Heisenberg equation (338b) for the external operators $\hat{b}(\omega;t)$, but now in terms of a final condition $\hat{b}(\omega;T) \equiv \hat{b}_T(\omega)$ at some long time $T > t$ (backwards integration). Using (251) we easily obtain

$$\hat{b}(\omega;t) = \hat{b}_T(\omega)e^{-{\rm i}\omega(t-T)} - \sqrt{\frac{\gamma}{\pi}}\int_t^T dt'\hat{a}(t')e^{-{\rm i}\omega(t-t')}. \tag{469}$$

Performing a frequency integral, we obtain

$$\int_{-\infty}^{+\infty} d\omega\hat{b}(\omega;t) = \int_{-\infty}^{+\infty} d\omega\hat{b}_T(\omega)e^{-{\rm i}\omega(t-T)} - \sqrt{\frac{\gamma}{\pi}}\int_t^T dt'\hat{a}(t')\underbrace{\int_{-\infty}^{+\infty} d\omega e^{{\rm i}\omega(t'-t)}}_{2\pi\delta(t'-t)} = \int_{-\infty}^{+\infty} d\omega\hat{b}_T(\omega)e^{-{\rm i}\omega(t-T)} - \sqrt{\gamma\pi}\hat{a}(t). \tag{470}$$

On the other hand, using the formal solution (339) in terms of the initial condition $\hat{b}(\omega;0) = \hat{b}_0(\omega)$ at time $0 < t$ (forward integration), we obtain

$$\int_{-\infty}^{+\infty} d\omega\hat{b}(\omega;t) = \underbrace{\int_{-\infty}^{+\infty} d\omega\hat{b}_0(\omega)e^{-{\rm i}\omega t}}_{-\sqrt{2\pi}\hat{b}_{\rm in}(t)} + \sqrt{\frac{\gamma}{\pi}}\int_0^t dt'\hat{a}(t')\underbrace{\int_{-\infty}^{+\infty} d\omega e^{{\rm i}\omega(t'-t)}}_{2\pi\delta(t'-t)} = -\sqrt{2\pi}\hat{b}_{\rm in}(t) + \sqrt{\gamma\pi}\hat{a}(t). \tag{471}$$

Combining Eqs. (470) and (471), we obtain

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} d\omega\hat{b}_T(\omega)e^{-{\rm i}\omega(t-T)} = \sqrt{2\gamma}\hat{a}(t) - \hat{b}_{\rm in}(t). \tag{472}$$

Thus, comparing this equation with (466), we obtain an alternative form of the output operator

$$\hat{b}_{\rm out}(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} d\omega\hat{b}_T(\omega)e^{-{\rm i}\omega(t-T)}, \tag{473}$$

in terms of the external field at a later time T. This allows us to prove the canonical commutation relations in time of Eq. (484) in a straightforward manner, simply using the equal-time canonical commutation relations in frequency of the external bosonic operators, particularized to the final time, that is, $[\hat{b}_T(\omega), \hat{b}_T^\dagger(\omega')] = \delta(\omega-\omega')$ and $[\hat{b}_T(\omega), \hat{b}_T(\omega')] = 0$.

In order to discuss causality, it is interesting to write the quantum Langevin equation for the intracavity operator in terms of the output operator. To this aim, we simply insert $\hat{b}_{\rm in}(t) = \sqrt{2\gamma}\hat{a}(t) - \hat{b}_{\rm out}(t)$ in the quantum Langevin equation (344), leading to

$$\partial_t\hat{a} = (\gamma - {\rm i}\omega_{\rm c})\,\hat{a} - \sqrt{2\gamma}\hat{b}_{\rm out}(t), \tag{474}$$

where it is interesting to note that the damping term $-\gamma\hat{a}$ has turned into an amplification term $\gamma\hat{a}$. This is natural once we realize that, for consistency with (469), this equation must be solved backwards in time starting from a final condition $\hat{a}(T)$. It is then common to call (357) and (474) the *forward* and *backwards quantum Langevin equations*, respectively.

With this at hand, we are in conditions to talk about causality in this *input-output theory*. In particular, note that since the quantum Langevin equations are local in time, intracavity operators can only depend on $\hat{b}_{\rm in}(t')$ at times $t' \leq t$, and on $\hat{b}_{\rm out}(t')$ at times $t' \geq t$. Hence, since both the input and output operators commute at different times, we see that a generic intracavity operator $\hat{c}(t)$, which is therefore a function of $\hat{a}(t)$ and $\hat{a}^\dagger(t)$, commutes with $\hat{b}_{\rm in}(t')$ for $t' > t$, and with $\hat{b}_{\rm out}(t')$ when $t' < t$. This proves Eqs. (468).

We can go even further, noting that when $t' > t$ we can use the *input-output relation* to write $[\hat{c}(t), \hat{b}_{\rm out}(t')] = [\hat{c}(t), \sqrt{2\gamma}\hat{a}(t') - \hat{b}_{\rm in}(t')] = \sqrt{2\gamma}[\hat{c}(t), \hat{a}(t')]$. Similarly, when $t' < t$ we have $[\hat{c}(t), \hat{b}_{\rm in}(t')] = [\hat{c}(t), \sqrt{2\gamma}\hat{a}(t') - \hat{b}_{\rm out}(t')] = \sqrt{2\gamma}[\hat{c}(t), \hat{a}(t')]$. In addition, when $t' = t$ we simply use (471), together with the fact that external operators commute with intracavity operators at equal times, obtaining $[\hat{c}(t), \hat{b}_{\rm in}(t)] = \sqrt{\gamma/2}[\hat{c}(t), \hat{a}(t)] - \int_{-\infty}^{+\infty} d\omega [\hat{c}(t), \hat{b}(\omega; t)]/\sqrt{2\pi} = \sqrt{\gamma/2}[\hat{c}(t), \hat{a}(t)]$. And then, using the input-output relation (466), $[\hat{c}(t), \hat{b}_{\rm out}(t)] = \sqrt{2\gamma}[\hat{c}(t), \hat{a}(t)] - [\hat{c}(t), \hat{b}_{\rm in}(t)] = \sqrt{\gamma/2}[\hat{c}(t), \hat{a}(t)]$. Putting everything together, we can rewrite all commutators in terms of intracavity operators only,

$$[\hat{c}(t), \hat{a}_{\rm in}(t')] = \begin{cases} \sqrt{2\gamma}[\hat{c}(t), \hat{a}(t')] & \text{for } t > t' \\ \sqrt{\gamma/2}[\hat{c}(t), \hat{a}(t)] & \text{for } t = t' \\ 0 & \text{for } t < t' \end{cases}, \tag{475}$$

and

$$[\hat{c}(t), \hat{a}_{\rm out}(t')] = \begin{cases} 0 & \text{for } t > t' \\ \sqrt{\gamma/2}[\hat{c}(t), \hat{a}(t)] & \text{for } t = t' \\ \sqrt{2\gamma}[\hat{c}(t), \hat{a}(t')] & \text{for } t \leq t' \end{cases}. \tag{476}$$

3. *The output field radiated by an atom*

Let us now do a similar procedure for the field radiated by a two-level atom. In this case, there is a subtlety related to the fact that the atom radiates in all directions, whereas the cavity emits radiation along a well defined optical axis defined by the partially transmitting mirror. Usually, one doesn't have access to all this emitted light, but only to part of it (this is evident in 3D, we cannot put detectors filling the whole space!). In our 1D model, we then assume that we have access only to light radiated towards the right (this will allow us to understand the effect that missing part of the emitted has on the detection), whose corresponding electric field we can write, using (430), as

$$\hat{\mathbf{E}}^{(+)}_{\rm out}(z,t) = \mathrm{i}\mathbf{e}_x \int_0^{+\infty} dk \sqrt{\frac{\hbar c k}{4\pi\varepsilon_0 S}} \hat{a}(k,t) e^{\mathrm{i}kz} \approx \mathrm{i}\mathbf{e}_x \sqrt{\frac{\hbar\varepsilon}{4\pi\varepsilon_0 S}} \int_0^{+\infty} dk \hat{a}(k,t) e^{\mathrm{i}kz}, \tag{477}$$

where we have again used the fact that $\sqrt{ck}$ is a slowly varying function of k, so we can approximate it by its value $\sqrt{\varepsilon}$ at the atomic resonance ε. Following the same procedure as with the field coming out of the cavity, we next use the Heisenberg equations of motion of the field operators to relate $\hat{a}(k,t)$ with the fields at the initial time $\hat{a}(k,0)$, and with the atomic operator $\hat{\sigma}(t)$. Reminding the Hamiltonians of the field and the atom-field interaction, (429) and (433), respectively, we obtain (for $k > 0$)

$$\partial_t \hat{a}(k) = -\mathrm{i}ck a(k) + \sqrt{\frac{\gamma c}{2\pi}} \hat{\sigma} \quad \Rightarrow \quad \hat{a}(k,t) = \hat{a}_0(k) e^{-\mathrm{i}ckt} + \sqrt{\frac{\gamma c}{2\pi}} \int_0^t dt' e^{\mathrm{i}ck(t'-t)} \hat{\sigma}(t'), \tag{478}$$

where we have made the frequency-independent approximation for the atom-field coupling and defined $\hat{a}_0(k) = \hat{a}(k,0)$, the annihilation operators at the initial time. Introducing this in the radiated field (477) we obtain

$$\hat{\mathbf{E}}^{(+)}_{\rm out}(z,t) = \mathrm{i}\mathbf{e}_x \sqrt{\frac{\hbar\varepsilon}{4\pi\varepsilon_0 S}} \int_0^{+\infty} dk \left[\hat{a}_0(k) e^{-\mathrm{i}ckt_R} + \sqrt{\frac{\gamma c}{2\pi}} \int_0^t dt' e^{\mathrm{i}ck(t'-t_R)} \hat{\sigma}(t') \right]. \tag{479}$$

Next we perform the same approximations as before. First, we extend the lower integration limit to $-\infty$, understanding that the negative values of k do not refer to modes propagating to the left, but to fictitious modes with negative frequency propagating to the right. As usual, this is a convenient mathematical trick which does not affect the physics because only modes with frequencies around the atomic transition contribute. Defining the input operator

$$\hat{b}_{\rm in}(t) = -\sqrt{\frac{c}{2\pi}} \int_{-\infty}^{+\infty} dk \hat{a}_0(k) e^{-\mathrm{i}ckt}, \tag{480}$$

which, just as the one defined for the open cavity, satisfies canonical commutation relations in time (343) and the statistical properties (356) for thermal fields, we then obtain

$$\hat{\mathbf{E}}^{(+)}_{\rm out}(z,t) = \mathrm{i}\mathbf{e}_x\sqrt{\frac{\hbar\varepsilon}{4\pi\varepsilon_0 S}}\Bigg[\underbrace{\int_{-\infty}^{+\infty} dk\hat{a}_0(k)e^{-\mathrm{i}ckt_R}}_{-\sqrt{2\pi/c}\hat{a}_{\rm in}(t_R)} + \sqrt{\frac{\gamma c}{2\pi}}\int_0^t dt'\hat{\sigma}(t')\underbrace{\int_{-\infty}^{+\infty} dke^{\mathrm{i}ck(t'-t_R)}}_{2\pi\delta(t'-t_R)/c}\Bigg] = \mathrm{i}\mathbf{e}_x\sqrt{\frac{\hbar\varepsilon}{2c\varepsilon_0 S}}\hat{b}_{\rm out}(t_R), \quad (481)$$

with

$$\hat{b}_{\rm out}(t) = \sqrt{\gamma}\hat{\sigma}(t) - \hat{b}_{\rm in}(t). \quad (482)$$

This result is similar to the one for the field leaking out of the cavity except for one subtle issue: while in both cases γ denotes the damping rate appearing in master or quantum Langevin equations, in the case of the cavity we have a $\sqrt{2\gamma}\hat{a}$ contribution to the output field, see (466), while in the case of the atom we have $\sqrt{\gamma}\hat{\sigma}$. This $\sqrt{2}$ mismatch comes from the fact that we are considering only half of the radiation emitted by the atom, so this output operator contains only half of the field lost from the atom. This can have enormous consequences for the detection and use of certain quantum properties of the output field, as we shall see.

B. Observing the output: photodetection, correlation functions, and the quantum regression theorem

1. *Photodetection and correlation functions*

Let us now move on to the characterization of the output field. The traditional way of analyzing optical fields is by using photodetectors, whose principle of action we pass to describe now. As we will see with the example of homodyne detection later, any other measurement technique aimed at characterizing optical fields makes use of photodetectors in one way or another.

Photodetection is based on the photoelectric effect or variations of it, see Fig. **ToDo**. The idea is that when the light beam that we want to detect impinges the detector, photons are able to release some of its bound electrons, which are accelerated towards a series of metallic plates at increasing positive voltages, releasing then more electrons which contribute to generate a measurable electric pulse. Each photon is then capable of releasing one electron which eventually produces a single pulse, named *photopulse*. The combination of all the generated photopulses leads to a macroscopic current $j(t)$, which is a classical random[47] signal that we can monitor and process.

Though not trivially (see [5, 60] and references therein), when measuring the field radiated by an open system, it is possible to show that the moments of this current are related to moments of the number operator $\hat{n}_{\rm out}(t) = \hat{b}^\dagger_{\rm out}(t)\hat{b}_{\rm out}(t)$ by

$$\overline{j(t_1)j(t_2)...j(t_N)} \propto \langle :\hat{n}_{\rm out}(t_1)\hat{n}_{\rm out}(t_2)...\hat{n}_{\rm out}(t_N):\rangle, \quad (483)$$

where the double dots denote normal ordering[48] of the operators. Hence, the quantum statistics of the number of photons coming out of the system per unit time are imprinted in the stochastic fluctuations of the photocurrent.

Let us for the upcoming discussions introduce a nomenclature that will gather the open cavity and radiating atom. We will refer to the cavity mode or the atom as the *system*. We will introduce an operator $\hat{s}$ which will denote the annihilation operator $\hat{a}$ or the raising operator $\hat{\sigma}$ depending on the context. On the other hand, we will call *environment* to the field outside the cavity and the field surrounding the atom, and we will introduce a rate κ which equals 2γ for the cavity case and γ for the atomic case, so that the input-output relation takes the general form

$$\hat{b}_{\rm out}(t) = \sqrt{\kappa}\hat{s}(t) - \hat{b}_{\rm in}. \quad (484)$$

Moreover, for reasons that will be obvious shortly, it is convenient to work with an output operator from which we remove the coherent part of the input operator, that is,

$$\hat{a}_{\rm out}(t) = \sqrt{\kappa}\hat{s}(t) - \hat{a}_{\rm in} = \hat{b}_{\rm out}(t) + \langle\hat{b}_{\rm in}(t)\rangle. \quad (485)$$

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[47] It is random, because the exact number of electrons ripped out during the amplification stage, as well as the exact time when the photoelectron and photopulse are generated, are all random, in the sense that fluctuate from realization to realization.

[48] Annihilation operators are moved to the right and creation operators to the left as if they would commute. For example, $\langle :\hat{n}_{\rm out}(t_1)\hat{n}_{\rm out}(t_2):\rangle = \langle\hat{b}^\dagger_{\rm out}(t_1)\hat{b}^\dagger_{\rm out}(t_2)\hat{b}_{\rm out}(t_2)\hat{b}_{\rm out}(t_1)\rangle$.

Making use of lasers mixed with the output field and several detectors, it is then clear that the most general quantity that we can observe takes the form

$$G_{\rm out}^{(N,M)}(t_1,t_2,...,t_{N+M})=\langle \hat{a}_{\rm out}^\dagger(t_1)\hat{a}_{\rm out}^\dagger(t_2)...\hat{a}_{\rm out}^\dagger(t_N)\hat{a}_{\rm out}(t_{N+1})...\hat{a}_{\rm out}(t_{N+M-1})\hat{a}_{\rm out}(t_{N+M})\rangle. \tag{486}$$

We call these the *field correlation functions*, which were introduced by Glauber in his seminal 1963 papers [63–65] in order to produce a definitive quantum-mechanical explanation of the coherence properties of lasers, masers, and thermal sources (the last ones corresponding to the famous experiments of Hanbury-Brown and Twiss [69]). Without loss of generality, we can assume time-ordering in this expression, that is, $t_1<t_2<...<t_{N-1}$ and $t_{N+M}<t_{N+M-1}<...<t_{N+1}$, because output operators at different times commute. This will turn out to be very useful for reasons that we explain next.

Note that, while we have defined correlation functions in terms of the output operator because it is the one usually measured, the dynamics is usually solved for operators of the system by using the master or quantum Langevin equations. Hence, it is interesting to rewrite the correlation functions in terms of system operators. In general, the best we can do is using (485) to write $G_{\rm out}^{(N)}(t_1,t_2,...,t_{2N})$ in terms of correlation functions of system and input operators. However, in the particular case in which the environment is at zero temperature, this connection is straightforward. In particular, reminding that $[\hat{s}(t),\hat{a}_{\rm in}(t')]=0$ when $t<t'$ (causality) and that operators are time ordered, we can bring all the input annihilation operators to the right and input creation operators to the left, and annihilate vacuum, so that the only remaining correlation function is the one involving system operators,

$$G^{(N,M)}(t_1,t_2,...,t_{N+M})=\langle \hat{s}^\dagger(t_1)\hat{s}^\dagger(t_2)...\hat{s}^\dagger(t_N)\hat{s}(t_{N+1})...\hat{s}(t_{N+M-1})\hat{s}(t_{N+M})\rangle, \tag{487}$$

and we obtain

$$G_{\rm out}^{(N,M)}(t_1,t_2,...,t_{N+M})=\kappa^{(N+M)/2}G^{(N,M)}(t_1,t_2,...,t_{N+M}). \tag{488}$$

Finally, it is interesting to consider normalized versions of the correlation functions. In particular, given the interpretation of $\hat{n}_{\rm out}(t)$ as the number of output photons per unit time, it is obvious that the absolute value of a given correlation function will be larger the larger the emission of the system is, as we will see through specific examples. Hence, in order to compare the properties of sources that emit at different rates, we introduce

$$g_{\rm out}^{(N)}(t_1,t_2,...,t_{2N})=\frac{G_{\rm out}^{(N,N)}(t_1,t_2,...,t_{2N})}{\sqrt{G_{\rm out}^{(1,1)}(t_1,t_1)G_{\rm out}^{(1,1)}(t_2,t_2)...G_{\rm out}^{(1,1)}(t_{2N},t_{2N})}}. \tag{489}$$

Of course, we can also define the same type of normalized correlation function for the system

$$g^{(N)}(t_1,t_2,...,t_{2N})=\frac{G^{(N,N)}(t_1,t_2,...,t_{2N})}{\sqrt{G^{(1,1)}(t_1,t_1)G^{(1,1)}(t_2,t_2)...G^{(1,1)}(t_{2N},t_{2N})}}. \tag{490}$$

Note that whenever (488) holds, these two normalized correlation functions coincide. Note also that $G_{\rm out}^{(1)}(t,t)=\langle\hat{n}_{\rm out}(t)\rangle$ is nothing but the average photon number radiated per unit time, and hence the normalization factors simply help bringing to the same value correlation functions of sources with different emission rates but same qualitative properties otherwise. For example, we shall see shortly that systems emitting coherent light will all have $g_{\rm out}^{(N)}=1$, irrespective of how much light they emit.

2. *Quantum regression theorem*

Let us now focus on the correlation functions of the system (487). In particular, we consider two-time correlators of various types, which are the most important for our purposes and in typical experiments, as we will see. Given three system operators $\{\hat{A},\hat{B},\hat{C}\}$, we will focus on the correlation function $\langle\hat{A}(t)\hat{B}(t')\hat{C}(t)\rangle$. The aim of this section is to relate this Heisenberg picture expression to a Schrödinger picture one. This is known as the *quantum regression theorem*, and, while it might sound like a trivial exercise, we will see that it provides a route towards efficient and simple ways towards the evaluation of such correlation functions, as well as towards their interpretation.

In order to make the notation lighter, we will not make an explicit distinction between Heisenberg or Schrödinger operators, instead the picture will be evident from the time dependence of the operators: time-dependent states must be understood as Schrödinger picture, while time-independent ones as Heisenberg picture; similarly, operators (other than the state) must be understood as Heisenberg picture or Schrödinger picture depending on whether they are explicitly time dependent or not, respectively.

With this in mind, consider an open system evolving according to a master equation with a general time-dependent Lindbladian $\mathcal{L}^{(t)}$, where we denote the time-dependence as a superscript for later convenience. The quantum regression theorem reads then

$$\langle \hat{A}(t)\hat{B}(t+\tau)\hat{C}(t)\rangle = \mathrm{tr}\left\{\hat{B}\mathcal{U}^{(\tau)}[\hat{C}\hat{\rho}(t)\hat{A}]\right\}, \tag{491}$$

where

$$\mathcal{U}^{(\tau)} = 1 + \sum_{n=1}^{\infty}\frac{1}{(\mathrm{i}\hbar)^n}\int_0^{\tau} dt_1 \int_0^{t_1} dt_2 ... \int_0^{t_{n-1}} dt_n \mathcal{L}^{(t_1)}\mathcal{L}^{(t_2)}...\mathcal{L}^{(t_n)} = \mathcal{T}\left\{e^{\int_0^{\tau} dt\mathcal{L}^{(t)}}\right\}, \tag{492}$$

is the time-evolution superoperator associated to the master evolution induced by the master equation, and $\mathcal{T}$ is the time-ordering symbol, which in this case orders superoperators in chronological order

$$\mathcal{T}\left\{\mathcal{L}^{(t)}\mathcal{L}^{(t')}\right\} = \begin{cases} \mathcal{L}^{(t)}\mathcal{L}^{(t')} & \text{for } t > t' \\ \mathcal{L}^{(t')}\mathcal{L}^{(t)} & \text{for } t < t' \end{cases}. \tag{493}$$

Note that in the case of a time-independent Lindbladian, the time-evolution superoperator simply reads

$$\mathcal{U}^{(\tau)} = e^{\mathcal{L}\tau}. \tag{494}$$

The quantum regression theorem is very suggestive, and allows for an interesting interpretation of the two-time correlation function: at time t, operators $\hat{C}$ and $\hat{A}$ effect a change on the state, which then evolves for a time τ; this leads to an unnormalized state, which we then use to evaluate the expectation value of $\hat{B}$.

Before we prove the theorem, it is important to remark that the quantum regression theorem can be adapted to any intermediate picture we choose to work on. That is, if we work in a picture defined by some unitary transformation $\hat{U}_{\mathrm{c}}(t)$, where the transformed state $\hat{\rho}_{\mathrm{I}}(t) = \hat{U}_{\mathrm{c}}^{\dagger}(t)\hat{\rho}(t)\hat{U}_{\mathrm{c}}(t)$ evolves according to a master equation $\partial_t\hat{\rho}_{\mathrm{I}} = \mathcal{L}_{\mathrm{I}}^{(t)}[\hat{\rho}_{\mathrm{I}}]$, with $\mathcal{L}_{\mathrm{I}}^{(t)}$ obtained from $\mathcal{L}^{(t)}$ as explained in Section V A 6, we can turn () into

$$\langle \hat{A}(t)\hat{B}(t+\tau)\hat{C}(t)\rangle = \mathrm{tr}\left\{\hat{B}_{\mathrm{I}}\mathcal{U}_{\mathrm{I}}^{(\tau)}[\hat{C}_{\mathrm{I}}\hat{\rho}_{\mathrm{I}}(t)\hat{A}_{\mathrm{I}}]\right\}, \tag{495}$$

where $\hat{A}_{\mathrm{I}}(t) = \hat{U}_{\mathrm{c}}^{\dagger}(t)\hat{A}\hat{U}_{\mathrm{c}}(t)$ is an intermediate-picture operator (similarly for $\hat{B}$ and $\hat{C}$), and $\mathcal{U}_{\mathrm{I}}^{(\tau)} = \mathcal{T}\left\{e^{\int_0^{\tau} dt\mathcal{L}_{\mathrm{I}}^{(t)}}\right\}$. This is a useful expression, as it allows us to evaluate the correlation function in the most convenient picture, for example, one in which the Lindbladian is time-independent, and the system reaches a time-independent (stationary) asymptotic state $\lim_{t\to\infty}\hat{\rho}_{\mathrm{I}}(t) = \bar{\rho}_{\mathrm{I}}$. Under such circumstances, we obtained the steady-state correlation functions

$$\lim_{t\to\infty}\langle \hat{A}(t)\hat{B}(t+\tau)\hat{C}(t)\rangle = \mathrm{tr}\left\{\hat{B}_{\mathrm{I}}e^{\mathcal{L}_{\mathrm{I}}\tau}[\hat{C}_{\mathrm{I}}\bar{\rho}_{\mathrm{I}}\hat{A}_{\mathrm{I}}]\right\}, \tag{496}$$

which will be the expression that we will use the most, since this is the typical object that experiments are interested in.

Let us now pass to prove the quantum regression theorem. In order to do this, let us introduce some notation. First, we denote the time-evolution operator of the whole universe (system and environment) by $\hat{U}_{\mathrm{SE}}(t)$. Similarly, we denote by $\hat{\rho}_{\mathrm{SE}}$ the state of the whole universe, while $\hat{\rho}_{\mathrm{E}}$ is the reduced state of the environment (taken as a thermal state within the Born approximation in our examples), leaving the name $\hat{\rho}$ for the state of the system. Consequently, we will denote the trace over the whole universe by $\mathrm{tr}_{\mathrm{SE}}$, over the environment by tr_{E}, and over the system simply by tr. Consider then an operator $\hat{W}$ acting on the whole universe. Within the framework introduced in the previous chapter (Born-Markov, non-backaction, and Markov approximations), it is clear that we can make the following approximation for the reduced dynamics

$$\mathrm{tr}_{\mathrm{E}}\left\{\hat{U}_{\mathrm{SE}}(\tau)\hat{W}\hat{U}_{\mathrm{SE}}^{\dagger}(\tau)\right\} = \mathcal{U}^{(\tau)}[\mathrm{tr}_{\mathrm{E}}\{\hat{W}\}], \tag{497}$$

which is just the integral form of the master equation. Keeping this in mind, it is then straightforward to prove the quantum regression theorem as

$$\begin{aligned}\langle \hat{A}(t)\hat{B}(t+\tau)\hat{C}(t)\rangle &= \mathrm{tr}_{\mathrm{SE}}\left\{\hat{\rho}_{\mathrm{SE}}\hat{U}_{\mathrm{SE}}^{\dagger}(t)\hat{A}\hat{U}_{\mathrm{SE}}(t)\hat{U}_{\mathrm{SE}}^{\dagger}(t+\tau)\hat{B}\hat{U}_{\mathrm{SE}}(t+\tau)\hat{U}_{\mathrm{SE}}^{\dagger}(t)\hat{C}\hat{U}_{\mathrm{SE}}(t)\right\} \\ &= \mathrm{tr}_{\mathrm{SE}}\left\{\hat{B}\hat{U}_{\mathrm{SE}}(\tau)\hat{C}\hat{\rho}_{\mathrm{SE}}(t)\hat{A}\hat{U}_{\mathrm{SE}}^{\dagger}(\tau)\right\} \approx \mathrm{tr}\left\{\hat{B}\mathcal{U}^{(\tau)}[\mathrm{tr}_{\mathrm{E}}\{\hat{C}\hat{\rho}_{\mathrm{SE}}(t)\hat{A}\}]\right\},\end{aligned} \tag{498}$$

where in the first step we just written the Heisenberg evolution of the operators explicitly, in the second step we have used the cyclic property of the trace and the composition property of the time-evolution operator, $\hat{U}^\dagger_{\rm SE}(t_2)\hat{U}_{\rm SE}(t_1) = \hat{U}^\dagger_{\rm SE}(t_2-t_1)$, and in the final step we have applied (497). The proof is completed by noting that $\mathrm{tr}_{\rm E}\{\hat{C}\hat{\rho}_{\rm SE}(t)\hat{A}\} = \hat{C}\mathrm{tr}_{\rm E}\{\hat{\rho}_{\rm SE}(t)\}\hat{A} = \hat{C}\hat{\rho}(t)\hat{A}$, since $\hat{A}$ and $\hat{C}$ act as the identity on the Hilbert space of the environment (hence, $\hat{A}\otimes\hat{I}$ would be a more rigorous notation, which we avoid when there is no room for confusion). This is easily proven by representing the state in a basis $\{|e^{\rm S}_m\rangle\otimes|e^{\rm E}_n\rangle\}^{n=1,...,d_{\rm E}}_{m=1,...,d_{\rm S}}$ of the full universe

$$\begin{aligned}\mathrm{tr}_{\rm E}\{\hat{C}\hat{\rho}_{\rm SE}(t)\hat{A}\} &= \mathrm{tr}_{\rm E}\left\{\hat{C}\otimes\hat{I}\left(\sum_{mm'=1}^{d_{\rm S}}\sum_{nn'=1}^{d_{\rm E}}\rho_{mm';nn'}(t)|e^{\rm S}_m\rangle\langle e^{\rm S}_{m'}|\otimes|e^{\rm E}_n\rangle\langle e^{\rm E}_{n'}|\right)\hat{A}\otimes\hat{I}\right\} \\ &\mathrm{tr}_{\rm E}\left\{\left(\sum_{mm'=1}^{d_{\rm S}}\sum_{nn'=1}^{d_{\rm E}}\rho_{mm';nn'}(t)\hat{C}|e^{\rm S}_m\rangle\langle e^{\rm S}_{m'}|\hat{A}\otimes|e^{\rm E}_n\rangle\langle e^{\rm E}_{n'}|\right)\right\} \\ &= \sum_{mm'=1}^{d_{\rm S}}\sum_{lnn'=1}^{d_{\rm E}}\rho_{mm';nn'}(t)\hat{C}|e^{\rm S}_m\rangle\langle e^{\rm S}_{m'}|\hat{A}\underbrace{\langle e^{\rm E}_l|e^{\rm E}_n\rangle}_{\delta_{ln}}\underbrace{\langle e^{\rm E}_{n'}|e^{\rm E}_l\rangle}_{\delta_{ln'}} \\ &= \hat{C}\underbrace{\left[\sum_{mm'=1}^{d_{\rm S}}\left(\sum_{l=1}^{d_{\rm E}}\rho_{mm';ll'}(t)\right)|e^{\rm S}_m\rangle\langle e^{\rm S}_{m'}|\right]}_{\mathrm{tr}_{\rm E}\{\hat{\rho}_{\rm SE}(t)\}}\hat{A}.\end{aligned} \tag{499}$$

As a final remark, note that this proof and the quantum regression theorem can be generalized to higher-order correlators with not too much effort. In particular, it's easy to prove, along the lines of the proof in Eqs. (498), the following connection between multi-time correlation functions in the Heisenberg and Shcrödinger pictures

$$\begin{aligned}&\langle\hat{A}_0(t_0)\hat{A}_1(t_1)...\hat{A}_n(t_n)\hat{C}_n(t_n)...\hat{C}_1(t_1)\hat{C}_0(t_0)\rangle \\ &\qquad = \mathrm{tr}\left\{\hat{A}_n\hat{C}_n\mathcal{U}^{(t_n-t_{n-1})}\left[\hat{C}_{n-1}\mathcal{U}^{(t_{n-1}-t_{n-2})}\left[...\hat{C}_1\mathcal{U}^{(t_1-t_0)}\left[\hat{C}_0\hat{\rho}(t_0)\hat{A}_0\right]\hat{A}_1...\right]\hat{A}_{n-1}\right]\right\},\end{aligned} \tag{500}$$

where $t_0 < t_1 < ... < t_n$. This is the most general type of multi-time correlation function that one can consider. Of course, this expression can also be written with all the operators, the state, and the time-evolution superoperator written in any intermediate picture, as we did in Eq. (495).

3. *Quantum regression formula*

We can use the quantum regression theorem to develop a way of finding the correlation functions from the evolution equations of expectation values of system operators. In particular, consider a *closed set* of system operators $\{\hat{B}_j\}_{j=1,2,...,L}$, 'closed' in the sense that their expectation values evolve according to a closed linear system

$$\partial_\tau\langle\hat{\mathbf{B}}(\tau)\rangle = M(\tau)\langle\hat{\mathbf{B}}(\tau)\rangle, \tag{501}$$

where $\hat{\mathbf{B}} = (\hat{B}_1,\hat{B}_2,...,\hat{B}_L)^T$, $M(\tau)$ is some $L\times L$ matrix (generically time dependent), and we denote the time by τ for later convenience. Note that, for a Hilbert space of dimension d, this is always possible with $L\sim d^2$ in the worst case (number of elements of the density operator). But, of course, the method will only be practical (either analytically or numerically) when L is small enough, either naturally, or by doing some approximate truncation to the most relevant operators. We will see examples of this shortly, but as a generic one, we already saw in the previous chapter that the first and second order moments of bosonic modes form a closed set of linear equations when the master equation is quadratic in annihilation and creation operators (Gaussian dynamics).

Next, we prove that the two-time correlators $\langle\hat{A}(t)\hat{B}_j(t+\tau)\hat{C}(t)\rangle$ at a given time t satisfy the same equations of motion as the expectation values, that is,

$$\partial_\tau\langle\hat{A}(t)\hat{\mathbf{B}}(t+\tau)\hat{C}(t)\rangle = M(\tau)\langle\hat{A}(t)\hat{\mathbf{B}}(t+\tau)\hat{C}(t)\rangle, \tag{502}$$

with the difference that now the initial condition is given by $\langle\hat{A}(t)\hat{\mathbf{B}}(t)\hat{C}(t)\rangle = \mathrm{tr}\left\{\hat{A}\hat{\mathbf{B}}\hat{C}\hat{\rho}(t)\right\}$. This expression, known as the *quantum regression formula*, allows us to find any desired two-time correlator by solving a linear system, which we will to be highly practical.

Let us now pass to prove (502). It follows easily by rewriting the left-hand-side and right-hand-side of (501) in the Schrödinger picture as

$$\partial_\tau \mathrm{tr}\left\{\hat{\mathbf{B}}\hat{\rho}(\tau)\right\} = \mathrm{tr}\left\{\hat{\mathbf{B}}\partial_\tau \mathcal{U}^{(\tau)}[\hat{\rho}]\right\} = \mathrm{tr}\left\{\hat{\mathbf{B}}\mathcal{L}^{(\tau)}\mathcal{U}^{(\tau)}\left[\hat{\rho}\right]\right\}, \tag{503a}$$

$$M(\tau)\langle\hat{\mathbf{B}}(\tau)\rangle = M(\tau)\mathrm{tr}\left\{\hat{\mathbf{B}}\hat{\rho}(\tau)\right\} = M(\tau)\mathrm{tr}\left\{\hat{\mathbf{B}}\mathcal{U}^{(\tau)}[\hat{\rho}]\right\}. \tag{503b}$$

. Note that this expression holds for any choice of initial-condition operator $\hat{\rho}$, and therefore the relation between the upper and lower lines in the previous equations must be a property of the set $\hat{\mathbf{B}}$ and the Lindblad superoperator alone. It is not even required that $\hat{\rho}$ is Hermitian, positive, or even normalized. In other words, the relation

$$\partial_\tau \mathrm{tr}\left\{\hat{\mathbf{B}}\mathcal{U}^{(\tau)}\hat{S}\right\} = M(\tau)\mathrm{tr}\left\{\hat{\mathbf{B}}\mathcal{U}^{(\tau)}[\hat{S}]\right\}, \tag{504}$$

must hold for any system operator $\hat{S}$ (as long as the operator inside the trace remains in the trace class, of course). Choosing $\hat{S} = \hat{A}\hat{\rho}(t)\hat{C}$, we then obtain

$$\partial_\tau \mathrm{tr}\{\hat{\mathbf{B}}\mathcal{U}^{(\tau)}[\hat{A}\hat{\rho}(t)\hat{C}]\} = M(\tau)\mathrm{tr}\{\hat{\mathbf{B}}\mathcal{U}^{(\tau)}[\hat{A}\hat{\rho}(t)\hat{C}]\}, \tag{505}$$

which using the quantum regression theorem (491) leads to the desired expression (502).

4. *Interpretation of the photodetection two-time correlation function*

Before we move on to examples, it is interesting to provide an interpretation for the two-time correlators in a physical situation. In particular, we consider the two-time correlator associated with the photocurrent obtained by direct photodetection of the output field in the stationary limit $t \to \infty$. This is the simplest dynamical object that one can study for a source after it reaches its asymptotic state, and we will see shortly that it has a clear and interesting physical interpretation. According to (483), the corresponding correlation function is

$$\lim_{t\to\infty} \overline{j(t)j(t+\tau)} \propto \lim_{t\to\infty} \langle \hat{s}^\dagger(t)\hat{s}^\dagger(t+\tau)\hat{s}(t+\tau)\hat{s}(t)\rangle = \lim_{t\to\infty} G^{(2,2)}(t,t+\tau,t+\tau,t) \equiv \bar{G}^{(2)}(\tau), \tag{506}$$

where we have assumed $\tau \geq 0$ for definiteness, a vacuum state for the environment so we can use (488), and we introduce the notation $\bar{G}^{(2)}(\tau)$ for this correlation function because we will use it a lot in what follows. Note that this has exactly the form given in (498) and (502), with $\hat{A} = \hat{s}^\dagger$, $\hat{B} = \hat{s}^\dagger\hat{s}$, and $\hat{C} = \hat{s}$.

The interpretation of this correlation function follows straightforwardly from the atomic case, for which $\hat{s} = \hat{\sigma} = |g\rangle\langle e|$, and considering a time-independent Lindbladian, so the system reaches a stationary state asymptotically. Using the quantum regression theorem (496), we can write the correlation function as

$$\bar{G}^{(2)}(\tau) = \mathrm{tr}\Big\{ \underbrace{\hat{\sigma}^\dagger\hat{\sigma}}_{|e\rangle\langle e|}\, e^{\mathcal{L}\tau} \underbrace{[\hat{\sigma}\bar{\rho}\hat{\sigma}^\dagger]}_{|g\rangle\langle e|\bar{\rho}|e\rangle\langle g|} \Big\} = \bar{p}_e \times \underbrace{\langle e|\left(e^{\mathcal{L}\tau}[|g\rangle\langle g|]\right)|e\rangle}_{p_e(\tau)|_{|\psi(0)\rangle=|g\rangle}} = \bar{p}_e \times p_e(\tau)|_{|\psi(0)\rangle=|g\rangle}\,. \tag{507}$$

Where $\bar{p}_e = \langle e|\bar{\rho}|e\rangle$ is the probability of finding the atom in the excited state once its state has reached its asymptotic limit, while $p_e(\tau)|_{|\psi(0)\rangle=|g\rangle}$ is the probability of finding the atom excited at time τ, starting from the ground state at time 0, since $e^{\mathcal{L}\tau}[|g\rangle\langle g|]$ is the state evolved during a time τ from the ground state. Now, when the atom is in the ground state, the probability of recording a photopulse in the detector is clearly zero. Hence, assuming a perfect photodetector that turns all photons into photopulses without errors, the probability of being excited is equivalent to the probability of recording a *click!* in the photodetector (after which the atom must be in the ground state according to collapse axiom of quantum mechanics). Therefore, the two-time correlation function (506) arising naturally from direct photodetection must be interpreted as the probability of getting two consecutive photodetection events separated by a time interval τ. In other words, this correlation function provides the waiting statistics for the arrival of photons to the photodetector. Hence, we will call *coincidence correlation function* to (506).

This interpretation is easily generalized to higher-order correlation functions. In particular, consider the multi-time correlation function

$$\begin{aligned}\lim_{t\to\infty} \overline{j(t)j(t+\tau_1)...j(t+\tau_{N-1})} &\propto \lim_{t\to\infty} \langle \hat{s}^\dagger(t)\hat{s}^\dagger(t+\tau_1)...\hat{s}^\dagger(t+\tau_{N-1})\hat{s}(t+\tau_{N-1})...\hat{s}(t+\tau_1)\hat{s}(t)\rangle \\ &= \lim_{t\to\infty} G^{(N,N)}(t,t+\tau_1,...,,t+\tau_{N-1},t+\tau_{N-1},...,t+\tau_1,t) \equiv \bar{G}^{(N)}(\tau_1,...,\tau_{N-1}),\end{aligned} \tag{508}$$

where we have assumed $\tau_1 \leq \tau_2 \leq ... \leq \tau_{N-1}$ for definiteness. Particularizing this expression again to the atomic case with a time-independent Lindbladian, and using the multi-time form of the quantum regression theorem of Eq. (500), it's easy to find

$$\bar{G}^{(N)}(\tau_1, \tau_2, ..., \tau_{N-1}) = \bar{p}_e \times p_e(\tau_1)|_{|\psi(0)\rangle=|g\rangle} \times p_e(\tau_2 - \tau_1)|_{|\psi(0)\rangle=|g\rangle} \times ... \times p_e(\tau_{N-1} - \tau_{N-2})|_{|\psi(0)\rangle=|g\rangle}\,, \tag{509}$$

which is then interpreted as the probability of getting N consecutive photodetection events separated by time intervals $\{\tau_j - \tau_{j-1}\}_{j=1,2,...,N-1}$ (with $\tau_0 = 0$), once the atom has reached its asymptotic state.

C. Open cavity: coherent sources and photon bunching

As a first example we consider the light emitted by an empty, monochromatically-driven cavity. We saw in Section V A 6 that the corresponding master equation, in a picture rotating at the laser frequency, is given by

$$\partial_t \hat{\rho}_{\rm I} = \left[{\rm i}\Delta\hat{a}^\dagger\hat{a} + \mathcal{E}\hat{a}^\dagger - \mathcal{E}^*\hat{a}, \hat{\rho}_{\rm I}\right] + (\bar{n}+1)\gamma\left(2\hat{a}\hat{\rho}_{\rm I}\hat{a}^\dagger - \hat{a}^\dagger\hat{a}\hat{\rho}_{\rm I} - \hat{\rho}_{\rm I}\hat{a}^\dagger\hat{a}\right) + \bar{n}\gamma\left(2\hat{a}^\dagger\hat{\rho}_{\rm I}\hat{a} - \hat{a}\hat{a}^\dagger\hat{\rho}_{\rm I} - \hat{\rho}_{\rm I}\hat{a}\hat{a}^\dagger\right) \equiv \mathcal{L}_{\rm I}[\hat{\rho}_{\rm I}], \tag{510}$$

which has a time-independent Lindbladian $\mathcal{L}_{\rm I}$. On the other hand, note that the interaction-picture annihilation operators read as $\hat{a}_{\rm I}(t) = \hat{U}_{\rm c}^\dagger(t)\hat{a}\hat{U}_{\rm c}(t) = e^{-{\rm i}\omega_{\rm L}t}\hat{a}$, so that using Eq. (496), the coincidence correlation function (506) can be written as

$$\bar{G}^{(2)}(\tau) = {\rm tr}\left\{\hat{a}_{\rm I}^\dagger\hat{a}_{\rm I}e^{\mathcal{L}_{\rm I}\tau}[\hat{a}_{\rm I}\bar{\rho}_{\rm I}\hat{a}_{\rm I}^\dagger]\right\} = {\rm tr}\left\{\hat{N}e^{\mathcal{L}_{\rm I}\tau}[\hat{a}\bar{\rho}_{\rm I}\hat{a}^\dagger]\right\}, \tag{511}$$

where we remind that $\bar{\rho}_{\rm I} = \lim_{t\to\infty}\tilde{\rho}(t)$ is the stationary state in the rotating picture, that is, that satisfying $\mathcal{L}_{\rm I}[\bar{\rho}_{\rm I}] = 0$.

As we saw in Section V A 6, the stationary state is the displaced thermal state, $\bar{\rho}_{\rm I} = \hat{D}(\bar{\alpha})\hat{\rho}_{\rm th}(\bar{n})\hat{D}^\dagger(\bar{\alpha})$ with $\bar{\alpha} = \mathcal{E}/(\gamma - {\rm i}\Delta)$. It is interesting though, to consider separately the case in which the environment is at zero temperature ($\bar{n} = 0$), and the case in which the driving is zero ($\mathcal{E} = 0$).

1. *Zero temperature: Poissonian light*

In the $\bar{n} = 0$ case, the steady state is coherent $\bar{\rho} = |\bar{\alpha}\rangle\langle\bar{\alpha}|$ and we thus easily find

$$\bar{G}^{(2)}(\tau) = {\rm tr}\left\{\hat{N}e^{\mathcal{L}_{\rm I}\tau}[\underbrace{\hat{a}|\bar{\alpha}\rangle\langle\bar{\alpha}|\hat{a}^\dagger}_{|\bar{\alpha}|^2|\bar{\alpha}\rangle\langle\bar{\alpha}|}]\right\} = |\bar{\alpha}|^2{\rm tr}\left\{\hat{a}^\dagger\hat{a}\underbrace{e^{\mathcal{L}_{\rm I}\tau}[|\bar{\alpha}\rangle\langle\bar{\alpha}|]}_{|\bar{\alpha}\rangle\langle\bar{\alpha}|}\right\} = |\bar{\alpha}|^2\langle\bar{\alpha}|\hat{N}|\bar{\alpha}\rangle = |\bar{\alpha}|^4. \tag{512}$$

(by definition of steady state)

We observe that the probability of getting two consecutive clicks in the photodetector is independent of their time delay. This means that the photodetection events are statistically independent: photons arrive to the detector at random times, with no correlation whatsoever. Indeed, this is consistent with the fact that the photon number probability distribution is Poissonian for a coherent state, since this distribution is the one corresponding to statistically independent events. On the other hand, we have $\lim_{t\to\infty} G^{(1,1)}(t,t) = \lim_{t\to\infty}\langle\hat{N}(t)\rangle = \langle\bar{\alpha}|\hat{N}|\bar{\alpha}\rangle = |\bar{\alpha}|^2$, leading to a normalized correlation function

$$\bar{g}^{(2)}(\tau) \equiv \lim_{t\to\infty} g^{(2)}(t, t+\tau, t+\tau, t) = \frac{\bar{G}^{(2)}(\tau)}{\left[\lim_{t\to\infty}\langle\hat{a}^\dagger(t)\hat{a}(t)\rangle\right]^2} = 1. \tag{513}$$

Moreover, the generalization of this calculation to higher-order correlators is straightforward, and leads to the result $\bar{G}^{(N)}(\tau_1, ..., \tau_{N-1}) = |\bar{\alpha}|^{2N}$, so that

$$\bar{g}^{(N)}(\tau_1, ..., \tau_{N-1}) \equiv \lim_{t\to\infty} g^{(N)}(t, t+\tau_1, ..., t+\tau_{N-1}, t+\tau_{N-1}, ..., t+\tau_1, t) = 1. \tag{514}$$

This value of 1 for the normalized photodetection correlation functions is not unique to coherent states, but, more generally, it is characteristic of sources whose steady-state number distribution is Poissonian. This is easy to prove as

follows. First, note that the most general state whose photon-number distribution is Poissonian must be necessarily written as a mixture of coherent states with the same amplitude α but arbitrary phases, say

$$\hat{\rho}_{\text{Poisson}} = \int_0^{2\pi} d\phi P(\phi) |\alpha e^{\mathrm{i}\phi}\rangle\langle \alpha e^{\mathrm{i}\phi}|, \qquad \text{with } P(\phi) > 0 \, \forall \phi \text{ and } \int_0^{2\pi} d\phi P(\phi) = 1. \tag{515}$$

Note that the a mixture of K coherent states with phases $\{\phi_k\}_{k=1,2,...,K}$ is obtained setting $P(\phi) = \sum_{k=1}^K w_k \delta(\phi - \phi_k)$, with $w_k > 0 \forall k$ and $\sum_{k=1}^K w_k = 1$. Indeed, note that the photon number distribution $\langle n|\hat{\rho}_{\text{Poisson}}|n\rangle = \exp(-\alpha^2)\alpha^{2n}/n!$ is Poissonian for any choice of $P(\phi)$. This is obviously not the case for any other type of state. Using the Schrödinger-picture expression (500) for the $\bar{G}^{(N)}(\tau_1, ..., \tau_{N-1})$ correlation function (508), assuming that the stationary state of the system has the form (515), so that $\lim_{t\to\infty} \hat{\rho}(t) = \hat{\rho}_{\text{Poisson}}$ with $\mathcal{L}[\hat{\rho}_{\text{Poisson}}] = 0$, it is then immediate to obtain $\bar{G}^{(N)}(\tau_1, ..., \tau_{N-1}) = \alpha^{2N}$ for any choice of $P(\phi)$, which together with $\lim_{t\to\infty} G^{(1,1)}(t,t) = \text{tr}\{\hat{N}\hat{\rho}_{\text{Poisson}}\} = \alpha^2$, leads to (514).

2. *Non-driven cavity: thermal light and bunching*

Let us now move on to the $\mathcal{E} = 0$ case, such that the steady state of the cavity is thermal, $\bar{\rho} = \hat{\rho}_{\text{th}}(\bar{n})$ with $\lim_{t\to\infty} G^{(1)}(t,t) = \text{tr}\left\{\hat{a}^\dagger \hat{a} \hat{\rho}_{\text{th}}(\bar{n})\right\} = \bar{n}$. Note that without driving, the master equation is time-independent in the original picture, so there is no need to refer everything to a rotating picture.

This case provides a perfect example for the use the quantum regression formula. In particular, note that the expectation value of the photon number satisfies the evolution equation

$$\partial_t \left\langle \hat{a}^\dagger \hat{a} \right\rangle = -2\gamma \left\langle \hat{a}^\dagger \hat{a} \right\rangle + 2\bar{n}\gamma, \tag{516}$$

as we proved in (402). We can rewrite this equation in the form (501) by choosing $\hat{B}_1 = \hat{a}^\dagger \hat{a}$ and $\hat{B}_2 = \bar{n}$ (constant), which form then a closed set with

$$\mathcal{M} = \begin{pmatrix} -2\gamma & 2\gamma \\ 0 & 0 \end{pmatrix}. \tag{517}$$

Therefore, according to the quantum regression formula (502) with $\hat{A} = \hat{a}^\dagger$ and $\hat{C} = \hat{a}$, we get

$$\partial_\tau \begin{pmatrix} \langle \hat{a}^\dagger(t) \hat{a}^\dagger(t+\tau) \hat{a}(t+\tau) \hat{a}(t) \rangle \\ \bar{n} \langle \hat{a}^\dagger(t) \hat{a}(t) \rangle \end{pmatrix} = \mathcal{M} \begin{pmatrix} \langle \hat{a}^\dagger(t) \hat{a}^\dagger(t+\tau) \hat{a}(t+\tau) \hat{a}(t) \rangle \\ \bar{n} \langle \hat{a}^\dagger(t) \hat{a}(t) \rangle \end{pmatrix}, \tag{518}$$

which taking the $t \to \infty$ limit, leads to

$$\partial_\tau \begin{pmatrix} \bar{G}^{(2)}(\tau) \\ \bar{n}^2 \end{pmatrix} = \mathcal{M} \begin{pmatrix} \bar{G}^{(2)}(\tau) \\ \bar{n}^2 \end{pmatrix} \Rightarrow \frac{d\bar{G}^{(2)}}{d\tau} = -2\gamma \bar{G}^{(2)} + 2\bar{n}^2 \gamma. \tag{519}$$

Using (251), we obtain the solution

$$\bar{G}^{(2)}(\tau) = e^{-2\gamma\tau} \bar{G}^{(2)}(0) + \bar{n}^2 \left(1 - e^{-2\gamma\tau}\right). \tag{520}$$

The initial condition of this expression is given by

$$\bar{G}^{(2)}(0) = \text{tr}\left\{\hat{a}^{\dagger 2} \hat{a}^2 \hat{\rho}_{\text{th}}(\bar{n})\right\} = \underbrace{\left|\text{tr}\left\{\hat{a}^2 \bar{\rho}_{\text{th}}(\bar{n})\right\}\right|^2}_{0} + 2 \underbrace{\text{tr}\left\{\hat{a}^\dagger \hat{a} \bar{\rho}_{\text{th}}(\bar{n})\right\}^2}_{\bar{n}^2} = 2\bar{n}^2, \tag{521}$$

where we have used the fact that the thermal state is Gaussian, and hence it satisfies the Gaussian moment theorem (139), which we conveniently generalize here as follows. Consider any set of operators $\{\hat{L}_1, \hat{L}_2, ..., \hat{L}_N\}$, all linear in annihilation and creation operators. Then, defining the fluctuation operators $\delta\hat{L}_j = \hat{L}_j - \langle \hat{L}_j \rangle$, Gaussian states satisfy

$$\langle \delta\hat{L}_1 \delta\hat{L}_2 ... \delta\hat{L}_N \rangle = \begin{cases} \sum\limits_{\substack{\{j_1, ..., j_N\} \in \text{all} \\ (N-1)!! \text{pairings}}} \langle \delta\hat{L}_{j_1} \delta\hat{L}_{j_2} \rangle ... \langle \delta\hat{L}_{j_{N-1}} \delta\hat{L}_{j_N} \rangle & \text{for even } N \\ 0 & \text{for odd } N \end{cases}. \tag{522}$$

Noting that $\langle \hat{a} \rangle$ for the thermal state, this version of the Gaussian-moment theorem leads directly to (521). Inserting then the latter in (520), we obtain the normalized coincidence correlation function

$$\bar{g}^{(2)}(\tau) = \frac{\bar{G}^{(2)}(\tau)}{\bar{n}^2} = 1 + e^{-2\gamma\tau}. \tag{523}$$

Interestingly, in this case $\bar{g}^{(2)}(\tau)$ starts at 2 for $\tau = 0$ and decays monotonically to 1 as time goes by. In other words, it is more likely to detect two photons at the same time, than spaced in time: photons arrive in bunches. We then call this phenomenon *bunching*.

D. Resonance fluorescence and antibunching

For the next example, let us discuss now the properties of the light radiated by a driven two-level atom, a problem known as *resonance fluorescence*. The general master equation of this problem is given by Eq. (434), but here we will focus on the zero-temperature case ($\bar{n} = 0$) for simplicity, and assume the driving to be monochromatic, that is $\mathcal{A}(t) = \mathcal{E}e^{-\mathrm{i}\omega_\mathrm{L} t}$.

Let us start by moving to a picture rotating at the laser frequency, where the Hamiltonian becomes time independent. This Hamiltonian is defined the transformation operator $\hat{U}_\mathrm{c}(t) = e^{-\mathrm{i}\omega_\mathrm{L} t\hat{\sigma}_z/2}$, leading to an interaction-picture lowering operator $\hat{\sigma}_\mathrm{I}(t) = \hat{U}_\mathrm{c}^\dagger(t)\hat{\sigma}\hat{U}_\mathrm{c}(t) = e^{-\mathrm{i}\omega_\mathrm{L} t}\hat{\sigma}$, and keeping $\hat{\sigma}_z$ invariant. The transformed state $\hat{\rho}_\mathrm{I}(t) = \hat{U}_\mathrm{c}^\dagger(t)\hat{\rho}(t)\hat{U}_\mathrm{c}(t)$ evolves then according to the master equation

$$\partial_t \hat{\rho}_\mathrm{I} = \left[\mathrm{i}\frac{\Delta}{2}\hat{\sigma}_z + \mathcal{E}\hat{\sigma}^\dagger - \mathcal{E}^*\hat{\sigma}, \hat{\rho}_\mathrm{I}\right] + \gamma\left(2\hat{\sigma}\hat{\rho}_\mathrm{I}\hat{\sigma}^\dagger - \hat{\sigma}^\dagger\hat{\sigma}\hat{\rho}_\mathrm{I} - \hat{\rho}_\mathrm{I}\hat{\sigma}^\dagger\hat{\sigma}\right) = \mathcal{L}_\mathrm{I}[\hat{\rho}_\mathrm{I}], \tag{524}$$

where $\Delta = \omega_\mathrm{L} - \varepsilon$.

In order to find the coincidence correlation function, we could proceed by showing that the operators $\{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z, \hat{I}\}$ form a closed set (Bloch equations), applying then the quantum regression formula similarly to how we did in the previous example. However, in the atomic case we have an easier route based on (507): we only need to evaluate the evolution of the excited-state probability. We will then follow this route.

We start by writing down the Bloch equations. Using the same notation as in Sec. V A 3 for expectation values in the interaction picture, that is, $\tilde{b}(t) = \langle\hat{\sigma}\rangle_\mathrm{I} = \mathrm{tr}\{\hat{\sigma}\hat{\rho}_\mathrm{I}(t)\}$, and noting that $b_z(t) = \mathrm{tr}\{\hat{\sigma}_z\hat{\rho}(t)\} = \mathrm{tr}\{\hat{\sigma}_z\hat{\rho}_\mathrm{I}(t)\}$, we can use the general expression (399) to find

$$\partial_t\tilde{b} = \mathrm{i}\frac{\Delta}{2}\langle[\hat{\sigma}, \hat{\sigma}_z]\rangle_\mathrm{I} + \mathcal{E}\left\langle\left[\hat{\sigma}, \hat{\sigma}^\dagger\right]\right\rangle_\mathrm{I} + \gamma\left\langle\left[\hat{\sigma}^\dagger, \hat{\sigma}\right]\hat{\sigma}\right\rangle_\mathrm{I} = -\mathcal{E}b_z - (\gamma - \mathrm{i}\Delta)\tilde{b}, \tag{525a}$$

$$\partial_t b_z = \mathcal{E}\left\langle\left[\hat{\sigma}_z, \hat{\sigma}^\dagger\right]\right\rangle_\mathrm{I} - \mathcal{E}^*\langle[\hat{\sigma}_z, \hat{\sigma}]\rangle_\mathrm{I} + \gamma\left(\left\langle\left[\hat{\sigma}^\dagger, \hat{\sigma}_z\right]\hat{\sigma}\right\rangle_\mathrm{I} + \left\langle\hat{\sigma}^\dagger\left[\hat{\sigma}_z, \hat{\sigma}\right]\right\rangle_\mathrm{I}\right) = 4\mathrm{Re}\{\mathcal{E}^*\tilde{b}\} - 4\gamma b_z - 4\gamma. \tag{525b}$$

Since we are ultimately interested in the excited-state population, it is best to write this equations in terms of it already. Using $p_e(t) = [1 + b_z(t)]/2$, we obtain

$$\partial_t\tilde{b} = -(\gamma - \mathrm{i}\Delta)\tilde{b} - 2\mathcal{E}p_e + \mathcal{E}, \tag{526a}$$

$$\partial_t p_e = 2\mathrm{Re}\{\mathcal{E}^*\tilde{b}\} - 4\gamma p_e. \tag{526b}$$

Before solving the full dynamics, it is interesting to evaluate the asymptotic state predicted by these equations. Since the Lindbladian is time independent, we expect a such state to be stationary. Then, we simply set the derivatives to zero, and solve the remaining linear system in a straightforward manner (just write $\tilde{b}$ in terms of p_e from the first equation, and substitute it in the second equation). Introducing the parameter $P = |\mathcal{E}|^2/(\gamma^2 + \Delta^2)$, we obtain

$$\bar{p}_e \equiv \lim_{t\to\infty} p_e(t) = \frac{P}{2(1+P)} \quad \text{and} \quad \lim_{t\to\infty}\tilde{b}(t) = \frac{\sqrt{P}}{1+P}e^{\mathrm{i}(\arg\{\mathcal{E}\} + \arg\{\gamma + \mathrm{i}\Delta\})}. \tag{527}$$

This shows that the atom remains in the ground state when the driving rate is negligible with respect to the damping rate or the detuning ($P \ll 1$), while in the limit where it dominates ($P \gg 1$), it can only bring half the population to the excited state[49]. This is interesting because it tells us that just through driving, it is impossible to fully invert the steady-state population of an atom, so more ingenious ways are required.

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[49] Why only half? Since $|\mathcal{E}|$ dominates, the atom starts performing perfect Rabi oscillations between the ground and excited states. However, on a much longer time scale, dissipation kicks in, and the corresponding noise starts shifting randomly the phase of the oscillations, until eventually they average out to half the population on each state.

Let us now move on to the coincidence correlation function (507), focusing on the normalized form

$$\bar{g}^{(2)}(\tau) = \frac{p_e(\tau)|_{|\psi(0)\rangle_{\rm I}=|g\rangle}}{\bar{p}_e}, \tag{528}$$

where we have taken into account that $\lim_{t\to\infty}\langle\hat{\sigma}^\dagger(t)\hat{\sigma}(t)\rangle = \mathrm{tr}\{\hat{\sigma}^\dagger\hat{\sigma}\bar{\rho}\} = \bar{p}_e$ for the normalization. There are very interesting things that we can see already in this expression without the need to evaluate it at all times. First, note that $\bar{g}^{(2)}(\tau\to\infty) = 1$, while $\bar{g}^{(2)}(\tau = 0) = 0$, since the probability of being in the excited state at time zero when starting from the ground state vanishes. Hence, we see that the probability of obtaining two simultaneous photons is identically zero, while the photodetection events become independent for long times. This is a phenomenon known as *antibunching*, and it is rooted in the quantization of the atom: once it decays, it requires some time to get re-excited (we call it *reloading time*), which means that it can emit only one photon at a time.

Let us now find the full time evolution of the coincidence correlation function. This analytically difficult in the general case, but quite easy in the resonant case, $\Delta = 0$, which we consider next. Taking the derivative of Eq. (526b), and using also Eq. (526a) to write $\tilde{b}$ and $\partial_t\tilde{b}$ as a function of p_e and $\partial_t p_e$, it is straightforward to find

$$\ddot{p}_e + 5\gamma\dot{p}_e + 4\gamma^2(1+P)p_e = 2\gamma^2 P. \tag{529}$$

Together with the initial conditions $p_e(0) = 0 = \dot{p}_e(0)$, this is a second order differential equation with constant coefficients that is easily solved, leading to

$$\bar{g}^{(2)}(\tau) = 1 - e^{-5\gamma\tau/2}\left[\cosh(r\gamma\tau/2) - \frac{5\sinh(r\gamma\tau/2)}{r}\right], \tag{530}$$

where we have defined $r = \sqrt{9-16P}$. We show this function in Fig. **soon**, for different values of P. As expected, the function starts at 0 and goes to 1 for long times. For intermediate times, the behavior depends on P. The most interesting case occurs under strong driving conditions, that is, $P \gg 1$ or, equivalently, $|\mathcal{E}| \gg \gamma$. In this case, $r \approx 4\mathrm{i}|\mathcal{E}|$ becomes imaginary, and leads to

$$\bar{g}^{(2)}(\tau) \approx 1 - e^{-5\gamma\tau/2}\cos(2|\mathcal{E}|\tau). \tag{531}$$

This result is very much connected to Rabi oscillations, which are clearly visible for several cycles, until dissipation washes them out. Hence, in order to measure Rabi oscillations, it is not required to initialize the atom in the ground state and monitoring the populations. Instead, we can simply let the strongly-driven atom relax to its asymptotic state, and then check the Rabi oscillations in the delay between photodetection events.

E. Homodyne detection and output squeezing

We have seen that direct photodetection provides normally-ordered moments of the output number operator. Hence, in loose terms, direct photodetection allows to measure only the number operator and related photon counting statistics. However, we can design clever measurement schemes involving different sources and photodetectors such that the moments of the combined photocurrents give us access to the moments of diffferent observables of the output light. As a most relevant example, in this section we study homodyne detection. As we will see, this type of measurement will allow us to determine the statistics of the quadratures of the field. We will also apply it to one specific source, the so-called below-threshold optical parametric oscillator, which can be modeled as an open cavity whose intracavity mode is fed via down-conversion in a nonlinear medium.

1. *Homodyne detection and the squeezing spectrum*

The scheme for homodyne detection is shown in Fig. **ToDo**. The output field of the source that we want to characterize is mixed in a balanced beam splitter with a strong laser field (dubbed *local oscillator*); the two fields emerging from the beam splitter are photodetected and their photocurrents are subtracted, leading to the so-called *homodyne photocurrent* $j_H(t)$. In the following we show that the stochastic correlation functions of this photocurrent are proportional to normally-ordered correlation functions of output quadratures.

We start by modeling the local oscillator field. We assume that it is the output of a monochromatic coherent source (that is, a source whose asymptotic state is coherent). This is indeed the commonly used model of a laser[50]. We write

[50] However, as we shall see in a later chapter, lasers are a bit more subtle, and this model only holds under some specific conditions.

the vector potential of the corresponding output field as

$$\hat{\mathbf{A}}_{\mathrm{LO}}^{(+)}(z,t)=\mathbf{e}_x\sqrt{\frac{\hbar}{2c\varepsilon_0 S\omega_{\mathrm{LO}}}}\hat{a}_{\mathrm{LO}}(t), \tag{532}$$

characterized by the correlation functions

$$\langle\hat{a}_{\mathrm{LO}}^{\dagger}(t_1)...\hat{a}_{\mathrm{LO}}^{\dagger}(t_N)\hat{a}_{\mathrm{LO}}(t_{N+1})...\hat{a}_{\mathrm{LO}}(t_{N+M})\rangle=e^{\mathrm{i}\omega_{\mathrm{LO}}(t_1+...+t_N-t_{N+1}-...-t_{N+M})}|\alpha_{\mathrm{LO}}|^{N+M}e^{\mathrm{i}\phi_{\mathrm{LO}}(M-N)}, \tag{533}$$

where ω_{LO} is the frequency of the coherent source (laser frequency) and $\alpha_{\mathrm{LO}}=|\alpha_{\mathrm{LO}}|e^{\mathrm{i}\phi_{\mathrm{LO}}}$ is a complex amplitude (specifically, if we denote by $|\bar{\beta}e^{-\mathrm{i}\omega_{\mathrm{LO}}t}\rangle$ the amplitude of the asymptotic coherent state reached by the cavity associated to this source, with decay rate Γ, then $\alpha_{\mathrm{LO}}=\sqrt{2\Gamma}\bar{\beta}$, as we have seen in previous results). We assume that both of this quantities are controllable in experiments.

Let us also note that, obviously, these local oscillator operators commute with those of the source at all times, since they act on different Hilbert spaces and do not interact. Moreover, since they are generated from independent sources, the states of the output field we want to study and the local oscillator fields are not correlated, meaning that the expectation value of the product of any output operator $\hat{B}_{\mathrm{out}}(t)$ of the relevant source with any local oscillator operator $\hat{B}_{\mathrm{LO}}(t')$ factorizes as $\langle\hat{B}_{\mathrm{out}}(t)\hat{B}_{\mathrm{LO}}(t')\rangle=\langle\hat{B}_{\mathrm{out}}(t)\rangle\langle\hat{B}_{\mathrm{LO}}(t')\rangle$.

Let us now consider the fields emerging from the beam splitter. Considering a balanced beam splitter (50% transmission and reflection), these fields are just the sum and difference of the fields entering its input ports. We denote them by

$$\hat{\mathbf{A}}_{\pm}(z,t)=\frac{1}{\sqrt{2}}\left[\hat{\mathbf{A}}_{\mathrm{out}}(z,t)\pm\hat{\mathbf{A}}_{\mathrm{LO}}(z,t)\right]. \tag{534}$$

Obviously, in order for the local oscillator to have any effect on the source that we want to characterize, ω_{LO} must be close to the central frequency of the light emitted by that source (in particular, usually in experiments one makes them match). Under such circumstances, we can write the these fields in the usual form

$$\hat{\mathbf{A}}_{\pm}^{(+)}(z,t)\approx\mathbf{e}_x\sqrt{\frac{\hbar}{2c\varepsilon_0 S\omega_{\mathrm{LO}}}}\hat{a}_{\pm}(t_R), \tag{535}$$

with

$$\hat{a}_{\pm}(t)=\frac{1}{\sqrt{2}}\left[\hat{a}_{\mathrm{out}}(t)\pm\hat{a}_{\mathrm{LO}}(t)\right]. \tag{536}$$

Let us write the number operators associated to any of these fields as

$$\hat{n}_{\pm}(t)=\hat{a}_{\pm}^{\dagger}(t)\hat{a}_{\pm}(t)=\frac{1}{2}\left[\hat{n}_{\mathrm{out}}(t)+\hat{n}_{\mathrm{LO}}(t)\pm\hat{h}(t)\right], \tag{537}$$

where we have defined the operator

$$\hat{h}(t)=\hat{a}_{\mathrm{LO}}^{\dagger}(t)\hat{a}_{\mathrm{out}}(t)+\hat{a}_{\mathrm{LO}}(t)\hat{a}_{\mathrm{out}}^{\dagger}(t). \tag{538}$$

Note that, using (533), it is simple to show that

$$\langle:\hat{h}(t_1)\hat{h}(t_2)...\hat{h}(t_N):\rangle=|\alpha_{\mathrm{LO}}|^N\langle:\tilde{X}_{\mathrm{out}}^{\phi_{\mathrm{LO}}}(t_1)\tilde{X}_{\mathrm{out}}^{\phi_{\mathrm{LO}}}(t_2)...\tilde{X}_{\mathrm{out}}^{\phi_{\mathrm{LO}}}(t_N):\rangle, \tag{539}$$

where we have defined slowly-varying quadratures of the output field

$$\tilde{X}_{\mathrm{out}}^{\phi}(t)=e^{\mathrm{i}\omega_{\mathrm{LO}}t-\mathrm{i}\phi}\hat{a}_{\mathrm{out}}(t)+e^{-\mathrm{i}\omega_{\mathrm{LO}}t+\mathrm{i}\phi}\hat{a}_{\mathrm{out}}^{\dagger}(t). \tag{540}$$

We call them 'slowly varying' because the factors $e^{\pm\mathrm{i}\omega_{\mathrm{LO}}t}$ cancel the fast oscillations of the output operators. Hence, we see two things. First, the detection scheme is only sensitive to the slowly-varying envelopes of the field (this is quite common to all measurement schemes: resolving optical oscillations is hard and only reserved to very specific state-of-the-art techniques). Second, we see that the operator $\hat{h}$ encodes the information about the statistics of the output quadratures. Essentially, the rest of the steps in the detection scheme are designed to remove all information but the one corresponding to this operator, as we see next by analyzing the homodyne photocurrent, for what we need one more result from photodetection theory.

Similarly to the case of direct photodetection, it is possible to prove (though not trivially) that the cross correlation between two photocurrents is related to quantum cross correlation functions between their corresponding detected photon number operators,

$$\overline{j_m(t)j_{m'}(t')} \propto \langle : \hat{n}_m(t)\hat{n}_{m'}(t') : \rangle. \tag{541}$$

This is indeed natural, because we expect two photodetection signals to be statistically independent only when the underlaying measured fields are.

We can now proceed to evaluate the first and second order stochastic correlation functions of the homodyne photocurrent $j_H(t) = j_+(t) - j_-(t)$. We obtain

$$\overline{j_H(t)} = \overline{j_+(t)} + \overline{j_-(t)} \propto \langle \hat{n}_+(t) \rangle - \langle \hat{n}_-(t) \rangle, \tag{542a}$$

$$\begin{aligned}\overline{j_H(t)j_H(t')} &= \overline{j_+(t)j_+(t')} + \overline{j_-(t)j_-(t')} - \overline{j_+(t)j_-(t')} - \overline{j_-(t)j_+(t')} \\ &\propto \langle : \hat{n}_+(t)\hat{n}_+(t') : \rangle + \langle : \hat{n}_-(t)\hat{n}_-(t') : \rangle - \langle : \hat{n}_+(t)\hat{n}_-(t') : \rangle - \langle : \hat{n}_-(t)\hat{n}_+(t') : \rangle.\end{aligned} \tag{542b}$$

Expanding each term using (537) and (533), it is then straightforward to obtain

$$\overline{j_H(t)} \propto |\alpha_{\mathrm{LO}}| \langle \tilde{X}_{\mathrm{out}}^{\phi_{\mathrm{LO}}}(t) \rangle, \tag{543a}$$

$$\overline{j_H(t)j_H(t')} \propto |\alpha_{\mathrm{LO}}|^2 \langle : \tilde{X}_{\mathrm{out}}^{\phi_{\mathrm{LO}}}(t)\tilde{X}_{\mathrm{out}}^{\phi_{\mathrm{LO}}}(t') : \rangle, \tag{543b}$$

which is precisely the result we advanced above.

It is usual to work with photocurrent fluctuations $\delta j_H(t) = j_H(t) - \overline{j_H(t)}$, since in quantum mechanics we are usually interested in how noise is distributed around the average value of an observable, as we have discussed before. The expressions above allow us to write then

$$\overline{\delta j_H(t)\delta j_H(t')} \propto |\alpha_{\mathrm{LO}}|^2 \langle : \delta\tilde{X}_{\mathrm{out}}^{\phi_{\mathrm{LO}}}(t)\delta\tilde{X}_{\mathrm{out}}^{\phi_{\mathrm{LO}}}(t') : \rangle. \tag{544}$$

Before moving on to an example where homodyne detection plays an important role, it is important to point out that most photodetectors do not allow to measure instantaneous photocurrents (some state-of-the-art ones do, though). In particular, a more detailed model of the photodetection process for common photodetectors [60] would show that the variance of the photocurrent, $\overline{\delta j_H^2(t)}$ in this case, is infinite at all times, meaning that the instantaneous signal $j_H(t)$ is completely hidden by a massive noise wall. Therefore, most experiments deal with a different quantity, namely the power spectrum, given by

$$\frac{1}{T}\int_0^T dt \int_0^T dt' \cos[\Omega(t-t')]\overline{\delta j_H(t)\delta j_H(t')}, \tag{545}$$

where T is the *detection time* and Ω is commonly known as the *noise* or *detection frequency*. The massive instantaneous noise is now confined to the spectral region $\Omega \in [0, \sim T^{-1}]$, and hence one gets a sensible signal for noise frequencies outside that region.

Consider a source that reaches a stationary state in which $\lim_{t\to\infty} \overline{\delta j_H(t)\delta j_H(t+\tau)}$ is a function only of $|\tau|$, which is the most common case. If we also consider sufficiently long detection times, it is then simple to prove that the previous expression can be written as the simple Fourier transform

$$\int_{-\infty}^{+\infty} d\tau e^{-\mathrm{i}\Omega\tau} \lim_{t\to\infty} \overline{\delta j_H(t)\delta j_H(t+\tau)}. \tag{546}$$

Related to the power spectrum of the homodyne photocurrent, we then define in quantum optics the so-called *quadrature noise spectrum*, given by

$$V^{\phi}(\Omega) = \int_{-\infty}^{+\infty} d\tau e^{-\mathrm{i}\Omega\tau} \lim_{t\to\infty} \langle \delta\tilde{X}_{\mathrm{out}}^{\phi}(t)\delta\tilde{X}_{\mathrm{out}}^{\phi}(t+\tau) \rangle, \tag{547}$$

which is the usual object measured in an experiment involving homodyne detection. Note that we have assumed that the two-time correlation function of the quadrature depends only on $|\tau|$, as it is usually the case in stationary quantum optical problems; if that's not the case, then the simple Fourier integral must be replaced by the more general integral (545). Using the commutation relations of the output operators (484), we can write the quadrature product in normal order as $\delta\tilde{X}_{\mathrm{out}}^{\phi}(t)\delta\tilde{X}_{\mathrm{out}}^{\phi}(t') = \delta(t-t') + : \delta\tilde{X}_{\mathrm{out}}^{\phi}(t)\delta\tilde{X}_{\mathrm{out}}^{\phi}(t') :$. Using then the input-output relations

under the assumption of a zero-temperature environment (so that the terms with input operators vanish), we then obtain the quadrature noise spectrum in terms of system correlation functions,

$$V^{\phi}(\Omega) = 1 + \underbrace{\kappa \int_{-\infty}^{+\infty} d\tau e^{-\mathrm{i}\Omega\tau} \lim_{t\to\infty} \langle : \delta\tilde{X}^{\phi}(t)\delta\tilde{X}^{\phi}(t+\tau) : \rangle}_{S^{\phi}(\Omega)}, \tag{548}$$

where we have defined the slowly-varying quadratures of the system

$$\tilde{X}^{\phi}(t) = e^{\mathrm{i}\omega_{\mathrm{LO}}t - \mathrm{i}\phi}\hat{s}(t) + e^{-\mathrm{i}\omega_{\mathrm{LO}}t + \mathrm{i}\phi}\hat{s}^{\dagger}(t). \tag{549}$$

The normally-ordered part of the noise spectrum, $S^{\phi}(\Omega)$, is known as *squeezing spectrum*.

Finally, let us discuss the concept of squeezing in the output light of an open system. As explained in Section III, some of the most common applications of light are sensing or communication. In both cases, a signal is encoded as a low-frequency (compared to optical frequencies) modulation of some quadrature. This signal would then appear as a peak at the corresponding frequency in the power spectrum of a homodyne signal, or, equivalently, in the quadrature noise spectrum. On the other hand, note that for a vacuum or coherent stationary state of the system we get $V^{\phi_{\mathrm{LO}}}(\Omega) = 1$ for all *noise frequencies* Ω and all local oscillator's phases ϕ_{LO}. This then sets a base value that limits the signal-to-noise ratio with which we will be able to observe the peak (see Fig. **ToDo**a). We call this the *shot noise.* Therefore, in order to increase the signal-to-noise ratio it is desirable to work with states that have $V^{\phi_{\mathrm{LO}}}(\Omega) < 1$ for some values of the noise frequency and the local oscillator's phase (see Fig. **ToDo**b). This is what we call *squeezed states* in the context of the light radiated by a open systems.

It's interesting to point out that, similarly to the position and momentum of a single harmonic oscillator, we can derive a sort of uncertainty relation between the noise spectra of orthogonal quadratures, namely

$$V^{\phi}(\Omega)V^{\phi+\pi/2}(\Omega) \geq 1. \tag{550}$$

Hence, the squeezing of an output quadrature must be accompanied by the antisqueezing of its canonical conjugate. Let us prove this relation... **soon**.

Next we proceed to put all this in action with a paradigmatic example: the optical parametric oscillator.

2. *Squeezing from the optical parametric oscillator*

Consider an open cavity at zero temperature containing a dielectric medium with second order nonlinearity such as the one we studied in Section IV C. Such system is known as optical parametric oscillator (we will fully understand the reason for the name in a chapter to come), and we now show now that it allows for the generation of highly-squeezed output light.

We worked out the previous examples through different approaches in the Schrödinger picture. Hence, in order to show a different method, we work in the Heisenberg picture in this case. We then consider the quantum Langevin equations (357) for the cavity mode, using

$$\hat{H}_{\mathrm{intra}}(t) = \mathrm{i}\frac{\hbar g}{2}(e^{\mathrm{i}\omega_2 t}\hat{a}^{\dagger 2} - e^{\mathrm{i}\omega_2 t}\hat{a}^{\dagger 2})$$

as the intracavity Hamiltonian, corresponding to down-conversion under the parametric approximation. Note that, for convenience, we have chosen a different phase for the pump compared to the Hamiltonian of Eq. (310). The quantum Langevin equation then becomes

$$\partial_t\hat{a} = -(\gamma + \mathrm{i}\omega_0)\hat{a} + ge^{\mathrm{i}\omega_2 t}\hat{a}^{\dagger} + \sqrt{2\gamma}\hat{a}_{\mathrm{in}}(t). \tag{551}$$

In order to turn the equation into a time-independent one, we define the slowly-varying operator[51] $\tilde{a}(t) = e^{\mathrm{i}\omega_2 t/2}\hat{a}(t)$, which evolves according to the equation

$$\partial_t\tilde{a} = -(\gamma + \mathrm{i}\Delta)\tilde{a} + g\tilde{a}^{\dagger} + \sqrt{2\gamma}\tilde{a}_{\mathrm{in}}(t), \tag{552}$$

[51] Equivalent to moving to a picture rotating at half the pump frequency.

where $\Delta = \omega_0 - \omega_2/2$ and $\tilde{a}_{\rm in}(t) = e^{{\rm i}\omega_2 t/2}\hat{a}_{\rm in}(t)$ is a slowly-varying input operator, which satisfies the same statistical properties (356) and commutation relations (484) as the original one. It is also interesting to note that if we use a local oscillator of frequency $\omega_{\rm LO} = \omega_2/2$, then the slowly-varying quadratures of the system (549) can be written directly in terms of the slowly-varying operators as

$$\tilde{X}^{\phi}(t) = e^{-{\rm i}\phi}\tilde{a}(t) + e^{{\rm i}\phi}\tilde{a}^{\dagger}(t). \tag{553}$$

In order to simplify the problem and avoid spurious technical details, we consider the resonant case, $\Delta = 0$. In such case, the position $\tilde{X}^0 \equiv \tilde{X}$ and momentum $\tilde{X}^{\pi/2} \equiv \tilde{P}$ quadratures obey independent equations that can be easily treated. In particular, simply adding and subtracting (552) and it's Hermitian conjugate, we find

$$\partial_t \tilde{X} = -(\gamma - g)\tilde{X} + \sqrt{2\gamma}\tilde{X}_{\rm in}(t), \tag{554a}$$

$$\partial_t \tilde{P} = -(\gamma + g)\tilde{P} + \sqrt{2\gamma}\tilde{P}_{\rm in}(t), \tag{554b}$$

where we have defined the input quadratures $\tilde{X}^{\phi}_{\rm in}(t) = e^{-{\rm i}\phi}\tilde{a}_{\rm in}(t) + e^{{\rm i}\phi}\tilde{a}^{\dagger}_{\rm in}(t)$, which satisfy the statistical properties

$$\langle \tilde{X}^{\phi}_{\rm in}(t)\rangle = 0, \tag{555a}$$

$$\langle \tilde{X}^{\phi}_{\rm in}(t)\tilde{X}^{\phi'}_{\rm in}(t')\rangle = e^{{\rm i}(\phi'-\phi)}\delta(t-t'). \tag{555b}$$

These equations are readily solved using (251) as usual, obtaining

$$\tilde{X}(t) = \tilde{X}(0)e^{-(\gamma-g)t} + \sqrt{2\gamma}\int_0^t dt' e^{-(\gamma-g)(t-t')}\tilde{X}_{\rm in}(t'), \tag{556a}$$

$$\tilde{P}(t) = \tilde{P}(0)e^{-(\gamma+g)t} + \sqrt{2\gamma}\int_0^t dt' e^{-(\gamma+g)(t-t')}\tilde{P}_{\rm in}(t'). \tag{556b}$$

Interestingly, we see that when $g < \gamma$ (damping dominates over down conversion) the initial condition is washed out for long times, and the cavity mode reaches a stationary state as usual. However, when $g > \gamma$ the position quadrature increases exponentially with time, showing that we enter a special regime where, apparently, no stationary state is reached. We will see in one of the next chapters that what happens is that the parametric approximation breaks down for $g \geq \gamma$, and we have to consider pump depletion. Hence, in what follows we focus on the $g < \gamma$ regime, known as *below-threshold regime* for reasons that will become obvious along the next chapters. In this regime, we can write the asymptotic solution as

$$\lim_{t\to\infty}\tilde{X}(t) = \sqrt{2\gamma}\lim_{t\to\infty}\int_0^t d\tau e^{-(\gamma-g)\tau}\tilde{X}_{\rm in}(t-\tau), \tag{557a}$$

$$\lim_{t\to\infty}\tilde{P}(t) = \sqrt{2\gamma}\lim_{t\to\infty}\int_0^t d\tau e^{-(\gamma+g)\tau}\tilde{P}_{\rm in}(t-\tau). \tag{557b}$$

Before commenting on the squeezing properties of the output field, it is interesting to understand the type of asymptotic state reached by the intracavity mode. Since the quantum Langevin equations are linear, we know that the state will be Gaussian, and hence we only need to find the asymptotic mean vector and covariance matrix as usual. Using the statistical properties of the input quadratures (555), we get

$$\lim_{t\to\infty}\langle\tilde{X}(t)\rangle = 0 = \lim_{t\to\infty}\langle\tilde{P}(t)\rangle, \tag{558a}$$

$$\lim_{t\to\infty}\langle\tilde{X}^2(t)\rangle = 2\gamma\lim_{t\to\infty}\int_0^t d\tau\int_0^t d\tau' e^{-(\gamma-g)(\tau+\tau')}\underbrace{\langle\tilde{X}_{\rm in}(t-\tau)\tilde{X}_{\rm in}(t-\tau')\rangle}_{\delta(\tau-\tau')} = 2\gamma\lim_{t\to\infty}\int_0^t d\tau e^{-2(\gamma-g)\tau} = \frac{\gamma}{\gamma-g}, \tag{558b}$$

$$\lim_{t\to\infty}\langle\tilde{P}^2(t)\rangle = 2\gamma\lim_{t\to\infty}\int_0^t d\tau\int_0^t d\tau' e^{-(\gamma+g)(\tau+\tau')}\underbrace{\langle\tilde{P}_{\rm in}(t-\tau)\tilde{P}_{\rm in}(t-\tau')\rangle}_{\delta(\tau-\tau')} = 2\gamma\lim_{t\to\infty}\int_0^t d\tau e^{-2(\gamma+g)\tau} = \frac{\gamma}{\gamma+g}, \tag{558c}$$

$$\lim_{t\to\infty}\left\langle\left(\tilde{X}(t)\tilde{P}(t)\right)^{(s)}\right\rangle = 2\gamma\lim_{t\to\infty}\int_0^t d\tau\int_0^t d\tau' e^{-(\gamma-g)\tau-(\gamma+g)\tau'}\left(\underbrace{\langle\tilde{X}_{\rm in}(t-\tau)\tilde{P}_{\rm in}(t-\tau')\rangle}_{{\rm i}\delta(\tau-\tau')} + \underbrace{\langle\tilde{P}_{\rm in}(t-\tau')\tilde{X}_{\rm in}(t-\tau)\rangle}_{-{\rm i}\delta(\tau-\tau')}\right) = 0, \tag{558d}$$

, where we remind that $(\tilde{X}\tilde{P})^{(s)} = (\tilde{X}\tilde{P}+\tilde{X}\tilde{P})/2$ denotes symmetrization. This expressions lead to a (rotating-picture) Gaussian state with zero mean and covariance matrix

$$\lim_{t\to\infty} V(t) = \begin{pmatrix} (1-\sigma)^{-1} & 0 \\ 0 & (1+\sigma)^{-1} \end{pmatrix}. \tag{559}$$

Here we have defined the parameter $\sigma = g/\gamma$, which determines the distance to threshold. For $\sigma = 0$ (no pump) we then obtain a vacuum state as expected. On the other hand, as the threshold condition $\sigma = 1$ is approached, the momentum quadrature gets more and more squeezed until its variance reaches half the value found in vacuum (50% of quantum noise reduction), that is, $\Delta\tilde{P}^2 \to 0.5$. At the same time, the position quadrature gets antisqueezed, but far more dramatically as threshold is approached, where $\Delta\tilde{X} \to \infty$. Hence, the down-converted mode is in a squeezed state for $\sigma > 0$, but not a minimum-uncertainty one, since $\Delta\tilde{X}\Delta\tilde{P} > 1$.

We are now in conditions of evaluating the noise spectrum of the output field. In this case, instead of using the normally ordered expression (548), the calculation is easier if we use the general definition (547) together with the input-output relations (466), which allow us to write

$$\tilde{X}^{\phi}_{\rm out}(t) = \sqrt{2\gamma}\tilde{X}^{\phi}(t) - \tilde{X}^{\phi}_{\rm in}(t). \tag{560}$$

In addition, we will combine the position and momentum solutions (557) in the single expression

$$\lim_{t\to\infty} \tilde{X}^{\varphi}(t) = \sqrt{2\gamma}\lim_{t\to\infty}\int_0^t d\tau' e^{-\lambda_\varphi \tau'}\tilde{X}^{\varphi}_{\rm in}(t-\tau'), \qquad \varphi = 0, \frac{\pi}{2}. \tag{561}$$

where $\lambda_0 = \gamma - g$ and $\lambda_{\pi/2} = \gamma + g$. Let us start by evaluating the asymptotic two-time correlation functions of the output quadratures, which can be written as the $t \to \infty$ limit of

$$\langle \tilde{X}^{\varphi}_{\rm out}(t)\tilde{X}^{\varphi}_{\rm out}(t+\tau)\rangle = \Big[2\gamma\langle \tilde{X}^{\varphi}(t)\tilde{X}^{\varphi}(t+\tau)\rangle - \sqrt{2\gamma}\langle \tilde{X}^{\varphi}(t)\tilde{X}^{\varphi}_{\rm in}(t+\tau) + \tilde{X}^{\varphi}_{\rm in}(t)\tilde{X}^{\varphi}(t+\tau)\rangle + \langle \tilde{X}^{\varphi}_{\rm in}(t)\tilde{X}^{\varphi}_{\rm in}(t+\tau)\rangle\Big]. \tag{562}$$

We evaluate the different terms for the position and momentum quadratures by using (561) and (555). For the terms involving the input quadrature we get

$$\langle \tilde{X}^{\varphi}_{\rm in}(t)\tilde{X}^{\varphi}_{\rm in}(t+\tau)\rangle = \delta(\tau) \quad \forall(\varphi,t), \tag{563a}$$

$$\lim_{t\to\infty}\langle \tilde{X}^{\varphi}(t)\tilde{X}^{\varphi}_{\rm in}(t+\tau)\rangle = \sqrt{2\gamma}\lim_{t\to\infty}\int_0^t d\tau' e^{-\lambda_\varphi\tau'}\underbrace{\langle \tilde{X}^{\varphi}_{\rm in}(t-\tau')\tilde{X}^{\varphi}_{\rm in}(t+\tau)\rangle}_{\delta(\tau+\tau')} = \begin{cases} \sqrt{2\gamma}e^{\lambda_\varphi\tau} & \tau<0 \\ \sqrt{\gamma/2} & \tau=0 \\ 0 & \tau>0 \end{cases}, \tag{563b}$$

$$\lim_{t\to\infty}\langle \tilde{X}^{\varphi}_{\rm in}(t)\tilde{X}^{\varphi}(t+\tau)\rangle = \sqrt{2\gamma}\lim_{t\to\infty}\int_0^t d\tau' e^{-\lambda_\varphi\tau'}\underbrace{\langle \tilde{X}^{\varphi}_{\rm in}(t)\tilde{X}^{\varphi}_{\rm in}(t+\tau-\tau')\rangle}_{\delta(\tau-\tau')} = \begin{cases} 0 & \tau<0 \\ \sqrt{\gamma/2} & \tau=0 \\ \sqrt{2\gamma}e^{-\lambda_\varphi\tau} & \tau>0 \end{cases}. \tag{563c}$$

On the other hand, the term involving only intracavity quadratures requires a bit more attention

$$\langle \tilde{X}^{\varphi}(t)\tilde{X}^{\varphi}(t+\tau)\rangle = 2\gamma\lim_{t\to\infty}\int_0^t d\tau_1\int_0^{t+\tau} d\tau_2 e^{-\lambda_\varphi(\tau_1+\tau_2)}\underbrace{\langle \tilde{X}^{\varphi}_{\rm in}(t-\tau_1)\tilde{X}^{\varphi}_{\rm in}(t+\tau-\tau_2)\rangle}_{\delta(\tau_1+\tau-\tau_2)}. \tag{564}$$

Since the domain of integration of τ_2 is different than that of τ_1, we have to be careful with the application of the delta function, which provides the condition $\tau_1 = \tau_2 - \tau$ only as long as the domains of both sides of the expression overlap (otherwise gives a zero). When $\tau > 0$, the domain of τ_2 is larger than the domain of τ_1 (see Fig. **ToDo**a). In particular, the condition $\tau_1 = \tau_2 - \tau$ cannot be satisfied when $\tau_2 \in [0,\tau[$ since $\tau_1 \in [0,t]$. Hence we integrate only over the latter domain

$$\langle \tilde{X}^{\varphi}(t)\tilde{X}^{\varphi}(t+\tau)\rangle = 2\gamma\lim_{t\to\infty}\int_0^t d\tau_1 e^{-2\lambda_\varphi\tau_1-\lambda_\varphi\tau} = 2\gamma\lim_{t\to\infty}\frac{1-e^{-2\lambda_\varphi t}}{2\lambda_\varphi}e^{-\lambda_\varphi\tau} = \frac{\gamma}{\lambda_\varphi}e^{-\lambda_\varphi\tau}. \tag{565}$$

On the other hand, when $\tau < 0$, the domain of τ_1 is larger than that of τ_2 (see Fig. **ToDo**a). Now the condition $\tau_1 = \tau_2 - \tau = \tau_2 + |\tau|$ cannot be satisfied when $\tau_1 \in [0,|\tau|[$ since $\tau_2 \in [0, t-|\tau|]$. Hence, in this case we integrate over the domain of τ_2

$$\langle \tilde{X}^{\varphi}(t)\tilde{X}^{\varphi}(t+\tau)\rangle = 2\gamma\lim_{t\to\infty}\int_0^{t+\tau} d\tau_2 e^{-2\lambda_\varphi\tau_2+\lambda_\varphi\tau} = 2\gamma\lim_{t\to\infty}\frac{1-e^{-2\lambda_\varphi(t+\tau)}}{2\lambda_\varphi}e^{\lambda_\varphi\tau} = \frac{\gamma}{\lambda_\varphi}e^{\lambda_\varphi\tau}. \tag{566}$$

Therefore, putting both results together, we obtain

$$\langle \tilde{X}^{\varphi}(t)\tilde{X}^{\varphi}(t+\tau)\rangle = \frac{\gamma}{\lambda_{\varphi}} e^{-\lambda_{\varphi}|\tau|}. \tag{567}$$

Combining (563) and (567), we write the asymptotic two-time correlation function of the output quadratures (562) as

$$\lim_{t\to\infty} \langle \tilde{X}^{\varphi}_{\text{out}}(t)\tilde{X}^{\varphi}_{\text{out}}(t+\tau)\rangle = 2\gamma\left(\frac{\gamma}{\lambda_{\varphi}} - 1\right) e^{-\lambda_{\varphi}|\tau|} + \delta(\tau). \tag{568}$$

Note that this function is independent of t and it is symmetric in τ. Therefore, we can use the Fourier-transform expression (547) of the quadrature noise spectrum, obtaining

$$\begin{aligned} V^{\varphi}(\Omega) &= \int_{-\infty}^{+\infty} d\tau e^{-\mathrm{i}\Omega\tau}\left[2\gamma\left(\frac{\gamma}{\lambda_{\varphi}} - 1\right) e^{-\lambda_{\varphi}|\tau|} + \delta(\tau)\right] \\ &= 1 + 2\gamma\left(\frac{\gamma}{\lambda_{\varphi}} - 1\right)\left[\int_{-\infty}^{0} d\tau e^{(\lambda_{\varphi}-\mathrm{i}\Omega)\tau} + \int_{0}^{+\infty} d\tau e^{-(\lambda_{\varphi}+\mathrm{i}\Omega)\tau}\right] \\ &= 1 + 2\gamma\left(\frac{\gamma}{\lambda_{\varphi}} - 1\right)\left(\frac{1}{\lambda_{\varphi}-\mathrm{i}\Omega} + \frac{1}{\lambda_{\varphi}+\mathrm{i}\Omega}\right) = 1 + \frac{4\gamma\,(\gamma-\lambda_{\varphi})}{\lambda_{\varphi}^2+\Omega^2}. \end{aligned} \tag{569}$$

Hence, introducing again the parameter $\sigma = g/\gamma$, we finally get the quadrature noise spectrum of the position and momentum quadratures

$$V^{0}(\Omega) = 1 + \frac{4\sigma}{(1-\sigma)^2 + (\Omega/\gamma)^2}, \tag{570a}$$

$$V^{\pi/2}(\Omega) = 1 - \frac{4\sigma}{(1+\sigma)^2 + (\Omega/\gamma)^2}. \tag{570b}$$

For $\sigma = 0$ both spectra are equal to 1 for all noise frequencies Ω, which is consistent with the fact that the intracavity mode is in vacuum. On the other hand, for any other value of σ we get $V^{\pi/2}(\Omega) < 1$ and $V^{0}(\Omega) > 1$, showing that the output field is in a momentum-squeezed state. However, contrary to the intracavity field, as the threshold $\sigma = 1$ is approached, the squeezing of the output field becomes perfect at zero noise frequency, $V^{\pi/2}(\Omega = 0) \to 0$. Moreover, again in contrast to the intracavity field, the output field is in a minimum uncertainty state, as we see that $V^{0}(\Omega)V^{\pi/2}(\Omega) = 1 \quad \forall(\Omega,\sigma)$. Finally, note that the shape of the spectra is Lorentzian, with a width given by the cavity decay rate, which sets the spectral bandwidth around which we can expect quantum noise reduction.

Let us conclude by pointing out that these devices, optical parametric oscillators, are the ones currently used in quantum optics and quantum information experiments for the production of the highest quality squeezed light, reaching impressive squeezing levels (the current record standing at 97% of quantum noise reduction [70]).

VII. ELIMINATION OF SPURIOUS DEGREES OF FREEDOM: EFFECTIVE MODELS

Strictly speaking, all the models that we have used so far (and essentially all the models used in quantum optics, condensed matter, atomic physics, etc...) are effective, in the sense that they do not describe all their fundamental constituents and elementary interactions, but rather consider a few relevant degrees of freedom that emerge from them. While these relevant degrees of freedom appear very natural in many situations, it is interesting to understand more deeply the reasons under which they emerge, and design systematic ways of deriving the corresponding effective models.

We have already seen a few situations leading to effective models. First, when describing an atom, we implicitly assumed that the strong force confining quarks inside protons and neutrons, and even the strong nuclear force binding the nucleons into atomic nuclei, are so large compared with the frequencies and the powers of common lasers, that we can simply take the whole nuclei as a single particle. This is an example of strongly correlated systems in which many degrees of freedom merge into just a few effective ones. We went through another example when discussing open systems and the master equation in particular: the environment (external field) was so large as compared with the system (atom or cavity mode), that the latter had little-to-none effect on the former. Moreover, the dynamics of the environment occur on a much faster time scale than that of the system, as shown by the fact that environmental correlation functions decayed instantaneously within the Markov approximation. Hence, in such situations, one can find an effective description for the dynamics of the system, for which the environment is essentially frozen in some fixed state.

Hence, we see that the concept of effective theories is rooted at the heart of quantum optics, or more generally, quantum mechanics at low energies. Moreover, in recent decades we have stopped looking at effective theories as some kind of natural phenomena, but rather as something that we can exploit to engineer desired (effective) models in our experimental systems.

In this section we are going to analyze this scenario, showing systematic methods for the derivation of effective models both for closed and open systems. We apply these methods to two very relevant examples: the engineering of effective motional potentials and zero-temperature effective environments for an atom via its coupling to light.

A. Elimination in closed systems

There are many methods designed to find effective Hamiltonians in closed systems. Some of them are quite general, while others are more applied to particular scenarios. Which one of them is better, actually depends on the specific problem. However, there are two methods which have found a wide range of applicability. The first one, which we introduce next, is based on projector operators, and works very well when we can identify the sector of the Hilbert space we are interested in and captures most (ideally all) the system excitations. The second one, known as Schrieffer-Wolff or Frölich transformation, is essentially equivalent to Hamiltonian-eigensystem perturbation theory, but leading to explicit and simple expressions for the different perturbation terms directly in the Hamiltonian (**not shown yet in the notes**).

1. Projection operators method

With full generality, consider a closed system evolving according to a Hamiltonian $\hat{H}$, that is, its state $|\psi(t)\rangle$ satisfies the Schrödinger equation $\mathrm{i}\hbar\partial_t|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$. The idea of the method relies on the fact that we can divide the Hilbert space into a relevant sector (whose effective dynamics we want to describe) and an irrelevant one (whose dynamics is trivial, typically because it stays unpopulated). We then define the projector operator $\hat{P} = \hat{P}^2$, which projects onto the relevant subspace, and its complement $\hat{Q} = 1 - \hat{P}$. Applying this projectors onto the Schrödinger equation, we get the equations

$$\mathrm{i}\hbar\partial_t\hat{P}|\psi(t)\rangle = \hat{P}\hat{H}(\underbrace{\hat{P}+\hat{Q}}_{1})|\psi(t)\rangle = \hat{P}\hat{H}\hat{P}|\psi(t)\rangle + \hat{P}\hat{H}\hat{Q}|\psi(t)\rangle, \tag{571a}$$

$$\mathrm{i}\hbar\partial_t\hat{Q}|\psi(t)\rangle = \hat{Q}\hat{H}(\underbrace{\hat{P}+\hat{Q}}_{1})|\psi(t)\rangle = \hat{Q}\hat{H}\hat{Q}|\psi(t)\rangle + \hat{Q}\hat{H}\hat{P}|\psi(t)\rangle. \tag{571b}$$

which are two coupled equations for the projections $\hat{P}|\psi(t)\rangle$ and $\hat{Q}|\psi(t)\rangle$. We can formally solve the second equation[52], obtaining

$$\hat{Q}|\psi(t)\rangle = \frac{1}{\mathrm{i}\hbar}e^{\hat{Q}\hat{H}t/\mathrm{i}\hbar}\hat{Q}|\psi(0)\rangle + \int_0^t \frac{dt'}{\mathrm{i}\hbar}e^{\hat{Q}\hat{H}(t-t')/\mathrm{i}\hbar}\hat{Q}\hat{H}\hat{P}|\psi(t')\rangle. \tag{573}$$

Naturally, we assume that the system is in the relevant subspace initially, so that $\hat{Q}|\psi(0)\rangle = 0$. Hence, substituting this formal solution into the first equation, we obtain

$$\mathrm{i}\hbar\partial_t\hat{P}|\psi(t)\rangle = \hat{P}\hat{H}\hat{P}|\psi(t)\rangle + \int_0^t \frac{d\tau}{\mathrm{i}\hbar}\hat{P}\hat{H}e^{\hat{Q}\hat{H}\tau/\mathrm{i}\hbar}\hat{Q}\hat{H}\hat{P}|\psi(t-\tau)\rangle, \tag{574}$$

where we have made the integration variable change $t' = t - \tau$. We can rewrite this expression as an effective Schrödinger equation on the relevant part of the state, $\hat{P}|\psi(t)\rangle$. In particular, we know that $|\psi(t-\tau)\rangle = e^{-\hat{H}\tau/\mathrm{i}\hbar}|\psi(t)\rangle$, which allows us to write

$$\begin{aligned}\mathrm{i}\hbar\partial_t\hat{P}|\psi(t)\rangle &= \hat{P}\hat{H}\hat{P}|\psi(t)\rangle + \int_0^t \frac{d\tau}{\mathrm{i}\hbar}\hat{P}\hat{H}e^{\hat{Q}\hat{H}\tau/\mathrm{i}\hbar}\hat{Q}\hat{H}\hat{P}e^{-\hat{H}\tau/\mathrm{i}\hbar}|\psi(t)\rangle, \\ &= \hat{P}\hat{H}\hat{P}|\psi(t)\rangle + \int_0^t \frac{d\tau}{\mathrm{i}\hbar}\hat{P}\hat{H}e^{\hat{Q}\hat{H}\tau/\mathrm{i}\hbar}\hat{Q}\hat{H}\hat{P}e^{-\hat{H}\tau/\mathrm{i}\hbar}(\underbrace{\hat{P}+\hat{Q}}_{1})|\psi(t)\rangle.\end{aligned} \tag{575}$$

Reintroducing (573) and iterating this process, we then obtain $\mathrm{i}\hbar\partial_t\hat{P}|\psi(t)\rangle = \hat{H}_{\mathrm{eff}}(t)\hat{P}|\psi(t)\rangle$, with an effective Hamiltonian given by

$$\hat{H}_{\mathrm{eff}}(t) = \sum_{n=0}^{\infty}\hat{P}\hat{H}\left[\int_0^t \frac{d\tau}{\mathrm{i}\hbar}e^{\hat{Q}\hat{H}\tau/\mathrm{i}\hbar}\hat{Q}\hat{H}\hat{P}e^{-\hat{H}\tau/\mathrm{i}\hbar}\right]^n\hat{P}. \tag{576}$$

There are three interesting things to note about this expression. First, it is not Hermitian. This seems to be at odds with the fact that we take it as an effective Hamiltonian. In fact, this is telling us that, in general, one cannot simply write the effective dynamics of a closed system as another closed system, but rather as an open system, that is, as a mixed state evolving according to a master equation. In fact, we already saw examples of this in Chapter V, where we started from a system+environment model described by a Hamiltonian, but ended up with a master equation for the system, not with an effective Hamiltonian. However, in many situations it indeed occurs that (576) becomes approximately Hermitian under the physical conditions we work on, as we will see in the example we treat in the next section. In general terms, we can expect this to happen when the dynamics and physical conditions do not allow excitations of the system to leak out from the relevant subspace, which is clearly not the case for the open systems considered in Chapter V.

The second interesting thing is that (576) seems to be time-dependent. Hence, it looks like the effective Hamiltonian is time dependent, even if the original Hamiltonian wasn't. However, in most situations one can show that the time-dependent terms are negligible within rotating-wave like approximations. This will again become clear with the example of the next section.

The final and most interesting thing to note is that, in general we can decompose the Hamiltonian as $\hat{H} = \hat{H}_0 + \hat{H}_1$. $\hat{H}_0$ is denoted by *free Hamiltonian* and contains all the terms that do not connect the relevant and irrelevant subspaces, that is, $\hat{P}\hat{H}_0\hat{Q} = 0 = \hat{Q}\hat{H}_0\hat{P}$. On the other hand, $\hat{H}_1$ is denoted by *interaction Hamiltonian* and gathers the rest of the terms. Note that we can even assume without loss of generality that $\hat{P}\hat{H}_1\hat{P} = 0$, that is, the interaction Hamiltonian does not connect states within the relevant subspace. It is always possible to ensure such a property, for if that's not the case, we just need to redefine the interaction and free Hamiltonians as $\hat{H}_1 - \hat{P}\hat{H}_1\hat{P}$ and $\hat{H}_0 + \hat{P}\hat{H}_1\hat{P}$, which we can do because $\hat{Q}(\hat{P}\hat{H}_1\hat{P})\hat{P} = 0 = \hat{P}(\hat{P}\hat{H}_1\hat{P})\hat{Q}$. Effective theories are meaningful whenever one can treat $\hat{H}_1$ as a perturbation with respect to $\hat{H}_0$. Hence, we don't need to consider the full effective Hamiltonian (576), but rather terms up to a desired order in the interaction.

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[52] Note that it's formally like (251), but with operators. With full generality, consider the equation $\partial_t|\psi\rangle = \hat{V}|\psi\rangle + |\chi(t)\rangle$. The solution is found following similar steps as with (251). First we make the change $|\Psi(t)\rangle = e^{-\hat{V}t}|\psi(t)\rangle$, so that $\partial_t|\Psi\rangle = e^{-\hat{V}t}(\partial_t|\psi\rangle - \hat{V}|\psi\rangle) = e^{-\hat{V}t}|\chi(t)\rangle \Rightarrow |\Psi(t)\rangle = |\Psi(t_0)\rangle + \int_{t_0}^t dt' e^{-\hat{V}t'}|\chi(t')\rangle$. Then, undoing the variable change as $|\psi(t)\rangle = e^{\hat{V}t}|\Psi(t)\rangle$, we find

$$|\psi(t)\rangle = e^{\hat{V}(t-t_0)}|\psi(t_0)\rangle + \int_{t_0}^t dt' e^{\hat{V}(t-t')}|\chi(t')\rangle. \tag{572}$$

Terms of order larger than two require a Dyson expansion of the exponentials, which is not difficult, but rather cumbersome. Let us then consider here terms up to second order, which we find just by taking up $n = 1$ in the sum, and replacing $\hat{H}$ by $\hat{H}_0$ in the exponentials, obtaining

$$\hat{H}_{\rm eff}(t) = \hat{P}\hat{H}\hat{P} + \int_0^t \frac{d\tau}{\mathrm{i}\hbar}\hat{P}\hat{H}e^{\hat{Q}\hat{H}_0\tau/\mathrm{i}\hbar}\hat{Q}\hat{H}\hat{P}e^{-\hat{H}_0\tau/\mathrm{i}\hbar}\hat{P}. \tag{577}$$

This expression can be simplified even further by using $[\hat{P}, \hat{H}_0] = 0 = [\hat{Q}, \hat{H}_0]$, which follows directly from $0 = \hat{P}\hat{H}_0\hat{Q} - \hat{Q}\hat{H}_0\hat{P} = \hat{P}\hat{H}_0(\hat{1} - \hat{P}) - (\hat{1} - \hat{P})\hat{H}_0\hat{P} = [\hat{P}, \hat{H}_0]$. This ensures that the relevant subspace can be chosen as a subset of the eigenspace of the free Hamiltonian. Using this property, we can then move $\hat{Q}$ down from the first exponential as

$$e^{\hat{Q}\hat{H}_0\tau/\mathrm{i}\hbar} = \sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{\tau}{\mathrm{i}\hbar}\right)^k \underbrace{\hat{Q}\hat{H}_0\hat{Q}\hat{H}_0\ldots\hat{Q}\hat{H}_0}_{k\text{ times}} = \sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{\tau}{\mathrm{i}\hbar}\right)^k \underbrace{\hat{Q}^k}_{\hat{Q}}\hat{H}_0^k = \hat{Q}e^{\hat{H}_0\tau/\mathrm{i}\hbar}, \tag{578}$$

leading to

$$\hat{H}_{\rm eff}(t) = \hat{P}\hat{H}\hat{P} + \int_0^t \frac{d\tau}{\mathrm{i}\hbar}\hat{P}\hat{H}\hat{Q}e^{\hat{H}_0\tau/\mathrm{i}\hbar}\hat{Q}\hat{H}\hat{P}e^{-\hat{H}_0\tau/\mathrm{i}\hbar}\hat{P}. \tag{579}$$

Using next $\hat{P}\hat{H}\hat{P} = \hat{P}\hat{H}_0\hat{P}$, $\hat{P}\hat{H}\hat{Q} = \hat{P}\hat{H}_1\hat{Q} = \hat{P}\hat{H}_{AB}(1 - \hat{P}) = \hat{P}\hat{H}_{AB}$, and similarly $\hat{Q}\hat{H}\hat{P} = \hat{H}_{AB}\hat{P}$, we obtain the final form of the effective Hamiltonian up to second order in the interaction

$$\hat{H}_{\rm eff}(t) = \hat{P}\hat{H}_0\hat{P} + \int_0^t \frac{d\tau}{\mathrm{i}\hbar}\hat{P}\hat{H}_1\tilde{H}_1(t)\hat{P}, \tag{580}$$

where

$$\tilde{H}_1(\tau) = e^{\hat{H}_0\tau/\mathrm{i}\hbar}\hat{H}_1e^{-\hat{H}_0\tau/\mathrm{i}\hbar}. \tag{581}$$

This is a very simple expression whose use we put in practice next with an important example.

2. Optical motional potential on an atom

Let us now consider a particular example: an atom whose center of mass is free to move, interacts with a classical optical field very far detuned from the atomic transition. At a first sight, it might seem like nothing will happen, since the field is far detuned. However, we will see that a perturbative effective motional potential with the shape of the intensity of the optical beam is generated on the atomic motion.

The problem is defined by two degrees of freedom. First, the center-of-mass motion, whose position and momentum operators we denote, respectively, by $\hat{z}$ and $\hat{p}$ (as usual, we stick to the quasi-1D model we have been using), and evolves according to the Hamiltonian $\hat{p}^2/2m$, where m is the mass of the atom. The other degree of freedom refers to the relative atomic coordinate (sometimes denoted by *internal* or *electronic* degree of freedom), which we treat in the usual way defined in Chapter III within the two-level approximation, evolving according to the the Hamiltonian $\hbar\varepsilon\hat{\sigma}_z/2$. We connect these two degrees of freedom by using a laser whose power we allow to vary spatially, leading to an interaction Hamiltonian $\hbar\left[\Omega^*(\hat{z})e^{\mathrm{i}\omega_{\rm L}t}\hat{\sigma} + \Omega(\hat{z})e^{-\mathrm{i}\omega_{\rm L}t}\hat{\sigma}\right]/2$ within the rotating-wave approximation. Moving to a picture rotating at the laser frequency as usual, we then obtain the time-independent Hamiltonian

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} + \frac{\hbar\Delta}{2}\hat{\sigma}_z}_{\hat{H}_0} + \underbrace{\frac{\hbar}{2}\left[\Omega^*(\hat{z})\hat{\sigma} + \Omega(\hat{z})\hat{\sigma}^\dagger\right]}_{\hat{H}_1}, \tag{582}$$

where we have defined the detuning as $\Delta = \varepsilon - \omega_{\rm L}$. We are interested in the effective dynamics of the system when the laser is far off resonance, that is, $|\Delta| \gg |\Omega|$. As we learned in previous chapters, we don't expect anything to happen to the internal dynamics of the atom. In particular, initializing the atom in the ground state, we expect it to remain in that state, and hence we define the projector $\hat{P} = |g\rangle\langle g|$, which acts as the identity in the motional space. We will show, however, that some nontrivial effective dynamics will be induced in the center of mass motion of the atom.

Let us first note that $\hat{P}\hat{H}_1\hat{P} \propto \langle g|\hat{H}_1|g\rangle = 0$ in this case. On the other hand, defining the kinetic evolution operator $\hat{K}(\tau) = \exp\left(-\mathrm{i}\hat{p}^2\tau/2m\hbar\right)$, we can write

$$\tilde{H}_1(\tau) = \frac{\hbar}{2}\left[\hat{K}(\tau)\Omega^*(\hat{z})\hat{K}^\dagger(\tau)\hat{\sigma}e^{\mathrm{i}\Delta\tau} + \hat{K}(\tau)\Omega(\hat{z})\hat{K}^\dagger(\tau)\hat{\sigma}^\dagger e^{-\mathrm{i}\Delta\tau}\right], \tag{583}$$

and hence

$$\langle g|\hat{H}_1\tilde{H}_1(\tau)|g\rangle = \frac{\hbar^2}{4}e^{-\mathrm{i}\Delta\tau}\Omega^*(\hat{z})\hat{K}(\tau)\Omega(\hat{z})\hat{K}^\dagger(\tau), \tag{584}$$

where we have used $\hat{\sigma}^2 = 0 = \langle g|\hat{\sigma}^\dagger\hat{\sigma}|g\rangle$ and $\langle g|\hat{\sigma}\hat{\sigma}^\dagger|g\rangle = 1$. We then write the effective Hamiltonian (580) as

$$\hat{H}_{\mathrm{eff}}(t) = \Bigg[\underbrace{-\frac{\hbar\Delta}{2}}_{\frac{\hbar\Delta}{2}\langle g|\hat{\sigma}_z|g\rangle} + \frac{\hat{p}^2}{2m} - \frac{\mathrm{i}\hbar}{4}\int_0^t d\tau e^{-\mathrm{i}\Delta\tau}\Omega^*(\hat{z})\hat{K}(\tau)\Omega(\hat{z})\hat{K}^\dagger(\tau)\Bigg]|g\rangle\langle g|. \tag{585}$$

We finally assume that the atoms have been cooled down, so their kinetic energy is small in the sense $\langle\hat{p}^2\rangle/2m \ll \hbar|\Delta|$. We can then neglect the kinetic evolution inside the integral under a rotating-wave approximation, finally obtaining

$$\hat{H}_{\mathrm{eff}}(t) \approx \left[-\frac{\hbar\Delta}{2} + \frac{\hat{p}^2}{2m} - \frac{\hbar|\Omega(\hat{z})|^2}{4\Delta}\left(1 - e^{-\mathrm{i}\Delta t}\right)\right]|g\rangle\langle g| \approx \left[-\frac{\hbar\Delta}{2} + \frac{\hat{p}^2}{2m} - \frac{\hbar|\Omega(\hat{z})|^2}{4\Delta}\right]|g\rangle\langle g|, \tag{586}$$

where in the last step we have have dropped out the $e^{-\mathrm{i}\Delta t}$ term, again within a rotating-wave approximation, since $|\Omega(\hat{z})| \ll |\Delta|$. Hence, we see that the laser induces an effective potential $V_{\mathrm{opt}}(\hat{z}) = -\hbar|\Omega(\hat{z})|^2/4\Delta$ on the atom's motion, which is known as *optical potential*. Alternatively, this effect can be understood as an energy shift $V_{\mathrm{opt}}(\hat{z})$ of the ground-state energy, a phenomenon known as *AC Stark shift*, which occurs even when the atom's center of mass is fixed. Hence, even though the laser is not capable of transferring population from the ground to the excited state, it has a perturbative effect on the atomic energy levels in the form of a shift (it can be easily proven that the excited state feels an opposite AC Stark shift $-V_{\mathrm{opt}}$).

B. Elimination in open systems

1. *Projection superoperators method*

Let us now generalize the previous methods for obtaining effective models to open systems. The same kind of general principles can be applied to the von Neumann or master equations. Here, we focus on the generalization of the projector-operator method. Consider hence a system whose state $\hat{\rho}$ evolves according to a master equation $\partial_t\hat{\rho} = \mathcal{L}[\hat{\rho}]$, with a time-independent Liouvillian for simplicity as usual. Let us define a projector superoperator $\mathcal{P} = \mathcal{P}^2$, as well as its complement $\mathcal{Q} = 1 - \mathcal{P}$. In this case, it is more difficult to interpret such objects, since they do not directly project in the Hilbert space, but in the space of operators. Sometimes, though, their action is similar to the one of the projector operators that we encounter in the previous section: they simply divides the Hilbert space in relevant states and irrelevant states. However, since now we are dealing with mixed states, in general we need to do that by defining a set of relevant and irrelevant (density) operators. In any case, the meaning of these projection superoperators will become clearer through examples later. Acting on the master equation with this projectors, we then find

$$\partial_t\mathcal{P}[\hat{\rho}] = \mathcal{P}\mathcal{L}\underbrace{(\mathcal{P}+\mathcal{Q})}_{1}[\hat{\rho}] = \mathcal{P}\mathcal{L}\mathcal{P}[\hat{\rho}] + \mathcal{P}\mathcal{L}\mathcal{Q}[\hat{\rho}], \tag{587a}$$

$$\partial_t\mathcal{Q}[\hat{\rho}] = \mathcal{Q}\mathcal{L}\underbrace{(\mathcal{P}+\mathcal{Q})}_{1}[\hat{\rho}] = \mathcal{Q}\mathcal{L}\mathcal{Q}[\hat{\rho}] + \mathcal{Q}\mathcal{L}\mathcal{P}[\hat{\rho}]. \tag{587b}$$

Our goal is finding an effective evolution equation for the relevant part of the state $\mathcal{P}[\hat{\rho}]$. For that, we simply integrate formally the second equation[53], obtaining

$$\mathcal{Q}[\hat{\rho}(t)] = e^{\mathcal{Q}\mathcal{L}t}\mathcal{Q}[\hat{\rho}(0)] + \int_0^t dt' e^{\mathcal{Q}\mathcal{L}(t-t')}\mathcal{Q}\mathcal{L}\mathcal{P}[\hat{\rho}(t')]. \tag{589}$$

[53] We simply need to generalize (572) by interpreting operators as vectors in the space of operators, and superoperators as operators acting on such space. Hence, the solution to $\partial_t\hat{\rho} = \mathcal{M}[\hat{\rho}] + \hat{\chi}(t)$ is easily found as

$$\hat{\rho}(t) = e^{\mathcal{M}(t-t_0)}[\hat{\rho}(t_0)] + \int_{t_0}^t dt' e^{\mathcal{M}(t-t')}[\hat{\chi}(t')]. \tag{588}$$

The first term depends on the initial condition and can be eliminated under either one of the following physical assumptions: either the initial state belongs already to the relevant subspace, or we are interested in the asymptotic dynamics only, which should not depend on the initial condition for well-behaved open systems, as we have seen in previous chapters. Hence, substituting this expression into the first equation we obtain

$$\partial_t \mathcal{P}[\hat{\rho}] = \mathcal{P}\mathcal{L}\mathcal{P}[\hat{\rho}] + \int_0^t d\tau \mathcal{P}\mathcal{L}e^{\mathcal{Q}\mathcal{L}\tau}\mathcal{Q}\mathcal{L}\mathcal{P}[\hat{\rho}(t-\tau)], \tag{590}$$

where we made the integration variable change $\tau = t - t'$. Up to here, the derivation has followed exactly the same steps as with the closed system, just with the obvious generalizations. To continue the equivalence, we would now need to write the state $\hat{\rho}(t-\tau)$ as $\hat{\rho}(t)$ evolved backwards during a time τ. While for closed systems this is useful because the time-evolution is very simple, for open systems it doesn't really leads us to a practical form of the effective Liouvillian. Hence, it is better to proceed for now with this time-nonlocal equation.

Similarly to the closed system, we now expand the Liouvillian as $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$. The first term, denoted by *free Liouvillian*, contains only terms that do not connect the relevant and irrelevant subspaces, that is, $\mathcal{P}\mathcal{L}_0\mathcal{Q} = 0 = \mathcal{Q}\mathcal{L}_0\mathcal{P}$. The second term, denoted by *interaction Liouvillian*, contains the rest of terms, and we can assume that $\mathcal{P}\mathcal{L}_1\mathcal{P} = 0$ with full generality, following the arguments given for closed systems. Just as with the latter, also for open systems effective theories only make sense as long as the interaction Liouvillian can be treated as a perturbation. We then truncate to second order in $\mathcal{L}_1$ and follow similar steps as we did for the closed case, obtaining the effective (time-nonlocal) master equation

$$\partial_t \mathcal{P}[\hat{\rho}] \approx \mathcal{P}\mathcal{L}_0\mathcal{P}[\hat{\rho}] + \int_0^t d\tau \mathcal{P}\mathcal{L}_1 e^{\mathcal{L}_0\tau}\mathcal{L}_1\mathcal{P}[\hat{\rho}(t-\tau)]. \tag{591}$$

In order to proceed forward, we consider now one specific situation that it's usually the most interesting one in open quantum optical settings. We consider a bipartite scenario consisting on a *system* and an *environment* with Hilbert spaces $\mathcal{H}_\mathrm{S}$ and $\mathcal{H}_\mathrm{E}$ respectively, so that the total Hilbert space is $\mathcal{H} = \mathcal{H}_\mathrm{S} \otimes \mathcal{H}_\mathrm{E}$. The notation already suggests that we will treat the case in which the environment remains essentially frozen from the point of view of the system, so that we can find an effective master equation for the latter in a similar way how we did it in Chapter V. However, in contrast to that chapter, we will not assume here that the environment is a huge system, but rather study the conditions under which such effective theory can be developed. Indeed, we will see that even when the environment is 'small', one can still use it to induce effective dynamics on the system as long as it satisfies certain conditions (e.g., couple weakly to the system and decay much faster than it).

Let us then write the free Liouvillian as $\mathcal{L}_0 = \mathcal{L}_\mathrm{S} + \mathcal{L}_\mathrm{E}$, where $\mathcal{L}_\mathrm{S}$ acts nontrivially only onto system operators and $\mathcal{L}_\mathrm{E}$ onto environment operators, so that $[\mathcal{L}_\mathrm{S}, \mathcal{L}_\mathrm{E}] = 0$. As the reference state for the environment we take its asymptotic state $\bar{\rho}_\mathrm{E}$, defined by $\mathcal{L}_\mathrm{E}[\bar{\rho}_\mathrm{E}] = 0$. Consequently, we take as the relevant subspace the one defined by density operators that match this reference one for the environment, leading to a projector superoperator $\mathcal{P}$ defined by the following action on any operator $\hat{Y}$:

$$\mathcal{P}[\hat{Y}] = \mathrm{tr}_\mathrm{E}\{\hat{Y}\} \otimes \bar{\rho}_\mathrm{E}. \tag{592}$$

Denoting the system's state by $\hat{\rho}_\mathrm{S} = \mathrm{tr}_\mathrm{E}\{\hat{\rho}\}$, we then rewrite the effective master equation (591) as

$$\partial_t \hat{\rho}_\mathrm{S} \approx \mathcal{L}_\mathrm{S}[\hat{\rho}_\mathrm{S}] + \int_0^t d\tau \mathrm{tr}_\mathrm{E}\left\{\mathcal{L}_1 e^{\mathcal{L}_0\tau}\mathcal{L}_1[\hat{\rho}_\mathrm{S}(t-\tau)\otimes\bar{\rho}_\mathrm{E}]\right\}, \tag{593}$$

where we have performed a trace over the environment. In order to simplify further, we need to give a form to the interaction. Usually, we are interested in cases in which the system and the environment are connected by a Hamiltonian, say $\hat{H}_1$. We will assume this in the following, although the next steps are easily generalizable to any other situation. Moreover, we assume that the interaction admits some kind of polynomial expansion in terms of products of system and environment operators, that is

$$\hat{H}_1/\hbar = \sum_{m=1}^{M} g_m \hat{S}_m \otimes \hat{E}_m, \tag{594}$$

where we note that $\hat{H}_1 = \hat{H}_1^\dagger$ imposes a restriction on the set of operators, that is, each product must either be Hermitian or have its Hermitian-conjugate counterpart in the set. The interaction Liouvillian acts then as

$$\mathcal{L}_1[\hat{Y}] = \left[\frac{\hat{H}_1}{\mathrm{i}\hbar}, \hat{Y}\right] = -\mathrm{i}\sum_{m=1}^{M} g_m[\hat{S}_m \otimes \hat{E}_m, \hat{Y}], \tag{595}$$

which introduced in (593) leads to

$$\mathrm{tr}_E\left\{\mathcal{L}_1 e^{\mathcal{L}_0\tau}\mathcal{L}_1[\hat{\rho}_\mathrm{S}(t-\tau)\otimes\bar{\rho}_\mathrm{E}]\right\} = \sum_{m,n=1}^{M} g_m g_n \Big(\mathrm{tr}_\mathrm{E}\left\{\hat{E}_n e^{\mathcal{L}_\mathrm{E}\tau}\left[\bar{\rho}_\mathrm{E}\hat{E}_m\right]\right\}\hat{S}_n e^{\mathcal{L}_\mathrm{S}\tau}\left[\hat{\rho}_\mathrm{S}(t-\tau)\hat{S}_m\right] - \mathrm{tr}_\mathrm{E}\left\{\hat{E}_n e^{\mathcal{L}_\mathrm{E}\tau}\left[\hat{E}_m\bar{\rho}_\mathrm{E}\right]\right\}\hat{S}_n e^{\mathcal{L}_\mathrm{S}\tau}\left[\hat{S}_m\hat{\rho}_\mathrm{S}(t-\tau)\right]\Big) + \mathrm{H.c.}. \tag{596}$$

Invoking now the quantum regression theorem (496), we see that the terms involving traces over the environment are nothing but asymptotic two-time correlators that we denote by

$$\mathrm{tr}_\mathrm{E}\left\{\hat{E}_n e^{\mathcal{L}_\mathrm{E}\tau}\left[\bar{\rho}_\mathrm{E}\hat{E}_m\right]\right\} = \lim_{t\to\infty}\langle\hat{E}_m(t)\hat{E}_n(t+\tau)\rangle_\mathrm{E} = C_{mn}(\tau), \tag{597a}$$

$$\mathrm{tr}_\mathrm{E}\left\{\hat{E}_n e^{\mathcal{L}_\mathrm{E}\tau}\left[\hat{E}_m\bar{\rho}_\mathrm{E}\right]\right\} = \lim_{t\to\infty}\langle\hat{E}_n(t+\tau)\hat{E}_m(t)\rangle_\mathrm{E} = K_{nm}(\tau), \tag{597b}$$

where the subscript 'E' in the expectation value denotes that it is related to the free-environment Liouvillian, not to the whole Liouvillian. Note that $K_{nm}(\tau) = \lim_{t\to\infty}\langle\hat{E}_n(t)\hat{E}_m(t-\tau)\rangle_\mathrm{E} = C_{nm}(-\tau)$, which is sometimes useful. Inserting these correlators in the previous expression, we get to

$$\mathrm{tr}_\mathrm{E}\left\{\mathcal{L}_1 e^{\mathcal{L}_0\tau}\mathcal{L}_1[\hat{\rho}_\mathrm{S}(t-\tau)\otimes\bar{\rho}_\mathrm{E}]\right\} \approx \sum_{m,n=1}^{M} g_m g_n \left(C_{mn}(\tau)\hat{S}_n e^{\mathcal{L}_\mathrm{S}\tau}\left[\hat{\rho}_\mathrm{S}(t-\tau)\hat{S}_m\right] - K_{nm}(\tau)\hat{S}_n e^{\mathcal{L}_\mathrm{S}\tau}\left[\hat{S}_m\hat{\rho}_\mathrm{S}(t-\tau)\right]\right) + \mathrm{H.c.}. \tag{598}$$

We arrive then to the crucial assumption that will allow us to find a time-local effective master equation for the system: we assume that the correlation functions $C_{mn}(\tau)$ and $K_{nm}(\tau)$ are either zero or decay as a function of τ, at a much faster rate than any process affecting the system, except for some Hamiltonian term that we denote by $\hat{H}_\mathrm{S}$. Typically $\hat{H}_\mathrm{S}$ corresponds to some Hamiltonian terms of $\mathcal{L}_\mathrm{S}$. On the other hand, we must check this approximation carefully, estimating the rate of the processes taken into account both $\mathcal{L}_\mathrm{S}$ and the final effective Liouvillian, in a self-consistent manner. This will become clear in the example of the next section. Applied to the previous expression, this approximation amounts to

$$\hat{\rho}_\mathrm{S}(t-\tau) \approx e^{-\hat{H}_\mathrm{S}\tau/\mathrm{i}\hbar}\hat{\rho}_\mathrm{S}(t)e^{\hat{H}_\mathrm{S}\tau/\mathrm{i}\hbar}, \tag{599a}$$

$$e^{\mathcal{L}_\mathrm{S}\tau}[\hat{S}] \approx e^{\hat{H}_\mathrm{S}\tau/\mathrm{i}\hbar}\hat{S}e^{-\hat{H}_\mathrm{S}\tau/\mathrm{i}\hbar}, \tag{599b}$$

where $\hat{S}$ can be any system operators, finally obtaining the effective time-local master equation

$$\partial_t\hat{\rho}_\mathrm{S} \approx \mathcal{L}_\mathrm{S}[\hat{\rho}_\mathrm{S}] + \sum_{m,n=1}^{M} g_m g_n \int_0^t d\tau\left[C_{mn}(\tau)\hat{S}_n\hat{\rho}_\mathrm{S}(t)\tilde{S}_m(\tau) - K_{nm}(\tau)\hat{S}_n\tilde{S}_m(\tau)\hat{\rho}_\mathrm{S}(t)\right] + \mathrm{H.c.}, \tag{600}$$

with $\tilde{S}(\tau) = e^{\hat{H}_S\tau/\mathrm{i}\hbar}\hat{S}e^{-\hat{H}_S\tau/\mathrm{i}\hbar}$.

Note that, in general, the effective master equation is time dependent, even if we started with a time-independent problem. However, in most situations the time-dependent terms can be neglected by using either one of the following two arguments: either a rotating-wave approximation naturally arising from the fact that the interaction Liouvillian is small (similarly to the effective Hamiltonian of the previous section); or the fact that we are interested in the asymptotic limit, where the time dependent terms have already died off. This, and all the other steps of the procedure, will become clear with the example that we analyze next.

2. *Cooling and Purcell enhancement of the atomic decay*

Consider the following scenario. We have a two-level atom at a much higher temperature than we'd like, meaning that it is described by a master equation (434) with a relatively large $\bar{n}$, and radiating equally in all spatial directions (further, we assume that it is not driven, $\mathcal{E} = 0$). We now show how to cool down the atom effectively just by (strongly[54]) coupling it to an open cavity at zero temperature, which will also have the effect of directing most of the atomic spontaneous emission towards the direction defined by the cavity.

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[54] This refers to the *strong coupling regime*, which in this context is defined as that in which the coupling between light and matter exceeds the atomic spontaneous emission rate. The term *ultrastrong coupling regime* is reserved for when the coupling reaches the atomic transition energies, which has become available in recent implementations based on superconducting circuits.

Consider then the Jaynes-Cummings Hamiltonian (259). We will work in a picture rotating at the atomic frequency both for the atom and the cavity mode, defined by the transformation operator $\hat{U}_{\rm c}(t) = e^{\hat{H}_{\rm c} t/{\rm i}\hbar}$ with $\hat{H}_{\rm c} = \hbar\varepsilon(\hat{a}^\dagger\hat{a} + \hat{\sigma}_z/2)$. Defining the detuning $\Delta = \omega - \varepsilon$, and including the interaction of the cavity and the atom with their respective environments, the transformed state $\tilde{\rho}(t) = \hat{U}_{\rm c}^\dagger(t)\hat{\rho}(t)\hat{U}_{\rm c}(t)$ evolves according to the master equation

$$\frac{d\tilde{\rho}}{dt} = \underbrace{-{\rm i}\left[\Delta\hat{a}^\dagger\hat{a},\tilde{\rho}\right] + \kappa\mathcal{D}_a[\tilde{\rho}]}_{\mathcal{L}_{\rm E}[\tilde{\rho}]} + \underbrace{\gamma(\bar{n}+1)\mathcal{D}_\sigma[\tilde{\rho}] + \gamma\bar{n}\mathcal{D}_{\sigma^\dagger}[\tilde{\rho}]}_{\mathcal{L}_{\rm S}[\tilde{\rho}]} \underbrace{-{\rm i}\left[\underbrace{g(\hat{a}\sigma^\dagger + \hat{a}^\dagger\hat{\sigma})}_{\hat{H}_1/\hbar},\tilde{\rho}\right]}_{\mathcal{L}_1}. \tag{601}$$

Note that we have chosen a different phase for the coupling constant g with respect to (259), which means that in this case we take the dipole matrix element $\langle g|\hat{x}_A|e\rangle$ as purely imaginary. This will simplify the upcoming derivations but makes no fundamental difference for the results we will find. Note also that we have denoted the cavity decay rate by κ.

Let us first argue qualitatively how these equations predict that the atom will get cooled down. Set $\Delta = 0$ for simplicity, and imagine that before the interaction is switched on, we have the atom in equilibrium thermal state, and the cavity empty. Starting in such state, once we switch on the interaction, what will happen is that the $\hat{a}^\dagger\hat{\sigma}$ Jaynes-Cummings Hamiltonian will destroy an atomic excitation and create a photon in the cavity. Now, if $\kappa \gg g$, the photon will leave the cavity before the atom can reabsorb it. On the other hand, the environment will try to bring the atom to the thermal state, but if $g \gg \gamma$, then we expect the Jaynes-Cummings interaction to transfer any atomic excitation to the cavity before the atom can equilibrate with its environment. Hence, provided the hierarchy $\kappa \gg g \gg \gamma$ is satisfied, the atom will be effectively decoupled from its thermal environment, and loosing all excitations through the cavity.

Let us prove rigorously that the physical picture explained above is correct. Note that vacuum is the stationary state associated to the free optical problem, $\bar{\rho}_{\rm E} = |0\rangle\langle 0|$. This implies that $\mathcal{P}\mathcal{L}_1\mathcal{P} = 0$, since, acting on any general operator $\hat{Y}$, we obtain

$$\mathcal{P}\mathcal{L}_1\mathcal{P}[\hat{Y}] = \mathcal{P}\mathcal{L}_1\left[{\rm tr}_{\rm E}\{\hat{Y}\}\otimes|0\rangle\langle 0|\right] = -{\rm i}g\left[\underbrace{\langle 0|\hat{a}|0\rangle}_{0}\sigma^\dagger + \underbrace{\langle 0|\hat{a}^\dagger|0\rangle}_{0}\hat{\sigma}, {\rm tr}_E\{\hat{Y}\}\right]\otimes|0\rangle\langle 0|. \tag{602}$$

The interaction Hamiltonian can be written as (594) with the choices $g_1 = g_2 = g$, $\hat{E}_1 = \hat{a} = \hat{E}_2^\dagger$, and $\hat{S}_2 = \hat{\sigma} = \hat{S}_1^\dagger$. In order to evaluate the correlation functions (597), the easiest in this case is to resort to the quantum regression formula (502). In order to lighten up the notation, let us not write tildes on top of the expectation values taken with respect the rotating-picture state, that is, we simply denote ${\rm tr}\{\hat{B}\tilde{\rho}\}$ by $\langle\hat{B}\rangle$. The annihilation operator form a closed set by itself,

$$\frac{d\langle\hat{a}(\tau)\rangle_{\rm E}}{d\tau} = {\rm tr}\{\hat{a}\mathcal{L}_{\rm E}[\tilde{\rho}]\} = -(\kappa + {\rm i}\Delta)\langle\hat{a}(\tau)\rangle_{\rm E} \quad \Rightarrow \quad \begin{cases} \langle\hat{a}(\tau)\rangle_{\rm E} = \langle\hat{a}(0)\rangle_{\rm E}e^{-(\kappa+{\rm i}\Delta)\tau} \\ \langle\hat{a}^\dagger(\tau)\rangle_{\rm E} = \langle\hat{a}^\dagger(0)\rangle_{\rm E}e^{-(\kappa-{\rm i}\Delta)\tau} \end{cases}, \tag{603}$$

so that for any two environment operators $\hat{A}$ and $\hat{C}$, the quantum regression formula (502) tells us that ($\tau > 0$)

$$\lim_{t\to\infty}\langle\hat{C}(t)\hat{a}(t+\tau)\hat{D}(t)\rangle_{\rm E} = \langle 0|\hat{C}\hat{a}\hat{D}|0\rangle_{\rm E}e^{-(\kappa+{\rm i}\Delta)\tau}, \tag{604a}$$

$$\lim_{t\to\infty}\langle\hat{C}(t)\hat{a}^\dagger(t+\tau)\hat{D}(t)\rangle_{\rm E} = \langle 0|\hat{C}\hat{a}^\dagger\hat{D}|0\rangle_{\rm E}e^{-(\kappa-{\rm i}\Delta)\tau}. \tag{604b}$$

Applying these expressions to the relevant correlators, we then get

$$C_{mn}(\tau) = e^{-(\kappa+{\rm i}\Delta)\tau}\delta_{m1}\delta_{n2}, \tag{605a}$$

$$K_{nm}(\tau) = e^{-(\kappa-{\rm i}\Delta)\tau}\delta_{n1}\delta_{m2}, \tag{605b}$$

both of which decay at rate κ. Before substituting these expressions onto the effective master equation (600), note that in this case $\tilde{S}_m(\tau) = \hat{S}_m$, since there is no free atomic Hamiltonian in the picture we are working in. Remember that it is important to come back and check this approximation at the end. Taking also into account that

$$\int_0^t e^{-(\kappa\pm{\rm i}\Delta)\tau} = \frac{1 - e^{-(\kappa\pm{\rm i}\Delta)t}}{\kappa\pm{\rm i}\Delta}, \tag{606}$$

and assuming that we are only interested in times $t \gg \kappa^{-1}$, we obtain the effective master equation

$$\begin{aligned}\partial_t\tilde{\rho}_{\rm S} &\approx \mathcal{L}_{\rm S}[\tilde{\rho}_{\rm S}] + \frac{g^2}{\kappa+{\rm i}\Delta}\hat{\sigma}\tilde{\rho}_{\rm S}\hat{\sigma}^\dagger - \frac{g^2}{\kappa-{\rm i}\Delta}\hat{\sigma}^\dagger\hat{\sigma}\tilde{\rho}_{\rm S} + {\rm H.c.} \\ &= -{\rm i}\underbrace{\frac{g^2\Delta}{\kappa^2+\Delta^2}}_{\Delta\varepsilon}[\hat{\sigma}^\dagger\hat{\sigma},\tilde{\rho}_{\rm S}] + \underbrace{\left(\frac{g^2\kappa}{\kappa^2+\Delta^2}+\gamma(\bar{n}+1)\right)}_{\Gamma_-}\mathcal{D}_\sigma[\tilde{\rho}_{\rm S}] + \underbrace{\gamma\bar{n}}_{\Gamma_+}\mathcal{D}_{\sigma^\dagger}[\tilde{\rho}_{\rm S}].\end{aligned} \tag{607}$$

The notation stresses that $\Delta\varepsilon$ is an atomic energy shift, Γ_- the rate of loss of atomic excitations, and Γ_+ the rate of incoherent gain of atomic excitations. We can come back to the Schrödinger picture and write it in the even more suggestive form

$$\partial_t\hat{\rho}_{\rm S} = -{\rm i}\left[\frac{\varepsilon+\Delta\varepsilon}{2}\hat{\sigma}_z,\hat{\rho}_{\rm S}\right] + \Gamma_{\rm eff}(\bar{n}_{\rm eff}+1)\mathcal{D}_\sigma[\hat{\rho}_{\rm S}] + \Gamma_{\rm eff}\bar{n}_{\rm eff}\mathcal{D}_{\sigma^\dagger}[\hat{\rho}_{\rm S}], \tag{608}$$

with

$$\Gamma_{\rm eff} = \Gamma_- - \Gamma_+ = \gamma\left[1+\frac{g^2/\kappa\gamma}{1+(\Delta/\kappa)^2}\right], \tag{609a}$$

$$\bar{n}_{\rm eff} = \frac{\Gamma_+}{\Gamma_- - \Gamma_+} = \frac{\bar{n}}{1+\frac{g^2/\kappa\gamma}{1+(\Delta/\kappa)^2}}. \tag{609b}$$

This form shows that the atom feels now a different effective thermal environment, with effective thermal excitations $\bar{n}_{\rm eff}$ and effective rate $\Gamma_{\rm eff}$. It is common to define the cooperativity $C = g^2/\kappa\gamma$. Whenever this is large enough, in particular $C \gg \{\bar{n}, 1, 1+(\Delta/\kappa)^2\}$, we obtain $\bar{n}_{\rm eff} \ll 1$, which is exactly what we wanted: an effective temperature close to zero. Moreover, note that $\Gamma_{\rm eff}$ is the sum of two terms. The first one, γ, is related to losses of the atom to its original environment. On the other hand, the second term $\gamma C/[1+(\Delta/\kappa)^2]$ comes from losses through the optical mode into the environment of the cavity, that is, emission radiated through the partially transmitting mirror. Hence, together with cooling, we find that the emission gets redirected mostly in the direction defined by the cavity. This phenomenon is known as *Purcell effect*.

Finally, we need to be careful and check self-consistently that all the required approximations are satisfied in the limit of large cooperativity that we want to work with. In particular, in this case we essentially care about two approximations. First, we need the interaction term to be much smaller than the free term so that our perturbation theory makes sense. Since the dominant scale of the free terms is κ, we then require $\kappa \gg g$. Next, we need to make sure that the incoherent rate of evolution of the atom is much smaller than the correlation time of the environment, which is κ as well according to (605). This means that we require $\kappa \gg \Gamma_{\rm eff} < \gamma C = g^2/\kappa$, a condition that is always satisfied since $\kappa \gg g$ is already assumed. Related to this, there is also one subtle condition: since we have neglected the evolution provided by the effective energy shift in (608), we also require $\kappa \gg \Delta\varepsilon$. This condition is always satisfied, as can be easily argued by inspecting the limits $|\Delta| \ll \kappa$ and $|\Delta| \gg \kappa$. However, note that when $|\Delta| \gg |\kappa|$, the large cooperativity condition $(\Delta/\kappa)^2 \ll C = g^2/\kappa\gamma$ can only be achieved by increasing the coupling g with respect to the atomic spontaneous emission rate γ, which becomes unfeasible experimentally beyond some limit. In any case, while there is no fundamental problem with this cooling method, it is indeed very impractical, because the large cooperativity limit requires $g/\gamma \gg \bar{n}(\kappa/g)$, which is beyond what can be accomplished experimentally, except in some special platforms (certainly not atoms and light).

Appendix A: Review of classical mechanics, Hilbert spaces, and quantum mechanics

The purpose of this appendix is introducing the fundamental principles of quantum mechanics as are used throughout the lectures. The quantum framework is far from being intuitive, but somehow feels reasonable (and even inevitable) once one understands the context in which it was created, specifically: (*i*) the theories that were used to describe physical systems prior to its development, (*ii*) the experiments which did not fit in this context, and (*iii*) the mathematical language that accommodates the new quantum formulation of physical phenomena. We will then briefly review these context prior to introducing and discussing the principles conforming the quantum-mechanical framework.

1. Classical mechanics

In this section we go through a brief introduction to classical mechanics[55], with emphasis in analyzing the Hamiltonian formalism and how it treats observable magnitudes. We will see that a proper understanding of this formalism will make the transition to quantum mechanics more natural.

a. *The Lagrangian formalism*

In classical mechanics the state of a system is specified by the position of its constituent particles at all times, $\mathbf{r}_j(t) = [x_j(t), y_j(t), z_j(t)]$ with $j = 1, 2, ..., N$, being N the number of particles. Defining the kinetic momentum of the particles as $\mathbf{P}_j = m_j \dot{\mathbf{r}}_j$ (m_j is the mass of particle j), the evolution of the system is found from a set of initial positions and velocities by solving the Newton equations of motion $\dot{\mathbf{P}}_j = \mathbf{F}_j$, being $\mathbf{F}_j$ the forces acting onto particle j.

Most physical systems have further constraints that have to fulfill (for example, the distance between the particles of a rigid body cannot change with time, that is, $|\mathbf{r}_j - \mathbf{r}_l| = const$), and therefore the positions $\{\mathbf{r}_j\}_{j=1,...,N}$ are no longer independent, which makes Newton equations hard to solve. This calls for a new simpler theoretical framework: the so-called *analytical mechanics*. In the following we review this framework, but assuming, for simplicity, that the constrains are *holonomic*[56] and *scleronomous*[57], meaning that they can always be written in the form $f(\mathbf{r}_1, ..., \mathbf{r}_N) = 0$.

In analytical mechanics the state of the system at any time is specified by a vector $\mathbf{q}(t) = [q_1(t), q_2(t), ..., q_n(t)]$. n is the number of degrees of freedom of the system (the total number of coordinates, $3N$, minus the number of constraints), and the q_j's are called the *generalized coordinates* of the system, which are compatible with the constraints and related to the usual coordinates of the particles through some smooth functions $\mathbf{q}(\{\mathbf{r}_j\}_{j=1,...,N}) \Leftrightarrow \{\mathbf{r}_j(\mathbf{q})\}_{j=1,...,N}$. The space formed by the generalized coordinates is called *coordinate space*, and $\mathbf{q}(t)$ describes a *trajectory* on it.

The basic object in analytical mechanics is the *Lagrangian*, $L[\mathbf{q}(t), \dot{\mathbf{q}}(t), t]$, which is a function of the generalized coordinates and velocities, and can even have some explicit time dependence. In general, the Lagrangian must be built based on general principles like symmetries. However, if the forces acting on the particles of the system are conservative, that is, $\mathbf{F}_j = \boldsymbol{\nabla}_j V[\{\mathbf{r}_l\}_{l=1,...,N}] = (\partial_{x_j} V, \partial_{y_j} V, \partial_{z_j} V)$ for some *potential* $V[\{\mathbf{r}_l\}_{l=1,...,N}]$, one can choose a Lagrangian with the simple form $L = T(\dot{\mathbf{q}}, \mathbf{q}) - V(\mathbf{q})$, being $T(\dot{\mathbf{q}}, \mathbf{q}) = \sum_{j=1}^{N} m_j \dot{\mathbf{r}}_j^2(\mathbf{q})/2$ the kinetic energy of the system and $V(\mathbf{q}) = V[\{\mathbf{r}_l(\mathbf{q})\}_{l=1,...,n}]$. The dynamical equations of the system are then formulated as a *variational principle* on the *action*

$$S = \int_{t_1}^{t_2} dt L[\mathbf{q}(t), \dot{\mathbf{q}}(t), t], \tag{A1}$$

by asking the trajectory of the system $\mathbf{q}(t)$ between two fixed points $\mathbf{q}(t_1)$ and $\mathbf{q}(t_2)$ to be such that the action is an extremal, $\delta S = 0$. From this principle, it is straightforward to arrive to the well known Euler-Lagrange equations

$$\frac{\partial L}{\partial q_j} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} = 0, \tag{A2}$$

which are a set of second order differential equations for the generalized coordinates $\mathbf{q}$, and together with the conditions $\mathbf{q}(t_1)$ and $\mathbf{q}(t_2)$ provide the trajectory $\mathbf{q}(t)$.

b. *The Hamiltonian formalism*

As we have seen, the Euler-Lagrange equations are a set of second order differential equations which allows us to find the trajectory $\mathbf{q}(t)$ in coordinate space. We could reduce the order of the differential equations by taking the velocities $\dot{\mathbf{q}}$ as dynamical variables, arriving then to a set of $2n$ first-order differential equations. This is, however, a very naïve way of reducing the order, which leads to a non-symmetric system of equations for $\mathbf{q}$ and $\dot{\mathbf{q}}$. In this section we review Hamilton's approach to analytical mechanics, which leads to a symmetric-like first-order system of equations, and will play a major role in understanding the transition from classical to quantum mechanics.

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[55] For a deeper reading I recommend Goldstein's book [22], as well as Greiner's books [23, 24], or the one of Hand and Finch [25].

[56] A constrain is *holonomic* when it can be written as $f(\mathbf{r}_1, ..., \mathbf{r}_N, t) = 0$. Nonholonomic constrains correspond, for example, to the boundary imposed by a wall that particles cannot cross, which is usually expressed in terms of inequalities [22], and require a much more careful treatment.

[57] A constrain is called *scleronomous* when the it does not depend explicitly on time. Time-dependent constrains are called *rheonomous* and correspond, for example, to a situation in which the motion of the particles is restricted to a moving surface or curve [22].

Instead of using the velocities, the Hamiltonian formalism considers the *generalized momenta*

$$p_j = \frac{\partial L}{\partial \dot{q}_j}, \tag{A3}$$

as the dynamical variables. Note that this definition establishes a relation between these generalized momenta and the velocities $\dot{\mathbf{q}}(\mathbf{q},\mathbf{p}) \Leftrightarrow \mathbf{p}(\mathbf{q},\dot{\mathbf{q}})$. Note also that when the usual Cartesian coordinates of the system's particles are taken as the generalized coordinates, these momenta coincide with those of Newton's approach.

The theory is then built in terms of a new object called the *Hamiltonian*, which is defined as a Legendre transform of the Lagrangian,

$$H(\mathbf{q},\mathbf{p}) = \mathbf{p}\dot{\mathbf{q}}(\mathbf{q},\mathbf{p}) - L[\mathbf{q},\dot{\mathbf{q}}(\mathbf{q},\mathbf{p}),t], \tag{A4}$$

and coincides with the total energy[58] for conservative systems with scleronomous constrains, that is, $H(\mathbf{q},\mathbf{p}) = T(\mathbf{q},\mathbf{p}) + V(\mathbf{q})$, with $T(\mathbf{q},\mathbf{p}) = T[\mathbf{q},\dot{\mathbf{q}}(\mathbf{q},\mathbf{p})]$. Differentiating this expression and using the Euler-Lagrange equations (or using again the variational principle on the action), it is then straightforward to obtain the equations of motion for the generalized coordinates and momenta (the *canonical equations*),

$$\dot{q}_j = \frac{\partial H}{\partial p_j} \qquad \text{and} \qquad \dot{p}_j = -\frac{\partial H}{\partial q_j}, \tag{A5}$$

which together with some initial conditions $\{\mathbf{q}(t_0),\mathbf{p}(t_0)\}$ allow us to find the trajectory $\{\mathbf{q}(t),\mathbf{p}(t)\}$ in the space formed by the generalized coordinates and momenta, which is known as *phase space*.

Another important object in the Hamiltonian formalism is the *Poisson bracket*. Given two functions of the coordinates and momenta $F(\mathbf{q},\mathbf{p})$ and $G(\mathbf{q},\mathbf{p})$, their Poisson bracket is defined as

$$\{F,G\} = \sum_{j=1}^{n} \frac{\partial F}{\partial q_j}\frac{\partial G}{\partial p_j} - \frac{\partial F}{\partial p_j}\frac{\partial G}{\partial q_j}. \tag{A6}$$

The importance of this object is reflected in the fact that the evolution equation of any quantity $g(\mathbf{q},\mathbf{p},t)$ can be written as

$$\frac{dg}{dt} = \{g,H\} + \frac{\partial g}{\partial t}, \tag{A7}$$

and hence, if the quantity does not depend explicitly on time and its Poisson bracket with the Hamiltonian is zero, it is a *constant of motion*.

Of particular importance for the transition to quantum mechanics are the *canonical Poisson brackets*, that is, the Poisson brackets of the coordinates and momenta,

$$\{q_j,p_l\} = \delta_{jl},\ \{q_j,q_l\} = \{p_j,p_l\} = 0, \tag{A8}$$

which define the mathematical structure of phase space.

c. *Observables and their mathematical structure*

In this last section concerning classical mechanics we will discuss about the mathematical structure in which observables are embedded within the Hamiltonian formalism. We will see that the mathematical objects corresponding to physical observables form a well defined mathematical structure, a real Lie algebra. Moreover, the position and momentum will be shown to be the generators of a particular Lie group, the Heisenberg group. Understanding this internal structure of *classical observables* will give us the chance to introduce the quantum description of observables in a reasonable way. Let us start by defining the concept of Lie algebra.

A *real Lie algebra* is a real vector space[59] $\mathcal{L}$ equipped with an additional operation, the *Lie product*, which takes two vectors f and g from $\mathcal{L}$, to generate another vector also in $\mathcal{L}$ denoted by[60] $\{f,g\}$. This operation must satisfy the following properties:

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[58] The general conditions under which the Hamiltonian coincides with the system's energy can be found in [22].

[59] The concept of complex vector space is defined in the next section. The definition of a *real* vector space is the same, but replacing by real numbers the complex numbers that appear in the definitions there.

[60] Note that we are using the same notation for the general definition of the Lie product and for the Poisson bracket, which are a particular case of Lie product as we will learn shortly.

1. $\{f, g+h\} = \{f, g\} + \{f, h\}$ (linearity)
2. $\{f, f\} = 0 \overset{\text{together}}{\underset{\text{with 1}}{\Longrightarrow}} \{f, g\} = -\{g, f\}$ (anticommutativity)
3. $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$ (Jacobi identity)

Hence, in essence a real Lie algebra is a vector space equipped with a linear, non-commutative, non-associative product. They have been a subject of study for many years, and now we know a lot about the properties of these mathematical structures. They appear in many branches of physics and geometry, specially connected to continuous symmetry transformations, whose associated mathematical structures are actually called *Lie groups*. In particular, it is possible to show that given any Lie group with p parameters (like, e.g., the three-parameter groups of translations or rotations in real space), any transformation onto the system in which it is acting can be generated from a set of p elements of a Lie algebra $\{g_1, g_2, ..., g_p\}$, called the *generators* of the Lie group, which satisfy some particular relations

$$\{g_j, g_k\} = \sum_{l=1}^{p} c_{jkl} g_l. \tag{A9}$$

These relations are called the *algebra-group relations*, and the *structure constants* c_{jkl} are characteristic of the particular Lie group (for example, the generators of translations and rotations in real space are the momenta and angular momenta, respectively, and the corresponding structure constants are $c_{jkl} = 0$ for the translation group and $c_{jkl} = \epsilon_{jkl}$ for the rotation group[61]).

Coming back to the Hamiltonian formalism, we start by noting that *observables*, being *measurable* quantities, must be given by continuous, real functions in phase space. Hence they form a real vector space with respect to the usual addition of functions and multiplication of a function by a real number. It also appeared naturally in the formalism a linear, non-commutative, non-associative operation between phase-space functions, the Poisson bracket, which applied to real functions gives another real function. It is easy to see that the Poisson bracket satisfies all the requirements of a Lie product, and hence, observables form a Lie algebra within the Hamiltonian formalism.

Moreover, the fundamental Poisson brackets (A8) show that the generalized coordinates $\mathbf{q}$ and momenta $\mathbf{p}$, together with the identity in phase space, satisfy particular algebra-group relations, namely[62] $\{q_j, p_k\} = \delta_{jk} 1$ and $\{q_j, 1\} = \{p_j, 1\} = \{1, 1\} = 0$, and hence can be seen as the generators of a Lie group. This group is known as the *Heisenberg group*, and was introduced by Weyl when trying to prove the equivalence between the Schrödinger and Heisenberg pictures of quantum mechanics (about which we will learn later). It was later shown to have connections with the symplectic group, which is the basis of many physical theories. Note that we could have taken the Poisson brackets between the angular momenta associated to the possible rotations in the system of particles (which are certainly far more intuitive transformations than the one related to the Heisenberg group) as the fundamental ones. However, we have chosen the Lie algebra associated to the Heisenberg group just because it deals directly with position and momenta, allowing for a simpler connection to quantum mechanics.

Therefore, we arrive to the main conclusion of this review in classical mechanics:

⌈The mathematical framework of Hamiltonian mechanics associates physical observables with elements of a Lie algebra, being the phase-space coordinates themselves the generators of the Heisenberg group.⌋

Maintaining this structure for observables will help us introducing the laws of quantum mechanics in a coherent way.

2. The mathematical language of quantum mechanics

Just as classical mechanics is formulated in terms of the mathematical language of differential calculus and its extensions, quantum mechanics takes linear algebra (and Hilbert spaces in particular) as its fundamental grammar. In this section we will review the concept of Hilbert space, and discuss the properties of some operators which play important roles in the formalism of quantum optics.

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[61] $\epsilon_{j_1 j_2 ... j_M}$ with all the subindices going from 1 to M is the Levi-Civita symbol in dimension M, which has $\epsilon_{12...M} = 1$ and is completely antisymmetric, that is, changes its sign after permutation of any pair of indices.

[62] Ordering the generators as $\{\mathbf{q}, \mathbf{p}, 1\}$, the structure constants associated to this algebra-group relations are explicitly

$$c_{jkl} = \begin{cases} \Omega_{jk}\delta_{l,2n+1} & j,k = 1,2,...,2n \\ 0 & j = 2n+1 \text{ or } k = 2n+1 \end{cases}, \tag{A10}$$

being $\Omega = \begin{pmatrix} 0_{n\times n} & I_{n\times n} \\ -I_{n\times n} & 0_{n\times n} \end{pmatrix}$, with $I_{n\times n}$ and $0_{n\times n}$ the $n \times n$ identity and null matrices, respectively.

a. Finite-dimensional Hilbert spaces

In essence, a Hilbert space is a *complex vector space* in which an *inner product* is defined. Let us define first these terms as we use them in these lectures.

A *complex vector space* is a set $\mathcal{V}$, whose elements will be called *vectors* or *kets* and will be denoted by $\{|a\rangle, |b\rangle, |c\rangle, ...\}$ (a, b, and c may correspond to any suitable label), in which the following two operations are defined: the *vector addition*, which takes two vectors $|a\rangle$ and $|b\rangle$ and creates a new vector inside $\mathcal{V}$ denoted by $|a\rangle + |b\rangle$; and the *multiplication by a scalar*, which takes a complex number $\alpha \in \mathbb{C}$ (in this section Greek letters will represent complex numbers) and a vector $|a\rangle$ to generate a new vector in $\mathcal{V}$ denoted by $\alpha|a\rangle$.

The following additional properties must be satisfied:

1. The vector addition is commutative and associative, that is, $|a\rangle+|b\rangle = |b\rangle+|a\rangle$ and $(|a\rangle+|b\rangle)+|c\rangle = |a\rangle+(|b\rangle+|c\rangle)$
2. There exists a null vector $|null\rangle$ such that $|a\rangle + |null\rangle = |a\rangle$
3. $\alpha(|a\rangle + |b\rangle) = \alpha|a\rangle + \alpha|b\rangle$
4. $(\alpha + \beta)|a\rangle = \alpha|a\rangle + \beta|a\rangle$
5. $(\alpha\beta)|a\rangle = \alpha(\beta|a\rangle)$
6. $1|a\rangle = |a\rangle$

From these properties it can be proved that the null vector is unique, and can be built from any vector $|a\rangle$ as $0|a\rangle$; hence, in the following we denote it simply by $|null\rangle \equiv 0$. It is also readily proved that any vector $|a\rangle$ has a unique *antivector* $|-a\rangle$ such that $|a\rangle + |-a\rangle = 0$, which is given by $(-1)|a\rangle$ or simply $-|a\rangle$.

An *inner product* is an additional operation defined in the complex vector space $\mathcal{V}$, which takes two vectors $|a\rangle$ and $|b\rangle$ and associates them with a complex number. It will be denoted by $\langle a|b\rangle$ or sometimes also by $(|a\rangle, |b\rangle)$, and must satisfy the following properties:

1. $\langle a|a\rangle > 0 \quad \text{if} \quad |a\rangle \neq 0$
2. $\langle a|b\rangle = \langle b|a\rangle^*$
3. $(|a\rangle, \alpha|b\rangle) = \alpha\langle a|b\rangle$
4. $(|a\rangle, |b\rangle + |c\rangle) = \langle a|b\rangle + \langle a|c\rangle$

The following additional properties can be proved from these ones:

- $\langle null|null\rangle = 0$
- $(\alpha|a\rangle, |b\rangle) = \alpha^*\langle a|b\rangle$
- $(|a\rangle + |b\rangle, |c\rangle) = \langle a|c\rangle + \langle b|c\rangle$
- $|\langle a|b\rangle|^2 \leq \langle a|a\rangle\langle b|b\rangle$ (Cauchy-Schwarz)

Note that for any vector $|a\rangle$, one can define the object $\langle a| \equiv (|a\rangle, \cdot)$, which will be called a *dual vector* or a *bra*, and which takes a vector $|b\rangle$ to generate the complex number $(|a\rangle, |b\rangle) \in \mathbb{C}$. It can be proved that the set formed by all the dual vectors corresponding to the elements in $\mathcal{V}$ is also a vector space, which will be called the *dual space* and will be denoted by $\mathcal{V}^+$. Within this picture, the inner product can be seen as an operation which takes a bra $\langle a|$ and a ket $|b\rangle$ to generate the complex number $\langle a|b\rangle$, a *bracket*. This whole *bra-c-ket* notation is due to Dirac [26].

In the following we assume that any time a bra $\langle a|$ is applied to a ket $|b\rangle$, the complex number $\langle a|b\rangle$ is formed, so that objects like $|b\rangle\langle a|$ generate kets when applied to kets from the left, $(|b\rangle\langle a|)|c\rangle = (\langle a|c\rangle)|b\rangle$, and bras when applied to bras from the right, $\langle c|(|b\rangle\langle a|) = (\langle c|b\rangle)\langle a|$. Technically, $|b\rangle\langle a|$ is called an *outer product*.

A vector space equipped with an inner product is called a *Euclidean space* [27]. In the following we give some important definitions and properties which are needed in order to understand the concept of Hilbert space:

- The vectors $\{|a_1\rangle, |a_2\rangle, ..., |a_m\rangle\}$ are said to be *linearly independent* if the relation $\alpha_1|a_1\rangle+\alpha_2|a_2\rangle+...+\alpha_m|a_m\rangle = 0$ is satisfied only for $\alpha_1 = \alpha_2 = ... = \alpha_m = 0$, as otherwise one of them can be written as a linear combination of the rest.
- The *dimension* of the vector space is defined as the maximum number of linearly independent vectors that can be found in the space, and can be finite or infinite.

- If the dimension of a Euclidean space is $d < \infty$, it is always possible to build a set of d orthonormal vectors $E = \{|e_j\rangle\}_{j=1,2,..,d}$ satisfying $\langle e_j|e_l\rangle = \delta_{jl}$, such that any other vector $|a\rangle$ can be written as a linear superposition of them, that is, $|a\rangle = \sum_{j=1}^{d} a_j|e_j\rangle$, being the a_j's some complex numbers. This set is called an *orthonormal basis* of the Euclidean space $\mathcal{V}$, and the coefficients a_j of the expansion can be found as $a_j = \langle e_j|a\rangle$. The column formed with the expansion coefficients, which is denoted by $\mathrm{col}(a_1, a_2, ..., a_d)$, is called a *representation* of the vector $|a\rangle$ in the basis E.

  Note that the set $E^+ = \{\langle e_j|\}_{j=1,2,..,d}$ is an orthonormal basis in the dual space $\mathcal{V}^+$, so that any bra $\langle a|$ can be expanded then as $\langle a| = \sum_{j=1}^{d} a_j^*\langle e_j|$. The representation of the bra $\langle a|$ in the basis E corresponds to the row formed by its expansion coefficients, and is denoted by $(a_1^*, a_2^*, ..., a_n^*)$. Note that if the representation of $|a\rangle$ is seen as a $d \times 1$ matrix, the representation of $\langle a|$ can be obtained as its $1 \times d$ conjugate-transpose matrix.

  Note finally that the inner product of two vectors $|a\rangle$ and $|b\rangle$ reads $\langle a|b\rangle = \sum_{j=1}^{d} a_j^* b_j$ when represented in the same basis, which is the matrix product of the representations of $\langle a|$ and $|b\rangle$.

For finite dimension, a Euclidean space is a *Hilbert space*. However, in most applications of quantum mechanics one has to deal with infinite-dimensional vector spaces. We will treat them after the following section.

b. Linear operators in finite dimensions

We now discuss the concept of linear operator, as well as analyze the properties of some important classes of operators. Only finite-dimensional Hilbert spaces are considered in this section, and we will generalize the discussion to infinite-dimensional Hilbert spaces in the next section.

We are interested in maps $\hat{L}$ (operators are denoted by a 'hat' throughout the monograph) which associate to any vector $|a\rangle$ of a Hilbert space $\mathcal{H}$ another vector denoted by $\hat{L}|a\rangle$ in the same Hilbert space. If the map satisfies

$$\hat{L}(\alpha|a\rangle + \beta|b\rangle) = \alpha\hat{L}|a\rangle + \beta\hat{L}|b\rangle, \tag{A11}$$

then it is called a *linear operator*. For our purposes this is the only class of interesting operators, and hence we will simply call them *operators* in the following.

Before discussing the properties of some important classes of operators, we need some definitions:

- Given an orthonormal basis $E = \{|e_j\rangle\}_{j=1,2,..,d}$ in a Hilbert space $\mathcal{H}$ with dimension $d < \infty$, any operator $\hat{L}$ has a matrix representation. While bras and kets are represented by $d \times 1$ and $1 \times d$ matrices (rows and columns), respectively, an operator $\hat{L}$ is represented by a $d \times d$ matrix with *elements* $L_{jl} = (|e_j\rangle, \hat{L}|e_l\rangle) \equiv \langle e_j|\hat{L}|e_l\rangle$. An operator $\hat{L}$ can then be expanded in terms of the basis E as $\hat{L} = \sum_{j,l=1}^{d} L_{jl}|e_j\rangle\langle e_l|$. It follows that the representation of the vector $|b\rangle = \hat{L}|a\rangle$ is just the matrix multiplication of the representation of $\hat{L}$ by the representation of $|a\rangle$, that is, $b_j = \sum_{l=1}^{d} L_{jl}a_l$.

- The *addition* and *multiplication* of two operators $\hat{L}$ and $\hat{K}$, denoted by $\hat{L} + \hat{K}$ and $\hat{L}\hat{K}$, respectively, are defined by their action onto any vector $|a\rangle$: $(\hat{L} + \hat{K})|a\rangle = \hat{L}|a\rangle + \hat{K}|a\rangle$ and $\hat{L}\hat{K}|a\rangle = \hat{L}(\hat{K}|a\rangle)$. It follows that the representation of the addition and the product are, respectively, the sum and the multiplication of the corresponding matrices, that is, $(\hat{L} + \hat{K})_{jl} = L_{jl} + K_{jl}$ and $(\hat{L}\hat{K})_{jl} = \sum_{k=1}^{d} L_{jk}K_{kl}$.

- Note that while the addition is commutative, the product is not in general. This leads us to the notion of *commutator*, defined for two operators $\hat{L}$ and $\hat{K}$ as $[\hat{L}, \hat{K}] = \hat{L}\hat{K} - \hat{K}\hat{L}$. When $[\hat{L}, \hat{K}] = 0$, we say that the operators *commute*.

- Given an operator $\hat{L}$, its *trace* is defined as the sum of the diagonal elements of its matrix representation, that is, $\mathrm{tr}\{\hat{L}\} = \sum_{j=1}^{d} L_{jj}$. It may seem that this definition is basis-dependent, as in general the elements L_{jj} are different in different bases. However, we will see later that the trace is invariant under any change of basis.

  The trace has two important properties. It is *linear* and *cyclic*, that is, given two operators $\hat{L}$ and $\hat{K}$, $\mathrm{tr}\{\hat{L}+\hat{K}\} = \mathrm{tr}\{\hat{L}\} + \mathrm{tr}\{\hat{K}\}$ and $\mathrm{tr}\{\hat{L}\hat{K}\} = \mathrm{tr}\{\hat{K}\hat{L}\}$, as is trivially proved.

- Given an operator $\hat{L}$, we define its *determinant* as the determinant of its matrix representation, that is, $\det\{\hat{L}\} = \sum_{j_1,j_2,...,j_d=1}^{d} \epsilon_{j_1 j_2 ... j_d} L_{1j_1} L_{2j_2} ... L_{dj_d}$. Just as the trace, we will see that it does not depend on the basis used to represent the operator.

  The determinant is a multiplicative map, that is, given two operators $\hat{L}$ and $\hat{K}$, the determinant of the product is the product of the determinants, $\det\{\hat{L}\hat{K}\} = \det\{\hat{L}\}\det\{\hat{K}\}$.

- We say that a vector $|l\rangle$ is an *eigenvector* of an operator $\hat{L}$ if there exists a $\lambda \in \mathbb{C}$ (called its associated *eigenvalue*) such that $\hat{L}|l\rangle = \lambda|l\rangle$. The set of all the eigenvalues of an operator is called its *spectrum*.

We can pass now to describe some classes of operators which play important roles in quantum mechanics.

The identity operator. The *identity operator*, denoted by $\hat{I}$, is defined as the operator which maps any vector onto itself. Its representation in any basis is then $I_{jl} = \delta_{jl}$, so that it can be expanded as

$$\hat{I} = \sum_{j=1}^{d} |e_j\rangle\langle e_j|. \tag{A12}$$

This expression is known as the *completeness relation* of the basis E; alternatively, it is said that the set E forms a *resolution of the identity*.

Note that the expansion of a vector $|a\rangle$ and its dual $\langle a|$ in the basis E is obtained just by application of the completeness relation from the left and the right, respectively. Similarly, the expansion of an operator $\hat{L}$ is obtained by application of the completeness relation both from the right and the left at the same time.

The inverse of an operator. The *inverse* of an operator $\hat{L}$, denoted by $\hat{L}^{-1}$, is defined as that satisfying $\hat{L}^{-1}\hat{L} = \hat{L}\hat{L}^{-1} = \hat{I}$. Not every operator has an inverse. An inverse exists if and only if the operator does not have a zero eigenvalue, or, equivalently, when $\det\{\hat{L}\} \neq 0$.

An operator function. Consider a real, analytic function $f(x)$ which can be expanded in powers of x as $f(x) = \sum_{m=0}^{\infty} f_m x^m$. Given an operator $\hat{L}$, we define the *operator function* $\hat{f}(\hat{L}) = \sum_{m=0}^{\infty} f_m \hat{L}^m$, where $\hat{L}^m$ means the product of $\hat{L}$ with itself m times.

The adjoint of an operator. Given an operator $\hat{L}$, we define its *adjoint*, and denote it by $\hat{L}^\dagger$, as that satisfying $(|a\rangle, \hat{L}|b\rangle) = (\hat{L}^\dagger|a\rangle, |b\rangle)$ for any two vectors $|a\rangle$ and $|b\rangle$. Note that the representation of $\hat{L}^\dagger$ corresponds to the conjugate transpose of the matrix representing $\hat{L}$, that is, $(\hat{L}^\dagger)_{jl} = L^*_{lj}$. Note also that the adjoint of a product of two operators $\hat{K}$ and $\hat{L}$ is given by $(\hat{K}\hat{L})^\dagger = \hat{L}^\dagger\hat{K}^\dagger$.

Self-adjoint operators. We say that $\hat{H}$ is a *self-adjoint* when it coincides with its adjoint, that is, $\hat{H} = \hat{H}^\dagger$. A property of major importance for the construction of the laws of quantum mechanics is that the spectrum $\{h_j\}_{j=1,2,\ldots,d}$ of a self-adjoint operator is real. Moreover, its associated eigenvectors[63] $\{|h_j\rangle\}_{j=1,2,\ldots,d}$ form an orthonormal basis of the Hilbert space.

The representation of any operator function $\hat{f}(\hat{H})$ in the *eigenbasis* of $\hat{H}$ is then $[\hat{f}(\hat{H})]_{jl} = f(h_j)\delta_{jl}$, from which it follows

$$\hat{f}(\hat{H}) = \sum_{j=1}^{d} f(h_j)|h_j\rangle\langle h_j|. \tag{A13}$$

This result is known as the *spectral theorem*.

Unitary operators. We say that $\hat{U}$ is a *unitary operator* when $\hat{U}^\dagger = \hat{U}^{-1}$. The interest of this class of operators is that they preserve inner products, that is, for any two vectors $|a\rangle$ and $|b\rangle$ the inner product $(\hat{U}|a\rangle, \hat{U}|b\rangle)$ coincides with $\langle a|b\rangle$. Moreover, it is possible to show that given two orthonormal bases $E = \{|e_j\rangle\}_{j=1,2,..,d}$ and $E' = \{|e'_j\rangle\}_{j=1,2,..,d}$, there exists a unique unitary matrix $\hat{U}$ which connects them as $\{|e'_j\rangle = \hat{U}|e_j\rangle\}_{j=1,2,..,d}$, and then any basis of the Hilbert space is unique up to a unitary transformation.

We can now prove that both the trace and the determinant of an operator are basis-independent. Let us denote by $\mathrm{tr}\{\hat{L}\}_E$ the trace of an operator $\hat{L}$ in the basis E. The trace of this operator in the transformed basis can be written then as $\mathrm{tr}\{\hat{L}\}_{E'} = \mathrm{tr}\{\hat{U}^\dagger\hat{L}\hat{U}\}_E$, which, using the cyclic property of the trace and the unitarity of $\hat{U}$, is rewritten as $\mathrm{tr}\{\hat{U}\hat{U}^\dagger\hat{L}\}_E = \mathrm{tr}\{\hat{L}\}_E$, proving that the trace is equal in both bases. Similarly, in the case of

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[63] For simplicity, we will assume that the spectrum of any operator is non-degenerate, that is, all the eigenvectors possess a distinctive eigenvalue.

the determinant we have $\det\{\hat{L}\}_{E'} = \det\{\hat{U}^\dagger \hat{L} \hat{U}\}_E$, which using the multiplicative property of the determinant is rewritten as $\det\{\hat{U}^\dagger\}_E \det\{\hat{L}\}_E \det\{\hat{U}\}_E = \det\{\hat{L}\}_E$, where we have used $\det\{\hat{U}^\dagger\}_E \det\{\hat{U}\}_E = 1$ as follows from $\hat{U}^\dagger \hat{U} = \hat{I}$.

Note finally that a unitary operator $\hat{U}$ can always be written as the complex exponential a self-adjoint operator $\hat{H}$, that is, $\hat{U} = \exp(\mathrm{i}\hat{H})$.

Projection operators. In general, any self-adjoint operator $\hat{P}$ satisfying $\hat{P}^2 = \hat{P}$ is called a *projector*. We are interested only on those projectors which can be written as the outer product of a vector $|a\rangle$ with itself, that is, rank-1 projectors[64] $\hat{P}_a = |a\rangle\langle a|$. When applied to a vector $|b\rangle$, this gets *projected* along the 'direction' of $|a\rangle$ as $\hat{P}_a|b\rangle = \langle a|b\rangle\ |a\rangle$.

Note that given an orthonormal basis E, we can use the projectors $\hat{P}_j = |e_j\rangle\langle e_j|$ to extract the components of a vector $|a\rangle$ as $\hat{P}_j|a\rangle = a_j|e_j\rangle$. Note also that the completeness and orthonormality of the basis E implies that $\sum_{j=1}^d \hat{P}_j = \hat{I}$ and $\hat{P}_j \hat{P}_l = \delta_{jl}\hat{P}_j$, respectively.

Density operators. A self-adjoint operator $\hat{\rho}$ is called a *density operator* when it has unit trace and it is *positive semidefinite*, that is, $\langle a|\hat{\rho}|a\rangle \geq 0$ for any vector $|a\rangle$.

The interesting property of density operators is that they 'contain' probability distributions in the diagonal of its representation. To see this just note that given an orthonormal basis E, the self-adjointness and positivity of $\hat{\rho}$ ensure that all its diagonal elements $\{\rho_{jj}\}_{j=1,2,\ldots,d}$ are either positive or zero, that is, $\rho_{jj} \geq 0\ \forall j$, while the unit trace makes them satisfy $\sum_{j=1}^d \rho_{jj} = 1$. Hence, the diagonal elements of a density operator have all the properties required by a *probability distribution*.

c. *Generalization to infinite dimensions*

Unfortunately, not all the previous concepts and objects that we have introduced for the finite-dimensional case are trivially generalized to infinite dimensions. In this section we discuss this generalization.

The first problem that we meet when dealing with infinite-dimensional Euclidean spaces is that the existence of a basis $\{|e_j\rangle\}_{j=1,2,\ldots}$ in which any other vector can be represented as $|a\rangle = \sum_{j=1}^\infty a_j|e_j\rangle$ is not granted, because not all infinite sequences converge. The class of infinite-dimensional Euclidean spaces in which these infinite but countable bases exist are called *separable Hilbert spaces*, and are the ones relevant for the quantum description of physical systems.

The conditions that ensure that an infinite-dimensional Euclidean space is indeed a Hilbert space[65] can be found in, for example, reference [27]. Here we just want to stress that, quite intuitively, any infinite-dimensional Hilbert space[66] is *isomorphic* to the space called $l^2(\infty)$, which is formed by the column vectors $|a\rangle = \mathrm{col}(a_1, a_2, \ldots)$ where the set $\{a_j \in \mathbb{C}\}_{j=1,2,\ldots}$ satisfies the restriction $\sum_{j=1}^\infty |a_j|^2 < \infty$, and has the operations $|a\rangle + |b\rangle = \mathrm{col}(a_1 + b_1, a_2 + b_2, \ldots)$, $\alpha|a\rangle = \mathrm{col}(\alpha a_1, \alpha a_2, \ldots)$, and $\langle a|b\rangle = \sum_{j=1}^\infty a_j^* b_j$.

Most of the previous definitions are directly generalized to Hilbert spaces by taking $d \to \infty$ (dual space, representations, operators,...). However, there is one crucial property of self-adjoint operators which does not hold in this case: its eigenvectors may not form an orthonormal basis in the Hilbert space. The remainder of this section is devoted to deal with this problem.

Just as in finite dimension, given an infinite-dimensional Hilbert space $\mathcal{H}$, we say that one of its vectors $|d\rangle$ is an eigenvector of the self-adjoint operator $\hat{H}$ if $\hat{H}|d\rangle = \delta|d\rangle$, where $\delta \in \mathbb{R}$ is called its associated eigenvalue. Nevertheless, it can happen in infinite-dimensional spaces that some vector $|c\rangle$ not contained in $\mathcal{H}$ also satisfies the condition $\hat{H}|c\rangle = \chi|c\rangle$, in which case we call it a *generalized eigenvector*, being χ its *generalized eigenvalue*[67]. The set of all the

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[64] The term "rank" refers to the number of non-zero eigenvalues.

[65] From now on we will assume that all the Hilbert spaces we refer to are "separable", even if we don't write it explicitly.

[66] An example of infinite-dimensional complex Hilbert space consists in the vector space formed by the complex functions of real variable, say $|f\rangle = f(x)$ with $x \in \mathbb{R}$, with integrable square, that is

$$\int_{\mathbb{R}} dx |f(x)|^2 < \infty, \tag{A14}$$

together with the inner product

$$\langle g|f\rangle = \int_{\mathbb{R}} dx g^*(x) f(x). \tag{A15}$$

This Hilbert space is usually denoted by $\mathrm{L}^2(x)$.

[67] In $\mathrm{L}^2(x)$ we have two simple examples of self-adjoint operators with eigenvectors not contained in $\mathrm{L}^2(x)$: the so-called $\hat{X}$ (*position*) and $\hat{P}$ (*momentum*), which, given an arbitrary vector $|f\rangle = f(x)$, act as $\hat{X}|f\rangle = xf(x)$ and $\hat{P}|f\rangle = -\mathrm{i}\partial_x f$, respectively. This is simple to see, as the equations

$$x f_X(x) = X f_X(x) \qquad \text{and} \qquad -\mathrm{i}\partial_x f_P(x) = P f_P(x), \tag{A16}$$

have

$$f_X(x) = \delta(x - X) \qquad \text{and} \qquad f_P(x) = \exp(\mathrm{i}Px), \tag{A17}$$

as solutions, which are not square-integrable, and hence do not belong to $\mathrm{L}^2(x)$.

eigenvalues of the self-adjoint operator is called its *discrete* (or *point*) *spectrum* and it is a countable set, while the set of all its generalized eigenvalues is called its *continuous spectrum* and it is uncountable, that is, forms a continuous set [27] (see also [28]).

In this lectures we only deal with two extreme cases: either the observable, say $\hat{H}$, has a pure discrete spectrum $\{h_j\}_{j=1,2,...}$; or the observable, say $\hat{X}$, has a pure continuous spectrum $\{x\}_{x\in\mathbb{R}}$. It can be shown that in the first case the eigenvectors of the observable form an orthonormal basis of the Hilbert space, so that we can build a resolution of the identity as $\hat{I} = \sum_{j=1}^{\infty} |h_j\rangle\langle h_j|$, and proceed along the lines of the previous sections.

In the second case, the set of generalized eigenvectors cannot form a basis of the Hilbert space in the strict sense, as they do not form a countable set and do not even belong to the Hilbert space. Fortunately, there are still ways to treat the generalized eigenvectors of $\hat{X}$ 'as if' they were a basis of the Hilbert space. The idea was introduced by Dirac [26], who realized that normalizing the generalized eigenvectors as[68] $\langle x|y\rangle = \delta(x-y)$, one can define the following integral operator

$$\hat{I}_{\rm c} = \int_{\mathbb{R}} dx|x\rangle\langle x|, \tag{A19}$$

which acts as the identity onto the generalized eigenvectors, that is, $\hat{I}_{\rm c}|y\rangle = |y\rangle$. It is then conjectured that $\hat{I}_{\rm c}$ coincides with the identity in $\mathcal{H}$, so that any other vector $|a\rangle$ or operator $\hat{L}$ defined in the Hilbert space can be expanded as

$$|a\rangle = \int_{\mathbb{R}} dx a(x)|x\rangle \qquad \text{and} \qquad \hat{L} = \int_{\mathbb{R}^2} dxdy L(x,y)|x\rangle\langle y|, \tag{A20}$$

where the elements $a(x) = \langle x|a\rangle$ and $L(x,y) = \langle x|\hat{L}|y\rangle$ of these *continuous representations* form complex functions defined in $\mathbb{R}$ and $\mathbb{R}^2$, respectively. From now on, we will call *continuous basis* to the set $\{|x\rangle\}_{x\in\mathbb{R}}$.

Dirac introduced this continuous representation as a 'limit to the continuum' of the countable case. Even though this approach was very intuitive, it lacked mathematical rigor. Some decades after Dirac's proposal, Gel'fand showed how to generalize the concept of Hilbert space to include these generalized representations in full mathematical rigor [29]. The generalized spaces are called *rigged Hilbert spaces* (in which the algebra of Hilbert spaces joins forces with the theory of continuous probability distributions), and working on them it is possible to show that given any self-adjoint operator, one can use its eigenvectors and generalized eigenvectors to expand any vector of the Hilbert space, just as we did above. In other words, within the framework of rigged Hilbert spaces, one can prove the identity $\hat{I}_c = \hat{I}$ rigorously.

Note finally that given two vectors $|a\rangle$ and $|b\rangle$ of the Hilbert space, and a continuous basis $\{|x\rangle\}_{x\in\mathbb{R}}$, we can use their generalized representations to write their inner product as

$$\langle a|b\rangle = \int_{\mathbb{R}} dx a^*(x)b(x). \tag{A21}$$

It is also easily proved that the trace of any operator $\hat{L}$ can be evaluated from its continuous representation on $\{|x\rangle\}_{x\in\mathbb{R}}$ as

$$\mathrm{tr}\{\hat{L}\} = \int_{\mathbb{R}} dx L(x,x). \tag{A22}$$

This has important consequences for the properties of density operators, say $\hat{\rho}$ for the discussion which follows. We explained at the end of the last section that when represented on an orthonormal basis of the Hilbert space, its diagonal elements (which are real owed to its self-adjointness) can be seen as a probability distribution, because they satisfy $\sum_{j=1}^{\infty}\rho_{jj} = 1$ and $\rho_{jj} \geq 0 \ \ \forall j$. Similarly, because of its unit trace and positivity, the diagonal elements of its continuous representation satisfy $\int_{\mathbb{R}} dx\rho(x,x) = 1$ and $\rho(x,x) \geq 0 \ \ \forall x$, and hence, the real function $\rho(x,x)$ can be seen as a *probability density function*.

d. Composite Hilbert spaces

In many moments of this lectures, we will find the need to associate a Hilbert space to a composite system, the Hilbert spaces of whose parts we know. In this section we show how to build a Hilbert space $\mathcal{H}$ starting from a set of Hilbert spaces $\{\mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_C, ...\}$.

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[68] $\delta(x)$ is the so-called *Dirac delta distribution* which is defined by the conditions

$$\int_{x_1}^{x_2} dx\delta(x-y) = \begin{cases} 1 & \text{if } y\in[x_1,x_2] \\ 0 & \text{if } y\notin[x_1,x_2] \end{cases} . \tag{A18}$$

Let us start with only two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ with dimensions d_A and d_B, respectively (which might be infinite); the generalization to an arbitrary number of Hilbert spaces is straightforward. Consider a vector space $\mathcal{V}$ with dimension $\dim(\mathcal{V}) = d_A \times d_B$. We define a map called the *tensor product* which associates to any pair of vectors $|a\rangle \in \mathcal{H}_A$ and $|b\rangle \in \mathcal{H}_B$ a vector in $\mathcal{V}$ which we denote by $|a\rangle \otimes |b\rangle \in \mathcal{V}$. This tensor product must satisfy the following properties:

1. $(|a\rangle + |b\rangle) \otimes |c\rangle = |a\rangle \otimes |c\rangle + |b\rangle \otimes |c\rangle$
2. $|a\rangle \otimes (|b\rangle + |c\rangle) = |a\rangle \otimes |b\rangle + |a\rangle \otimes |c\rangle$
3. $(\alpha|a\rangle) \otimes |b\rangle = |a\rangle \otimes (\alpha|b\rangle)$

If we endorse the vector space $\mathcal{V}$ with the inner product $(|a\rangle \otimes |b\rangle, |c\rangle \otimes |d\rangle) = \langle a|c\rangle\langle b|d\rangle$, it is easy to show it becomes a Hilbert space, which in the following will be denoted by $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Given the bases $E_A = \{|e_j^A\rangle\}_{j=1,2,\ldots,d_A}$ and $E_B = \{|e_j^B\rangle\}_{j=1,2,\ldots,d_B}$ of the Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, a basis of the *tensor product Hilbert space* $\mathcal{H}_A \otimes \mathcal{H}_B$ can be built as $E = E_A \otimes E_B = \{|e_j^A\rangle \otimes |e_l^B\rangle\}_{l=1,2,\ldots,d_B}^{j=1,2,\ldots,d_A}$ (note that the notation after the first equality is symbolic).

We may use a more economic notation for the tensor product, namely $|a\rangle \otimes |b\rangle = |a, b\rangle$, except when the explicit tensor product symbol is needed for some special reason. With this notation the basis of the tensor product Hilbert space is written as $E = \{|e_j^A, e_l^B\rangle\}_{l=1,2,\ldots,d_B}^{j=1,2,\ldots,d_A}$.

The tensor product also maps operators acting on $\mathcal{H}_A$ and $\mathcal{H}_B$ to operators acting on $\mathcal{H}$. Given two operators $\hat{L}_A$ and $\hat{L}_B$ acting on $\mathcal{H}_A$ and $\mathcal{H}_B$, the *tensor product operator* $\hat{L} = \hat{L}_A \otimes \hat{L}_B$ is defined in $\mathcal{H}$ as that satisfying $\hat{L}|a, b\rangle = (\hat{L}_A|a\rangle) \otimes (\hat{L}_B|b\rangle)$ for any pair of vectors $|a\rangle \in \mathcal{H}_A$ and $|b\rangle \in \mathcal{H}_B$. When explicit subindices making reference to the Hilbert space on which operators act on are used, so that there is no room for confusion, we will use the shorter notations $\hat{L}_A \otimes \hat{L}_B = \hat{L}_A\hat{L}_B$, $\hat{L}_A \otimes \hat{I} = \hat{L}_A$, and $\hat{I} \otimes \hat{L}_B = \hat{L}_B$.

Note that the tensor product preserves the properties of the operators; for example, given two self-adjoint operators $\hat{H}_A$ and $\hat{H}_B$, unitary operators $\hat{U}_A$ and $\hat{U}_B$, or density operators $\hat{\rho}_A$ and $\hat{\rho}_B$, the operators $\hat{H}_A \otimes \hat{H}_B$, $\hat{U}_A \otimes \hat{U}_B$, and $\hat{\rho}_A \otimes \hat{\rho}_B$ are self-adjoint, unitary, and a density operator acting on $\mathcal{H}$, respectively. But keep in mind that this does not mean that all self-adjoint, unitary, or density operators acting on $\mathcal{H}$ can be written in a simple tensor product form $\hat{L}_A \otimes \hat{L}_B$.

3. The quantum-mechanical framework

In this section we review the basic postulates that describe how quantum mechanics treats physical systems. As the building blocks of the theory, these principles cannot be *proved*. They can only be formulated following *plausibility arguments* based on the *observation* of physical phenomena and the *connection* of the theory with previous theories which are known to work in some limit. We will try to motivate (and justify to a point) these principles as much as possible, starting with a brief historical introduction to the context in which they were created[69].

a. A brief historical introduction

By the end of the XIX century there was a great feeling of safety and confidence among the physics community: analytical mechanics (together with statistical mechanics) and Maxwell's electromagnetism (in the following *classical physics* altogether) seem to explain the whole range of physical phenomena that one could observe, and hence, in a sense, the foundations of physics were complete. There were, however, a couple of experimental observations which lacked explanation within this 'definitive' framework, which actually led to the construction of a whole new way of understanding physical phenomena: quantum mechanics.

Among these experimental evidences, the shape of the high-energy spectrum of the radiation emitted by a black body, the photoelectric effect which showed that only light exceeding some frequency can release electrons from a metal irrespective of its intensity, and the discrete set of spectral lines of hydrogen, were the principal triggers of the revolution to come in the first quarter of the XX century. The first two led Planck and Einstein, respectively, to suggest that electromagnetic energy is not continuous but divided in small packets of energy $\hbar\omega$ (ω being the angular frequency of the radiation), while Bohr succeeded in explaining the Hydrogen spectrum by assuming that the

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[69] For a thorough historical overview of the birth of quantum physics see [30].

electron orbiting the nucleus can occupy only a discrete set of orbits with angular momenta proportional to $\hbar$. The constant $\hbar = h/2\pi \sim 10^{-34}\mathrm{J}\cdot\mathrm{s}$, where h is now known as the Planck constant, appeared in both cases as somehow the 'quantization unit', the value separating the quantized values that energy or angular momentum are able to take.

Even though the physicists of the time tried to understand this quantization of the physical magnitudes within the framework of classical physics, it was soon realized that a completely new theory was required. The first attempts to build such a theory (which actually worked for some particular scenarios) were based on applying ad-hoc quantization rules to various mechanical variables of systems, but with a complete lack of physical interpretation for such rules [31]. However, between 1925 and 1927 the first real formulations of the needed theory were developed: the *wave mechanics* of Schrödinger [32] and the *matrix mechanics* of Heisenberg, Born and Jordan [33–35] (see [31] for English translations), which received also independent contributions by Dirac [36]. Even though in both theories the quantization of various observable quantities appeared naturally and in correspondence with experiments, they seemed completely different, at least until Schrödinger showed the equivalence between them both.

The new theory was later formalized mathematically using vector spaces by Dirac [26] (though not entirely rigorously), and a little later by von Neumann with more mathematical rigor using Hilbert spaces [37] ([38] for an English version). They developed the laws of *quantum mechanics* basically as we know them today [39–44]. In the next sections we will introduce these rules in the form of six principles that will set the structure of the theory of quantum mechanics as we will use it along the lectures.

b. Principle I: Observables and measurement outcomes

The experimental evidence for the quantization of some observable physical quantities motivates the first principle:

Principle I. ⌈Any physical observable quantity A corresponds to a self-adjoint operator $\hat{A}$ acting on an abstract Hilbert space. After a measurement of A, the only possible outcomes are the eigenvalues of $\hat{A}$.⌋

The quantization of physical observables is therefore directly introduced within the theory by this postulate. Note that it does not say anything about the dimension d of the Hilbert space corresponding to a given observable, and it even leaves open the possibility of observables having a continuous spectrum, rather than a discrete one. The problem of how to make the proper correspondence between observables and self-adjoint operators will be addressed in an principle to come.

In this lectures we use the name 'observable' both for the physical quantity A and its associated self-adjoint operator $\hat{A}$ indistinctly. Observables having purely-discrete or purely-continuous spectra will be referred to as *countable* and *continuous observables*, respectively.

c. Principle II: State of the system and statistics of measurements

The next principle follows from the following question: according to the previous principle the eigenvalues of an observable are the only values that can appear when measuring it, but what about the statistics of such a measurement? We know a class of operators in Hilbert spaces which act as probability distributions for the eigenvalues of any self-adjoint operator, density operators. This motivates the second principle:

Principle II. ⌈The state of the system is completely specified by a density operator $\hat{\rho}$. When measuring a countable observable A with eigenvectors $\{|a_j\rangle\}_{j=1,2,\ldots,d}$ (d might be infinite), it is associated to the possible outcomes $\{a_j\}_{j=1,2,\ldots,d}$ a probability distribution $\{p_j = \rho_{jj}\}_{j=1,2,\ldots,d}$ which determines the statistics of the experiment (*Born rule*). Similarly, when measuring a continuous observable X with eigenvectors $\{|x\rangle\}_{x\in\mathbb{R}}$, the probability density function $P(x) = \rho(x,x)$ is associated to the possible outcomes $\{x\}_{x\in\mathbb{R}}$ in the experiment.⌋

This principle has deep consequences that we analyze now. Contrary to classical mechanics (and intuition), even if the system is prepared in a given state, the value of an observable is in general not well defined. We can only specify with what probability a given value of the observable will come out in a measurement. Hence, this principle proposes a change of paradigm; determinism must be abandoned: the theory is no longer able to predict with certainty the outcome of a single run of an experiment in which an observable is measured, but rather gives the statistics that will be extracted after a large number of runs.

To be fair, there is a case in which the theory allows us to predict the outcome of the measurement of an observable with certainty: When the system is prepared such that its state is an eigenvector of the observable. This seems much like when in classical mechanics the system is prepared with a given value of its observables. However, we will

show that it is impossible to find a common eigenvector to *all* the available observables of a system, and hence the difference between classical and quantum mechanics is that in the later it is impossible to prepare the system in a state which would allow us to predict with certainty the outcome of a measurement of each of its observables. Let us try to elaborate on this in a more rigorous fashion.

Let us define the *expectation value* of a given operator $\hat{B}$ as

$$\langle \hat{B} \rangle = \mathrm{tr}\{\hat{\rho}\hat{B}\}. \tag{A23}$$

In the case of a countable observable $\hat{A}$ or a continuous observable $\hat{X}$, this expectation value can be written in their own eigenbases as

$$\langle \hat{A} \rangle = \sum_{j=1}^{d} \rho_{jj} a_j \qquad \text{and} \qquad \langle \hat{X} \rangle = \int_{-\infty}^{+\infty} dx \rho(x,x) x, \tag{A24}$$

which correspond to the mean value of the outcomes registered in large number of measurements of the observables. We define also the *variance* $V(A)$ of the observable as the expectation value of the square of its *fluctuation operator* $\delta\hat{A} = \hat{A} - \langle \hat{A} \rangle$, that is,

$$V(A) = \mathrm{tr}\{\hat{\rho}(\delta\hat{A})^2\} = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2, \tag{A25}$$

from which we obtain the *standard deviation* or *uncertainty* as $\Delta A = \sqrt{V(A)}$, which measures how much the outcomes of the experiment deviate from the mean, and hence, somehow specifies how 'well defined' is the value of the observable A.

Note that the probability of obtaining the outcome a_j when measuring A can be written as the expectation value of the projection operator $\hat{P}_j = |a_j\rangle\langle a_j|$, that is $p_j = \langle \hat{P}_j \rangle$. Similarly, the probability density function associated to the possible outcomes $\{x\}_{x\in\mathbb{R}}$ when measuring X can be written as $P(x) = \langle \hat{P}(x) \rangle$, where $\hat{P}(x) = |x\rangle\langle x|$.

Having written all these objects (probabilities, expectation values, and variances) in terms of traces is really useful, since the trace is invariant under basis changes, and hence can be evaluated in any basis we want to work with, see Section A 2 b.

These principles have one further counterintuitive consequence. It is possible to prove that irrespectively of the state of the system, the following relation between the variances of two non-commuting observables A and B is satisfied:

$$\Delta A \Delta B \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|. \tag{A26}$$

According to this inequality, known as the *uncertainty principle* (which was first derived by Heisenberg), in general, the only way in which the observable A can be perfectly defined ($\Delta A \to 0$) is by making completely undefined observable B ($\Delta B \to \infty$), or vice-versa. Hence, in the quantum formalism one cannot, in general, prepare the system in a state in which all its observables are well defined, what is completely opposite to our everyday experience.

Before moving to the third principle, let us comment on a couple more things related to the state of the system. It is possible to show that a density operator can always be expressed as a *statistical* or *convex mixture* of projection operators, that is, $\hat{\rho} = \sum_{m=1}^{M} w_m |\varphi_m\rangle\langle\varphi_m|$, where $\{w_m\}_{m=1,2,\ldots,M}$ is a probability distribution and the vectors $\{|\varphi_m\rangle\}_{m=1}^{M}$ are normalized to one, but do not need to be orthogonal (note that in fact M does not need to be equal to d). Hence, another way of specifying the state of the system is by a set of normalized vectors together with some statistical rule for mixing them, that is, the set $\{w_m, |\varphi_m\rangle\}_{m=1,2,\ldots,M}$, known as an *ensemble decomposition* of the state $\hat{\rho}$. Such decompositions are not unique, in the sense that different ensembles can lead to the same $\hat{\rho}$. It can be proved though [45] that two ensembles $\{w_m, |\varphi_m\rangle\}_{m=1,2,\ldots,M}$ and $\{v_n, |\psi_n\rangle\}_{n=1,2,\ldots,N}$ (we take $M \leq N$ for definiteness) give rise to the same density operator $\hat{\rho}$ if and only if there exists a left-unitary matrix[70] U with elements $\{U_{mn}\}_{m,n=1,2,\ldots,N}$ such that [45]

$$\sqrt{w_m}|\varphi_m\rangle = \sum_{n=1}^{N} U_{mn}\sqrt{v_n}|\psi_n\rangle, \qquad m = 1, 2, ..., N, \tag{A27}$$

where if $M \neq N$, $N - M$ zeros must be included in the ensemble with less states, so that $\mathcal{U}$ is a square matrix.

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[70] U is left-unitary if $U^\dagger U = I$ but $UU^\dagger$ might not be I, where I is the identity matrix of the corresponding dimension. It is easy to prove that finite-dimensional left-unitary matrices are unitary.

When only one vector $|a\rangle$ contributes to the mixture, $\hat{\rho} = |\varphi\rangle\langle\varphi|$ is completely specified by just this single vector, and we say that the density operator is *pure*; otherwise, we say that it is *mixed*. A necessary and sufficient condition for $\hat{\rho}$ to be pure is $\hat{\rho}^2 = \hat{\rho}$. Along the lectures we will learn that the mixedness of a state always comes from the fact that some of the information of the system has been lost to some other inaccessible system with which it has interacted for a while before becoming isolated or is interacting continuously. In other words, the state of a system is pure only when it has no correlations at all with other systems.

Note, finally, that when the state of the system is in a *pure state* $|\psi\rangle$, the expectation value of an operator $\hat{B}$ takes the simple form $\langle\psi|\hat{B}|\psi\rangle$. Moreover, the pure state can be expanded in the countable and continuous bases of two observables $\hat{A}$ and $\hat{X}$ as

$$|\psi\rangle = \sum_{j=1}^{d} \psi_j |a_j\rangle \qquad \text{and} \qquad |\psi\rangle = \int_{-\infty}^{+\infty} dx \psi(x)|x\rangle, \tag{A28}$$

respectively, being $\psi_j = \langle a_j|\psi\rangle$ and $\psi(x) = \langle x|\psi\rangle$. In this case, the probability distribution for the discrete outcomes $\{a_j\}_{j=1,2,\ldots,d}$ is given by $\{p_j = |\psi_j|^2\}_{j=1,2,\ldots,d}$, while the probability density function for the continuous outcomes $\{x\}_{x\in\mathbb{R}}$ is given by $P(x) = |\psi(x)|^2$.

d. Principle III: Composite systems

The next principle specifies how the theory accommodates dealing with composite systems within its mathematical framework. Of course, a composition of two systems is itself another system subject to the laws of quantum mechanics; the question is how can we construct it.

Principle III. ⌈Consider two systems A and B with associated Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. Then, the state of the composite system $\hat{\rho}_{AB}$ as well as its observables act onto the tensor product Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$.⌋

This principle has the following consequence. Imagine that the systems A and B interact during some time in such a way that they cannot be described anymore by independent states $\hat{\rho}_A$ and $\hat{\rho}_B$ acting on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, but by a state $\hat{\rho}_{AB}$ acting on the joint space $\mathcal{H}_{AB}$. After the interaction, system B is kept isolated from any other system, but system A is given to an observer, who is therefore able to measure observables defined in $\mathcal{H}_A$ only, and might not even know that system A is part of a larger system. The question is, is it possible to reproduce the statistics of the measurements performed on system A with some state $\hat{\rho}_A$ acting on $\mathcal{H}_A$ only? This question has a positive and *unique* answer: this state is given by the *reduced density operator* $\hat{\rho}_A = \mathrm{tr}_B\{\hat{\rho}_{AB}\}$, that is, by performing the partial trace[71] with respect system's B subspace onto the joint state.

e. Principle IV: Quantization rules

The introduction of the fourth principle is motivated by the following fact. The class of self-adjoint operators forms a real vector space with respect to the addition of operators and the multiplication of an operator by a real number. Using the commutator we can also build an operation that takes two self-adjoint operators $\hat{A}$ and $\hat{B}$ to generate another self-adjoint operator $\hat{C} = \mathrm{i}[\hat{A}, \hat{B}]$, which, in addition, satisfies all the properties required by a Lie product. Hence, even if classical and quantum theories seem fundamentally different, it seems that observables are treated similarly within their corresponding mathematical frameworks: they are elements of a Lie algebra.

On the other hand, we saw that the generalized coordinates and momenta have a particular mathematical structure in the Hamiltonian formalism, they are the generators of the Heisenberg group. It seems then quite reasonable to ask for the same in the quantum theory, so that at least in what concerns to observables both theories are equivalent. This motivates the fourth principle:

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[71] Given an orthonormal basis $\{|b_j\rangle\}_j$ of $\mathcal{H}_B$, this is defined by

$$\mathrm{tr}_B\{\hat{\rho}_{AB}\} = \sum_j \langle b_j|\hat{\rho}_{AB}|b_j\rangle, \tag{A29}$$

which is indeed an operator acting on $\mathcal{H}_A$.

Principle IV. ⌈Consider a physical system which is described classically within a Hamiltonian formalism by a set of generalized coordinates $\mathbf{q} = \{q_j\}_{j=1}^n$ and momenta $\mathbf{p} = \{p_j\}_{j=1}^n$ at a given time. Within the quantum formalism, the corresponding observables $\hat{\mathbf{q}} = \{\hat{q}_j\}_{j=1}^n$ and $\hat{\mathbf{p}} = \{\hat{p}_j\}_{j=1}^n$ satisfy the *canonical commutation relations*

$$[\hat{q}_j, \hat{p}_l] = \mathrm{i}\hbar\delta_{jl} \qquad \text{and} \qquad [\hat{q}_j, \hat{q}_l] = [\hat{p}_j, \hat{p}_l] = 0. \ \rfloor \tag{A30}$$

The constant $\hbar$ is included because, while the Poisson bracket $\{q_j, p_l\}$ has no units, the commutator $[\hat{q}_j, \hat{p}_l]$ has units of action. That it is exactly $\hbar$ the proper constant can be seen only once the theory is compared with experiments.

We can now discuss how to build the self-adjoint operator corresponding to a given observable. In general, meaningful observables are built from symmetry principles [44], e.g., the kinetic and angular momenta as the generators of space translations and rotations, respectively. An alternative route might be taken when the observable is well-defined classically. Suppose that in the Hamiltonian formalism the observable A is represented by the real phase-space function $A(\mathbf{q}, \mathbf{p})$. It seems quite natural to use then $A(\hat{\mathbf{q}}, \hat{\mathbf{p}})$ as the corresponding quantum operator. However, this correspondence faces a lot of troubles resulting from the fact that, while coordinates and momenta commute in classical mechanics, they do not in quantum mechanics. For example, given the classical observable $A = qp = pq$, we could be tempted to assign to it any of the quantum operators $\hat{A}_1 = \hat{q}\hat{p}$ or $\hat{A}_2 = \hat{p}\hat{q}$. These two operators are not equivalent (they do not commute) and they are not even self-adjoint, and hence cannot represent observables. One possible solution to this problem, at least for observables with a series expansion, is to always symmetrize the classical expressions with respect to coordinates and momenta, so that the resulting operator is self-adjoint. Applied to our previous example, we should take $\hat{A} = (\hat{p}\hat{q} + \hat{q}\hat{p})/2$ according to this rule. This simple procedure leads to the correct results most of the times, and when it fails (for example, if the classical observable does not have a series expansion) it was proved by Groenewold [46] that it is possible to make a faithful systematic correspondence between classical observables and self-adjoint operators by using more sophisticated correspondence rules.

Of course, when the observable corresponds to a degree of freedom which is not defined in a classical context (like *spin*), it must be built from scratch based on experimental observations and/or first principles.

Note that the commutation relations between coordinates and momenta makes them satisfy the uncertainty relation $\Delta q \Delta p \geq \hbar/2$, and hence, if one of them is well defined in the system, the other must have statistics very spread around the mean.

f. Principle V: Free evolution of the system

The previous principles have served to define the mathematical structure of the theory and its relation to physical systems. We have not said anything yet about how quantum mechanics treats the evolution of the system. As we are about to see, the formalism treats very differently the evolution due to a measurement performed by an observer, and the *free* evolution of the system when it is not subject to observation. The following principle specifies how to deal with the latter case. Just as with the previous principle, it feels pretty reasonable to keep the analogy with the Hamiltonian formalism, a motivation which comes also from the fact that, as stated, quantum mechanics must converge to classical mechanics in some limit. In the Hamiltonian formalism, observables evolve according to (A7), so that making the correspondence between the classical and quantum Lie products as in the previous principle, we enunciate the fifth principle:

Principle V. ⌈The evolution of an observable $\hat{A}(\hat{\mathbf{q}}, \hat{\mathbf{p}}, ...; t)$ is given by

$$\mathrm{i}\hbar\frac{d\hat{A}}{dt} = [\hat{A}, \hat{H}] + \frac{\partial\hat{A}}{\partial t}, \tag{A31}$$

which is known as the Heisenberg equation, and where $\hat{H}(\hat{\mathbf{q}}, \hat{\mathbf{p}}, ...; t)$ is the self-adjoint operator corresponding to the Hamiltonian of the system. Note that the notation "$\hat{\mathbf{q}}, \hat{\mathbf{p}}, ...$" emphasizes the fact that the observable may depend on fundamental operators other than the generalized coordinates, e.g., purely-quantum degrees of freedom such as spin.⌋

For the case of an observable and a Hamiltonian with no explicit time-dependence (as will be assumed from now on), this evolution equation admits the explicit solution

$$\hat{A}(t) = \hat{U}^\dagger(t)\hat{A}(0)\hat{U}(t), \quad \text{being } \hat{U}(t) = \exp[\hat{H}t/\mathrm{i}\hbar], \tag{A32}$$

a unitary operator called the *evolution operator*. For explicitly time-dependent Hamiltonians it is still possible to solve formally the Heisenberg equation as a *Dyson series*, but we will not worry about this case, as it does not appear

throughout the lectures. Let us remark that this type of evolution ensures that if the canonical commutation relations (A30) are satisfied at some time, they will be satisfied at all times.

Note that within this formalism the state $\hat{\rho}$ of the system is fixed in time, the observables are the ones which evolve. On the other hand, we have seen that, on what concerns to observations (experiments), only expectation values of operators are relevant; and for an observable $\hat{A}$ at time t, these can be written as

$$\langle \hat{A}(t) \rangle = \mathrm{tr}\{\hat{\rho}\hat{A}(t)\} = \mathrm{tr}\{\hat{U}(t)\hat{\rho}\hat{U}^{\dagger}(t)\hat{A}(0)\}, \tag{A33}$$

where in the last equality we have used the cyclic property of the trace. This expression shows that, instead of treating the observable as the evolving operator, we can define a new state at time t given by

$$\rho(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^{\dagger}(t), \tag{A34}$$

while keeping fixed the operator. In differential form, this expression reads

$$\mathrm{i}\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}], \tag{A35}$$

which is known as the *von Neumann equation*. When the system is in a pure state $|\psi\rangle$, the following evolution equation is derived for the state vector itself

$$\mathrm{i}\hbar \frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle, \tag{A36}$$

which is known as the *Schrödinger equation*, from which the state at time t is found as $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$.

Therefore, we have two different but equivalent evolution formalisms or *pictures*. In one, which we shall call *Heisenberg picture*, the state of the system is fixed, while observables evolve according to the Heisenberg equation. In the other, which we will denote by *Schrödinger picture*, observables are fixed, while states evolve according to the von Neumann equation.

We can even define intermediate pictures in which both the state and the observables evolve, the so-called *interaction pictures*. To show how this is done, let us denote by $\hat{A}$ and $\hat{\rho}\,(t)$ an observable and the state of the system in the Schrödinger picture (the same kind of transformation can be performed from the Heisenberg picture). The expectation value of an observable A is written as $\mathrm{tr}\{\hat{\rho}(t)\hat{A}\}$. We can define a unitary operator $\hat{U}_{\mathrm{c}} = \exp[\hat{H}_{\mathrm{c}}t/\mathrm{i}\hbar]$, with $\hat{H}_{\mathrm{c}}$ some self-adjoint operator, and then a transformed state $\tilde{\rho} = \hat{U}_{\mathrm{c}}^{\dagger}\hat{\rho}\hat{U}_{\mathrm{c}}$ and a transformed observable $\tilde{A} = \hat{U}_{\mathrm{c}}^{\dagger}\hat{A}\hat{U}_{\mathrm{c}}$. This transformation leaves invariant the expectation value, which can be evaluated as $\mathrm{tr}\{\tilde{\rho}\,(t)\,\tilde{A}\,(t)\}$, but now the evolution equations of the state and the observable read

$$\mathrm{i}\hbar \frac{d\tilde{\rho}}{dt} = [\hat{H}_{\mathrm{I}}, \tilde{\rho}] \qquad \text{and} \qquad \mathrm{i}\hbar \frac{d\tilde{A}}{dt} = [\tilde{A}, \hat{H}_{\mathrm{c}}], \tag{A37}$$

so that within this new picture states evolve according to the *interaction-picture Hamiltonian* $\hat{H}_{\mathrm{I}} = \hat{U}_{\mathrm{c}}^{\dagger}\hat{H}\hat{U}_{\mathrm{c}} - \hat{H}_{\mathrm{c}}$, while observables evolve according to the *transformation Hamiltonian* $\hat{H}_{\mathrm{c}}$.

The same kind of game can be played from the Heisenberg picture. Let us denote in this case by $\hat{A}(t)$ and $\hat{\rho}$ an observable and the state in the Heisenberg picture. The transformed state $\tilde{\rho} = \hat{U}_{\mathrm{c}}^{\dagger}\hat{\rho}\hat{U}_{\mathrm{c}}$ and observable $\tilde{A} = \hat{U}_{\mathrm{c}}^{\dagger}\hat{A}\hat{U}_{\mathrm{c}}$ satisfy then the evolution equations

$$\mathrm{i}\hbar \frac{d\tilde{\rho}}{dt} = [\hat{H}_{\mathrm{c}}, \tilde{\rho}] \qquad \text{and} \qquad \mathrm{i}\hbar \frac{d\tilde{A}}{dt} = [\tilde{A}, \hat{H}_{\mathrm{I}}]. \tag{A38}$$

g. Principle VI: Post-measurement state

The previous postulate specifies how the free evolution of the system is taken into account in the quantum mechanical formalism. It is then left to specify how the state of the system evolves after a measurement is performed on it. For reasons that we will briefly review after enunciating the principle, this is probably the most controversial point in the quantum formalism. Indeed, while in classical physics we assume that it is possible to perform measurements onto the system without disturbing its state, this final quantum-mechanical principle states:

Principle VI. ⌈If upon a measurement of a countable observable A the outcome a_m is obtained, then immediately after the measurement the state of the system *collapses* to $|a_m\rangle$.⌋

The principle assumes that, after the measurement, the observer gains knowledge about the measurement outcome, what we will denote as a *selective* measurement. However, suppose that for some reason the user interface of the measurement device does not allow us to distinguish between a set of outcomes $\{a_{m_k}\}_{k=1,2,\ldots,K}$, what we will denote by a *partially-selective* measurement. Then, after the corresponding experimental outcome is obtained, the best estimate that the observer can assign to the post-measurement state is the ensemble decomposition $\{\bar{p}_{m_k}, |a_{m_k}\rangle\}_{k=1,2,\ldots,K}$ with relative probabilities $\bar{p}_{m_k} = p_{m_k}/\sum_{k=1}^{K} p_{m_k}$, since the real outcome is unknown, but the *a priori* probabilities p_m of the possible outcomes are known. Hence, in such case we would assign the post-measurement state $\hat{\rho}_{\{m_1,m_2,\ldots,m_K\}} = \sum_{k=1}^{K} \bar{p}_{m_k}|a_{m_k}\rangle\langle a_{m_k}|$ to the system. The extreme case in which the outcome of the measurement is simply not recorded, so that we cannot know which outcome occurred and the best estimate for the post-measurement state is $\hat{\rho}' = \sum_{m=1}^{d} p_m|a_m\rangle\langle a_m|$, is known as a *non-selective* measurement.

So far we have considered the post-measurement state in the case of measuring a countable observable. The continuous case is tricky, since, as mentioned in Sec. A 2 c, the eigenvectors of a continuous observable cannot correspond to physical states (they cannot be normalized). On the other hand, one can always argue that the detection of a single definite value out of the spectrum $\{x\}_{x\in\mathbb{R}}$ of a continuous observable $\hat{X}$ would require an infinite precision, whereas detectors always have some finite precision. Consequently, there are two natural ways of dealing with such problem:

- Accepting that measuring continuous observables is simply not possible, and what is measured in real experiments is always some countable version of them, which only in some unphysical limit reproduce the continuous measurement precisely. An example of this consists in the process of *bining* the continuous observable, which assumes that the detector can only distinguish between pixels with width Δ_x centered at certain points $\{x_k = k\Delta_x\}_{k\in\mathbb{Z}}$ in the spectrum of the continuous observable, so what is measured is instead the countable observable

$$\hat{X}_{\text{count}} = \sum_{k=-\infty}^{\infty} x_k|x_k\rangle\langle x_k|, \qquad \text{with } |x_k\rangle = \frac{1}{\sqrt{\Delta_x}}\int_{x_k-\Delta_x/2}^{x_k+\Delta_x/2} dx|x\rangle. \tag{A39}$$

- Allowing for the possible outcomes of the measurement to still be continuous, but with an uncertainty given by the precision of the measurement device. In the case of starting with a pure state, this would simply mean that the post-measurement state is not an eigenvector of the continuous operator, but a normalizable superposition of several of them, spanning around the measured value with a width given by the measurement's precision. This intuitive approach can be formalized with the theory of generalized quantum measurements [47, 48].

In any case, it is sometimes useful for theoretical calculations to proceed as if perfectly precise measurements were possible, with the system collapsing to one eigenvector of the continuous observable. However, it is important to keep in mind that this is just an unphysical idealization, whose corrections have to be taken into account when applying it to a real situation.

We can pass now to discuss the controversial aspects of this principle, of which a pedagogical introduction can be found in [43] (see also [49] and Appendix E of [28]). In short, the problem is that, even though it leads to predictions which fully agree with the observations, the principle somehow creates an *inconsistency* in the theory because of the following argument. According to Principle V, the unitary evolution of a system not subject to observation is *reversible*, that is, one can always change the sign of the relevant terms of the Hamiltonian which contributed to the evolution (at least conceptually), and come back to the original state. On the other hand, the *collapse* principle claims that when the system is put in contact with a measurement device and an observable is measured, the state of the system collapses to some other state in an *irreversible* way[72]. However, coming back to Principle V, the whole measurement process could be described reversibly by considering, in addition to the system's particles, the evolution of all the particles forming the measurement device (or even the human who is observing the measurement outcome if needed!), that is, the Hamiltonian for the whole 'observed system + measurement device' scenario. Hence, it seems that, when including the collapse principle, quantum mechanics allows for two completely different descriptions of the measurement process, one reversible and one irreversible, without giving a clear rule for when to apply each. It is in this sense that the theory contains an inconsistency.

There are three[73] main positions that physicists have taken regarding how this inconsistency might be solved, which we will refer too as *objective*, *subjective*, and *apparent* collapse interpretations, and whose (highly simplified) main

[72] Note that in the literature the terms *reversible* and *irreversible* are sometimes replaced by *linear* and *nonlinear*, referring to the fact that unitary evolution comes from a linear equation (Schrödinger or von Neumann equations), while measurement-induced dynamics becomes nonlinear through its dependence on the probability of the possible outcomes, which in turn depend on the state.

[73] But each with many sub-interpretations differing in subtle, or even not so subtle points. In essence, one can find a lot of truth to the say "Give me a room with N physicists and I'll find you $N+1$ different interpretations of quantum mechanics".

ideas we hereby discuss[74]:

- **Objective collapse.** There is a clear boundary (yet to be found) between the quantum and the classical worlds. In the classical world, to which measurement devices and observers belong, there exists some *decoherence mechanism* that prevents systems from being in a superposition of states corresponding to mutually exclusive values of their observables. When the measurement device enters in contact with the quantum system, the latter becomes a part of the classical world, and the aforementioned decoherence mechanism forces its collapse. Hence, within this interpretation the collapse is pretty much a real physical process that we still need to understand along with the quantum/classical boundary. There are several *collapse theories* available at the moment [49], part of which we expect to be able to falsify or confirm in the near future with modern quantum technologies based on, for example, opto-, electro-, or magneto-mechanics [52].

- **Subjective collapse.** The state is simply a mathematical object which conveniently describes the statistics of experiments, but that otherwise has no physical significance. As such, what the quantum formalism provides is simply a set of rules for how to update our best estimate to the state according to the information that we have about the system. In this sense, the collapse is just the way that an observer subjectively updates the state of the system after gathering the information concerning the outcome. Quantum Bayesianism or *QBism* [53, 54] is possibly the most refined of such interpretations, which has gathered a lot of momentum in the last years.

- **Apparent collapse.** The measurement can be described without the need of abandoning the framework of Principle V as a joint unitary transformation onto the system and the measurement device (even including the observer), leading to a final entangled state[75] between these in which the eigenstates of the system's observable are in one-to-one correspondence with a set of macroscopically distinct *pointer* states of the measurement device [43]. Hence, after a measurement, reality splits into many *branches* where observers experience different outcomes and which stay in a quantum superposition, and collapse appears just an illusion coming from the fact that we only see the effective dynamics projected into the corresponding branch that we are experiencing. This approach finds its best-developed expression in the so-called *many-worlds interpretation* [55], which describes the quantum-mechanical framework as unitary evolution of a pure state (*wave function*) of the whole universe, which includes all the branches or *worlds*[76].

In any case whether of objective, subjective, or apparent value, it is clear that the collapse principle is of great *operational* value, that is, it is currently the easiest successful way of analyzing schemes involving measurements, and hence we will apply it when needed.

h. Classical versus quantum correlations: entanglement

Consider two systems A and B (named after Alice and Bob, two observers which are able to interact locally with their respective system) with associated Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ of dimension d_A and d_B, respectively. The systems are prepared in some state $\hat{\rho}_{AB}$ acting on the joint space $\mathcal{H}_A \otimes \mathcal{H}_B$. Recall from the discussion after Principle III that Alice and Bob can reproduce the statistics of measurements performed on their subsystems via the reduced states $\hat{\rho}_A = \mathrm{tr}_B\{\hat{\rho}_{AB}\}$ and $\hat{\rho}_B = \mathrm{tr}_A\{\hat{\rho}_{AB}\}$, respectively.

When the state of the joint system is of the type $\hat{\rho}_{AB}^{(\mathrm{prod})} = \hat{\rho}_A \otimes \hat{\rho}_B$, that is, a tensor product of two arbitrary density operators, the actions performed by Alice on system A won't affect Bob's system, the statistics of which are given by $\hat{\rho}_B$, no matter the actual state $\hat{\rho}_A$. In this case A and B are completely *uncorrelated*. For any other type of joint state, A and B will share some kind of correlation.

Correlations are not strange in classical mechanics. Hence, a problem of paramount relevance in quantum mechanics is understanding which type of correlations can appear at a classical level, and which are purely quantum. This is because only if the latter are present, one can expect the correlated systems to be useful for quantum-mechanical applications which go beyond what is classically possible, the paradigmatic example being the exponential speed up of computational algorithms.

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[74] One interpretation of quantum mechanics that is formulated with a completely different set of principles, and hence does not fit this list is *Bohmian mechanics* [50, 51], in which particles follow deterministic trajectories, but determined from a *guiding wave* that obeys the Schrödinger equation.

[75] We will discuss in detail about the concept of entanglement towards the end of this chapter.

[76] Believers of the many-worlds interpretation, or even people who are not sure of their quantum-mechanical beliefs (better safe than sorry), are strongly encouraged to use the *quantum world splitter* when in need of choosing between equally reasonable options in life: www.qol.tau.ac.il.

Intuitively, the state of the system will induce only classical correlations between A and B when it can be written in the form

$$\hat{\rho}_{AB}^{(\mathrm{sep})} = \sum_{k=1}^{M} w_k \hat{\rho}_A^{(k)} \otimes \hat{\rho}_B^{(k)}, \tag{A40}$$

where the $\hat{\rho}^{(k)}$'s are density operators, $\{w_k\}_{k=1,2,\ldots,M}$ is a probability distribution, M can be infinite, and the index k can even be continuous in some range, in which case the sum turns into an integral in that range and the probability distribution into a probability density function. Indeed, a state of the type (A40) can be prepared by a protocol involving only local actions and classical correlations: Alice and Bob can share a classical machine which randomly picks a value of k according to the distribution $\{w_k\}_{k=1,2\ldots,M}$ to trigger the preparation of the states $\hat{\rho}_A^{(k)}$ and $\hat{\rho}_B^{(k)}$, what can be done locally, and hence cannot induce further correlations. If the process is automatized so that Alice and Bob do not learn the outcome k of the random number generator, the best estimate that they can assign to the state in order to reproduce the statistics of any forthcoming experiments is the mixture $\hat{\rho}_{AB}^{(\mathrm{sep})}$. In other words, the state does not contain quantum correlations if it can be prepared using only *local operations and classical communication*.

There is yet another intuitive way of justifying that states which cannot be written in the separable form (A40) will make A and B share quantum correlations. The idea is that arguably the most striking difference between classical and quantum mechanics is the *superposition principle*, that is, the possibility of states corresponding to *mutually exclusive* properties of the system to *interfere* (e.g., two different colors, $|\mathrm{blue}\rangle + |\mathrm{red}\rangle$). Hence, it is intuitive that correlations should have a quantum nature only when they come from some kind of superposition of joint states corresponding to mutually exclusive properties of the correlated systems (e.g., color in one system and flavor in the other, $|\mathrm{blue}\rangle\otimes|\mathrm{sweet}\rangle + |\mathrm{red}\rangle\otimes|\mathrm{sour}\rangle$), in which case the state cannot be written as a tensor product of two independent states ($|\mathrm{blue}\rangle \otimes |\mathrm{sour}\rangle$) or as a purely classical statistical mixture of these ($|\mathrm{blue}\rangle\langle\mathrm{blue}| \otimes |\mathrm{sweet}\rangle\langle\mathrm{sweet}| + |\mathrm{red}\rangle\langle\mathrm{red}| \otimes |\mathrm{sour}\rangle\langle\mathrm{sour}|$).

States of the type $\hat{\rho}_{AB}^{(\mathrm{sep})}$ are called *separable*. Any state which cannot be written in this form will induce quantum correlations between A and B. These correlations which cannot be generated by classical means are known as *entanglement*, and states which are not separable are called *entangled states*.

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