Quantum Information and Quantum Noise

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Contents

Chapter 1

Review of quantum mechanics

Quantum mechanics is all about **states** and **operators**. States represent the instantaneous configuration of your system. You have probably seen them in the form of kets, such as $|\psi\rangle$ and $|i\rangle$, or as wave-functions $\psi(x)$. However, as we will soon learn, the real state in quantum mechanics is specified by an object called a **density matrix**, ρ. Density matrices encompass all the information you can have about a physical system, with kets and wave-functions being simply particular cases.

You have also probably seen several examples of operators, such as H, $\hat{p}$, $a^\dagger$, σ_z, etc. *Operators act on states to produce new states.* For instance, the operator σ_x flips the 0 and 1's of a qubit, whereas the operator $a^\dagger a$ counts the number of photons in the state. Understanding the action of operators on states is the key to understanding the physics behind the mathematics. After you gain some intuition, by simply looking at a Hamiltonian you will already be able to draw a bunch of conclusions about your system, without having to do any calculations.

Operators also fall into different categories, depending on what they are designed to do. The two most important classes are Hermitian and Unitary operators. Hermitian operators always have real eigenvalues and are used to describe quantities that can be observed in the lab. Unitary operators, on the other hand, preserve probabilities for kets and are used to describe the evolution of closed quantum systems. The evolution of an open quantum system, on the other hand, is described by another type of process known as **Quantum Operation** where instead of operators we use *super-operators* (which, you have to admit, sounds cool).

Finally, we have **measurements**. Measurements are also implemented by operators. For instance, that wave-function collapse idea is what we call a *projective measurements* and is implemented by a projection operator. In this course you will also learn about **generalized measurements and POVMs**. We will actually have a lot to say about measurements in general. Not only are they the least intuitive aspect of quantum mechanics, but they are also the source of all weird effects. If measurements did not exist, quantum mechanics would be quite simple. For many decades, the difficulties concerning the process of measurement were simply swept under the rug. But in the last 4 decades, partially due to experimental advances and fresh new theoretical ideas, this subject has seen a revival of interest. In this course I will adopt the so-called

Darwinistic approach: *measurements result from the interaction of a system with its environment*. This interaction is what enables amplification (the process in which quantum signals reach our classical human eyes) and ultimately defines the transition from quantum to classical. But I should probably stop here. I promise we will discuss more about this later.

Before getting our hands dirty, I just want to conclude by saying that, in a simplified view, the above discussion essentially summarizes quantum mechanics, as being formed of three parts: **states, evolutions and measurements**. You have probably seen all three in the old-fashioned way. In this course you will learn about their modern generalizations and how they can be used to construct new technologies. Even though I would love to jump right in, we must start slow. In this chapter I will review most of the linear algebra used in quantum mechanics, together with some results you may have seen before, such as projective measurements and Schrödinger's equation. This will be essential to all that will be discussed in the remaining chapters.

1.1 Hilbert spaces and states

To any physical system we can associated an abstract complex vector space with inner product, known as a **Hilbert space**, such that the state of the system at an given instant can be described by a vector in this space. This is the first and most basic postulate of quantum mechanics. Following Dirac, we usually denote vectors in this space as $|\psi\rangle$, $|i\rangle$, etc., where the quantity inside the $|\rangle$ is nothing but a *label* to specify which state we are referring to.

A Hilbert space can be both finite or infinite dimensional. The dimension d is defined by the number of linearly independent vectors we need to span the vector space. A set $\{|i\rangle\}$ of linearly independent vectors that spans the vector space is called a basis. With this basis any state may be expressed as

$$|\psi\rangle = \sum_{i=0}^{d-1} \psi_i |i\rangle, \tag{1.1}$$

where ψ_i can be arbitrary complex numbers.

A Hilbert space is also equipped with an **inner product**, $\langle\phi|\psi\rangle$, which converts pairs of vectors into complex numbers, according to the following rules:

1. If $|\psi\rangle = a|\alpha\rangle + b|\beta\rangle$ then $\langle\gamma|\psi\rangle = a\langle\gamma|\alpha\rangle + \langle\gamma|\beta\rangle$.
2. $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$.
3. $\langle\psi|\psi\rangle \geq 0$ and $\langle\psi|\psi\rangle = 0$ if and only if $|\psi\rangle = 0$.

A set of basis vectors $|i\rangle$ is called **orthonormal** when it satisfies

$$\langle i|j\rangle = \delta_{i,j}. \tag{1.2}$$

Exploring the 3 properties of the inner product, one may then show that given two states written in this basis, $|\psi\rangle = \sum_i \psi_i|i\rangle$ and $|\phi\rangle = \sum_i \phi_i|i\rangle$, the inner product becomes

$$\langle\psi|\phi\rangle = \sum_i \psi_i^* \phi_i. \tag{1.3}$$

We always work with orthonormal bases. And even though the basis set is never unique, the basis we are using is usually clear from the context. A general state such as (1.1) is then generally written as a column vector

$$|\psi\rangle = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{d-1} \end{pmatrix}. \tag{1.4}$$

The object $\langle\psi|$ appearing in the inner product, which is called a **bra**, may then be written as a row vector

$$\langle\psi| = \begin{pmatrix} \psi_0^* & \psi_1^* & \dots & \psi_{d-1}^* \end{pmatrix}. \tag{1.5}$$

The inner product formula (1.3) can now be clearly seen to be nothing but the multiplication of a row vector by a column vector. Notwithstanding, I am obligated to emphasize that when we write a state as in Eq. (1.4), we are making specific reference to a basis. If we were to use another basis, the coefficients would be different. The inner product, on the other hand, does not depend on the choice of basis. If you use a different basis, each term in the sum (1.3) will be different, but the total sum will be the same.

The vectors in the Hilbert space which represent physical states are also constructed to satisfy the **normalization** condition

$$\langle\psi|\psi\rangle = 1. \tag{1.6}$$

This, as we will see, is related to the probabilistic nature of quantum mechanics. It means that if two states differ only by a global phase $e^{i\theta}$, then they are physically equivalent.

You may also be wondering about wave-functions. Wave-functions are nothing but the inner product of a ket with the position state $|x\rangle$:

$$\psi(x) = \langle x|\psi\rangle \tag{1.7}$$

Wave-functions are not very useful in this field. In fact, I don't think we will ever need them again in this course. So bye-bye $\psi(x)$.

1.2 Qubits and Bloch's sphere

The simplest quantum system is one whose Hilbert space has dimension $d = 2$, which is what we call a **qubit**. In this case we only need two states that are usually labeled as $|0\rangle$ and $|1\rangle$ and are often called the **computational basis**. Note that when we refer to a qubit, we don't make any mention to the physical system it represents. In fact, a qubit may represent many physical situations, the two most common being spin 1/2 particles, two-level atoms and the two polarization directions of a photon. A spin 1/2 particle is characterized by spin projections ↑ and ↓ in a given direction, so we can label $|0\rangle \equiv |\uparrow\rangle$ and $|1\rangle \equiv |\downarrow\rangle$. Atoms, on the other hand, have very many energy levels.

However, sometimes it is reasonable to assume that only the ground state and the first excited state are important, which will be reasonable when the other excited states live too far up the energy ladder. In this case we can make the association $|0\rangle \equiv |g\rangle$, the ground-state, and $|1\rangle \equiv |e\rangle$, the first excited state. Finally, for the polarization of a photon we can call $|0\rangle = |x\rangle$ and $|1\rangle = |y\rangle$, which mean a photon polarized either in the x or y direction. We will play back and forth with these physical representations of a qubit. So let me summarize the main notations:

$$\begin{aligned} |0\rangle &= |\uparrow\rangle = |g\rangle = |x\rangle, \\ |1\rangle &= |\downarrow\rangle = |e\rangle = |y\rangle. \end{aligned} \tag{1.8}$$

An arbitrary state of a qubit may be written as

$$|\psi\rangle = a|0\rangle + b|1\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \tag{1.9}$$

where a and b are complex numbers which, according to Eq. (1.6), should satisfy

$$|a|^2 + |b|^2 = 1 \tag{1.10}$$

A convenient way to parametrize a and b is as

$$a = \cos(\theta/2), \qquad b = e^{i\phi}\sin(\theta/2), \tag{1.11}$$

where θ and ϕ are arbitrary real parameters. While this parametrization may not seem unique, it turns out that it is since any other choice will only differ by a global phase and hence will be physically equivalent. It also suffices to consider the parameters in the range $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$, as other values would just give the same state up to a global phase.

You can probably see a similarity here with the way we parametrize a sphere in terms of a polar and a azimutal angle. This is somewhat surprising since these are completely different things. A sphere is an object in $\mathbb{R}^3$, whereas in our case we have a vector in $\mathbb{C}^2$. But since our vector is constrained by the normalization (1.10), it is possible to map one representation into the other. That is the idea of **Bloch's sphere**, which is illustrated in Fig. 1.1. In this representation, the state $|0\rangle$ is the north pole, whereas $|1\rangle$ is the south pole. In this figure I also highlight two other states which appear often, called $|\pm\rangle$. They are defined as

$$|\pm\rangle = \frac{|0\rangle \pm |1\rangle}{\sqrt{2}}. \tag{1.12}$$

In terms of the angles θ and ϕ in Eq. (1.11), this corresponds to $\theta = \pi/2$ and $\phi = 0, \pi$. Thus, these states lie in the *equator*, as show in Fig. 1.1. Also, I should mention a possible source of confusion between the states $|\pm\rangle$ and the up-down states of spin 1/2 particles. I will discuss a way to lift this confusion below, when we talk about Pauli matrices.

A word of warning: Bloch's sphere is only used as a way to represent a complex vector as something real, so that we humans can visualize it. Be careful not to take this mapping too seriously. For instance, if you look blindly at Fig. 1.1 you will think $|0\rangle$ and $|1\rangle$ are parallel to each other, whereas in fact they are orthogonal, $\langle 0|1\rangle = 0$.

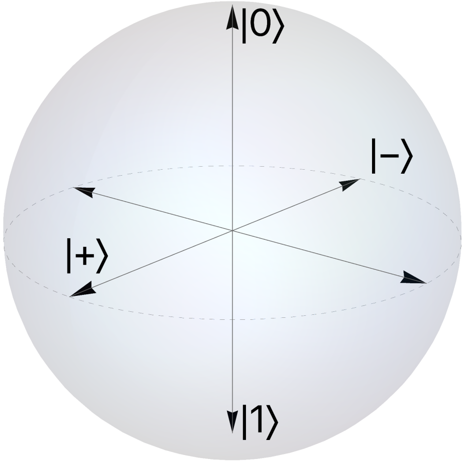

Figure 1.1: Example of Bloch's sphere which maps the general state of a qubit into a sphere of unit radius.

1.3 Outer product and completeness

The inner product gives us a recipe to obtain numbers starting from vectors. As we have seen, to do that, we simply multiply row vectors by column vectors. We could also think about the opposite operation of multiplying a column vector by a row vector. The result will be a matrix. For instance, if $|\psi\rangle = a|0\rangle + b|1\rangle$ and $|\phi\rangle = c|0\rangle + d|1\rangle$, then

$$|\psi\rangle\langle\phi| = \begin{pmatrix} a \\ b \end{pmatrix} \begin{pmatrix} c^* & d^* \end{pmatrix} = \begin{pmatrix} ac^* & ad^* \\ bc^* & bd^* \end{pmatrix}. \tag{1.13}$$

This is the idea of the **outer product**. In linear algebra the resulting object is usually referred to as a rank-1 matrix.

Let us go back now to the decomposition of an arbitrar state in a basis, as in Eq. (1.1). Multiplying on the left by $\langle j|$ and using the orthogonality (1.2) we see that

$$\psi_i = \langle i|\psi\rangle. \tag{1.14}$$

Substituting this back into Eq. (1.1) then gives

$$|\psi\rangle = \sum_i |i\rangle\langle i|\psi\rangle.$$

This has the form $x = ax$, whose solution must be $a = 1$. Thus

$$\boxed{\sum_i |i\rangle\langle i| = 1 = \mathbb{I}} \tag{1.15}$$

This is the **completeness relation**. It is a direct consequence of the orthogonality of a basis set: all orthogonal bases satisfy this relation. In the right-hand side of Eq. (1.15) I wrote both the symbol $\mathbb{I}$, which stands for the identity matrix, and the number 1. Using the same symbol for a matrix and a number can feel strange sometimes. The point is that the identity matrix and the number 1 satisfy exactly the same properties and therefore it is not necessary to distinguish between the two.

To make the idea clearer, consider first the basis $|0\rangle$ and $|1\rangle$. Then

$$|0\rangle\langle 0| + |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

which is the completeness relation, as expected since $|0\rangle, |1\rangle$ form an orthonormal basis. But we can also do this with other bases. For instance, the states (1.12) also form an orthogonal basis, as you may check. Hence, they must also satisfy completeness:

$$|+\rangle\langle +| + |-\rangle\langle -| = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The completeness relation (1.15) has an important interpretation in terms of **projection onto orthogonal subspaces**. Given a Hilbert space, one may sub-divide it into several sub-spaces of different dimensions. The number of basis elements that you need to span each sub-space is called the rank of the sub-space. For instance, the space spanned by $|0\rangle$, $|1\rangle$ and $|2\rangle$ may be divided into a rank-1 sub-spaced spanned by the basis element $|0\rangle$ and a rank-2 sub-space spanned by $|1\rangle$ and $|2\rangle$. Or it may be divided into 3 rank-1 sub-spaces.

Each term in the sum in Eq. (1.15) may now be thought of as a projection onto a rank-1 sub-space. In fact, we define **rank-1 projectors**, as operators of the form

$$P_i = |i\rangle\langle i|. \tag{1.16}$$

They are called projection operators because if we apply them onto a general state of the form (1.1), they will only take the part of $|\psi\rangle$ that lives in the sub-space $|i\rangle$:

$$P_i|\psi\rangle = \psi_i|i\rangle.$$

They also satisfy

$$P_i^2 = P_i, \qquad P_i P_j = 0 \quad \text{if } i \neq j, \tag{1.17}$$

which are somewhat intuitive: if you project twice, you gain nothing new and if you project first on one sub-space and then on another, you get nothing since they are orthogonal.

We can construct projection operators of higher rank simply by combining rank-1 projectors. For instance, the operator $P_0 + P_{42}$ projects onto a sub-space spanned by the vectors $|0\rangle$ and $|42\rangle$. An operator which is a sum of r rank-1 projectors is called a rank-r projector. The completeness relation (1.15) may now also be interpreted as saying that if you project onto the full Hilbert space, it is the same as not doing anything.

1.4 Operators

The outer product is our first example of a linear operator. That is, an operator that acts linearly on vectors to produce other vectors:

$$A\bigg(\sum_i \psi_i|i\rangle\bigg) = \sum_i \psi_i A|i\rangle.$$

Such a linear operator is completely specified by knowing its action on all elements of a basis set. The reason is that, when A acts on an element $|j\rangle$ of the basis, the result will also be a vector and must therefore be a linear combination of the basis entries:

$$A|j\rangle = \sum_i A_{i,j}|i\rangle \tag{1.18}$$

The entries $A_{i,j}$ are called the matrix elements of the operator A in the basis $|i\rangle$. The quickest way to determine them is by taking the inner product of Eq. (1.18) with $\langle j|$, which gives

$$A_{i,j} = \langle i|A|j\rangle. \tag{1.19}$$

However, I should mention that using the inner product is not strictly necessary to determine matrix elements. It is also possible to define matrix elements for operators acting on vector spaces that are not equipped with inner products. After all, we only need the list of results in Eq. (1.18).

We can also use the completeness (1.15) twice to write

$$A = 1A1 = \sum_{i,j} |i\rangle\langle i|A|j\rangle\langle j| = \sum_{i,j} A_{i,j}|i\rangle\langle j|. \tag{1.20}$$

We therefore see that the matrix element $A_{i,j}$ is the coefficient multiplying the outer product $|i\rangle\langle j|$. Knowing the matrix form of each outer product then allows us to write A as a matrix. For instance,

$$A = \begin{pmatrix} A_{0,0} & A_{0,1} \\ A_{1,0} & A_{1,1} \end{pmatrix} \tag{1.21}$$

Once this link is made, the transition from abstract linear operators to matrices is simply a matter of convenience. For instance, when we have to multiply two linear operators A and B we simply need to multiply their corresponding matrices.

Of course, as you well know, with matrix multiplication you have to be careful with the ordering. That is to say, in general, $AB \neq BA$. This can be put in more elegant terms by defining the **commutator**

$$[A, B] = AB - BA. \tag{1.22}$$

When $[A, B] \neq 0$ we then say the two operators do not commute. Commutators appear all the time. The commutation relations of a given set of operators is called the **algebra** of that set. And the algebra defines all properties of an operator. So in order to specify a physical theory, essentially all we need is the underlying algebra. We will see how that appears when we work out specific examples.

Commutators appear so often that it is useful to memorize the following formula:

$$[AB, C] = A[B, C] + [A, C]B \tag{1.23}$$

This formula is really easy to remember: first A goes out to the left then B goes out to the right. A similar formula holds for $[A, BC]$. Then B exists to the left and C exists to the right.

1.5 Eigenvalues and eigenvectors

When an operator acts on a vector, it produces another vector. But every once in a while, if you get lucky the operator may act on a vector and produce the same vector, up to a constant. When that happens, we say this vector is an eigenvector and the constant in front is the eigenvalue. In symbols,

$$A|\lambda = \lambda|\lambda\rangle. \tag{1.24}$$

The eigenvalues are the numbers λ and $|\lambda\rangle$ is the eigenvector associated with the eigenvalue λ.

Determining the structure of the eigenvalues and eigenvectors for an arbitrary operator may be a difficult task. One class of operators that is super well behaved are the **Hermitian operators**. Given an operator A, we define its adjoint as the operator $A^\dagger$ whose matrix elements are

$$(A^\dagger)_{i,j} = A^*_{j,i} \tag{1.25}$$

That is, we transpose and then take the complex conjugate. An operator is then said to be Hermitian when $A^\dagger = A$. Projection operators, for instance, are Hermitian.

The eigenvalues and eigenvectors of Hermitian operators are all well behaved and predictable:

1. Every Hermitian operator of dimension d always has d (not necessarily distinct) eigenvalues.
2. The eigenvalues are always real.
3. The eigenvectors can always be chosen to form an orthonormal basis.

An example of a Hermitian operator is the rank-1 projector $P_i = |i\rangle\langle i|$. It has one eigenvalue $\lambda = 1$ and all other eigenvalues zero. The eigenvector corresponding to $\lambda = 1$ is precisely $|i\rangle$ and the other eigenvectors are arbitrary combinations of the other basis vectors.

I will not prove these properties, since they can be found in any linear algebra textbook or on Wikipedia. The proof that the eigenvalues are real, however, is cute and simple, so we can do it. Multiply Eq. (1.24) by $\langle\lambda|$, which gives

$$\langle\lambda|A|\lambda\rangle = \lambda. \tag{1.26}$$

Because of the relation (1.25), it now follows for any state that,

$$\langle\psi|A|\phi\rangle = \langle\phi|A^\dagger|\psi\rangle^*. \tag{1.27}$$

Taking the complex conjugate of Eq. (1.26) then gives

$$\langle\lambda|A^\dagger|\lambda\rangle = \lambda^*.$$

If $A^\dagger = A$ then we immediately see that $\lambda^* = \lambda$, so the eigenvalues are real. This result also shows that when A is not Hermitian, if λ happens to be an eigenvalue, then λ^* will also be an eigenvalue.

Since the eigenvectors $|\lambda\rangle$ form a basis, we can decompose an operator A as in (1.20), but using the basis λ. We then get

$$A = \sum_\lambda \lambda|\lambda\rangle\langle\lambda|. \tag{1.28}$$

Thus, an operator A is diagonal when written in its own basis. That is why the procedure for finding eigenvalues and eigenvectors is called **diagonalization**.

1.6 Unitary matrices

A unitary matrix U is one that satisfies:

$$UU^\dagger = U^\dagger U = 1, \tag{1.29}$$

where, as above, here 1 means the identity matrix. Unitary matrices play a pivotal role in quantum mechanics. One of the main reasons for this is that they preserve the normalization of vectors. That is, if $|\psi'\rangle = U|\psi\rangle$ then $\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle$. Unitaries are the complex version of **rotation matrices**: when you rotate a vector, you don't change its magnitude, just the direction. The idea is exactly the same, except it is in $\mathbb{C}^d$ instead of $\mathbb{R}^3$.

Unitary matrices also appear naturally in the diagonalization of Hermitian operators that we just discussed [Eq. (1.24)]. Given the set of d eigenvectors $|\lambda_i\rangle$, construct a matrix where each column is an eigenvector:

$$U = \begin{pmatrix} \vdots & \vdots & \dots & \vdots \\ \vdots & \vdots & \dots & \vdots \\ |\lambda_0\rangle & |\lambda_1\rangle & \dots & |\lambda_{d-1}\rangle \\ \vdots & \vdots & \dots & \vdots \\ \vdots & \vdots & \dots & \vdots \end{pmatrix} \tag{1.30}$$

Then

$$U^\dagger = \begin{pmatrix} \dots & \dots & \langle\lambda_0| & \dots & \dots \\ \dots & \dots & \langle\lambda_1| & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & \dots & \langle\lambda_{d-1}| & \dots & \dots \end{pmatrix} \tag{1.31}$$

But since A is Hermitian, the eigenvectors form an orthonormal basis, $\langle\lambda_i|\lambda_j\rangle = \delta_{i,j}$. You may then verify that this U satisfies (1.29). That is, it is unitary.

To finish the diagonalization procedure, let us also define a diagonal matrix containing the eigenvalues:

$$\Lambda = \text{diag}(\lambda_0, \lambda_1, \ldots, \lambda_{d-1}) \tag{1.32}$$

Then, I will leave for you to check that the matrix A in (1.28) may be written as

$$A = U\Lambda U^\dagger \tag{1.33}$$

Thus, we see that any Hermitian matrix may be diagonalized by a Unitary transformation. That is to say, there is always a "rotation" that makes A diagonal. The eigenvector basis $|\lambda_i\rangle$ is the "rotated" basis, where A is diagonal.

1.7 Projective measurements and expectation values

As you know, in quantum mechanics measuring a system causes the wave-function to collapse. The basic measurement describing this (and which we will later generalize) is called a projective measurement. It can be postulated in two ways, either as *measuring in a basis* or *measuring an observable*. Both are actually equivalent. Let $|\psi\rangle$ be the state of the system at any given time. The postulate then goes as follows: If we measure in a certain basis $\{|i\rangle\}$, we will find the system in a given element $|i\rangle$ with probability

$$p_i = |\langle i|\psi\rangle|^2 \tag{1.34}$$

Moreover, if the system was found in state $|i\rangle$, then due to the action of the measurement its state has collapsed to the state $|i\rangle$. That is, the measurement transforms the state as $|\psi\rangle \to |i\rangle$. The quantity $\langle i|\psi\rangle$ is the *probability amplitude* to find the system in $|i\rangle$. The modulus squared of the probability amplitude is the actual probability. The probabilities (1.34) are clearly non-negative. Moreover, they will sum to 1 when the state $|\psi\rangle$ is properly normalized:

$$\sum_i p_i = \sum_i \langle\psi|i\rangle\langle i|\psi\rangle = \langle\psi|\psi\rangle = 1.$$

This is why we introduced Eq. (1.6) back then.

Now let A be a Hermitian operator with eigenstuff $|\lambda_i\rangle$ and λ_i. If we measure in the basis $|\lambda_i\rangle$ then we can say that, with probability p_i the operator A was found in the eigenvalue λ_i. This is the idea of *measuring an observable*: we say an observable (Hermitian operator) can take on a set of values given by its eigenvalues λ_i, each occurring with probability $p_i = |\langle\lambda_i|\psi\rangle|^2$. Since any basis set $\{|i\rangle\}$ can always be associated with some observable, measuring in a basis or measuring an observable is actually the same thing.

Following this idea, we can also define the **expectation value** of the operator A. But to do that, we must define it as an *ensemble average*. That is, we prepare many identical copies of our system and then measure each copy, discarding it afterwards. If we measure the same system sequentially, we will just obtain the same result over and over again, since in a measurement we collapsed the state.[1] From the data we collect, we construct the probabilities p_i. The expectation value of A will then be

$$\langle A\rangle := \sum_i \lambda_i p_i \tag{1.35}$$

I will leave for you to show that using Eq. (1.34) we may also write this as

$$\langle A\rangle := \langle\psi|A|\psi\rangle \tag{1.36}$$

The expectation value of the operator is therefore the **sandwich** (yummmm) of A on $|\psi\rangle$.

The word "projective" in projective measurement also becomes clearer if we define the projection operators $P_i = |i\rangle\langle i|$. Then the probabilities (1.34) become

$$p_i = \langle\psi|P_i|\psi\rangle. \tag{1.37}$$

The probabilities are therefore nothing but the expectation value of the projection operators on the state $|\psi\rangle$.

1.8 Pauli matrices

As far as qubits are concerned, the most important matrices are the Pauli matrices. They are defined as

$$\boxed{\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.} \tag{1.38}$$

The Pauli matrices are both Hermitian, $\sigma_i^\dagger = \sigma_i$ and unitary, $\sigma_i^2 = 1$. The operator σ_z is diagonal in the $|0\rangle, |1\rangle$ basis:

$$\sigma_z|0\rangle = |0\rangle, \qquad \sigma_z|1\rangle = -|1\rangle. \tag{1.39}$$

The operators σ_x and σ_y, on the other hand, flip the qubit. For instance,

$$\sigma_x|0\rangle = |1\rangle, \qquad \sigma_x|1\rangle = |0\rangle. \tag{1.40}$$

The action of σ_y is similar, but gives a factor of $\pm i$ depending on the flip.

Another set of operators that are commonly used are the **lowering and raising operators**:

$$\boxed{\sigma_+ = |0\rangle\langle 1| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \text{and} \qquad \sigma_- = |1\rangle\langle 0| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}} \tag{1.41}$$

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[1] To be more precise, after we collapse, the state will start to evolve in time. If the second measurement occurs right after the first, nothing will happen. But if it takes some time, we may get something non-trivial. We can also keep on measuring a system on purpose, to always push it to a given a state. That is called the Zeno effect.

They are related to $\sigma_{x,y}$ according to

$$\sigma_x = \sigma_+ + \sigma_- \qquad \text{and} \qquad \sigma_y = -i(\sigma_+ - \sigma_-) \tag{1.42}$$

or

$$\sigma_\pm = \frac{\sigma_x \pm i\sigma_y}{2} \tag{1.43}$$

The action of these operators on the states $|0\rangle$ and $|1\rangle$ can be a bit counter-intuitive:

$$\sigma_+|1\rangle = |0\rangle, \qquad \text{and} \qquad \sigma_-|0\rangle = |1\rangle \tag{1.44}$$

This confusion is partially my fault since I defined $|0\rangle = |\uparrow\rangle$ and $|1\rangle = |\downarrow\rangle$. In terms of $\uparrow$ and $\downarrow$ they make sense: the operator σ_- lowers the spin value whereas σ_+ raises it.

In the way we defined the Pauli matrices, the indices x, y and z may seem rather arbitrary. They acquire a stronger physical meaning in the theory of angular momentum, where the Pauli matrices appear as the spin operators for spin 1/2 particles. As we will see, this will allow us to make nice a connection with Bloch's sphere. The commutation relations between the Pauli matrices are

$$[\sigma_i, \sigma_j] = 2i\epsilon_{i,j,k}\sigma_k, \tag{1.45}$$

which is the angular momentum algebra, except for the factor of 2. Based on our little table (1.8), we then see that $|0\rangle = |\uparrow\rangle$ and $|1\rangle = |\downarrow\rangle$ are the eigenvectors of σ_z, with eigenvalues $+1$ and -1 respectively. The states $|\pm\rangle$ in Eq. (1.12) are then the eigenstates of σ_x, also with eigenvalues ± 1. To avoid the confusion a good notation is to call the eigenstates of σ_z as $|z_\pm\rangle$ and those of σ_x as $|x_\pm\rangle$. That is, $|0\rangle = |z_+\rangle$, $|1\rangle = |z_-\rangle$ and $|\pm\rangle = |x_\pm\rangle$.

As mentioned, the operator σ_i is the spin operator at direction i. Of course, the orientation of $\mathbb{R}^3$ is a matter of choice, but once we choose a coordinate system, we can then define 3 independent spin operators, one for each of the orthogonal directions. We can also define spin operators in an arbitrary orientation in space. Such an orientation can be defined by a unit vector in spherical coordinates

$$\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \tag{1.46}$$

where $\theta \in [0, \pi)$ and $\phi \in [0, 2\pi]$. The spin operator at an arbitrary direction $\boldsymbol{n}$ is then defined as

$$\sigma_{\boldsymbol{n}} = \boldsymbol{\sigma} \cdot \boldsymbol{n} = \sigma_x n_x + \sigma_y n_y + \sigma_z n_z \tag{1.47}$$

Please take a second to check that we can recover $\sigma_{x,y,z}$ just by taking appropriate choices of θ and ϕ. In terms of the parametrization (1.46) this spin operator becomes

$$\sigma_{\boldsymbol{n}} = \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} = \begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{pmatrix} \tag{1.48}$$

I will leave for you to compute the eigenvalues and eigenvectors of this operator. The eigenvalues are ± 1, which is quite reasonable from a physical perspective since the eigenvalues are a property of the operator and thus should not depend on our choice of orientation in space. In other words, the spin components in any direction in space are always ±1. As for the eigenvectors, they are

$$|\boldsymbol{n}_+\rangle = \begin{pmatrix} e^{-i\phi/2}\cos\frac{\theta}{2} \\ e^{i\phi/2}\sin\frac{\theta}{2} \end{pmatrix}, \qquad |\boldsymbol{n}_-\rangle = \begin{pmatrix} -e^{-i\phi/2}\sin\frac{\theta}{2} \\ e^{i\phi/2}\cos\frac{\theta}{2} \end{pmatrix} \tag{1.49}$$

If we stare at this for a second, then the connection with Bloch's sphere in Fig. 1.1 starts to appear: the state $|\boldsymbol{n}_+\rangle$ is exactly the same as the Bloch sphere parametrization (1.11), except for a global phase $e^{-i\phi/2}$. Moreover, the state $|\boldsymbol{n}_-\rangle$ is simply the state opposite to $|\boldsymbol{n}_+\rangle$.

Another connection to Bloch's sphere is obtained by computing the expectation values of the spin operators in the state $|\boldsymbol{n}_+\rangle$. They read

$$\langle\sigma_x\rangle = \sin\theta\cos\phi, \qquad \langle\sigma_y\rangle = \sin\theta\sin\phi, \qquad \langle\sigma_z\rangle = \cos\theta \tag{1.50}$$

Thus, the average of σ_i is simply the i-th component of $\boldsymbol{n}$: it makes sense! We have now gone full circle: we started with $\mathbb{C}^2$ and made a parametrization in terms of a unit sphere in $\mathbb{R}^3$. Now we defined a point $\boldsymbol{n}$ in $\mathbb{R}^3$, as in Eq. (1.46), and showed how to write the corresponding state in $\mathbb{C}^2$, Eq. (1.49).

To finish, let us also write the diagonalization of $\sigma_{\boldsymbol{n}}$ in the form of Eq. (1.33). To do that, we construct a matrix whose columns are the eigenvectors $|\boldsymbol{n}_+\rangle$ and $|\boldsymbol{n}_-\rangle$. This matrix is then

$$G = \begin{pmatrix} e^{-i\phi/2}\cos\frac{\theta}{2} & -e^{-i\phi/2}\sin\frac{\theta}{2} \\ e^{i\phi/2}\sin\frac{\theta}{2} & e^{i\phi/2}\cos\frac{\theta}{2} \end{pmatrix} \tag{1.51}$$

The diagonal matrix Λ in Eq. (1.33) is the matrix containing the eigenvalues ±1. Hence it is precisely σ_z. Thus, we conclude that

$$\sigma_{\boldsymbol{n}} = G\sigma_z G^\dagger \tag{1.52}$$

We therefore see that G is the unitary matrix that "rotates" a spin operator from an arbitrary direction towards the z direction.

1.9 General two-level systems

As we mentioned above, two-state systems appear all the time. And when writing operators for these systems, it is always convenient to express them in terms of Pauli matrices σ_x, σ_y, σ_z and $\sigma_0 = 1$ (the identity matrix), which can be done for any 2×2 matrix. We can write this in an organized way as

$$A = a_0 + \boldsymbol{a}\cdot\boldsymbol{\sigma}, \tag{1.53}$$

for a certain set of four numbers a_0, a_x, a_y and a_z. Next define $a = |\boldsymbol{a}| = \sqrt{a_x^2 + a_y^2 + a_z^2}$ and $\boldsymbol{n} = \boldsymbol{a}/a$. Then A can be written as

$$A = a_0 + a(\boldsymbol{n}\cdot\boldsymbol{\sigma}) \tag{1.54}$$

Now suppose we wish to find the eigenvalues and eigenvectors of A. The eigenvalues are always easy, but the eigenvectors can become somewhat ugly, even in this 2×2 case. Writing in terms of Pauli matrices makes this more organized. For the eigenvalues, the following silly properties are worth remembering:

1. If $A|\lambda\rangle = \lambda|\lambda\rangle$ and $B = \alpha A$ then the eigenvalues of B will be $\lambda_B = \alpha\lambda$.
2. If $A|\lambda\rangle = \lambda|\lambda\rangle$ and $B = A + c$ then the eigenvalues of B will be $\lambda_B = \lambda + c$.

Moreover, in both cases, the eigenvectors of B are the same as those of A. Looking at Eq. (1.54), we then see that

$$\text{eigs}(A) = a_0 \pm a \tag{1.55}$$

As for the eigenvectors, they will be given precisely by Eq. (1.49), where the angles θ and ϕ are defined in terms of the unit vector $\boldsymbol{n} = \boldsymbol{a}/a$. Thus, we finally conclude that any 2×2 matrix may be diagonalized as

$$A = G(a_0 + a\sigma_z)G^\dagger \tag{1.56}$$

This gives an elegant way of writing the eigenvectors of 2×2 matrices.

1.10 Functions of operators

Let A be some Hermitian operator, decomposed as in Eq. (1.28):

$$A = \sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i|.$$

Now let us compute A^2. Since $\langle\lambda_i|\lambda_j\rangle = \delta_{i,j}$ it follows that

$$A^2 = \sum_i \lambda_i^2 |\lambda_i\rangle\langle\lambda_i|.$$

Thus, we see that the eigenvalues of A^2 are λ_i^2, whereas the eigenvectors are the same as those of A. Of course, this is also true for A^3 or any other power. Now let $f(x)$ be an arbitrary function which can be expanded in a Taylor series, $f(x) = \sum_n c_n x^n$. We can always define the action of this function on operators, instead of numbers, by assuming that the same Taylor series holds for the operators. That is, we define

$$f(A) := \sum_n c_n A^n \tag{1.57}$$

If we now write A in diagonal form, we then see that

$$f(A) = \sum_i f(\lambda_i)|\lambda_i\rangle\langle\lambda_i| \tag{1.58}$$

This is a very useful formula for computing functions of operators.

We can also derive this formula for the case when A is diagonalized as in Eq. (1.33): $A = U\Lambda U^\dagger$. Then, since $UU^\dagger = U^\dagger U = 1$, it follows that $A^2 = U\Lambda^2 U^\dagger$ and so on. By writing A like this, we can now apply any function we want, by simply applying the function to the corresponding eigenvalues:

$$f(A) = U f(\Lambda) U^\dagger \tag{1.59}$$

Since Λ is diagonal, the action of f on Λ is equivalent to applying f to each diagonal entry.

The most important example is by far the exponential of an operator, defined as

$$e^A = 1 + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \dots, \tag{1.60}$$

Using our two basic formulas (1.58) and (1.59) we then get

$$e^A = \sum_i e^{\lambda_i} |\lambda_i\rangle\langle\lambda_i| = U e^\Lambda U^\dagger \tag{1.61}$$

Another useful example is the inverse:

$$A^{-1} = U \Lambda^{-1} U^\dagger \tag{1.62}$$

To practice, let us compute the exponential of some Pauli operators. We start with σ_z. Since it is diagonal, we simply exponentiate the entries:

$$e^{i\alpha\sigma_z} = \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix}$$

Next we do the same for σ_x. The eigenvectors of σ_x are the $|\pm\rangle$ states in Eq. (1.12). Thus

$$e^{i\alpha\sigma_x} = e^{i\alpha}|+\rangle\langle+| + e^{-i\alpha}|-\rangle\langle-| = \begin{pmatrix} \cos\alpha & i\sin\alpha \\ i\sin\alpha & \cos\alpha \end{pmatrix} = \cos\alpha + i\sigma_x \sin\alpha \tag{1.63}$$

It is also interesting to compute this in another way. Recall that $\sigma_x^2 = 1$. In fact, this is true for any Pauli matrix $\sigma_{\boldsymbol{n}}$. We can use this to compute $e^{i\alpha\sigma_{\boldsymbol{n}}}$ via the definition of the exponential in Eq. (1.60). Collecting the terms proportional to $\sigma_{\boldsymbol{n}}$ and $\sigma_{\boldsymbol{n}}^2 = 1$ we get:

$$e^{i\alpha\sigma_{\boldsymbol{n}}} = \Big[1 - \frac{\alpha^2}{2} + \frac{\alpha^4}{4!} + \dots\Big] + \sigma_{\boldsymbol{n}}\Big[i\alpha - i\frac{\alpha^3}{3!} + \dots\Big].$$

Thus, we readily see that

$$e^{i\alpha\sigma_{\boldsymbol{n}}} = \cos\alpha + i\sigma_{\boldsymbol{n}} \sin\alpha, \tag{1.64}$$

where I remind you that the first term in Eq. (1.64) is actually $\cos\alpha$ multiplying the identity matrix. If we now replace $\sigma_{\boldsymbol{n}}$ by σ_x, we recover Eq. (1.63). It is interesting to point out that nowhere did we use the fact that the matrix was 2×2. If you are ever given a matrix, of arbitrary dimension, but such that $A^2 = 1$, then the same result will also apply.

In the theory of angular momentum, we learn that the operator which affects a rotation around a given axis, defined by a vector $\boldsymbol{n}$, is given by $e^{-i\alpha\sigma_{\boldsymbol{n}}/2}$. We can use this to construct the state $|\boldsymbol{n}_+\rangle$ in Eq. (1.49). If we start in the north pole, we can get to a general point in the $\mathbb{R}^3$ unit sphere by two rotations. First you rotate around the y axis by an angle θ and then around the z axis by an angle ϕ (take a second to imagine how this works in your head). Thus, one would expect that

$$|\boldsymbol{n}_+\rangle = e^{-i\phi\sigma_z/2}e^{-i\theta\sigma_y/2}|0\rangle. \tag{1.65}$$

I will leave for you to check that this is indeed Eq. (1.49). Specially in the context of more general spin operators, these states are also called **spin coherent states**, since they are the closest analog to a point in the sphere. The matrix G in Eq. (1.51) can also be shown to be

$$G = e^{-i\phi\sigma_z/2}e^{-i\theta\sigma_y/2} \tag{1.66}$$

The exponential of an operator is defined by means of the Taylor series (1.60). However, that does not mean that it behaves just like the exponential of numbers. In fact, the exponential of an operator *does not* satisfy the exponential property:

$$e^{A+B} \neq e^A e^B. \tag{1.67}$$

In a sense this is obvious: the left-hand side is symmetric with respect to exchanging A and B, whereas the right-hand side is not since e^A does not necessarily commute with e^B. Another way to see this is by means of the interpretation of $e^{i\alpha\sigma_{\boldsymbol{n}}}$ as a rotation: rotations between different axes do not in general commute.

Exponentials of operators is a serious business. There is a vast mathematical literature on dealing with them. In particular, there are a series of popular formulas which go by the generic name of Baker-Campbell-Hausdorff (BCH) formulas. For instance, there is a BCH formula for dealing with e^{A+B}, which in Wikipedia is also called Zassenhaus formula. It reads

$$e^{t(A+B)} = e^{tA}e^{tB}e^{-\frac{t^2}{2}[A,B]}e^{\frac{t^3}{3!}(2[B,[A,B]]+[A,[A,B]])}\dots, \tag{1.68}$$

where t is just a parameter to help keep track of the order of the terms. From the fourth order onwards, things just become mayhem. There is really no mystery behind this formula: it simply summarizes the *ordering* of non-commuting objects. You can derive it by expanding both sides in a Taylor series and grouping terms of the same order in t. It is a really annoying job, so everyone just trusts the result of Dr. Zassenhaus. Notwithstanding, we can extract some physics out of this. In particular, suppose t is a tiny parameter. Then Eq. (1.68) can be seen as a series expansion in t: the error you make in writing $e^{t(A+B)}$ as $e^{tA}e^{tB}$ will be a term proportional to t^2. A particularly important case of Eq. (1.68) is when $[A, B]$ commutes with both A and B. That generally means $[A, B] = c$, a number. But it can also be that $[A, B]$ is just some fancy matrix which happens to commute with both A and B. We see in Eq. (1.68) that in this case all higher order terms commute and the series truncates. That is

$$e^{t(A+B)} = e^{tA}e^{tB}e^{-\frac{t^2}{2}[A,B]}, \qquad \text{when } [A,[A,B]] = 0 \text{ and } [B,[A,B]] = 0 \tag{1.69}$$

There is also another BCH formula that is very useful. It deals with the sandwich of an operator between two exponentials, and reads

$$e^{tA}Be^{-tA} = B + t[A,B] + \frac{t^2}{2!}[A,[A,B]] + \frac{t^3}{3!}[A,[A,[A,B]]] + \dots \tag{1.70}$$

Again, you can derive this formula by simply expanding the left-hand side and collecting terms of the same order in t. I suggest you give it a try in this case, at least up to order t^2. That will help give you a feeling of how messy things can get when dealing with non-commuting objects.

Finally, I wanna mention a trick that is very useful when dealing with general functions of operators. Let A be some operator and define $B = UAU^\dagger$, where U is unitary. Then $B^2 = UA^2U^\dagger$ and etc. Consequently, when we apply a unitary sandwich to any function $f(A)$, we can infiltrate the unitary inside the function:

$$Uf(A)U^\dagger = f(UAU^\dagger). \tag{1.71}$$

This is a little bit more general than (1.59), in which Λ was diagonal. But the idea is exactly the same. For instance, with Eq. (1.52) in mind, we can write

$$e^{i\alpha\sigma_{\boldsymbol{n}}} = Ge^{i\alpha\sigma_z}G^\dagger$$

1.11 The Trace

The trace of an operator is defined as the sum of its diagonal entries:

$$\text{tr}(A) = \sum_i \langle i|A|i\rangle. \tag{1.72}$$

It turns out that the trace is the same no matter which basis you use. You can see that using completeness: for instance, if $|a\rangle$ is some other basis then

$$\sum_i \langle i|A|i\rangle = \sum_i\sum_a \langle i|a\rangle\langle a|A|i\rangle = \sum_i\sum_a \langle a|A|i\rangle\langle i|a\rangle = \sum_a \langle a|A|a\rangle.$$

Thus, we conclude that

$$\text{tr}(A) = \sum_i \langle i|A|i\rangle = \sum_a \langle a|A|a\rangle. \tag{1.73}$$

The trace is a property of the operator, not of the basis you choose. Since it does not matter which basis you use, let us choose the basis $|\lambda_i\rangle$ which diagonalizes the operator A. Then $\langle\lambda_i|A|\lambda_i\rangle = \lambda_i$ will be an eigenvalue of A. Thus, we also see that

$$\boxed{\text{tr}(A) = \sum_i \lambda_i = \text{sum of all eigenvalues of } A}. \tag{1.74}$$

Perhaps the most useful property of the trace is that it is *cyclic*:

$$\text{tr}(AB) = \text{tr}(BA). \tag{1.75}$$

I will leave it for you to demonstrate this. You can do it, as with all demonstrations in quantum mechanics, by inserting a convenient completeness relation in the middle of

AB. Using the cyclic property (1.75) you can also move around an arbitrary number of operators, but only in cyclic permutations. For instance:

$$\mathrm{tr}(ABC) = \mathrm{tr}(CAB) = \mathrm{tr}(BCA). \tag{1.76}$$

Note how I am moving them around in a specific order: $\mathrm{tr}(ABC) \neq \mathrm{tr}(BAC)$. An example that appears often is a trace of the form $\mathrm{tr}(UAU^\dagger)$, where U is unitary operator. In this case, it follows from the cyclic property that

$$\mathrm{tr}(UAU^\dagger) = \mathrm{tr}(AU^\dagger U) = \mathrm{tr}(A)$$

Thus, the trace of an operator is invariant by unitary transformations. This is also in line with the fact that the trace is the sum of the eigenvalues and unitaries preserve eigenvalues.

Finally, let $|\psi\rangle$ and $|\phi\rangle$ be arbitrary kets and let us compute the trace of the outer product $|\psi\rangle\langle\phi|$:

$$\mathrm{tr}(|\psi\rangle\langle\phi|) = \sum_i \langle i|\psi\rangle\langle\phi|i\rangle = \sum_i \langle\phi|i\rangle\langle i|\psi\rangle$$

The sum over $|i\rangle$ becomes a 1 due to completeness and we conclude that

$$\boxed{\mathrm{tr}(|\psi\rangle\langle\phi|) = \langle\phi|\psi\rangle.} \tag{1.77}$$

Notice how this follows the same logic as Eq. (1.75), so you can pretend you just used the cyclic property. This formula turns out to be extremely useful, so it is definitely worth remembering.

1.12 Schrödinger's equation

So far nothing has been said about how states evolve in time. The equation governing the time evolution is called Schödinger's equation. This equation cannot be derived from first principles. It is a postulate of quantum mechanics. Interestingly, however, we don't need to postulate the equation itself. Instead, all we need to postulate is that the transformation caused by the time evolution is a *linear* operation, in the sense that it corresponds to the action of a linear operator on the original state. That is, we can write the time evolution from time t_0 to time t as

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle, \tag{1.78}$$

where $U(t, t_0)$ is the operator which affects the transformation between states. This assumption of linearity is one of the most fundamental properties of quantum mechanics and, in the end, is really based on experimental observations.

In addition to the assumption of linearity, we also have that states must remain normalized. That is, they must always satisfy $\langle\psi|\psi\rangle = 1$ at all times. Looking at Eq. (1.78), we see that this will only be true when the matrix $U(t, t_0)$ is unitary. Hence, we conclude that *time evolution must be described by a unitary matrix.*

Eq. (1.78) doesn't really look like the Schrödinger equation you know. We can get to that by assuming we do a tiny evolution, from t to $t + \Delta t$. The operator U must of course satisfy $U(t, t) = 1$ since this means we haven't evolved at all. Thus we can expand it in a Taylor series in Δt, which to first order can be written as

$$U(t + \Delta t, t) \simeq 1 - i\Delta t H(t) \tag{1.79}$$

where $H(t)$ is some operator which, as you of course know, is called the **Hamiltonian** of your system. The reason why I put the i in front is because then H is Hermitian. I also didn't introduce Planck's constant $\hbar$. In this course $\hbar = 1$. This simply means that time and energy have the same units:

$$\boxed{\text{In this course we always set } \hbar = 1}$$

Inserting Eq. (1.79) in Eq. (1.78), dividing by Δt and then taking the limit $\Delta t \to 0$ we get

$$\partial_t |\psi(t)\rangle = -iH(t)|\psi(t)\rangle \tag{1.80}$$

which is Schrödinger's equation.

What we have therefore learned is that, once we postulate normalization and linearity, the evolution of a physical system *must* be given by an equation of the form (1.80), where $H(t)$ is some operator. Thus, the structure of Schrödinger's equation is really a consequence of these two postulates. Of course, the really hard question is what is the operator $H(t)$. The answer is usually a mixture of physical principles and experimental observations. We will explore several Hamiltonians along the way.

If the Hamiltonian is time-independent, then the solution of Eq. (1.80) is given by the time-evolution operator

$$U(t, t_0) = e^{-iH(t-t_0)}. \tag{1.81}$$

Even when the Hamiltonian is time-dependent, it is also possible to write a solution that looks like this, but we need to introduce something called the time-ordering operator. We will discuss this later. Eq. (1.81) also has an interesting interpretation concerning the quantization of classical mechanics. When a unitary is written like the exponential of something, we say the quantity in the exponent is the *generator* of that transformation. Thus, **the Hamiltonian is the generator of time-translations**. According to Nöether's theorem in classical mechanics, to every symmetry there is a corresponding conserved quantity. Thus, for instance, when a system is invariant under time translations (i.e. has a time-independent Hamiltonian) then energy is a conserved quantity. In quantum mechanics, the conserved quantity is promoted to an operator and becomes the generator of the symmetry.

To take another example, we know that if a classical system is invariant under rotations, the angular momentum is conserved. Consequently, in the quantum theory, angular momentum will be promoted to an operator and will become the generator of translations. Indeed, as we have already seen, $e^{-i\phi\sigma_z/2}$ is the operator that rotates a ket around the z axis by an angle ϕ.

Next let us define the eigenstuff of the Hamiltonian as

$$H|n\rangle = E_n|n\rangle. \tag{1.82}$$

Then, using the tricks of Sec. 1.10, we may write the time-evolution operator in Eq. (1.81) as

$$U(t,t_0) = \sum_n e^{-iE_n(t-t')}|n\rangle\langle n|. \tag{1.83}$$

An arbitrary initial state $|\psi_0\rangle$ may always be decomposed in the eigenbasis $|n\rangle$ as $|\psi_0\rangle = \sum_n \psi_n|n\rangle$. Then, the time-evolved state will be

$$|\psi_t\rangle = \sum_n e^{-iE_n(t-t_0)}\psi_n|n\rangle \tag{1.84}$$

Each component in the eigenbasis of the Hamiltonian simply evolves according to a simple exponential. Consequently, if the system starts in an eigenstate of the Hamiltonian, it stays there forever. On the other hand, if the system starts in a state which is not an eigenstate, it will oscillate back and forth forever.

1.13 The Schrödinger Lagrangian

It is possible to cast Schrödinger's equation as a consequence of the **principle of least action**, similar to what we do in classical mechanics. This is fun because it formulates quantum mechanics as a classical theory, as weird as that may sound. There is no particular reason why I will introduce this idea here. I just think it is beautiful and I wanted to share it with you.

Let us start with a brief review of classical mechanics. Consider a system described by a set of generalized coordinates q_i and characterized by a Lagrangian $L(q_i, \partial_t q_i)$. The action is defined as

$$S = \int_{t_1}^{t_2} L(q_i, \partial_t q_i)\,\mathrm{d}t. \tag{1.85}$$

The motion of the system is then generated by the principle of least action; ie, by requiring that the actual path should be an extremum of S. We can find the equations of motion (the Euler-Lagrange equations) by performing a tiny variation in S and requiring that $\delta S = 0$ (which is the condition on any extremum point; maximum or minimum). To do that we write $q_i \to q_i + \eta_i$, where $\eta_i(t)$ is supposed to be an infinitesimal distortion of the original trajectory. We then compute

$$\begin{aligned}
\delta S &= S[q_i(t) + \eta_i(t)] - S[q_i(t)] \\
&= \int_{t_1}^{t_2} \mathrm{d}t \sum_i \left\{ \frac{\partial L}{\partial q_i}\eta_i + \frac{\partial L}{\partial(\partial_t q_i)}\partial_t \eta_i \right\} \\
&= \int_{t_1}^{t_2} \mathrm{d}t \sum_i \left\{ \frac{\partial L}{\partial q_i} - \partial_t\left(\frac{\partial L}{\partial(\partial_t q_i)}\right)\right\}\eta_i.
\end{aligned}$$

where, in the last line, I integrated by parts the second term. Setting each term proportional to η_i to zero then gives us the **Euler-Lagrange equations**

$$\boxed{\frac{\partial L}{\partial q_i} - \partial_t\Big(\frac{\partial L}{\partial(\partial_t q_i)}\Big) = 0.} \tag{1.86}$$

The example you are probably mostly familiar with is the case when

$$L = \frac{1}{2}m(\partial_t q)^2 - V(q), \tag{1.87}$$

with $V(q)$ being some potential. In this case Eq. (1.86) gives Newton's law

$$m\partial_t^2 q = -\frac{\partial V}{\partial q}. \tag{1.88}$$

Another example, which you may not have seen before, but which will be interesting for us, is the case when we write L with both the position q and the momenta p as generalized coordinates; , ie $L(q, \partial_t q, p, \partial_t p)$. For instance,

$$L = p\partial_t q - H(q, p), \tag{1.89}$$

where H is the Hamiltonian function. In this case there will be two Euler-Lagrange equations for the coordinates q and p:

$$\begin{aligned}
\frac{\partial L}{\partial q} - \partial_t\Big(\frac{\partial L}{\partial(\partial_t q)}\Big) &= -\frac{\partial H}{\partial q} - \partial_t p = 0\\
\frac{\partial L}{\partial p} - \partial_t\Big(\frac{\partial L}{\partial(\partial_t p)}\Big) &= \partial_t q - \frac{\partial H}{\partial p} = 0.
\end{aligned}$$

Rearranging, this gives us Hamilton's equations

$$\partial_t p = -\frac{\partial H}{\partial q}, \qquad \partial_t q = \frac{\partial H}{\partial p}. \tag{1.90}$$

Another thing we will need is the **conjugated momentum** π_i associated to a generalized coordinate q_i. It is always defined as

$$\pi_i = \frac{\partial L}{\partial(\partial_t q_i)}. \tag{1.91}$$

For the Lagrangian (1.87) we get $\pi = m\partial_t q$. For the Lagrangian (1.89) we have two variables, $q_1 = q$ and $q_2 = p$. The corresponding conjugated momenta are $\pi(q) = p$ and $\pi(p) = 0$ (there is no momentum associated with the momentum!). Once we have the momentum we may construct the Hamiltonian from the Lagrangian using the Legendre transform:

$$H = \sum_i \pi_i \partial_t q_i - L \tag{1.92}$$

For the Lagrangian (1.87) we get

$$H = \frac{p^2}{2m} + V(q),$$

whereas for the Lagrangian (1.89) we get

$$H = \pi(q)\partial_t q + \pi(p)\partial_t p - L = p\partial_t q + 0 - p\partial_t q + H = H,$$

as of course expected.

Now consider Schrödinger's equation (1.80) and let us write it in terms of the components ψ_n in some basis:

$$i\partial_t\psi_n = \sum_m H_{n,m}\psi_m, \tag{1.93}$$

where $H_{n,m} = \langle n|H|m\rangle$. We now ask the following question: can we cook up a Lagrangian and an action such that the corresponding Euler-Lagrange equations give Eq. (1.93)? The answer, of course, is yes.[2] The "variables" in this case are all components ψ_n. But since they are complex variables, we actually have ψ_n and ψ_n^* as an independent set. That is, $L = L(\psi_n, \partial_t\psi_n, \psi_n^*, \partial_t\psi_n^*)$. and the action is

$$S[\psi_n^*, \psi_n] = \int_{t_1}^{t_2} L(\psi_n, \partial_t\psi_n, \psi_n^*, \partial_t\psi_n^*)\, \mathrm{d}t. \tag{1.94}$$

The correct Lagrangian we should use is

$$L = \sum_n i\psi_n^*\partial_t\psi_n - \sum_{n,m} H_{n,m}\psi_n^*\psi_m. \tag{1.95}$$

where ψ_n and ψ_n^* are to be interpreted as independent variables. Please take notice of the similarity with Eq. (1.89): ψ_n plays the role of q and ψ_n^* plays the role of p. To check that this works we use the Euler-Lagrange equations for the variable ψ_n^*:

$$\frac{\partial L}{\partial\psi_n^*} - \partial_t\left(\frac{\partial L}{\partial(\partial_t\psi_n^*)}\right) = 0.$$

The second term is zero since $\partial_t\psi_n^*$ does not appear in Eq. (1.95). The first term then gives

$$\frac{\partial L}{\partial\psi_n^*} = i\partial_t\psi_n - \sum_m H_{n,m}\psi_m = 0.$$

which is precisely Eq. (1.93). Thus, we have just cast Schrödinger's equation as a principle of least action for a weird action that depends on the quantum state $|\psi\rangle$. I will leave to you as an exercise to compute the Euler-Lagrange equation for ψ_n; you will simply find the complex conjugate of Eq. (1.93).

---

[2] If the answer was no, I would be a completely crazy person, because I just spent more than two pages describing Lagrangian mechanics, which would have all been for nothing.

Eq. (1.95) is written in terms of the components ψ_n of a certain basis. We can also write it in a basis independent way, as

$$\boxed{L = \langle\psi|(i\partial_t - H)|\psi\rangle} \tag{1.96}$$

This is what I call the Schrödinger Lagrangian. Isn't it beautiful? If this abstract version ever confuse you, simply refer back to Eq. (1.95).

Let us now ask what is the conjugated momentum associated with the variable ψ_n for the Lagrangian (1.95). Using Eq. (1.91) we get,

$$\pi(\psi_n) = \frac{\partial L}{\partial(\partial_t \psi_n)} = i\psi_n^*, \qquad \pi(\psi_n^*) = 0 \tag{1.97}$$

This means that ψ_n and $i\psi_n^*$ are conjugated variables. As a sanity check, we can now find the Hamiltonian using the definition (1.92):

$$H = \sum_n i\psi_n^* \partial_t \psi_n - L \tag{1.98}$$

which, substituting (1.95) gives just the actual Hamiltonian.

Chapter 2

Density matrices and composite systems

In this chapter we will take a step further in our description of quantum systems. First we will show that quantum information can be combined with classical information in a new object ρ, called the density matrix, which generalizes the idea of a ket. Then we show how to describe systems composed of multiple parts. At first these two things will seem unrelated. But in Sec. **??** we will connect the dots and show that there is an intimate relation between the two. The remainder of the chapter is then dedicated to the basic toolbox of Quantum Information; that is, the basic tools used to quantify information-theoretic measures in quantum systems.

2.1 The density matrix

A ket $|\psi\rangle$ is actually not the most general way of defining a quantum state. To motivate this, consider the state $|\boldsymbol{n}_+\rangle$ in Eq. (1.49) and the corresponding expectation values computed in Eq. (1.50). This state always points *somewhere*: it points at the direction $\boldsymbol{n}$ of the Bloch sphere. It is never possible to find a quantum ket $|\psi\rangle$ where the state doesn't point somewhere specific; that is, where it is isotropic. That sounds strange since, if we put the spin in a high temperature oven without any magnetic fields, then we certainly expect that it will never have a preferred magnetization direction. The solution to this paradox is that, when we put a spin in an oven, we are actually adding a *classical uncertainty* to the problem, whereas kets are only able to encompass quantum uncertainty.

The most general representation of a quantum system is written in terms of an operator ρ called the *density operator*, or *density matrix*. It is built in such a way that it naturally encompasses both quantum and classical probabilities. In this section I want to introduce the idea of density matrix by looking at a system which mixes quantum and classical probabilities. There is also another cool way of introducing the density matrix as stemming from the **entanglement** between two sub-systems. We will deal with that in Sec. **??**.

Suppose we have an apparatus which prepares quantum systems in certain states. For instance, this could be an oven producing spin 1/2 particles, or a quantum optics setup producing photons. But suppose that this apparatus is imperfect, so it does not always produces the same state. That is, suppose that it produces a state $|\psi_1\rangle$ with a certian probability q_1 or a state $|\psi_2\rangle$ with a certain probability q_2 and so on. Notice how we are introducing here a *classical uncertainty*. We can have as many q's as we want. All we assume is that they behave like classical probabilities:

$$q_i \in [0, 1], \qquad \text{and} \qquad \sum_i q_i = 1 \tag{2.1}$$

Now let A be an observable. If the state is $|\psi_1\rangle$, then the expectation value of A will be $\langle\psi_1|A|\psi_1\rangle$. But if it is $|\psi_2\rangle$ then it will be $\langle\psi_2|A|\psi_2\rangle$. To compute the actual expectation value of A we must therefore perform an average of quantum averages:

$$\langle A\rangle = \sum_i q_i \langle\psi_i|A|\psi_i\rangle \tag{2.2}$$

What is important to realize is that this type of average *cannot* be writen as $\langle\phi|A|\phi\rangle$ for some ket $|\phi\rangle$. If we want to attribute a "state" to our system, then we must generalize the idea of ket. To do that, we use Eq. (1.77) to write

$$\langle\psi_i|A|\psi_i\rangle = \text{tr}\Big[A|\psi_i\rangle\langle\psi_i|\Big]$$

Then Eq. (2.2) may be written as

$$\langle A\rangle = \sum_i q_i \,\text{tr}\Big[A|\psi_i\rangle\langle\psi_i|\Big] = \text{tr}\Big\{A\sum_i q_i|\psi_i\rangle\langle\psi_i|\Big\}$$

This motivates us to define the **density matrix** as

$$\boxed{\rho = \sum_i q_i|\psi_i\rangle\langle\psi_i|} \tag{2.3}$$

Then we may finally write Eq. (2.2) as

$$\boxed{\langle A\rangle = \text{tr}(A\rho)} \tag{2.4}$$

which, by the way, is the same as $\text{tr}(\rho A)$ since the trace is cyclic [Eq. (1.75)].

With this idea, we may now recast *all* of quantum mechanics in terms of density matrices, instead of kets. If it happens that a density matrix can be written as $\rho = |\psi\rangle\langle\psi|$, we say we have a **pure state**. And in this case it is not necessary to use ρ at all. One may simply continue to use $|\psi\rangle$. For instance, Eq. (2.4) reduces to the usual result: $\text{tr}(A\rho) = \langle\psi|A|\psi\rangle$. A state which is not pure is usually called a **mixed state**. In this case kets won't do us no good and we must use ρ.

Examples

To start, suppose a machine tries to produce qubits in the state $|0\rangle$. But it is not very good so it only produces $|0\rangle$ with probability q. And, with probability $1-q$ it produces a state $|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}|1\rangle$, where θ may be some small angle (just for the sake of example). The density matrix for this system will then be

$$\rho = q|0\rangle\langle 0| + (1-q)|\psi\rangle\langle\psi| = \begin{pmatrix} q + (1-q)\cos^2\frac{\theta}{2} & (1-q)\sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ (1-q)\sin\frac{\theta}{2}\cos\frac{\theta}{2} & (1-q)\sin^2\frac{\theta}{2} \end{pmatrix} \tag{2.5}$$

which is a just a very ugly guy. We could generalize it as we wish For instance, we can have a machine that produces $|0\rangle$, $|\psi_1\rangle$ and $|\psi_2\rangle$, and so on. Of course, the more terms we add, the uglier will the result be, but the idea is the same.

Next I want to discuss with you something called the **ambiguity of mixtures**. The idea is quite simple: if you mix stuff, you generally loose information, so you don't always know where you started at. To see what I mean, consider a state which is a 50-50 mixture of $|0\rangle$ and $|1\rangle$. The corresponding density matrix will then be

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Alternatively, consider a 50-50 mixture of the states $|\pm\rangle$ in Eq. (1.12). In this case we get

$$\rho = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

We see that both are identical. Hence, we have *no way to tell* if we began with a 50-50 mixture of $|0\rangle$ and $|1\rangle$ or of $|+\rangle$ and $|-\rangle$. By mixing stuff, we have lost information.

Properties of the density matrix

The density matrix satisfies a bunch of very special properties. We can figure them out using only the definition (2.3) and recalling that $q_i \in [0,1]$ and $\sum_i q_i = 1$ [Eq. (2.1)]. First, the density matrix is a Hermitian operator:

$$\rho^\dagger = \rho. \tag{2.6}$$

Second,

$$\operatorname{tr}(\rho) = \sum_i q_i \operatorname{tr}(|\psi_i\rangle\langle\psi_i|) = \sum_i q_i \langle\psi_i|\psi_i\rangle = \sum_i q_i = 1. \tag{2.7}$$

This is the *normalization* condition of the density matrix. Another way to see this is from Eq. (2.4) by choosing $A = 1$. Then, since $\langle 1\rangle = 1$ we again get $\operatorname{tr}(\rho) = 1$.

We also see from Eq. (2.9) that $\langle\phi|\rho|\phi\rangle$ is a sum of quantum probabilities $|\langle\phi|\psi_i\rangle|^2$ averaged by classical probabilities q_i. This entails the following interpretation: for an arbitrary state $|\phi\rangle$,

$$\boxed{\langle\phi|\rho|\phi\rangle = \text{Prob. of finding the system at state } |\phi\rangle \text{ given that it's state is } \rho} \tag{2.8}$$

Besides normalization, the other big property of a density matrix is that it is **positive semi-definite**, which we write symbolically as $\rho \geq 0$. What this means is that *its sandwich in any quantum state is always non-negative*. In symbols, if $|\phi\rangle$ is an arbitrary quantum state then

$$\langle\phi|\rho|\phi\rangle = \sum_i q_i |\langle\phi|\psi_i\rangle|^2 \geq 0. \tag{2.9}$$

Of course, this makes sense in view of the probabilistic interpretation of Eq. (2.8). Please note that this does *not* mean that all entries of ρ are non-negative. Some of them may be negative. It does mean, however, that the diagonal entries are always non-negative, no matter which basis you use.

Another equivalent definition of a positive semi-definite operator is one whose **eigenvalues are always non-negative**. In Eq. (2.3) it already looks as if ρ is in diagonal form. However, we need to be a bit careful because the $|\psi_i\rangle$ are arbitrary states and do not necessarily form a basis [which can be seen explicitly in the example in Eq. (2.5)]. Thus, in general, the diagonal structure of ρ will be different. Notwithstanding, ρ is Hermitian and may therefore be diagonalized by some orthonormal basis $|k\rangle$ as

$$\rho = \sum_k p_k |k\rangle\langle k|, \tag{2.10}$$

for certain eigenvalues p_k. Since Eq. (2.9) must be true for any state $|\phi\rangle$ we may choose, in particular, $|\phi\rangle = |k\rangle$, which gives

$$p_k = \langle k|\rho|k\rangle \geq 0.$$

Thus, we see that the statement of positive semi-definiteness is equivalent to saying that the eigenvalues are non-negative. In addition to this, we also have that $\text{tr}(\rho) = 1$, which implies that $\sum_k p_k = 1$. Thus we conclude that the eigenvalues of ρ behave like probabilities:

$$p_k \in [0, 1], \qquad \sum_k p_k = 1. \tag{2.11}$$

But they are not the same probabilities q_i. They just behave like a set of probabilities, that is all.

For future reference, let me summarize what we learned in a big box: the basic properties of a density matrix are

$$\boxed{\text{Defining properties of a density matrix:} \qquad \text{tr}(\rho) = 1 \quad \text{and} \quad \rho \geq 0.} \tag{2.12}$$

Any normalized positive semi-definite matrix is a valid candidate for a density matrix.

Purity

Next let us look at ρ^2. The eigenvalues of this matrix are p_k^2 so

$$\text{tr}(\rho^2) = \sum_k p_k^2 \leq 1 \tag{2.13}$$

The only case when $\text{tr}(\rho^2) = 1$ is when ρ is a pure state. In that case it can be written as $\rho = |\psi\rangle\langle\psi|$ so it will have one eigenvalue $p_1 = 1$ and all other eigenvalues equal to zero. Hence, the quantity $\text{tr}(\rho^2)$ represents the **purity** of the quantum state. When it is 1 the state is pure. Otherwise, it will be smaller than 1:

$$\boxed{\text{Purity} = \mathcal{P} := \text{tr}(\rho^2) \leq 1} \tag{2.14}$$

As a side note, when the dimension of the Hilbert space d is finite, it also follows that $\text{tr}(\rho^2)$ will have a lower bound:

$$\frac{1}{d} \leq \text{tr}(\rho^2) \leq 1 \tag{2.15}$$

This lower bound occurs when ρ is the **maximally disordered state**

$$\rho = \frac{\mathbb{I}_d}{d} \tag{2.16}$$

where $\mathbb{I}_d$ is the identity matrix of dimension d.

The von Neumann equation

The time evolution of any ket $|\psi\rangle$ under unitary dynamics is given by Eq. (1.78): $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$. Any density operator may be written in the form (2.3) so its time evolution will be

$$\rho(t) = \sum_i q_i e^{-iHt}|\psi_i(0)\rangle\langle\psi_i(0)|e^{iHt} = e^{-iHt}\rho(0)e^{iHt}.$$

Differentiating with respect to t we then get

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = (-iH)e^{-iHt}\rho(0)e^{iHt} + e^{-iHt}\rho(0)e^{iHt}(iH) = -iH\rho(t) + i\rho(t)H$$

Thus, we reach von Neumann's equation:

$$\boxed{\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho], \qquad \rho(t) = e^{-iHt}\rho(0)e^{iHt}} \tag{2.17}$$

This is equivalent to Schrödinger's equation, but written in terms of the density matrix. Thus, in this sense, it is more general than Schrödinger's equation. But, of course, that is a bit of an exaggeration since if we solve one, we solve the other. Also, in practice, the best thing is just solve for U. That is, to compute $U = e^{-iHt}$. Then it doesn't matter if we apply this to a ket or a density matrix.

2.2 Bloch's sphere and coherence

The density matrix for a qubit will be 2×2 and may therefore be parametrized as

$$\rho = \begin{pmatrix} p & q \\ q^* & 1-p \end{pmatrix}, \tag{2.18}$$

where $p \in [0,1]$ and I used $1-p$ in the last entry due to the normalization $\mathrm{tr}(\rho^2) = 1$. If the state is pure then it can be written as $|\psi\rangle = a|0\rangle + b|1\rangle$, in which case the density matrix becomes

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}. \tag{2.19}$$

This is the density matrix of a system which is in a *superposition* of $|0\rangle$ and $|1\rangle$. Conversely, we could construct a state which can be in $|0\rangle$ **or** $|1\rangle$ with different probabilities. According to the very definition of the density matrix in Eq. (2.3), this state would be

$$\rho = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1| = \begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix}. \tag{2.20}$$

This is a classical state, obtained from classical probability theory. The examples in Eqs. (2.19) and (2.20) reflect well the difference between quantum superpositions and classical probability distributions.

We can also make this more operational by defining the idea of **coherence**. Coherence is a basis dependent concept. Given a certain basis (here the computational basis), we say a state is *incoherent* if it is diagonal in that basis:

$$\rho = \sum_i p_i |i\rangle\langle i|. \tag{2.21}$$

Any state that is not diagonal contains a certain amount of coherence (with respect to the chosen basis). Coherence plays a central role in quantum information and has seen a boom of interest in the last few years. It is seen as the ultimate **quantum resource**, from which other resources such as entanglement (which will be discussed below) can be extracted. It is also a central concept in the transition from quantum to classical.

The origin of this transition lies in the *interaction of a system with its environment*, a process known as **decoherence**. Decoherence is the process through which the system looses the coherence (off-diagonal entries) in pure states such as (2.19) to end up in mixed states such as (2.20). All system are in contact with their surroundings, so this process is really unavoidable. In fact, even if the system is in the middle of space, with nothing around it, it will still be in contact with the **electromagnetic vacuum**. For this reason, isolating quantum systems turns out to be quite a difficult task and constitutes an active topic of research nowadays. In fact, decoherence is not something that can be avoided. All we can hope to do is to delay it long enough to be able to do something interesting with our state.

When we first learn about quantum mechanics, we use Schrödinger's equation to solve, for instance, for the Hydrogen atom, from which we find the allowed energy levels for the electron. In principle quantum mechanics would allow us to place an electron into a superposition of these eigenstates. However, we *never* do that: I am sure you never heard someone saying "the electron is in a superposition of 1s and 3p" [which would represent a state of the form (2.19)]. Instead, we always assume a situation similar to Eq. (2.20). For instance, when we use the Hydrogen energy levels to construct (approximately) the periodic table, we simply "put" the electrons into the energy levels, stacking them one on top of each other. The reason why this works is because for electrons the decoherence rate is usually really high, so that even if we were to prepare the electron in a pure superposition state, it would quickly decohere to a mixture.

You may also be wondering, if coherence is a basis dependent concept, then how can we talk about decoherence as a physical effect, independent of *our* choice of basis? I mean, what makes one basis more important than another. The answer, again, is the environment. The environment and, in particular, the system-environment interaction, singles out a specific basis.

Models of decoherence are usually based on **master equations**. This name which, admittedly, is a bit weird, corresponds to modifications of the von Neumann Eq. (2.17) to include also the effects of the environment. There is an infinite number of different such models and we will explore them in this course in quite some detail. Here I want to study the simplest model of a master equation, called the **dephasing noise**. We consider a qubit with some Hamiltonian $H = \frac{\Omega}{2}\sigma_z$ and subject it to the equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho] + \frac{\gamma}{2}(\sigma_z\rho\sigma_z - \rho) \tag{2.22}$$

The first part is Eq. (2.17) and the second part describes the action of the environment. In this case γ is a constant specifying the *coupling strength* to the environment: if you set $\gamma \to 0$ you isolate your system and recover the unitary dynamics of the von Neumann Eq. (2.17).

The solution of Eq. (2.22) is really easy. We assume that the density matrix can be parametrized as in Eq. (2.18), with $p_\pm(t)$ and $q(t)$ being just time-dependent functions. Plugging this into Eq. (2.22) and doing all the silly 2×2 matrix multiplications we get the following system of equations:

$$\frac{\mathrm{d}p_\pm}{\mathrm{d}t} = 0 \tag{2.23}$$

$$\frac{\mathrm{d}q}{\mathrm{d}t} = -(i\Omega + \gamma)q \tag{2.24}$$

Thus, we see that the dephasing noise does not change the populations, but only affects the off-diagonal elements. In particular, the solution for q is

$$q(t) = e^{-(i\Omega+\gamma)t}q(0) \tag{2.25}$$

so that $|q|$ decays exponentially. Thus, the larger the coupling strength γ the faster the system looses coherence. If we start in a pure state such as (2.19) then after a time t the state will be

$$\rho(t) = \begin{pmatrix} |a|^2 & ab^* e^{-(i\Omega+\gamma)t} \\ a^* b e^{-(-i\Omega+\gamma)t} & |b|^2 \end{pmatrix}. \tag{2.26}$$

Thus, after a sufficiently long time, coherence will be completely lost and eventually the system will reach

$$\lim_{t\to\infty} \rho(t) = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}. \tag{2.27}$$

This is no longer a superposition, but simply a classical statistical mixture, just like (2.20). The action of the environment therefore changed quantum probabilities into classical probabilities.

The above example illustrates well I think, how the environment acts to destroy quantum features. Of course, that is not the only way that the bath can act. The dephasing model is very special in that it does not change the populations. In general, the interaction with the environment will induce both decoherence *and* changes in populations. A qubit model which captures that is the **amplitude damping** described by the master equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho] + \gamma\Big[\sigma_-\rho\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-,\rho\}\Big] \tag{2.28}$$

where $\{A, B\} = AB - BA$ is the anti-commutator. I will leave the study of this model for you as an exercise. As you will find, in this case $q(t)$ continues to decay exponentially, but $p_\pm$ change as well.

Let us now go back to Bloch's sphere. So far we have seen that a pure state can be described as point on the surface of a unit sphere. Now let us see what happens for mixed states. Another convenient way to write the state (2.18) is as

$$\boxed{\rho = \frac{1}{2}(1 + \boldsymbol{s}\cdot\boldsymbol{\sigma}) = \frac{1}{2}\begin{pmatrix} 1+s_z & s_x - is_y \\ s_x + is_y & 1 - s_z \end{pmatrix}.} \tag{2.29}$$

where $\boldsymbol{s} = (s_x, s_y, s_z)$ is a vector. The physical interpretation of $\boldsymbol{s}$ becomes evident from the following relation:

$$s_i = \langle \sigma_i \rangle = \mathrm{tr}(\sigma_i \rho). \tag{2.30}$$

The relation between these parameters and the parametrization in Eq. (2.18) is

$$\begin{aligned} \langle \sigma_x \rangle &= q + q^*, \\ \langle \sigma_y \rangle &= i(q - q^*), \\ \langle \sigma_z \rangle &= 2p - 1. \end{aligned}$$

Next we look at the purity of a qubit density matrix. From Eq. (2.29) one also readily finds that

$$\mathrm{tr}(\rho^2) = \frac{1}{2}(1 + \boldsymbol{s}^2). \tag{2.31}$$

Thus, due to Eq. (2.13), it also follows that

$$\boldsymbol{s}^2 = s_x^2 + s_y^2 + s_z^2 \leq 1. \tag{2.32}$$

When $\boldsymbol{s}^2 = 1$ we are in a pure state. In this case the vector $\boldsymbol{s}$ lays on the surface of the Bloch sphere. For mixed states $\boldsymbol{s}^2 < 1$ and the vector is inside the Bloch sphere. Thus, we see that the purity can be directly associated with the radius in Bloch's sphere. The smaller the radius, the more mixed is the state. In particular, the maximally disordered state occurs when $s = 0$ and reads

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{2.33}$$

In this case the state lies in the center of the sphere. A graphical representation of pure and mixed states in the Bloch sphere is shown in Fig. 2.1.

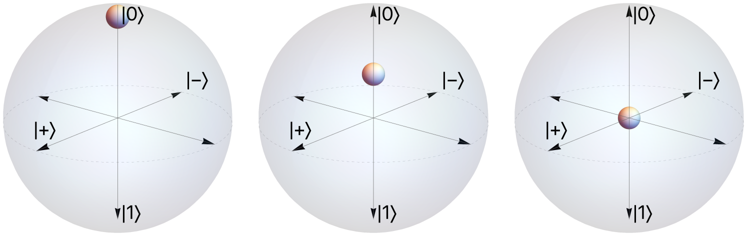

Figure 2.1: Examples of pure and mixed states in the z axis. Left: a pure state. Center: an arbitrary mixed state. Right: the maximally mixed state (2.33).

2.3 Composite systems and the almighty kron

So far we have considered only a single quantum system described by a basis $|i\rangle$. Now we turn to the question of how to describe mathematically a system composed of two or more sub-systems. Suppose we have two sub-systems, which we call A and B. They can be, for instance, two qubits: one on earth and the other on mars. We use a basis $|i\rangle_A$ to describe the sub-system A and a basis $|j\rangle_B$ to describe sub-system B. In general, each sub-system can have different dimensions, $d_A \neq d_B$.

If we now wish to describe the composite system A+B, we could use as a basis set, states labeled as $|i, j\rangle_{AB}$, where i is the quantum number of A and j is the quantum number of B. That makes sense: suppose A and B are spins which can be up or down. Then a state such as $|\uparrow, \downarrow\rangle_{AB}$ means the first is up and the second is down, and so on. But how do we operate with these states? That is, how do we construct operators which act on these states to produce new states?

The intuition is that A and B represent separate universes: things related to A have nothing to do with things related to B. After all, they can be on different planets. Thus, for instance, we know that for one qubit the operator σ_x flips the bit: $\sigma_x|0\rangle = |1\rangle$. Now suppose two qubits are in a state $|0, 0\rangle$. Then we expect that there should be an operator σ_x^A which flips the first qubit and an operator σ_x^B that flips only the second. That is,

$$\sigma_x^A|0,0\rangle = |1,0\rangle, \qquad \sigma_x^B|0,0\rangle = |0,1\rangle \tag{2.34}$$

The mathematical structure to do this is called the **tensor product** or **Kronecker product**. It is, in essence, a way to glue together two vector spaces to form a larger space. The tensor product between two states $|i\rangle_A$ and $|j\rangle_B$ is written as

$$|i, j\rangle_{AB} = |i\rangle_A \otimes |j\rangle_B. \tag{2.35}$$

The symbol $\otimes$ separates the two universes. Sometimes this is read as "i tens j" or "i kron j". I like the "kron" since it reminds me of a Transformers villain. Sometimes the notation $|i\rangle_A|j\rangle_B$ is also used for convenience, just to avoid using the symbol $\otimes$ over and over again. Let me summarize the many notations we use:

$$\boxed{|i, j\rangle_{AB} = |i\rangle_A \otimes |j\rangle_B = |i\rangle_A|j\rangle_B} \tag{2.36}$$

When is clear from the context, we also sometimes omit the suffix AB and write only $|i, j\rangle$.

Eq. (2.36) is still not very useful since we haven't specified how to operate on a tensor product of states. That is, we haven't yet specified what is the tensor structure of operators. In order to do that, we must have a rule for how objects behave when there is an $\otimes$ around. There is only one rule that you need to remember: *stuff to the left of $\otimes$ only interact with stuff to the left and stuff to the right only interact with stuff to the right*. We write this as

$$\boxed{(A \otimes B)(C \otimes D) = (AC) \otimes (BD),} \tag{2.37}$$

In this rule A, B, C and D can be arbitrary objects. For instance, this rule applies if they are all matrices. Or, they apply if you want to multiply a vector by a matrix. In that case we get instead

$$(A \otimes B)(|\psi\rangle \otimes |\phi\rangle) = (A|\psi\rangle) \otimes (B|\phi\rangle), \tag{2.38}$$

From this we now define operators which act only on A or act only on B as

$$O_A \otimes 1_B = \text{an operator that acts only on space A} \tag{2.39}$$

$$1_A \otimes O_B = \text{an operator that acts only on space B} \tag{2.40}$$

where 1_A means the identity operator on system A and similarly for 1_B.

For instance, going back to the example in Eq. (2.34), we can define the Pauli matrices for qubits A and B as

$$\sigma_x^A = \sigma_x \otimes 1_2, \qquad \sigma_x^B = 1_2 \otimes \sigma_x, \tag{2.41}$$

Combining the definition (2.36) with the rule (2.37) we can now repeat the computation in example (2.34) using the $\otimes$ notation:

$$\sigma_x^A|i, j\rangle_{A,B} = (\sigma_x \otimes 1_2)(|i\rangle_A \otimes |j\rangle_B) = (\sigma_x|i\rangle_A) \otimes |j\rangle_B.$$

We can also consider other operators, such as

$$\sigma_x^A\sigma_x^B = \sigma_x \otimes \sigma_x.$$

which is an operator that simultaneously flips both spins:

$$\sigma_x^A \sigma_x^B |0,0\rangle_{AB} = |1,1\rangle_{AB} \tag{2.42}$$

You can also use the $\otimes$ notation to combine weird objects. The only rule is that the combination makes sense in each space separated by the $\otimes$. For instance, the object $\langle 0| \otimes |0\rangle$ is allowed, although it is a bit strange. But if you want to operate with it on something, that operation must make sense. For instance

$$(\langle 0| \otimes |0\rangle)(\sigma_x \otimes \sigma_x)$$

makes no sense because even though $\langle 0|\sigma_x$ makes sense, the operation $|0\rangle\sigma_x$ does not. On the other hand, a weird operation which does make sense is

$$(\langle 0| \otimes |0\rangle)(|0\rangle \otimes \langle 0|) = (\langle 0|0\rangle) \otimes |0\rangle\langle 0| = |0\rangle\langle 0|$$

In particular, in the last equality I used the fact that $\langle 0|0\rangle = 1$ is a number and the tensor product of a number with something else, is just the multiplication of the something else by the number.

I am also obliged to say that everything I said extends naturally to systems composed of more than two parts. For instance, if we have a system of 4 qubits, then we can define $\sigma_x^1 = \sigma_x \otimes 1 \otimes 1 \otimes 1$ or $\sigma_x^3 = 1 \otimes 1 \otimes \sigma_x \otimes 1$, and so on. We will for now focus only on bipartite systems. But you have plenty of opportunities to play with multipartite systems in the future.

Matrix representation of the Kronecker product

If A and B are two matrices, then in order to satisfy Eq. (2.37), the components of the Kronecker product must be given by

$$A \otimes B = \begin{pmatrix} a_{1,1}B & \dots & a_{1,N}B \\ \vdots & \ddots & \vdots \\ a_{M,1}B & \dots & a_{M,N}B \end{pmatrix}. \tag{2.43}$$

This is one of those things that you sort of just have to convince yourself that is true. At each entry $a_{i,j}$ you introduce the full matrix B (and then get rid of the parenthesis lying around). For instance

$$\sigma_x \otimes \sigma_x = \begin{pmatrix} 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ 1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{2.44}$$

This provides an automated way to construct tensor product matrices. Such functionality is implemented in any computer library (Mathematica, Matlab, etc.), which is a very convenient tool to use.

We can also do the same for vectors. For instance

$$|0,0\rangle = |0\rangle \otimes |0\rangle = \begin{pmatrix} 1\begin{pmatrix}1\\0\end{pmatrix} \\ 0\begin{pmatrix}1\\0\end{pmatrix} \end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \tag{2.45}$$

You can proceed similarly to find the others basis elements. You will then find

$$|0,0\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \qquad |0,1\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \qquad |1,0\rangle = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \qquad |1,1\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix} \tag{2.46}$$

Thus, from the rule (2.43) we therefore see that the correct order of the basis elements is $|0,0\rangle$, $|0,1\rangle$, $|1,0\rangle$ and $|1,1\rangle$. This is known as *lexicographic* order. As an exercise, try to use the rule (2.43) to compute $\langle 0| \otimes |0\rangle$.

The operation highlighted by Eq. (2.43) is implemented in any numerical library. In MATLAB they call it `kron()` whereas in Mathematica they call it `KroneckerProduct[]`. These functions are really useful. You should really try to play with them a bit.

2.4 Entanglement

If qubit A is on Earth and quibit B is on Mars, it makes sense to attribute to them *local states*. For instance, we could have

$$|\psi\rangle_A = \alpha|0\rangle_A + \beta|1\rangle_A, \qquad |\phi\rangle_B = \gamma|0\rangle_B + \delta|1\rangle_B.$$

Then, the global state of AB will be

$$\begin{aligned}|\psi\rangle_A \otimes |\phi\rangle_B &= \Big[\alpha|0\rangle_A + \beta|1\rangle_A\Big] \otimes \Big[\gamma|0\rangle_B + \delta|1\rangle_B\Big] \\ &= \alpha\gamma|0,0\rangle_{AB} + \alpha\delta|0,1\rangle_{AB} + \beta\gamma|1,0\rangle_{AB} + \beta\delta|1,1\rangle_{AB}.\end{aligned}$$

This state looks just like a linear combination of the global basis $|i,j\rangle_{AB}$. However, it is not an arbitrary linear combination because it contains a very special choice of parameters which are such that you can perfectly factor the state into something related to A times something related to B. This is what we call a **product state**. However, quantum theory also allows us to have more general linear combinations which are not necessarily factorable into a product. Such a general linear combination has the form

$$|\psi\rangle_{AB} = \sum_{i,j} C_{i,j}|i,j\rangle_{AB}, \tag{2.47}$$

where $C_{i,j}$ are a set of coefficients. If it happens that we can write $C_{i,j} = f_i g_j$, then the state (2.47) can be factored into a product and is therefore a product state. Otherwise, it is called an **entangled state**.

An important set of entangled states are the so called **Bell states**:

$$|\Phi_1\rangle = \frac{1}{\sqrt{2}}\Big[|0,0\rangle + |1,1\rangle\Big], \tag{2.48}$$

$$|\Phi_2\rangle = \frac{1}{\sqrt{2}}\Big[|0,0\rangle - |1,1\rangle\Big], \tag{2.49}$$

$$|\Phi_3\rangle = \frac{1}{\sqrt{2}}\Big[|0,1\rangle + |1,0\rangle\Big], \tag{2.50}$$

$$|\Phi_4\rangle = \frac{1}{\sqrt{2}}\Big[|0,1\rangle - |1,0\rangle\Big]. \tag{2.51}$$

These states *cannot* be factored into a product of local states (please try to convince yourself). In fact, they are what is known as **maximally entangled states**: we don't have the tools yet to *quantify* the degree of entanglement, so we are not ready yet to properly define the term "maximally". We will get to that later.

In order to better understand the meaning of entanglement, let us discuss what happens when a composite system is in an entangled state and we measure one of the parts. We have seen in Sec. 1.7 of the previous chapter that in order to measure in a basis we define a projection operator $P_i = |i\rangle\langle i|$ such that, if the system is in a state $|\psi\rangle = \sum_i \psi_i |i\rangle$, then the outcome $|i\rangle$ is obtained with probability

$$p_i = \langle\psi|P_i|\psi\rangle = |\psi_i|^2 \tag{2.52}$$

Moreover, if $|i\rangle$ was found, then the state of the system after the measurement is of course $|i\rangle$. We can write that in a slightly different way as follows:

$$|\psi\rangle \to \frac{P_i|\psi\rangle}{\sqrt{p_i}} \tag{2.53}$$

Since $P_i|\psi\rangle = \psi_i|i\rangle$, this is of course the same as the state $|i\rangle$, up to a global phase which is not important.

We now use this to define what is the operation of making a projective measurement on one of the two sub-systems. The operation performing a projective measurement on B will also be a projection operator, but will have the form

$$P_i^B = 1 \otimes |i\rangle\langle i|, \tag{2.54}$$

You can check that this is a valid projection operator ($P_i^B P_j^B = P_i^B \delta_{i,j}$). Thus, with this definition, the rules (2.52) and (2.53) continue to be valid, provided we use this modified projection operator.

As an example, suppose that AB are prepared in the Bell state (2.48). And suppose Bob measures B in the computational basis $\{|0\rangle, |1\rangle\}$. Then we get outcomes 0 or 1 with probabilities

$$p_0 = \langle\Phi_1|P_0^A|\Phi_1\rangle = \frac{1}{2} = p_1 \tag{2.55}$$

Moreover, if B happened to be found in state $|0\rangle_B$, then the global state after the measurement will be

$$|\Phi_1\rangle \to \frac{P_0^A|\Phi_1}{\sqrt{p_0}} = |0,0\rangle \tag{2.56}$$

whereas if the output $|1\rangle_B$ was found, then the state has collapsed to

$$|\Phi_1\rangle \to \frac{P_1^A|\Phi_1}{\sqrt{p_1}} = |1,1\rangle \tag{2.57}$$

Before the measurement system A could have been found in either 0 or 1. But after the measurement, A will be found with certainty in state 0 or with certainty in state 1. We have changed A even though B could have been 100 light years away. This "spooky action at a distance" is the source of a century of debates and research. Of course, the key question is whether Alice, the person that has system A in her lab, can know whether this happened or not. We will see in a second that she cannot, unless Bob sent her a classical communication (like an e-mail) telling her what he found. Thus, information cannot be transmitted faster than the speed of light. There was definitely a change in the state of A and this change was non-local: it took place during a very short time (the time it took to make the measurement) even if A and B are arbitrarily far apart. But no information was transmitted. We will get back to this discussion over and over again, during this chapter and the next ones.

2.5 Mixed states and entanglement

I want you now to recall our construction of a density matrix in Sec. 2.1. What we did there was mix quantum states with classical uncertainty, which was done by considering a machine which is not very good at producing quantum states. As a result, we found that a density matrix could be written as

$$\rho = \sum_i q_i |\psi_i\rangle\langle\psi_i| \tag{2.58}$$

where the $|\psi_i\rangle$ are arbitrary states and the q_i are arbitrary probabilities. This construction may have left you with the impression that the density matrix is only necessary when we want to mix quantum and classical stuff. That is, that a density matrix is not really a quantum thing. Now I want to show you that this is not the case. I will show you that there is an intimate relation between mixed states and entanglement. And this relation is one the key steps relating quantum mechanics and information theory.

Essentially, the connection is made by the notion of **reduced state** or **reduced density matrix**. When a composite system is in a product state $|\psi\rangle_A \otimes |\phi\rangle_B$, then we can attribute the ket $|\psi\rangle_A$ as representing the state of A and $|\phi\rangle_B$ as the state of B. But if the composite system is in an entangled state, like (2.47), then that is no longer possible. As we will show, *if AB are entangled, the reduced state of A and B are mixed states, described by density matrices.*

Suppose we have a bipartite system and, for simplicity, assume that the two parts are identical. Let $|i\rangle$ denote a basis for any such part and assume that the composite system is in a state of the form

$$|\psi\rangle = \sum_i c_i |i\rangle \otimes |i\rangle \tag{2.59}$$

for certain coefficients c_i.[1] If $c_1 = 1$ and all other $c_i = 0$ then $|\psi\rangle = |i\rangle \otimes |i\rangle$ becomes a **product state**. When more than one c_i is non-zero, then the state can never be written as a product. Whenever a state of a bipartite system cannot be written as a product state, we say it is **entangled**.

Now let A be an operator which acts only on system A. Then, its expectation value in the state (2.59) will be

$$\langle A\rangle = \langle\psi|(A \otimes 1)|\psi\rangle \tag{2.60}$$

Carrying out the calculation we get:

$$\begin{aligned}
\langle A\rangle &= \sum_{i,j} c_i^* c_j \langle i, i|(A \otimes 1)|j, j\rangle \\
&= \sum_{i,j} c_i^* c_j \langle i|A|j\rangle\langle i|j\rangle \\
&= \sum_i |c_i|^2 \langle i|A|i\rangle
\end{aligned}$$

If we now define the density matrix of system A as

$$\rho_A = \sum_i |c_i|^2 |i\rangle\langle i| \tag{2.61}$$

then the expectation value of A becomes

$$\langle A\rangle = \text{tr}(A\rho_A) \tag{2.62}$$

This result is quite remarkable. Note how Eq. (2.61) has *exactly* the same form as Eq. (2.58), with the classical probabilities q_i replaced by $|c_i|^2$. But there are no classical probabilities at play here: we started with a pure state. Moreover, we also see that in general the state of A will be a mixed state. The only exception is when the original state was a product state. Then one $c_i = 1$ and all other $c_j = 0$, so that $\rho_A = |i\rangle\langle i|$. Thus, we conclude that whenever the global AB state is entangled, the reduced state of a given part will be a mixed state. Eq. (2.61) is what we call a **reduced density matrix**, a concept which is fundamental in the theory of Quantum Information and which we will use throughout this course. In the above calculation I introduced it in a not so formal way. But don't worry, in the next section we will go back to it and see how to define it more generally.

But before we do so, I just want to give one example, which will also connect with our discussion of entanglement in Sec. 2.4, in particular Eq. (2.57). Suppose again that

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[1] This is called the Schmidt form of a bipartite state. We will talk more about this in Sec. 2.8.

AB is in the Bell state (2.48). This state has the form of Eq. (2.59) with $c_i = 1/\sqrt{2}$. Thus, it is easy to apply Eq. (2.61), which gives

$$\rho_A = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{2.63}$$

We therefore see that the reduced state of A is actually the maximally mixed state (2.16). This is a feature of all Bell states and it is the reason we call them maximally entangled states: we will learn soon that *the degree of entanglement can be quantified by how mixed the reduced state is*.

Now let us ask what is the state of A after we measure B. As we have seen in Eq. (2.57), the composite state after the measurement can be either $|0,0\rangle$ or $|1,1\rangle$, both occurring with probability 1/2. Thus, if Alice does not know the outcomes of the measurements that B performed, then best possible guess to the state of A will be a classical probabilistic combination

$$\rho_A = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{2.64}$$

which is exactly the same state as (2.63). Hence, from the point of view of Alice, it is impossible to know if the state of A is mixed because of entanglement or if it is mixed because Bob performed some measurements. All Alice can know is that the density matrix of A has the form of a maximally mixed state. This is called **the ambiguity of mixtures**. Even though the global AB state is affected by the measurement, from the point of view of Alice, she has no way of knowing. The only way that A would know is if she receives a *classical communication* from B. That is, if Bob sends an e-mail to Alice saying "Hey Alice, are you going to the party tonight? Oh, by the way, I measured my qubit and found it in 0."

2.6 The partial trace

The calculation that led us to Eq. (2.61) is what we call a partial trace. The trace, which we studied in Sec. 1.11, is an operation that receives an operator and spits out a number. The partial trace is an operation which receives a tensor product of operators and spits another operator, but living in a smaller Hilbert space. Why this is the correct procedure to be used in defining a reduced density matrix will be explained shortly.

Consider again a composite system AB. Let $|a\rangle$ and $|b\rangle$ be basis sets for A and B. Then a possible basis for AB is the tensor basis $|a,b\rangle$. What I want to do is investigate the trace operation within the full AB space. To do that, let us consider a general operator of the form $O = A \otimes B$. After we learn how to deal with this, then we can generalize for an arbitrary operator, since any operator on AB can always be written as

$$O = \sum_\alpha A_\alpha \otimes B_\alpha \tag{2.65}$$

for some index α and some set of operators A_α and B_α.

Let us then compute the trace of $O = A \otimes B$ in the $|a, b\rangle$ basis:

$$\begin{aligned}
\mathrm{tr}(O) &= \sum_{a,b} \langle a, b|O|a, b\rangle \\
&= \sum_{a,b} (\langle a| \otimes \langle b|)(A \otimes B)(|a\rangle \otimes |b\rangle) \\
&= \sum_{a,b} \langle a|A|a\rangle \otimes \langle b|B|b\rangle \\
&= \sum_{a} \langle a|A|a\rangle \sum_{b} \langle b|B|b\rangle
\end{aligned}$$

I got rid of the $\otimes$ in the last line because the kron of two numbers is a number. The two terms in this formula are simply the trace of the operators A and B in their respective Hilbert spaces. Whence, we conclude that

$$\boxed{\mathrm{tr}(A \otimes B) = \mathrm{tr}(A)\,\mathrm{tr}(B)} \tag{2.66}$$

Now we can imagine an operation where we only trace over a part of the system. This is what we call the **partial trace**. It is defined as

$$\boxed{\mathrm{tr}_A(A \otimes B) = \mathrm{tr}(A)B, \qquad \mathrm{tr}_B(A \otimes B) = A\,\mathrm{tr}(B)} \tag{2.67}$$

When you "trace over A", you eliminate the variables pertaining to A and what you get left is an operator acting only on $\mathscr{H}_B$. This is something we often forget, so please pay attention: the result of a partial trace is still an operator. More generally, for an arbitrary operator O as defined in Eq. (2.65), we have

$$\mathrm{tr}_A\, O = \sum_\alpha \mathrm{tr}(A_\alpha) B_\alpha \qquad \mathrm{tr}_B\, O = \sum_\alpha A_\alpha\, \mathrm{tr}(B_\alpha) \tag{2.68}$$

As an example, suppose we have two qubits, with Pauli operators σ_x^A and σ_x^B. Then we would have, for instance,

$$\mathrm{tr}_A(\sigma_x^A \sigma_x^B) = \mathrm{tr}(\sigma_x)\sigma_x^B$$

Note how in the right-hand side I wrote σ_x instead of σ_x^A. The partial trace acts only on the single-spin subspace, so it does not matter which notation I use. Of course, this example I just gave is a bit silly because $\mathrm{tr}(\sigma_x) = 0$. But still, you get the idea. As another example, consider the partial trace of $\boldsymbol{\sigma}_A \cdot \boldsymbol{\sigma}_B = \sigma_x^A\sigma_x^B + \sigma_y^A\sigma_y^B + \sigma_z^A\sigma_z^B$. To compute it we need to use the linearity of the trace:

$$\mathrm{tr}_A(\boldsymbol{\sigma}_A \cdot \boldsymbol{\sigma}_B) = \mathrm{tr}(\sigma_x)\sigma_B^x + \mathrm{tr}(\sigma_y)\sigma_B^y + \mathrm{tr}(\sigma_z)\sigma_B^z$$

Again, all terms are zero in the end, so sorry again for the silly example. In principle every operator may be written in the form (2.65) so linearity solves all problems. However, that does not mean that writing down such an expansion is easy. For instance, suppose you want to compute the partial trace of $e^{\sigma_A\cdot\sigma_B}$. This turns out to be a quite clumsy calculation. For two qubits the matrices will be 4×4, so albeit clumsy, this is something a computer can readily do. For N qubits things become more difficult.

We can also write down the partial trace in terms of components. For instance, the partial trace over B reads:

$$\boxed{\operatorname{tr}_B O = \sum_b \langle b|O|b\rangle} \tag{2.69}$$

This notation may be a bit confusing at first. Actually, when we write $|b\rangle$ here, what we really mean is $1 \otimes |b\rangle$. So the full formula would be

$$\operatorname{tr}_B O = \sum_b (1 \otimes \langle b|) O (1 \otimes |b\rangle) \tag{2.70}$$

We can check that this works using $O = A \otimes B$. We then get

$$\begin{aligned}
\operatorname{tr}_B O &= \sum_b (1 \otimes \langle b|)(A \otimes B)(1 \otimes |b\rangle) \\
&= \sum_b (1A1) \otimes (\langle b|B|b\rangle) \\
&= A \sum_b \langle b|B|b\rangle \\
&= A \operatorname{tr}(B)
\end{aligned}$$

Eq. (2.69) with $1 \otimes |b\rangle$ is a convenient way to implement the partial trace in a computer.

Finally we could also write down a general formula for the partial trace in terms of the components of O in a basis. To do that, note that we may always insert two identities to decompose O as

$$O = \sum_{a,b,a',b'} |a, b\rangle\langle a, b|O|a', b'\rangle\langle a', b'| \tag{2.71}$$

To perform the partial trace over B, for instance, we sum over the diagonal entries of the B part ($b' = b$) :

$$\operatorname{tr}_B O = \sum_{a,b,a'} |a\rangle\langle a, b|O|a', b\rangle\langle a'| \tag{2.72}$$

The result is an operator acting on A, which we can see from the fact that this is a sum of outer products of the form $|a\rangle\langle a'|$:

$$\boxed{\operatorname{tr}_B O = \sum_{a,a'} \bigg[\sum_b \langle a, b|O|a', b\rangle\bigg] |a\rangle\langle a'|} \tag{2.73}$$

An example that is often encountered is the partial trace of some outer product, such as $|a,b\rangle\langle a',b'|$. To take the partial trace, remember that this can be written as

$$|a,b\rangle\langle a',b'| = |a\rangle\langle a'| \otimes |b\rangle\langle b'|$$

The partial trace over B, for instance, will simply go right through the first part and act only on the second part; i.e.,

$$\begin{aligned}\mathrm{tr}_B\, |a,b\rangle\langle a',b'| &= |a\rangle\langle a'|\, \mathrm{tr}\Big\{ |b\rangle\langle b'| \Big\} \\ &= |a\rangle\langle a'| \Big\{ \langle b'|b\rangle \Big\}\end{aligned}$$

Thus, we conclude that

$$\boxed{\mathrm{tr}_A\, |a,b\rangle\langle a',b'| = \delta_{a,a'} |b\rangle\langle b'|, \qquad \mathrm{tr}_B\, |a,b\rangle\langle a',b'| = |a\rangle\langle a'| \delta_{b,b'}} \tag{2.74}$$

2.7 Reduced density matrices

We are now ready to introduce the idea of a reduced density matrix in a more formal way. Given a bipartite system ρ_{AB} we define the reduced density matrix of A and B as

$$\boxed{\rho_A = \mathrm{tr}_B\, \rho_{AB}, \qquad \rho_B = \mathrm{tr}_A\, \rho_{AB}} \tag{2.75}$$

Thus, with the tools described in the previous section, it is now a matter of practice to play around and find reduced density matrices. It is also important to note that the partial trace works for both pure and mixed states. If we are dealing with pure states, then we simply write the density matrix as $|\psi\rangle\langle\psi|$ and continue as usual.

To warm up consider again the Bell state example that led us from the bipartite state (2.48) to the reduced state (2.63). Then

$$\rho_{AB} = |\Phi_1\rangle\langle\Phi_1| = \frac{1}{2}\Big\{ |0,0\rangle\langle 0,0| + |0,0\rangle\langle 1,1| + |1,1\rangle\langle 0,0| + |1,1\rangle\langle 1,1| \Big\} \tag{2.76}$$

To take the partial trace we use Eq. (2.74). We then get

$$\rho_A = \frac{1}{2}\Big\{ |0\rangle\langle 0| + |1\rangle\langle 1| \Big\} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{2.77}$$

with an identical result for ρ_B.

Let us look at some further examples. For instance, if we have a state which is of the form $\rho_{AB} = \rho_A \otimes \rho_B$, then Eq. (2.67) directly gives us $\mathrm{tr}_B\, \rho_{AB} = \rho_A$ and $\mathrm{tr}_A\, \rho_{AB} = \rho_B$, as of course expected. So any density matrix which is a product of the form $\rho_{AB} = \rho_A \otimes \rho_B$ represents *uncorrelated* systems, irrespective of whether the state is pure or not. However, it is very important to note that in general we *cannot* recover the full density matrix ρ_{AB} from the reduced density matrices ρ_A and ρ_B. The operation of taking the partial trace is **irreversible** and in general looses information. To put that more precisely, given a general ρ_{AB} and its reduced density matrices (2.75), we have

$$\rho_A \otimes \rho_B \neq \rho_{AB} \tag{2.78}$$

This is only true when ρ_{AB} was already originally uncorrelated. Thus, in general, we see that information is lost whenever AB are correlated.

To given an example, suppose we have two qubits in a state of the form

$$\rho_{AB} = \rho_A^0 \otimes \rho_B^0 + \chi \tag{2.79}$$

where

$$\chi = \alpha \Big\{ |0,1\rangle\langle 1,0| + |1,0\rangle\langle 0,1| \Big\} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha & 0 \\ 0 & \alpha & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{2.80}$$

with α being a parameter.[2] What I like about (2.79) is that the partial trace of χ is always zero: $\text{tr}_A(\chi) = \text{tr}_B(\chi) = 0$. Thus, the reduced density matrices are $\rho_A = \rho_A^0$ and $\rho_B = \rho_B^0$. This means that from the perspective of A and B, it is as if χ doesn't even exist. But from a *global* perspective, you have a certain degree of correlations.

The partial trace is the quantum analog of *marginalizing* a probability distribution. To see that in first hand, consider a bipartite state of the form

$$\rho_{AB} = \sum_{i,j} p_{i,j} |i, j\rangle\langle i, j| \tag{2.81}$$

which will be a valid quantum state provided $p_{i,j} \in [0, 1]$ and $\sum_{i,j} p_{i,j} = 1$. This state is as close as one gets from a *classical* probability distribution. To compute the partial trace over B we use Eq. (2.74), which gives

$$\rho_A = \text{tr}_B\, \rho_{AB} = \sum_{i,j} p_{i,j} |i\rangle\langle i| = \sum_i p_i |i\rangle\langle i|$$

In the last equality I carried out the sum over j and defined

$$p_i = \sum_j p_{i,j} \tag{2.82}$$

This is exactly the marginalization procedure in classical probability theory. We simply sum over all probabilities of B to obtain a reduced probability distribution only for A.

Finally, let us talk about *why* this partial trace operation works. Or, putting it more precisely, why does the rule (2.67) works. What we really require of the partial trace operation is that

$$\text{tr}_{\text{AB}}\Big[(A \otimes 1)\rho_{AB}\Big] = \text{tr}_A\Big[A\rho_A\Big] \tag{2.83}$$

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[2] The allowed values of α depend on ρ_A^0 and ρ_B^0 in order for te purity to be within the bounds $\frac{1}{4} \leq \mathcal{P} \leq 1$.

That is, taking expectation values of A operators over the full Hilbert space or over the reduced Hilbert space give the same result. This is clearly true for the partial trace as we defined. What is a bit more subtle, is to show that the partial trace is the unique operation satisfying this criteria. This is demonstrated in Sec. 2.4.3 of Nielsen and Chuang.

2.8 Singular value and Schmidt decompositions

Consider a bipartite system AB with basis $|a, b\rangle$. The most general pure state in this system can be written as

$$|\psi\rangle = \sum_{a,b} \psi_{ab} |a, b\rangle, \tag{2.84}$$

where ψ_{ab} are coefficients. This state will in general be entangled. To see that in first hand, let us look at the reduced density matrices of A and B. I will leave for you as an exercise to show that

$$\rho_A = \mathrm{tr}_B\, |\psi\rangle\langle\psi| = \sum_{a,a'} \bigg[\sum_b \psi^*_{ab} \psi_{a'b} \bigg] |a\rangle\langle a'|, \tag{2.85}$$

$$\rho_B = \mathrm{tr}_A\, |\psi\rangle\langle\psi| = \sum_{b,b'} \bigg[\sum_a \psi^*_{ab} \psi_{ab'} \bigg] |b\rangle\langle b'|. \tag{2.86}$$

Of course, these are kind of ugly because ρ_A and ρ_B are not diagonal. But what I want to stress is that in general these states will be mixed. The only case in which these states will be pure is when the $\psi_{a,b}$ factor as a product of coefficients $\psi_{a,b} = f_a g_b$. Then one can already see from (2.84) that $|\psi\rangle$ will also factor as a product.

Suppose we now have a N-partite system with basis elements $|s_1, \ldots, s_N\rangle$. Then the most general state pure state of this system will be

$$|\psi\rangle = \sum_{s_1,\ldots,s_N} \psi_{s_1 \ldots s_N} |s_1, \ldots, s_N\rangle. \tag{2.87}$$

The coefficients $\psi_{s_1 \ldots s_N}$ contain all the information about this system. It says, for instance, that 3 is entangled to 25 but 1 is not entangled with 12. Or that $1, 2, 3$ taken as a block, is completely independent of $4, 5, \ldots, N$. Everything is encoded in $\psi_{s_1,\ldots,s_N}$. Understanding how to extract the physics from this messy ψ is one of the most important questions of modern research.

If we think about it for a second, we also see that $\psi_{s_1,\ldots,s_N}$ can be viewed as a **tensor**. It is a rank-N tensor where each index has dimension d (the dimension of the local Hilbert space). Thus, there are in total d^N possible entries in this tensor. The physics of the state is then encoded inside this very very messy tensor structure. And that is a big problem because for $d = 2$ and $N = 300$, 2^{300} represents more particles than there are in the universe. Thus, if we want to characterize the entanglement properties of only 300 qubits, we are already in huge trouble because this is not a computational limitation that will be solved with the next generation of processors. It is a fundamental constraint.

The difficulties underlying the complex entanglement structure of states such as (2.87) has given rise to a new field of research known as **tensor networks**. The idea is two-fold. First, to create tools (such as diagrams and numerical libraries) which are efficient at dealing with complex tensors and give us intuition on what to do. Second, and most importantly, to understand what types of tensor structures appear most often. You see, *the many-body Hilbert space is enormous, but that does not mean that all of it is equally important.* It may very well be that in most typical scenarios, only a small part of the full Hilbert space is occupied. Figuring out what parts of the many-body Hilbert space are relevant is a million dollar question. Substantial progress has been done recently for certain classes of quantum systems, such as one-dimensional chains with short-range interactions. But the problem is nonetheless still in its infancy.

Singular Value Decomposition

In this section we will introduce some tools for dealing with the entanglement properties of quantum states. We start with a linear algebra tool that also has applications in many other fields of research, called the **singular value decomposition (SVD)**. Twenty years ago no one would teach the SVD for undergraduates. In twenty years from now, I guarantee you, SVD will be standard textbook material. The SVD theorem is as follows. Let A be an arbitrary rectangular $M \times N$ matrix. Then it is always possible to decompose A as

$$\boxed{A = USV^\dagger,} \tag{2.88}$$

where

- U is $M \times \min(M,N)$ and has *orthogonal columns* $U^\dagger U = 1$. If $M \leq N$ then U will be square and unitary, $UU^\dagger = 1$.
- V is $N \times \min(M,N)$ and has *orthogonal columns* $V^\dagger V = 1$. If $M \geq N$ then V will be square and unitary, $VV^\dagger = 1$.
- S is $\min(M,N) \times \min(M,N)$ and diagonal, with entries $S_{\alpha\alpha} = \sigma_\alpha \geq 0$, which are called the **singular values** of the matrix A. It is convention to always order the singular values in decreasing order, $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0$. The number of non-zero singular values, called r, is known as the *Schmidt rank* of the matrix.

When the matrix is square, $M = N$, then both U and V become unitary. The sizes of A, U, S and V are shown in Fig. 2.2. For future reference, I will also write down Eq. (2.88) in terms of the components of A:

$$A_{ij} = \sum_{\alpha=1}^{r} U_{i\alpha}\sigma_\alpha V^*_{j\alpha} \tag{2.89}$$

where the sum extends only up the Schmidt rank r (after that the σ_α are zero so we don't need to include them).

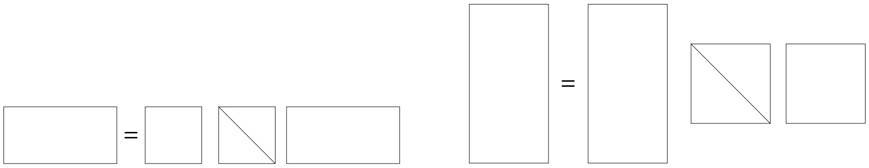

Figure 2.2: The size of the matrices appearing in Eq. (2.88). Left: A is short and fat ($M \leq N$). Right: A is thin and tall ($M \geq N$).

The SVD is not in general related to eigenvalues of A. In fact, it is defined even for rectangular matrices. Instead, the SVD is actually related to the eigenvalues of $A^\dagger A$ and $AA^\dagger$. Starting from Eq. (2.88) and using the fact that $U^\dagger U = 1$ we see that

$$A^\dagger A = V^\dagger S^2 V \tag{2.90}$$

By construction, the matrix $A^\dagger A$ is Hermitian and positive semi-definite. Hence, we see that V forms its eigenvectors and σ_α^2 its eigenvalues. Similarly, using the fact that $VV^\dagger = 1$ we get

$$AA^\dagger = US^2U^\dagger \tag{2.91}$$

Thus, σ_α^2 are also the eigenvalues of $AA^\dagger$. It is interesting to note that when A is rectangular, $A^\dagger A$ and $AA^\dagger$ will have different dimensions. The point is that the largest of the two will have the same eigenvalues as the smaller one, plus a bunch of zero eigenvalues. The only type of matrix for which the singular values are identically equal to the eigenvalues are positive semi-definite matrices, like density matrices ρ.

One of the most important applications of the SVD is in making **low rank approximations** of matrices. To do that, suppose A is $N \times N$. Then it will have N^2 entries which, if N is large, will mean a bunch of entries. But now let $\boldsymbol{u}$ and $\boldsymbol{v}$ be vectors of size N and consider the outer product $\boldsymbol{u}\boldsymbol{v}^\dagger$, which is also an $N \times N$ matrix with entries $(\boldsymbol{u}\boldsymbol{v}^\dagger)_{ij} = u_i v_j^*$. We then see that even though this is $N \times N$, the entries of this matrix are not independent, but are completely specified by the $2N$ numbers u_i and v_i. A matrix of this form is called a rank-1 matrix (just like the rank-1 projectors we studied before).

Going back now to Eq. (2.89), let $\boldsymbol{u}_\alpha$ denote a column vector with entries $U_{i\alpha}$ and, similarly, let $\boldsymbol{v}_\alpha$ denote a column vector with entries $V_{j\alpha}$. Then it is easy to verify that the matrix A in Eq. (2.89) can be written as

$$A = \sum_{\alpha=1}^{r} \sigma_\alpha \boldsymbol{u}_\alpha \boldsymbol{v}_\alpha^\dagger. \tag{2.92}$$

We have therefore decomposed the matrix A into a sum of rank-1 matrices, weighted by the singular values σ_α. Since the singular values are always non-negative and appear in decreasing order, we can now think about retaining only the largest singular values. That is, instead of summing over the full Schmidt rank r, we sum only up to a smaller number of singular values $r' < r$ to get an approximate representation of A:

$$A' = \sum_{\alpha=1}^{r'} \sigma_\alpha \boldsymbol{u}_\alpha \boldsymbol{v}_\alpha^\dagger.$$

This is called a rank-r' approximation for the matrix A. If we consider just the largest singular value (a rank-1 approximation) then we replaced N^2 elements by $2N$, which can be an enormous improvement if N is large. It turns out that this approximation is controllable in the sense that the matrix A' is the *best rank-r' approximation* of A given the Frobenius norm, defined as $||A|| = \sum_{ij} |A_{ij}|^2$. That is, A' is the rank-r' matrix which minimizes $||A - A'||$.

Schmidt decomposition

I have introduced above the SVD as a general matrix decomposition, which is useful to know since it appears often in many fields of research. Now I want to apply the SVD to extract properties of quantum states. Consider again a bipartite system described by the pure state

$$|\psi\rangle = \sum_{a,b} \psi_{ab} |a, b\rangle. \tag{2.93}$$

With a moment of though we see that ψ_{ab} can also be interpreted as a matrix of coefficients. In fact, this matrix will in general be rectangular when the dimensions d_A and d_B are different. We may then apply the SVD to the matrix with entries ψ_{ab}. Using Eq. (2.89) we see that this decomposition will have the form

$$\psi_{ab} = \sum_{\alpha} \sigma_\alpha U_{a\alpha} V^*_{b\alpha}. \tag{2.94}$$

The matrix ψ_{ab} is special in that the state $|\psi\rangle$ must be normalized. This means that $\sum_{ab} |\psi_{ab}|^2 = 1$ which in turn implies that

$$\sum_{\alpha=1}^{r} \sigma_\alpha^2 = 1. \tag{2.95}$$

In general the singular values are simply non-negative. But for states ψ_{ab} they are also normalized in this way.

Inserting Eq. (2.94) back into (2.93) now gives

$$|\psi\rangle = \sum_{a,b,\alpha} \sigma_\alpha U_{a\alpha} V^*_{b\alpha} |a, b\rangle = \sum_{\alpha} \sigma_\alpha \Big[\sum_a U_{a\alpha} |a\rangle \Big] \otimes \Big[\sum_b V^*_{b\alpha} |b\rangle \Big]. \tag{2.96}$$

We now define new sets of states for systems A and B, as

$$|\alpha_A\rangle = \sum_a U_{a\alpha} |a\rangle, \tag{2.97}$$

$$|\alpha_B\rangle = \sum_b V^*_{b\alpha} |b\rangle. \tag{2.98}$$

Note how these states are labeled by the same index α, even though they may be completely different (recall that we can even have $d_A \neq d_B$). Notwithstanding, we notice that these states are orthonormal because of the properties of the SVD matrices U and V.

Thus, we can now write our entangled state $|\psi\rangle$ as

$$\boxed{|\psi\rangle = \sum_\alpha \sigma_\alpha |\alpha_A\rangle \otimes |\alpha_B\rangle.} \tag{2.99}$$

This is way better than (2.93) because now we only have a single sum. It is a bit like we diagonalized something (but what we did was find the singular values of ψ_{ab}). Note also that this is exactly the type of state that we used in Eq. (2.59) when we first introduced the connection between mixed states and entanglement. The step in going from a general entangled state (2.93) to a state of the form (2.99) is called the **Schmidt decomposition** of the state. The square of the singular values, $\lambda_\alpha := \sigma_\alpha^2$, are also called Schmidt coefficients. As we will see, all the information about entanglement is contained in these guys.

We have seen that a general state such as (2.93) will be a product state when $\psi_{ab} = f_a g_b$ is a product of coefficients. But that can in practice be a hard thing to check. If we look at the Schmidt form (2.99), however, it is now trivial to know when the state will be a product or not: it will only be a product if $\sigma_1 = 1$ and all other $\sigma_\alpha = 0$. That is, they will be in a product state when the Schmidt rank is $r = 1$. We can even go further and use the singular values/Schmidt coefficients to quantify the the *degree* of entanglement. To do that, we compute the reduced density matrices of A and B, starting from the state (2.99). Since the states $|\alpha_A\rangle$ and $|\alpha_B\rangle$ are orthonormal, it is straightforward to find that

$$\rho_A = \sum_\alpha \sigma_\alpha^2 |\alpha_A\rangle\langle\alpha_A|, \tag{2.100}$$

$$\rho_B = \sum_\alpha \sigma_\alpha^2 |\alpha_B\rangle\langle\alpha_B|. \tag{2.101}$$

Once we have these reduced density matrices, we can now compute their purity:

$$\boxed{\mathrm{tr}(\rho_A^2) = \mathrm{tr}(\rho_B^2) = \sum_\alpha \sigma_\alpha^4 = \sum_\alpha \lambda_\alpha^2.} \tag{2.102}$$

Quite remarkably, we see that the purity of A and B are equal (which is true even if one has $d_A = 2$ and the other has $d_B = 1000$). Thus, we conclude that *the purity of the reduced states can be directly used as a quantifier of entanglement*. The more entangled are two systems, the more mixed are their reduced density matrices.

To summarize, I want to emphasize that *all* entanglement properties can be obtained from the singular values of ψ_{ab}. If one such singular value is $\sigma_1 = 1$ then the others must be zero so the two parties are in a product state. Otherwise, their degree of entanglement is quantified by the sum in Eq. (2.102). In particular, we now finally have the tools to define what a *maximally entangled state* is: a maximally entangled state is a state in which all singular values are equal. Due to the normalization (2.95), this then implies

$$\sigma_\alpha = \frac{1}{\sqrt{r}}. \tag{2.103}$$

As an example, consider a state of the form

$$|\psi\rangle = \cos(\theta/2)|0,1\rangle + \sin(\theta/2)|1,0\rangle. \tag{2.104}$$

We already know that if $\theta = 0, \pi$ the state will be a product and if $\theta = \pi/2$ the state will be a Bell state (2.50). In this case the matrix ψ_{ab} has coefficients $\psi_{01} = \cos(\theta/2)$ and $\psi_{10} = \sin(\theta/2)$. The singular values can be found either by asking semiconductors to do it for you or by computing the eigenvalues of $\psi^\dagger\psi$. In either case, they are

$$\sigma_1 = \cos(\theta/2), \qquad \sigma_2 = \sin(\theta/2). \tag{2.105}$$

Thus we see that when $\theta = 0, \pi$ we have one of the singular values equal to 1, which is the case of a product state. Conversely, we see that the singular values will be all equal when $\theta = \pi/2$. Thus, the Bell state (2.50) is the maximally entangled state.

So far we have only considered the entanglement between bipartite systems which are in *pure* states. A natural question therefore is how to quantify the degree of entanglement between parties that are in mixed states. That is, when not only are ρ_A and ρ_B mixed, but when ρ_{AB} itself is already mixed. This question is actually much harder and is still an open topic of research. The reason is that it is not easy to distinguish between *quantum correlations* and *classical correlations*. To see what I mean, have a look back at the state (2.81). This is a classical probability distribution. However, the sub-systems A and B are not statistically independent because $p_{i,j}$ cannot be factored as a product of two probability distributions. This is therefore an instance of classical correlations. For more general states, it is not easy to separate it from true quantum features. In fact, in this case there is even more than one type of quantum correlation (for instance, a famous one is the so called *quantum discord*). We will get back to this topic later in the course.

Multipartite entanglement

The quantification of entanglement in a multipartite system A, B, C, . . . is a difficult task and still an open research problem. One thing that can be done, though, is to look at the entanglement of all bipartitions. To see how that works, consider again a general N-partite state

$$|\psi\rangle = \sum_{s_1,\ldots,s_N} \psi_{s_1\ldots s_N} |s_1,\ldots,s_N\rangle. \tag{2.106}$$

The key now is to try to map this into the problem we just discussed, which can be done using the idea of *collective indices*. For instance, suppose we want to make a bipartition such as $1,\ldots,k$ and $k+1,\ldots,N$. Then we define two collective indeces

$$a = \{s_1,\ldots,s_k\}, \qquad b = \{s_{k+1},\ldots,s_N\} \tag{2.107}$$

so that the state (2.106) is now mapped back into state (2.93). We can then use the usual Schmidt procedure we just described.

This idea of collective indices is really important and really abstract at first. The point to remember is that this is only a *relabelling* of stuff. For instance, suppose we have two qubits with states $s_i = \{0, 1\}$. Then we can define a collective index by means of a correspondence table. For instance we can say $(0, 0)$ is $a = 1$,$(0, 1)$ is $a = 2$ and so on. We usually write this symbolically as follows:

$$\psi_{s_1 \ldots s_N} = \psi_{(s_1 \ldots s_k),(s_{k+1} \ldots s_N)}. \tag{2.108}$$

This means we have grouped the big tensor into two blocks and now it behaves as matrix with only two collective indices. This type of operation is really annoying to do by hand, but computationally it is not hard since it is simply a matter of relabelling.

State purification

We finish this section with the concept of purifying a state. Consider a physical system A described by a general mixed state ρ_A with diagonal form

$$\rho = \sum_a p_a |a\rangle\langle a|$$

By purification we mean writing this mixed state as a pure state in a larger Hilbert space. Of course, this can obviously always be done because we can always imagine that A is mixed because it was entangled with some other system B. All we need is to make that formal. One thing we note from the start is that this operation is certainly not unique since the system B can have any size. Thus, there is an infinite number of pure states which purify ρ_A. The simplest approach is then to consider B to be a copy of A. We then define the pure state

$$|\psi\rangle = \sum_a \sqrt{p_a} |a\rangle \otimes |a\rangle \tag{2.109}$$

Tracing over B we get

$$\operatorname{tr}_R |\psi\rangle\langle\psi| = \rho \tag{2.110}$$

Thus, $|\psi\rangle$ is a purified version of ρ, which lives in a doubled Hilbert space. Notice how the probabilities p_a appear naturally here as the Schmidt coefficients.

2.9 Entropy and mutual information

The concept of entropy plays a central role in classical and quantum information theory. In its simplest interpretation, entropy is a measure of the disorder (or mixedness) of a density matrix, a bit like the purity $\operatorname{tr}(\rho^2)$. But with entropy this disorder acquires a more informational sense. We will therefore start to associate entropy with questions like "how much information is stored in my system". Also like the purity, entropy can be used to quantify the degree of correlation between systems. And that makes sense because correlation is a measure of information: when two systems are correlated we can ask questions such as "how much information about A is stored in

B". Unlike the purity, however, entropy will also serve to quantify correlations of mixed states, which is done using the concept of **mutual information**. We will also introduce another concept called **relative entropy** which plays the role of a "distance" between two density matrices. It turns out that the relative entropy is not only useful in itself, but it is also useful as a tool to prove certain mathematical identities.

In thermodynamics we like to associate entropy with a unique physical quantity. In quantum information theory that is not exactly the case. There is one entropy, called the **von Neumann entropy**, which does have a prominent role. However, there are also other entropy measures which are also of relevance. An important family of such functions are the so-called **Rényi entropies**, which contain the von Neumann entropy as a particular case. We will also discuss them a bit.

The von Neumann entropy

Given a density matrix ρ, the von Neumann entropy is defined as

$$\boxed{S(\rho) = -\operatorname{tr}(\rho \ln \rho) = -\sum_k p_k \ln p_k.} \tag{2.111}$$

Working with the logarithm of an operator can be awkward. That is why in the last equality I expressed $S(\rho)$ in terms of the eigenvalues p_k of ρ. In information theory the last expression in (2.111) is also called the **Shannon entropy** (they usually use the log in base 2, but the idea is the same).

The entropy is seen to be a sum of functions of the form $-p\ln(p)$, where $p \in [0,1]$. The behavior of this function is shown in Fig. 2.3. It tends to zero both when $p \to 0$ and $p \to 1$, and has a maximum at $p = 1/e$. Hence, any state which has $p_k = 0$ *or* $p_k = 1$ will not contribute to the entropy (even though $\ln(0)$ alone diverges, $0\ln(0)$ is well behaved). States that are too deterministic therefore contribute little to the entropy. Entropy likes randomness.

Since each $-p\ln(p)$ is always non-negative, the same must be true for $S(\rho)$:

$$S(\rho) \geq 0. \tag{2.112}$$

Moreover, if the system is in a pure state, $\rho = |\psi\rangle\langle\psi|$, then it will have one eigenvalue $p_1 = 1$ and all others zero. Consequently, in a pure state the entropy will be zero:

$$\boxed{\text{The entropy of a pure state is zero.}} \tag{2.113}$$

In information theory the quantity $-\ln(p_k)$ is sometimes called the *surprise*. When an "event" is rare ($p_k \sim 0$) this quantity is big ("surprise!") and when an event is common ($p_k \sim 1$) this quantity is small ("meh"). The entropy is then interpreted as the *average surprise* of the system, which I think is a little bit funny.

As we have just seen, the entropy is bounded from below by 0. But if the Hilbert space dimension d is finite, then the entropy will also be bounded from above. I will

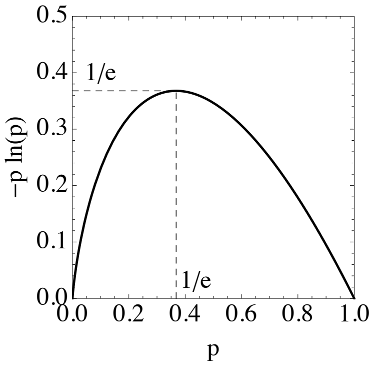

Figure 2.3: The function $-p\ln(p)$, corresponding to each term in the von Neumann entropy (2.111).

leave this proof for you as an exercise. What you need to do is maximize Eq. (2.111) with respect to the p_k, but using Lagrange multipliers to impose the constraint $\sum_k p_k = 1$. Or, if you are not in the mood for Lagrange multipliers, wait until Eq. (2.122) where I will introduce a much easier method to demonstrate the same thing. In any case, the result is

$$\max(S) = \ln(d). \qquad \text{Occurs when } \rho = \frac{\mathbb{I}}{d}. \tag{2.114}$$

The entropy therefore varies between 0 for pure states and $\ln(d)$ for maximally disordered states. Hence, it clearly serves as a measure of how mixed a state is.

Another very important property of the entropy (2.111) is that it is invariant under unitary transformations:

$$S(U\rho U^\dagger) = S(\rho). \tag{2.115}$$

This is a consequence of the infiltration property of the unitaries $Uf(A)U^\dagger = f(UAU^\dagger)$ [Eq. (1.71)], together with the cyclic property of the trace. Since the time evolution of closed systems are implemented by unitary transformations, this means that the entropy is a constant of motion. We have seen that the same is true for the purity: unitary evolutions do not change the mixedness of a state. Or, in the Bloch sphere picture, unitary evolutions keep the state on the same spherical shell. For open quantum systems this will no longer be the case.

As a quick example, let us write down the formula for the entropy of a qubit. Recall the discussion in Sec. 2.2: the density matrix of a qubit may always be written as in Eq. (2.29). The eigenvalues of ρ are therefore $(1 \pm s)/2$ where $s = \sqrt{s_x^2 + s_y^2 + s_z^2}$ represents the radius of the state in Bloch's sphere. Hence, applying Eq. (2.111) we get

$$S = -\left(\frac{1+s}{2}\right)\ln\left(\frac{1+s}{2}\right) - \left(\frac{1-s}{2}\right)\ln\left(\frac{1-s}{2}\right). \tag{2.116}$$

For a pure state we have $s = 1$ which then gives $S = 0$. On the other hand, for a maximally disordered state we have $s = 0$ which gives the maximum value $S = \ln 2$, the log of the dimension of the Hilbert space. The shape of S is shown in Fig. 2.4.

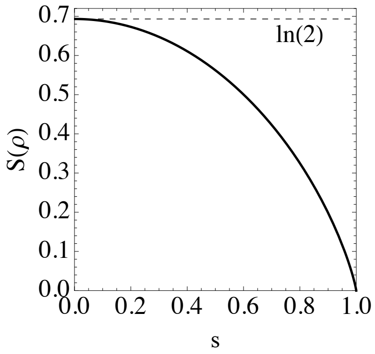

Figure 2.4: The von Neumann entropy for a qubit, Eq. (2.116), as a function of the Bloch-sphere radius s.

The quantum relative entropy

Another very important quantity in quantum information theory is the *quantum relative entropy* or *Kullback-Leibler divergence*. Given two density matrices ρ and σ, it is defined as

$$\boxed{S(\rho||\sigma) = \text{tr}(\rho\ln\rho - \rho\ln\sigma).} \tag{2.117}$$

This quantity is important for a series of reasons. But one in particular is that it satisfies the *Klein inequality*:

$$\boxed{S(\rho||\sigma) \geq 0, \qquad S(\rho||\sigma) = 0 \text{ iff } \rho = \sigma.} \tag{2.118}$$

The proof of this inequality is really boring and I'm not gonna do it here. You can find it in Nielsen and Chuang or even in Wikipedia.

Eq. (2.118) gives us the idea that we could use the relative entropy as a measure of the *distance* between two density matrices. But that is not entirely precise since the relative entropy does not satisfy the triangle inequality

$$d(x,z) \leq d(x,y) + +d(y,z). \tag{2.119}$$

This is something a true measure of distance must always satisfy. If you are wondering what quantities are actual distances, the *trace distance* is one of them[3]

$$\mathcal{T}(\rho,\sigma) = ||\rho-\sigma||_1 := \text{tr}\left[\sqrt{(\rho-\sigma)^\dagger(\rho-\sigma)}\right]. \tag{2.120}$$

But there are others as well.

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[3] The fact that $\rho-\sigma$ is Hermitian can be used to simplify this a bit. I just wanted to write it in a more general way, which also holds for non-Hermitian operators.

As I mentioned above, the relative entropy is very useful in proving some mathematical relations. For instance consider the result in Eq. (2.114). We can prove it quite easily by noting that

$$\begin{aligned} S(\rho||1/d) &= \operatorname{tr}(\rho\ln\rho) - \operatorname{tr}(\rho\ln(1/d)) \\ &= -S(\rho) + \ln(d). \end{aligned} \tag{2.121}$$

Because of (2.118) we see that

$$S(\rho) \leq \ln(d), \tag{2.122}$$

and $S(\rho) = \ln(d)$ iff $\rho = 1/d$, which is precisely Eq. (2.114). Oh, and by the way, if you felt a bit insecure with the manipulation of $1/d$ in Eq. (2.121), that's ok. The point is that here "1" stands for the identity matrix, but the identity matrix satisfies the *exact* same properties as the number one, so we can just use the usual algebra of logarithms in this case.

Unlike the entropy, which is always well behaved, the relative entropy may be infinite. The problem is in the last term of (2.117) because we may get a ln(0) which does not have a 0 in front to save the day. To take an example, suppose ρ is the general state (2.18) and suppose that $\sigma = \operatorname{diag}(f, 1-f)$ for some $f \in [0,1]$. Then

$$\begin{aligned} \operatorname{tr}(\rho\ln\sigma) &= \langle 0|\rho\ln\sigma|0\rangle + \langle 1|\rho\ln\sigma|1\rangle \\ &= p\ln f + (1-p)\ln(1-f). \end{aligned}$$

We can now see that if we happen to have $f = 0$, then the only situation where the first term will not explode is when $p = 0$ as well. This idea can be made mathematically precise as follows. Given a density matrix ρ, we define the **support** of ρ as the vector space spanned by eigenvectors which have non-zero eigenvalues. Moreover, we call the **kernel** as the complementary vector space; that is, the vector space spanned by eigenvectors having eigenvalue zero. Then we can say that $S(\rho||\sigma)$ will be infinite whenever the kernel of σ has an intersection with the support of ρ. If that is not the case, then $S(\rho||\sigma)$ is finite.

Sub-additivity and mutual information

Consider now a bipartite system prepared in a certain state ρ_{AB}. We have seen that if the two systems are not correlated then we can write $\rho_{AB} = \rho_A \otimes \rho_B$. Otherwise, that is not possible. Now we look at the entropy (2.111). When we have two operators separated by a tensor product $\otimes$, the log of the product becomes the sum of the logs:

$$\ln(\rho_A \otimes \rho_B) = (\ln\rho_A) \otimes 1_B + 1_A \otimes (\ln\rho_B). \tag{2.123}$$

This can be viewed more clearly by looking at the eigenvalues of $\rho_A \otimes \rho_B$, which are just of the form $p_k^A p_\ell^B$. Sometimes I'm lazy and I just write this relation as

$$\ln(\rho_A\rho_B) = \ln\rho_A + \ln\rho_B. \tag{2.124}$$

It is then implicit that ρ_A and ρ_B live on separate spaces and therefore commute.

From this it now follows that

$$\begin{aligned} S(\rho_A \otimes \rho_B) &= -\operatorname{tr}(\rho_A \rho_B \ln \rho_A) - \operatorname{tr}(\rho_A \rho_B \ln \rho_B) \\ &= -\operatorname{tr}_A(\rho_A \ln \rho_A) \operatorname{tr}_B(\rho_B) - \operatorname{tr}_B(\rho_B \ln \rho_B) \operatorname{tr}_A(\rho_A) \\ &= -\operatorname{tr}(\rho_A \ln \rho_A) - \operatorname{tr}(\rho_B \ln \rho_B). \end{aligned}$$

I know this calculation is a bit messy, but please try to convince yourself that it's ok. For instance, you can do everything with $\otimes$ and use Eq. (2.65). In any case, what we conclude is that

$$S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B). \tag{2.125}$$

Thus, the entropy is an *additive* quantity: if two systems are uncorrelated, the total entropy is simply the sum of the parts.

This is no longer true if ρ_{AB} is a correlated state. In fact, the entropy of ρ_{AB} is related to the entropy of the reduced density matrices $\rho_A = \operatorname{tr}_B \rho_{AB}$ and $\rho_B = \operatorname{tr}_A \rho_{AB}$ by the **subadditivity condition**

$$\boxed{S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B).} \tag{2.126}$$

where the equality holds only for a product state $\rho_{AB} = \rho_A \otimes \rho_B$. Another way to write this is as $S(\rho_{AB}) \leq S(\rho_A \otimes \rho_B)$. This has a clear interpretation: by taking the partial trace we *loose information* so that the entropy afterwards is larger.

The proof of Eq. (2.126) can be done easily using the relative entropy. We just need to convince ourselves that

$$S(\rho_{AB} || \rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}). \tag{2.127}$$

Then, because of (2.118), this quantity will always be non-negative. So let's do it: let's see that (2.127) is indeed correct.

$$\begin{aligned} S(\rho_{AB} || \rho_A \otimes \rho_B) &= = \operatorname{tr}(\rho_{AB} \ln \rho_{AB}) - \operatorname{tr}(\rho_{AB} \ln \rho_A \rho_B) \\ &= -S(\rho_{AB}) - \operatorname{tr}(\rho_{AB} \ln \rho_A) - \operatorname{tr}(\rho_{AB} \ln \rho_B). \end{aligned} \tag{2.128}$$

Now comes the key point: given any operator O we can always take the trace in steps:

$$\operatorname{tr}(O) = \operatorname{tr}_A(\operatorname{tr}_B(O)).$$

Then, to deal with $\operatorname{tr}(\rho_{AB} \ln \rho_A)$ we can first take the trace in B. This will only affect ρ_{AB} and it will turn it into ρ_A:

$$\operatorname{tr}(\rho_{AB} \ln \rho_A) = \operatorname{tr}_A \rho_A \ln \rho_A.$$

This is always true, even when ρ_{AB} is not a product. Plugging this in (2.128), we immediately see that (2.127) will hold.

Looking back now at Eqs. (2.126) and (2.127) we see that we have just found a quantity which is always non-negative and is zero exactly when the two systems are uncorrelated ($\rho_{AB} = \rho_A \otimes \rho_B$). Thus, we may use this as a quantifier of the **total degree of correlations**. We call this quantity the **mutual information**:

$$\boxed{\mathcal{I}(\rho_{AB}) := S(\rho_{AB}||\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}) \geq 0.} \tag{2.129}$$

This is one the central concepts in all of quantum information. *It represents the amount of information stored in AB which is not stored in A and B, when taken separately.* One thing I should warn, though, is that the mutual information quantifies the *total* degree of correlations, in the sense that it does not distinguish between classical and quantum contributions. A big question in the field is how to separate the mutual information in a quantum and a classical part. We will get back to that later.

Let me try to give an example of the mutual information. This is always a little bit tricky because even for two qubits, the formulas can get quite ugly (although asking Mathematica to write them down is really easy). So for the purpose of example, let us consider a state of the form:

$$\rho_{AB} = \begin{pmatrix} p^2 & 0 & 0 & 0 \\ 0 & p(1-p) & \alpha & 0 \\ 0 & \alpha & p(1-p) & 0 \\ 0 & 0 & 0 & (1-p)^2 \end{pmatrix}. \tag{2.130}$$

This has the structure of Eq. (2.79), but with ρ_A and ρ_B being equal and diagonal: $\rho_A = \rho_B = \text{diag}(p, 1-p)$. The constant α here is also not arbitrary, but is bounded by $|\alpha| < p(1-p)$, which is a condition so that the eigenvalues of ρ_{AB} are always non-negative. The mutual information is then

$$\mathcal{I}(\rho_{AB}) = p(1-p)\ln\left[\frac{p^2(1-p)^2 - \alpha^2}{p^2(1-p^2)}\right] + \alpha \ln\left[\frac{p(1-p)+\alpha}{p(1-p)-\alpha}\right]. \tag{2.131}$$

This function is plotted in Fig. 2.5. As expected, the larger the correlation α, the larger is the mutual information. The maximum value occurs when $|\alpha| = p(1-p)$ and has the value $\mathcal{I} = 2p(1-p)\ln(2)$.

Next suppose that $\rho_{AB} = |\psi\rangle\langle\psi|$ is actually a pure state. Then $S(\rho_{AB}) = 0$. Moreover, we have seen in Sec. 2.8 that the reduced density matrices of A and B can both be written in diagonal form in terms of the Schmidt coefficients, Eqs. (2.100) and (2.101). Thus, it follows that in this case

$$S(\rho_A) = S(\rho_B) \qquad \text{when } \rho_{AB} \text{ is pure.} \tag{2.132}$$

Hence, the mutual information becomes

$$\mathcal{I}(\rho_{AB}) = 2S(\rho_A) = 2S(\rho_B) \qquad \text{when } \rho_{AB} \text{ is pure.} \tag{2.133}$$

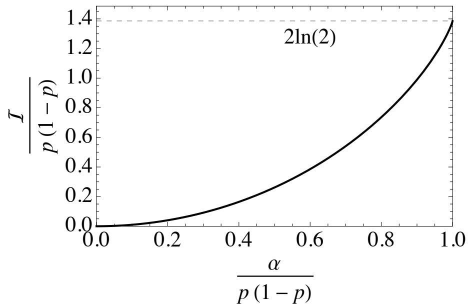

Figure 2.5: Eq. (2.131) plotted in terms of convenient quantities.

We therefore conclude that for pure states the maximum amount of information stored in non-local correlations is twice the information of each of the parts.

For the case of pure states, we saw that we could quantify the degree of entanglement by means of the purity of ρ_A or ρ_B. Another way to quantify entanglement is by means of the entropy $S(\rho_A)$ and $S(\rho_B)$. For this reason, this is sometimes referred to as the **entanglement entropy**. Eq. (2.133) then shows us that for pure states the mutual information is twice the entanglement entropy. On the other hand, if the state is not pure, than entanglement will be mixed with classical correlations. An important question is then what part of $\mathcal{I}$ is due to entanglement and what part is classical. We will get back to this later in the course.

In addition to the subadditivity inequality (2.126), the von Neumann entropy also satisfies the **strong subadditivitiy inequality**:

$$\boxed{S(\rho_{ABC}) + S(\rho_B) \leq S(\rho_{AB}) + S(\rho_{BC}).} \tag{2.134}$$

If B is a Hilbert space of dimension 1 this reduces to Eq. (2.126). The intuition behind this formula is as follows (Preskill): We can think as AB and BC as two overlapping systems, so that $S(\rho_{ABC})$ is the entropy of their union and $S(\rho_B)$ is the entropy of their intersection. Then Eq. (2.134) says this cannot exceed the sum of the entropies of the parts. Eq. (2.134) can also be stated in another way as

$$S(\rho_A) + S(\rho_B) \leq S(\rho_{AC}) + S(\rho_{BC}). \tag{2.135}$$

The strong subadditivity inequality turns out to be an essential property in quantum information tasks, such as communication protocols. The proof of Eq. (2.134), however, turns out to be quite difficult and we will not be shown here. You can find it, for instance, in Nielsen and Chuang, chapter 11.

Convexity of the entropy

Consider now a bipartite state of the form

$$\rho_{AB} = \sum_i p_i \rho_i \otimes |i\rangle\langle i|, \tag{2.136}$$

where ρ_i are valid density matrices and p_i are arbitrary probabilities. This type of state is what we call a *quantum-classical state*. It is like a mixture of classical probabilities from the point of view of B, but with (possibly) quantum density matrices from the point of view of A. That can be seen more clearly by looking at the reduced density matrices:

$$\rho_A = \operatorname{tr}_B \rho_{AB} = \sum_i p_i \rho_i, \tag{2.137}$$

$$\rho_B = \operatorname{tr}_A \rho_{AB} = \sum_i p_i |i\rangle\langle i|. \tag{2.138}$$

Each ρ_i may have quantum stuff inside them and what we are doing in ρ_A is making classical mixtures of these guys.

The entropy of ρ_B is now the **classical Shannon entropy** of the probability distribution p_i:

$$S(\rho_B) := H(p_i) = -\sum_i p_i \ln p_i. \tag{2.139}$$

The use of the letter H is not completely necessary. I just put it there to emphasize that we are talking about the entropy of a set of numbers $\{p_i\}$ and not a density matrix. Next let us compute the entropy of ρ_{AB}. Denote by $P_{i,j}$ the j-th eigenvalue of each ρ_i. Then the eigenvalues of ρ_{AB} will be $p_i P_{i,j}$. Thus

$$\begin{aligned} S(\rho_{AB}) &= -\sum_{i,j} p_i P_{i,j} \ln(p_i P_{i,j}) \qquad (2.140)\\ &= -\sum_{i,j} p_i P_{i,j} \ln p_i - \sum_{i,j} p_i P_{i,j} \ln P_{i,j} \qquad (2.141)\end{aligned}$$

In the first term we now use $\sum_j P_{i,j} = 1$, which is the normalization condition for each ρ_i. What is left is then $S(\rho_B) = S(p_i)$. In the second term, on the other hand, we note that for each i, the sum over j is just $S(\rho_i) = -\sum_j P_{i,j} \ln P_{i,j}$. Thus we finally get

$$S(\rho_{AB}) = H(p_i) + \sum_i p_i S(\rho_i). \tag{2.142}$$

We therefore see that in this case the total entropy has two clear contributions. The first is the disorder introduced by the probability distribution p_i and the second is the local disorder contained in each ρ_i.

Using now the subadditivity formula (2.126) together with the fact that $S(\rho_B) = H(p_i)$, we also see that

$$S\Big(\sum_i p_i \rho_i\Big) \geq \sum_i p_i S(\rho_i), \tag{2.143}$$

where I used the form of ρ_A in Eq. (2.137). The entropy is therefore a concave function of its arguments. The logic behind this formula is that $\sum_i p_i \rho_i$ contains not only ignorance about the ρ_i but also about the p_i. So its total entropy must be higher than the sum of the parts.

Eq. (2.143) provides a lower bound to the entropy of mixtures. It turns out that it is also possible to find an upper bound, so that instead of (2.143) we can write the more general result

$$\boxed{H(p_i) + \sum_i p_i S(\rho_i) \geq S\Big(\sum_i p_i \rho_i\Big) \geq \sum_i p_i S(\rho_i).} \tag{2.144}$$

The proof is given in chapter 11 of Nielsen and Chuang. The cool thing about this new bound is that it allows for an interpretation of entropy in terms of the **ambiguity of mixtures**. Remember that we discussed how the same density matrix ρ could be constructed from an infinite number of combinations of pure states

$$\rho = \sum_i q_i |\psi_i\rangle\langle\psi_i|. \tag{2.145}$$

In this formula there can be an arbitrary number of terms and the $|\psi_i\rangle$ do not need to be orthogonal or anything. All we require is that the q_i behave like probabilities. Hence, due to this flexibility, there is an infinite number of choices for $\{q_i, |\psi_i\rangle\}$ which give the same ρ. But note how this falls precisely into the category of Eq. (2.144), with $\rho_i = |\psi_i\rangle\langle\psi_i|$ and $p_i \to q_i$. Since $S(\rho_i) = 0$ for a pure state, we then find that

$$\boxed{S(\rho) \leq H(q_i).} \tag{2.146}$$

That is, *the von Neumann entropy is the entropy that minimizes the classical distribution of the probabilities* $H(q_i)$. In terms of the eigenvalues p_k of ρ, we have $S(\rho) = -\sum_k p_k \ln p_k$ so that the equality in Eq. (2.146) is obtained when the mixture is precisely that of the eigenvalues/eigenvectors of ρ.

Rényi entropy

A generalization of the von Neumann entropy that is also popular in quantum information are the so-called Rényi entropies,[4] defined as

$$\boxed{S_\alpha(\rho) = \frac{1}{1-\alpha} \ln \operatorname{tr} \rho^\alpha.} \tag{2.147}$$

where α is a tunable parameter in the range $[0, \infty)$. This therefore corresponds to a continuous family of entropies. The Rényi entropies appear here and there in quantum information. But a word of caution: S_α *does not* satisfy sub-additivity (2.126) in general.

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[4]

I particularly like $\alpha = 2$, which is simply minus the logarithm of the purity:

$$S_2(\rho) = -\ln \operatorname{tr} \rho^2. \tag{2.148}$$

Another special case is $\alpha = 1$, where we recover the von Neumann entropy. Note how this is tricky because of the denominator in Eq. (2.147). The safest way to do this is to expand x^α in a Taylor series in α around $\alpha = 1$. We have the following result from introductory calculus:

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} x^\alpha = x^\alpha \ln(x).$$

Thus, expanding x^α around $\alpha = 1$ we get:

$$x^\alpha \simeq x^1 + x^1 \ln(x)(\alpha - 1).$$

Now we substitute this into Eq. (2.147) to get

$$\begin{aligned} S_\alpha(\rho) &\simeq \frac{1}{1-\alpha} \ln \Big\{ \operatorname{tr} \rho + (\alpha - 1) \operatorname{tr}(\rho \ln \rho) \Big\} \\ &= \frac{1}{1-\alpha} \ln \Big\{ 1 + (\alpha - 1) \operatorname{tr}(\rho \ln \rho) \Big\}. \end{aligned}$$

Since we want the limit $\alpha \to 1$, we may expand the logarithm above using the formula $\ln(1 + x) \simeq x$. The terms $\alpha - 1$ will then cancel out, leaving us with

$$\lim_{\alpha \to 1} S_\alpha(\rho) = -\operatorname{tr}(\rho \ln \rho), \tag{2.149}$$

which is the von Neumann entropy. The Rényi entropy therefore forms a family of entropies which contains the von Neumann entropy as a particular case. Other particular cases of importance are $\alpha = 0$, which is called the *max entropy*, and $\alpha = \infty$ which is called the *min entropy*. Using the definition (2.147) we see that

$$S_0(\rho) = \ln(d), \tag{2.150}$$

$$S_\infty(\rho) = -\ln \max_k p_k. \tag{2.151}$$

As an example, consider a qubit with eigenvalues p and $1 - p$. Then $\operatorname{tr}(\rho^\alpha) = p^\alpha + (1 - p)^\alpha$ so that Eq. (2.147) becomes

$$S_\alpha(\rho) = \frac{1}{1-\alpha} \ln \Big\{ p^\alpha + (1-p)^\alpha \Big\}. \tag{2.152}$$

This result is plotted in Fig. 2.6 for several values of α. As can be seen, except for $\alpha \to 0$, which is kind of silly, the behavior of all curves is qualitatively similar.

Integral representations of $\ln(\rho)$

When dealing with more advanced calculations, sometimes dealing with $\ln(\rho)$ in terms of eigenvalues can be hard. An alternative is to write the logarithm of operators

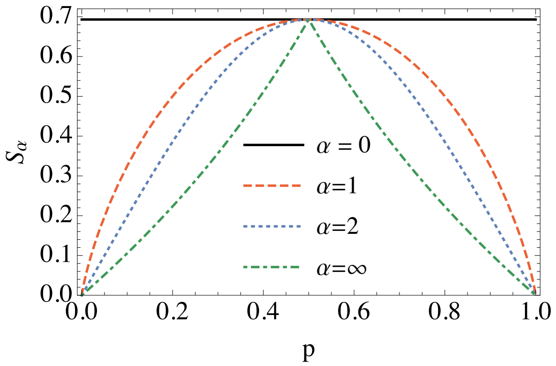

Figure 2.6: The Rényi entropies for a 2-state system, computed using Eq. (2.152) for different values of α.

as an integral representation. I know two of them. If you know more, tell me and I can add them here. A simple one is

$$\ln(\rho) = (\rho - 1)\int_0^1 \frac{\mathrm{d}x}{1 + x(\rho - 1)}. \tag{2.153}$$

Here whenever ρ appears in the denominator, what is meant is the matrix inverse. Another formula is[5]

$$\ln(\rho) = (\rho - 1)\int_0^\infty \frac{\mathrm{d}x}{(1 + x)(\rho + x)} \tag{2.154}$$

$$= \int_0^\infty \mathrm{d}x\left(\frac{1}{1+x} - \frac{1}{\rho + x}\right). \tag{2.155}$$

This last formula in particular can now be used as the starting point for a series expansion, based on the matrix identity

$$\frac{1}{A+B} = \frac{1}{A} - \frac{1}{A}B\frac{1}{A+B}. \tag{2.156}$$

For instance, after one iteration of Eq. (2.155) we get

$$\ln(\rho) = \int_0^\infty \mathrm{d}x\left(\frac{1}{1+x} - \frac{1}{x} + \frac{\rho}{x^2} - \frac{\rho^2}{x^2}\frac{1}{\rho + x}\right). \tag{2.157}$$

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[5] See M. Suzuki, *Prog. Theo. Phys*, **100**, 475 (1998)

2.10 Generalized measurements and POVMs

So far our discussion of measurements has been rather shallow. What I have done so far is simply postulate the idea of a projective measurement, without discussing the physics behind it. I know that this may be a bit frustrating, but measurements in quantum mechanics are indeed a hard subject and experience shows that it is better to postulate things first, without much discussion, and then later on study models which help justify these postulates.

Starting from next chapter, we will begin to work out several models of measurements, so I promise things will get better. What I would like to do now is discuss measurements from a mathematical point of view and try to answer the question "what is the most general structure a measurement may have?" We will further divide this in two questions. First, what is a measurement? Well, it is *an assignment from states to probabilities*. That is, given an arbitrary state ρ, we should ask what is the most general way of assigning probabilities to it? This will introduce us to the idea of **POVMs** (Positive Operator-Valued Measures). The next question is, what should be the state of the system after the measurement? That will lead us to the idea of **Kraus operators**.

Ok. So let's start. We have a system prepared in a state ρ. Then we use as our starting point the postulate that a measurement is a probabilistic event for which different outcomes can be obtained with different probabilities. Let us label the outcomes as $i = 1, 2, 3, \ldots$. At this point the number of possible outcomes has no relation in principle to the dimension of the Hilbert space or anything of that sort. All we want to do is find an operation which, given ρ, spits out a set of probabilities $\{p_i\}$. Well, from density matrices, information is always obtained by taking the expectation value of an operator, so this association must have the form

$$\boxed{p_i = \text{tr}(E_i \rho),} \tag{2.158}$$

where E_i are certain operators, the properties of which are determined once we impose that the p_i should behave like probabilities. First, the p_i must be non-negative for any ρ, which can only occur if the operators E_i are positive semi-definite. Second, $\sum_i p_i = 1$ so that $\sum_i E_i = 1$. We therefore conclude that if the rule to associate probabilities with quantum states has the structure of Eq. (2.158), the set of operators $\{E_i\}$ must satisfy

$$\boxed{E_i \geq 0, \qquad \sum_i E_i = 1.} \tag{2.159}$$

A set of operators satisfying this is called a **POVM**: Positive-Operator Valued Measure, a name which comes from probability theory. The set of POVMs also contain projective measurements as a special case: the projection operators P_i are positive semi-definite and add up to the identity.

POVMs for a qubit

Here is an example of a POVM we can construct by hand for a qubit:

$$\begin{aligned} E_1 &= \lambda|0\rangle\langle 0| \\ E_2 &= (1-\lambda)|0\rangle\langle 0| + |1\rangle\langle 1|. \end{aligned} \tag{2.160}$$

These guys form a POVM provided $\lambda \in [0,1]$: they are positive semi-definite and add up to the identity. However, this is in general not a projective measurement, unless $\lambda = 1$. The logic here is that outcome E_1 represents the system being found in $|0\rangle$, but outcome E_2 means it can be in either $|0\rangle$ or $|1\rangle$ with different probabilities. For a general qubit density matrix like (2.18), we get

$$p_1 = \text{tr}(E_1\rho) = \lambda p, \tag{2.161}$$

$$p_2 = \text{tr}(E_2\rho) = 1 - \lambda p. \tag{2.162}$$

So even if $p = 1$ (the system is for sure in $|0\rangle$), then we can still obtain the outcome E_2 with a certain probability. From such a silly example, you are probably wondering "can this kind of thing be implemented in the lab?" The answer is yes and the way to do it will turn out to be much simpler than you can imagine. So hang in there!

What is cool about POVMs is that we can choose measurement schemes with more than two outcomes, even though our qubit space is two-dimensional. For instance, here is an example of a POVM with 3 outcomes (taken from Nielsen and Chuang):

$$E_1 = q|0\rangle\langle 0| \tag{2.163}$$

$$E_2 = q|+\rangle\langle +| \tag{2.164}$$

$$E_3 = 1 - E_1 - E_2. \tag{2.165}$$

To illustrate what you can do with this, suppose you are walking down the street and someone gives you a state, telling you that *for sure* this state is either $|1\rangle$ or $|-\rangle$, but he/she doesn't know which one. Then if you measure the system and happen to find outcome E_1, you know for certain that the state you were given could not be $|1\rangle$, since $\langle 0|1\rangle = 0$. Hence, it must have been $|-\rangle$. A similar reasoning holds if you happen to measure E_2, since $|+\rangle$ and $|-\rangle$ are orthogonal. But if you happen to measure E_3, then you don't really know anything. So this is a POVM where the observer never makes a mistake about what it is measuring, but that comes at the cost that sometimes he/she simply doesn't learn anything.

Generalized measurements

We now come to the much harder question of what is the state of the system after the measurement. Unlike projective measurements, for which the state always collapses, for general measurements many other things can happen. So we should instead ask what is the most general mathematical structure that a state can have after a measurement. To do that, I will postulate something, which we will only prove on later chapters, but which I will try to give a reasonable justification below. You can take this next postulate as the ultimate measurement postulate: that is, it is a structure worth remembering because every measurement can be cast in this form. The postulate is as follows.

Measurement postulate: any quantum measurement is fully specified by a set of operators $\{M_i\}$, called **Kraus operators**, satisfying

$$\boxed{\sum_i M_i^\dagger M_i = 1.} \tag{2.166}$$

The probability of obtaining measurement outcome i is

$$\boxed{p_i = \text{tr}(M_i \rho M_i^\dagger),} \tag{2.167}$$

and, if the outcome of the measurement is i, then the state after the measurement will be

$$\boxed{\rho \to \frac{M_i \rho M_i^\dagger}{p_i}.} \tag{2.168}$$

Ok. Now breath! Let us analyze this in detail. First, for projective measurements $M_i = P_i$. Since $P_i^\dagger = P_i$ and $P_i^2 = P_i$ we then get $P_i^\dagger P_i = P_i$ so that Eqs. (2.166)-(2.168) reduce to

$$\sum_i P_i = 1, \qquad p_i = \text{tr}(P_i \rho), \qquad \rho \to \frac{P_i \rho P_i}{p_i}, \tag{2.169}$$

which are the usual projective measurement/collapse scenario. It also does not matter if the state is mixed or pure. In particular, for the latter $\rho = |\psi\rangle\langle\psi|$ so the state after the measurement becomes (up to a constant) $P_i|\psi\rangle$. That is, we have projected onto the subspace where we found the system in.

Next, let us analyze the connection with POVMs. Define

$$E_i = M_i^\dagger M_i. \tag{2.170}$$

Then Eqs. (2.166) and (2.167) become precisely Eqs. (2.158) and (2.159). You may therefore be wondering why define POVMs separately from these generalized measurements. The reason is actually simple: different sets of measurement operators $\{M_i\}$ can give rise to the same POVM $\{E_i\}$. Hence, if one is only interested in obtaining the probabilities of outcomes, then it doesn't matter which set $\{M_i\}$ is used, all that matters is the POVM $\{E_i\}$. However, states having the same POVM can lead to completely different post-measurement states.

Examples for a qubit

Consider the following measurement operators

$$M_1 = \begin{pmatrix} \sqrt{\lambda} & 0 \\ 0 & 0 \end{pmatrix}, \qquad M_2 = \begin{pmatrix} \sqrt{1-\lambda} & 0 \\ 0 & 1 \end{pmatrix}. \tag{2.171}$$

These operators satisfy (2.166). Moreover, $E_1 = M_1^\dagger M_1$ and $E_2 = M_2^\dagger M_2$ give exactly the same POVM as in Eq. (2.160). Suppose now that the system is initially in the pure state $|+\rangle = \frac{1}{\sqrt{2}}(1,1)$. Then the outcome probabilities and the states after the measurements will be

$$\begin{aligned} p_1 &= \frac{\lambda}{2} & \qquad |+\rangle &\to |0\rangle \\ p_2 &= 1 - \frac{\lambda}{2} & \qquad |+\rangle &\to \frac{\sqrt{1-\lambda}|0\rangle + |1\rangle}{\sqrt{2-\lambda}} \end{aligned} \tag{2.172}$$

Thus, unless $\lambda = 1$, the state after the measurement will not be a perfect collapse.

Next consider the measurement operators defined by

$$M_1' = \begin{pmatrix} 0 & 0 \\ \sqrt{\lambda} & 0 \end{pmatrix}, \qquad M_2' = M_2 = \begin{pmatrix} \sqrt{1-\lambda} & 0 \\ 0 & 1 \end{pmatrix}. \tag{2.173}$$

Compared to Eq. (2.171), we have only changed M_1. But note that $M_1'^\dagger M_1' = M_1^\dagger M_1$. Hence this gives the same POVM (2.160) as the set $\{M_i\}$. However, the final state after the measurement is completely different: if outcome 1 is obtained, then instead of (2.172), the state will now collapse to

$$|+\rangle \to |1\rangle. \tag{2.174}$$

To give a physical interpretation of what is going on here, consider an atom and suppose that $|0\rangle = |e\rangle$ is the excited state and $|1\rangle = |g\rangle$ is the ground-state. The system is then initially in the state $|+\rangle$, which is a superposition of the two. But if you measure and find the atom in the excited state, then that means it must have emitted a photon and therefore decayed to the ground-state. The quantity λ in Eq. (2.173) therefore represents the probability of emitting a photon *during the time-span* of the observation. If it emits, then the state is $|1\rangle = |g\rangle$ because it must have decayed to the ground-state. If it doesn't emit, then it continues in a superposition, but this superposition is now updated to $\sim \sqrt{1-\lambda}|0\rangle + |1\rangle$. This is really interesting because it highlights the fact that *if nothing happens, we still update our information about the atom*. In particular, if λ is very large, for instance $\lambda = 0.99$, then the state after the measurement will be very close to $|1\rangle$. This means that if the atom did not emit, there is a huge chance that it was actually in the ground-state $|1\rangle$ to begin with.

Origin of generalized measurements

Now I want to show you one mechanism through which generalized measurements appear very naturally: *a generalized measurement is implemented by making a projective measurement on an ancilla that is entangled with the system.* That is, instead of measuring A, we first entangle it with an auxiliary system B (which we call *ancilla*) and then measure B using projective measurements. Then, from the point of view of A, this will be translated into a generalized measurement.

To illustrate the idea, suppose we have a system in a state $|\psi\rangle_A$ and an ancilla prepared in a state $|0\rangle_B$. Then, to entangle the two, we first evolve them with a joint unitary U_{AB}. The joint state of AB, which was initially product, will then evolve to a generally entangled state

$$|\phi\rangle = U_{AB}\Big[|\psi\rangle_A \otimes |0\rangle_B\Big]. \tag{2.175}$$

We now perform a projective measurement on B, characterized by a set of projection operators $P_i^B = 1_A \otimes |i\rangle_B\langle i|$. Then outcome i is obtained with probability

$$p_i = \langle\phi|P_i^B|\phi\rangle, \tag{2.176}$$

and the state after the measurement, if this outcome was obtained, collapses to $P_i^B|\phi\rangle$.

Now let's see how all this looks from the perspective of A. The next calculations are a bit abstract, so I recommend some care. Have a first read all the way to the end and then come back and try to understand it in more detail. The point is that here the $\otimes$ can be a curse. It is better to get rid of it and write, for instance, $P_i^B = |i\rangle_B\langle i|$ where the fact that this is an operator acting only on Hilbert space B is implicit in the subscript. Similarly we write $|\psi\rangle_A \otimes |0\rangle_B = |\psi\rangle_A|0\rangle_B$. With this we then get, for instance,

$$p_i = {}_A\langle\psi|\, {}_B\langle 0|U_{AB}^\dagger|i\rangle_B\langle i|U_{AB}|\psi\rangle_A|0\rangle_B. \tag{2.177}$$

This quantity is a scalar, so we are contracting over everything. But what we could do is leave the contraction $\langle\psi|(\ldots)|\psi\rangle$ for last. Then the $(\ldots)$ will be an operator acting only on the Hilbert space of A. If we define the operators

$$\boxed{M_i = {}_B\langle i|U_{AB}|0\rangle_B = \Big(1 \otimes \langle i|\Big)U_{AB}\Big(1 \otimes |0\rangle\Big).} \tag{2.178}$$

acting only Hilbert space A, then we get

$$p_i = {}_A\langle\psi|M_i^\dagger M_i|\psi\rangle_A, \tag{2.179}$$

which is precisely Eq. (2.167) for the probabilities of a generalized measurement. Moreover, we can also check that the $\{M_i\}$ satisfy the normalization condition (2.166):

$$\begin{aligned}\sum_i M_i^\dagger M_i &= \sum_i {}_B\langle 0|U_{AB}^\dagger|i\rangle_B\langle i|U_{AB}|0\rangle_B \\ &= {}_B\langle 0|U_{AB}^\dagger U_{AB}|0\rangle_B \\ &= {}_B\langle 0|0\rangle_B \\ &= 1_A,\end{aligned}$$

so they indeed form a set of measurement operators.

We now ask what is the reduced density matrix ρ_A^i of system A, given that the outcome of the measurement on B was i. Well, this is simply obtained by taking the partial trace over B of the new state $P_i^B|\phi\rangle$:

$$\begin{aligned}\rho_A^i &= \mathrm{tr}_B\left\{P_i^B|\phi\rangle\langle\phi|P_i^B\right\}\\ &= {}_B\langle i|\phi\rangle\langle\phi|i\rangle_B\\ &= {}_B\langle i|U_{AB}|\psi\rangle_A|0\rangle_B\,{}_A\langle\psi|\,{}_B\langle 0|U_{AB}^\dagger|i\rangle_B\end{aligned}$$

Using Eq. (2.178) this may then be written as

$$\rho_A^i = M_i\Big(|\psi\rangle\langle\psi|\Big)M_i^\dagger, \tag{2.180}$$

which is exactly the post-measurement state (2.168). Thus, as we set out to prove, if we do a projective measurement on a ancila B which is entangled with A, from the point of view of A we are doing a generalized measurement.

The above calculations are rather abstract, I know. It is a good exercise to do them using $\otimes$ to compare. That can be done decomposition $U_{AB} = \sum_\alpha A_\alpha \otimes B_\alpha$. Eq. (2.177), for instance, then becomes:

$$p_i = \sum_{\alpha,\beta}\Big(\langle\psi|\otimes\langle 0|\Big)\Big(A_\alpha^\dagger \otimes B_\alpha^\dagger\Big)\Big(1\otimes|0\rangle\langle 0|\Big)\Big(A_\beta\otimes B_\beta\Big)\Big(|\psi\rangle\otimes|0\rangle\Big).$$

I will leave for you as an exercise to check that this indeed gives (2.179). Also, try to check that the same idea leads to Eq. (2.180).

Chapter 3

Continuous variables

Continuous variables is a fancy name we give to harmonic oscillators. So far we have talked about systems with a finite number of states, so that everything is discrete. Now we will talk about harmonic oscillators, which have an infinite number of levels. Of course, these levels are also discrete. However, it turns out that many things can be described in terms of continuous variables, such as coherent states and the quantum phase space representation.

Continuous variables systems occur naturally in many platforms. The most important example is quantum optics, where, it turns out, the quantum properties of the electromagnetic field can be represented in terms of harmonic oscillators. Other continuous variable platforms include trapped ions, nano- or micro-mechanical oscillators and Bose-Einstein condensates.

This chapter provides a first look into continuous variables. After this, we will start to work with both discrete and continuous variable systems, side by side. More advanced properties will be discussed later, or can be found in the excellent book by Alessio Serafini entitled *"Quantum Continuous Variables"*.

3.1 Creation and annihilation operators

The starting point of continuous variable systems is an operator a called the *annihilation operator* and its Hermitian conjugate $a^\dagger$, called the *creation operator*. They are defined so as to satisfy the following algebra:

$$\boxed{[a, a^\dagger] = 1.} \tag{3.1}$$

All properties of these operators and the Hilbert space they represent follow from this simple commutation relation, as we will see below. Another set of operators which can be used as the starting point of the discussion are the *position and momentum operators*

q and p. They satisfy

$$\boxed{[q, p] = i.} \tag{3.2}$$

In quantum optics, they no longer represent position and momentum, but are related to the electric and magnetic fields. In this case they are usually called *quadrature operators*. We define q and p to be dimensionless. Then they are related to the creation and annihilation operators according to

$$\begin{aligned} q &= \frac{1}{\sqrt{2}}(a^\dagger + a) & & & a &= \frac{1}{\sqrt{2}}(q + ip) \\ & & \Longleftrightarrow & & & \\ p &= \frac{i}{\sqrt{2}}(a^\dagger - a) & & & a^\dagger &= \frac{1}{\sqrt{2}}(q - ip)\,. \end{aligned} \tag{3.3}$$

From this it can be clearly seen that q and p are Hermitian operators, even though a is not. Also, please take a second to verify that with this relation Eq. (3.1) indeed implies (3.2) and vice-versa.

Mechanical oscillators

The operators a, $a^\dagger$, q and p appear in two main contexts: mechanical oscillators and second quantization. The latter will be discussed below. A mechanical oscillator is specified by the Hamiltonian

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 Q^2, \tag{3.4}$$

where m is the mass and ω is the frequency. Moreover Q and P are the position and momentum operators satisfying

$$[Q, P] = i\hbar. \tag{3.5}$$

Now define the dimensionless operators

$$q = \sqrt{\frac{m\omega}{\hbar}}Q, \qquad p = \frac{P}{\sqrt{m\hbar\omega}}. \tag{3.6}$$

Then Eq. (3.5) implies that q and p will satisfy (3.2). In terms of q and p, the Hamiltonian (3.4) becomes

$$H = \frac{\hbar\omega}{2}(p^2 + q^2), \tag{3.7}$$

which, you have to admit, is way more elegant than (3.4). Using now Eq. (3.3) we finally write the Hamiltonian as

$$H = \hbar\omega(a^\dagger a + 1/2). \tag{3.8}$$

Eqs. (3.7) and (3.8) show very well why $\hbar$ is not important: it simply redefines the energy scale. If we set $\hbar = 1$, as we shall henceforth do, we are simply measuring energy in units of frequency.

In the days of Schrödinger, harmonic oscillators were usually used either as toy models or as an effective description of some other phenomena such as, for instance, the vibration of molecules. In the last two decades this has change and we are now able to observe quantum effects in actual mechanical mesoscopic- (nano- or micro-) oscillators. This is usually done by engineering thin suspended membranes, which can then undergo mechanical vibrations. This field is usually known as **optomechanics** since most investigations involve the contact of the membranes with radiation. I find it absolutely fascinating that in our day and age we can observe quantum effects as awesome as entanglement and coherence in these mechanical objects. I love the century we live in!

An algebraic problem

In Eq. (3.8) we see the appearance of the Hermitian operator $a^\dagger a$, called the **number operator**. To find the eigenstuff of H we therefore only need to know the eigenstuff of $a^\dagger a$. We have therefore arrived at a very clean mathematical problem: *given a non-Hermitian operator* a*, satisfying* $[a, a^\dagger] = 1$*, find the eigenvalues and eigenvectors of* $a^\dagger a$. This is a really important problem that appears often in all areas of quantum physics: given an algebra, find the eigenstuff. Maybe you have seen this before, but I will nonetheless do it again, because I think this is one of those things that everyone should know.

Here we go. Since $a^\dagger a$ is Hermitian, its eigenvalues must be real and its eigenvectors can be chosen to form an orthonormal basis. Let us write them as

$$\boxed{a^\dagger a|n\rangle = n|n\rangle.} \tag{3.9}$$

Our goal is to find the allowed n and the corresponding $|n\rangle$. The first thing we notice is that $a^\dagger a$ must be positive semi-definite operator, so n cannot be negative:

$$n = \langle n|a^\dagger a|n\rangle \geq 0.$$

Next we use Eq. (3.1) to show that

$$\boxed{[a^\dagger a, a] = -a, \qquad\qquad [a^\dagger a, a^\dagger] = a^\dagger.} \tag{3.10}$$

This type of structure is a signature of a *ladder* like spectrum (that is, when the eigenvalues are equally spaced). To see that, we use these commutation relations to compute:

$$(a^\dagger a)a|n\rangle = [a(a^\dagger a) - a]|n\rangle = a(a^\dagger a - 1)|n\rangle = (n-1)a|n\rangle.$$

Hence, we conclude that if $|n\rangle$ is an eigenvector with eigenvalue n, then $a|n\rangle$ is also an eigenvector, but with eigenvalue $(n-1)$ [This is the key argument. Make sure you understand what this sentence means.]. However, I wouldn't call this $|n-1\rangle$ just yet because $a|n\rangle$ is not normalized. Thus we need to write

$$|n-1\rangle = \gamma a|n\rangle,$$

where γ is a normalization constant. To find it we simply write

$$1 = \langle n-1|n-1\rangle = |\gamma|^2 \langle n|a^\dagger a|n\rangle = |\gamma|^2 n.$$

Thus $|\gamma|^2| = 1/n$. The actual sign of γ is arbitrary so we choose it for simplicity as being real and positive. We then get

$$|n-1\rangle = \frac{a}{\sqrt{n}}|n\rangle.$$

From this analysis we conclude that a reduces the eigenvalues by unity:

$$a|n\rangle = \sqrt{n}|n-1\rangle.$$

We can do a similar analysis with $a^\dagger$. We again use Eq. (3.10) to compute

$$(a^\dagger a) a^\dagger |n\rangle = (n+1) a^\dagger |n\rangle.$$

Thus $a^\dagger$ raises the eigenvalue by unity. The normalization factor is found by a similar procedure: we write $|n+1\rangle = \beta a^\dagger |n\rangle$, for some constant β, and then compute

$$1 = \langle n+1|n+1\rangle = |\beta|^2 \langle n|a a^\dagger|n\rangle = |\beta|^2 \langle n|(1 + a^\dagger a)|n\rangle = |\beta|^2 (n+1).$$

Thus

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.$$

These results are important, so let me summarize them in a boxed equation:

$$\boxed{a|n\rangle = \sqrt{n}|n-1\rangle, \qquad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle}. \tag{3.11}$$

From this formula we can see why the operators a and $a^\dagger$ also receive the name *lowering and raising operators*.

Now comes the trickiest (and most beautiful) argument. We have seen that if n is an eigenvalue, then $n \pm 1$, $n \pm 2$, etc., will all be eigenvalues. But this doesn't mean that n itself should be an integer. Maybe we find one eigenvalue which is 42.42 so that the eigenvalues are 41.42, 43.42 and so on. Of course, you know that is not true and n must be integer. To show that, we proceed as follows. Suppose we start with some eigenstate $|n\rangle$ and keep on applying a a bunch of times. At each application we will lower the eigenvalue by one tick:

$$a^\ell |n\rangle = \sqrt{n(n-1)\ldots(n-\ell+1)}|n-\ell\rangle.$$

But this crazy party cannot continue forever because, as we have just discussed, the eigenvalues of $a^\dagger a$ cannot be negative. They can, at most, be zero. The only way for this to happen is if there exists a certain integer ℓ for which $a^\ell|n\rangle \neq 0$ but $a^{\ell+1}|n\rangle = 0$. And this can only happen if $\ell = n$ because, then

$$a^{\ell+1}|n\rangle = \sqrt{n(n-1)\ldots(n-\ell+1)(n-\ell)}|n-\ell-1\rangle = 0,$$

and the term $n - \ell$ will vanish. Since ℓ is an integer, we therefore conclude that n must also be an integer. Thus, we finally conclude that

$$\text{eigs}(a^\dagger a) = n \in \{0, 1, 2, 3, \ldots\}. \tag{3.12}$$

It is for this reason that $a^\dagger a$ is called the number operator: we usually say $a^\dagger a$ counts the number of quanta in a given state: given a state $|n\rangle$, you first apply a to annihilate one quant and then $a^\dagger$ to create it back again. The proportionality factor is the eigenvalue n. Curiously, this analysis seem to imply that if you want to count how many people there are in a room, you first need to annihilate one person and then create a fresh new human. Quantum mechanics is indeed strange.

This analysis also serves to define the state with $n = 0$, which we call the **vacuum**, $|0\rangle$. It is defined by

$$\boxed{a|0\rangle = 0.} \tag{3.13}$$

We can build all states starting from the vacuum and applying $a^\dagger$ successively:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle. \tag{3.14}$$

Using this and the algebra of a and $a^\dagger$ it then follows that the states $|n\rangle$ form an orthonormal basis, as expected:

$$\langle n|m\rangle = \delta_{n,m}.$$

The states $|n\rangle$ are called **Fock states**, although this nomenclature is more correctly employed in the case of multiple modes, as we will now discuss.

Multiple modes and second quantization

It is straightforward to generalize the idea of creation and annihilation operators to composite systems. We simply define a set of annihilation operators a_i, where $i = 1, 2, \ldots, N$. It is customary to use the word **mode** to label each i. Thus we say things like "mode a_2". These operators are defined to satisfy

$$[a_i, a_j^\dagger] = \delta_{i,j}, \qquad [a_i, a_j] = 0. \tag{3.15}$$

That is, a_i with $a_i^\dagger$ behaves just like before, whereas a_i with $a_j^\dagger$ commute if $j \neq i$. Moreover annihilation operators always commute among themselves. Taking the adjoint of $[a_i, a_j] = 0$ we see that the same will be true for the creation operators $[a_i^\dagger, a_j^\dagger] = 0$. Using the same transformation as in Eq. (3.3), but with indices everywhere, we can also define quadrature operators q_i and p_i, which will then satisfy

$$[q_i, p_j] = i\delta_{i,j}, \qquad [q_i, q_j] = [p_i, p_j] = 0. \tag{3.16}$$

Multi-mode systems can appear in mechanical contexts. For instance, consider two mechanical oscillators coupled by springs, as in Fig. 3.1. Each oscillator has a natural

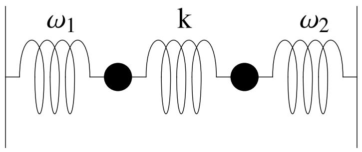

Figure 3.1: Two harmonic oscillators coupled by a harmonic spring.

frequency ω_1 and ω_2 and they are coupled by a spring constant k. Assuming unit mass, the Hamiltonian will then be

$$H = \left(p_1^2 + \frac{\omega_1^2}{2}q_1^2\right) + \left(p_2^2 + \frac{\omega_2^2}{2}q_2^2\right) + \frac{k}{2}(q_1 - q_2)^2. \tag{3.17}$$

If we want we can also transform this into a_i and $a_i^\dagger$, or we can extend it to multiple oscillators forming a chain. In fact, these "harmonic chains" are a widely studied topic in the literature because they can always be solved analytically and they are the starting point for a series of interesting quantum effects. We will have the opportunity to practice with some of these solutions later on.

But by far the most important use of multi-mode systems is in **second quantization**. Since operators pertaining to different modes commute, the Hilbert space of a multi-mode system will be described by a basis

$$|\boldsymbol{n}\rangle = |n_1, n_2, \ldots, n_N\rangle, \qquad n_i = 0, 1, 2, \ldots. \tag{3.18}$$

These are called **Fock states** and are the eigenstates of the number operators $a_i^\dagger a_i$:

$$a_i^\dagger a_i|\boldsymbol{n}\rangle = n_i|\boldsymbol{n}\rangle. \tag{3.19}$$

Thus, $a_i^\dagger a_i$ counts the number of quanta in mode i.

Second quantization is essentially a change of perspective from "quanta" to "particles". After all, what the hell is a quanta anyway? In second quantization we say $a_i^\dagger a_i$ is the operator counting the number of *particles* in mode i. Then $a_i^\dagger$ is the operator which creates a particle in mode i, whereas $a_i^\dagger$ annihilates. You may also be wondering what is a "mode" in this case. Well, there is actually an infinite number of choices. We could take for instance $i = x$, the position in space. Then $a_x^\dagger$ is the operator which creates a particle at position x. In quantum field theory we call it $\psi^\dagger(x)$ instead. But it's the same thing.

According to Eq. (3.19) each mode can have an arbitrary number n of particles. We then call a_i a **bosonic mode**. So whenever someone says "consider a set of bosonic modes" they mean a set of operators a_i satisfying (3.15). This is to be contrasted with Fermionic systems, for which the only allowed Fock states are $n = 0$ and $n = 1$ (due to the Pauli exclusion principle). We will not discuss much of fermionic systems in this course, but the idea is somewhat similar. We also define creation and annihilation operators, except that now they satisfy a different algebra:

$$\{c_i, c_j^\dagger\} = \delta_{i,j}, \qquad \{c_i, c_j\} = 0, \tag{3.20}$$

where $\{A, B\} = AB + BA$ is the anti-commutator. If we repeat the diagonalization procedure of the last section for this kind of algebra we will find a similar "Fock structure" but with the only allowed eigenvalues being $n_i = 0$ and $n_i = 1$.

The most important bosonic system is the electromagnetic field. The excitations are then the photons and the modes are usually chosen to be the momentum and polarization. Hence, we usually write an annihilation operator as $a_{\boldsymbol{k},\lambda}$ where $\boldsymbol{k} = (k_x, k_y, k_z)$ is the momentum and $\lambda = \pm 1$ is the polarization. Moreover, the Hamiltonian of the electromagnetic field is written as

$$H = \sum_{\boldsymbol{k},\lambda} \omega_{\boldsymbol{k}} a^{\dagger}_{\boldsymbol{k},\lambda} a_{\boldsymbol{k},\lambda}, \tag{3.21}$$

where $\omega_{\boldsymbol{k}}$ is the frequency of each mode and is given by[1] $\omega_{\boldsymbol{k}} = c|\boldsymbol{k}|$ where c is the speed of light.

You have noticed that my discussion of second quantization was rather shallow. I apologize for that. But I have to do it like this, otherwise we would stray too far. Second quantization is covered in many books on condensed matter, quantum many-body and quantum field theory. A book which I really like is Feynman's *Statistical mechanics: a set of lectures*".

3.2 Some important Hamiltonians

In this section we briefly discuss some important Hamiltonians that appear often in controlled quantum experiments.

Optical cavities

Many controlled experiments take place inside optical cavities, like the one represented in my amazing drawing in Fig. 3.2 (it took me 30 minutes to draw it!). The cavity is made up of highly reflective mirrors allowing the photons to survive for some time, forming standing wave patterns. Unlike in free space, where all radiation modes can exist equally, the confinement inside the cavity favors those radiation modes whose frequencies are close to the *cavity frequency* ω_c, which is related to the geometry of the cavity. It is therefore common to consider only one radiation mode, with operator a and frequency ω_c.

The photons always have a finite lifetime so more photons need to be injected all the time. This is usually done by making one of the mirrors semi-transparent and pumping it with a laser from the outside, with frequency ω_p. Of course, since photons can come in, they can also leak out. This leakage is an intrinsically irreversible process and can only be described using the theory of open quantum systems, which we will get to in the next chapter. Hence, we will omit the process of photon losses for now. The Hamiltonian describing a single mode pumped externally by a laser then has the form

$$H = \omega_c a^{\dagger} a + \epsilon a^{\dagger} e^{-i\omega_p t} + \epsilon^* a e^{i\omega_p t}, \tag{3.22}$$

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[1] If we define $\omega = 2\pi\nu$ and $|\boldsymbol{k}| = 2\pi/\lambda$ we see that this is nothing but the relation $\nu = \lambda c$ that you learned in high school.

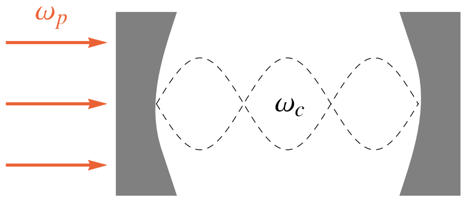

Figure 3.2: An optical cavity of frequency ω_c, pumped from the outside by a laser of frequency ω_p.

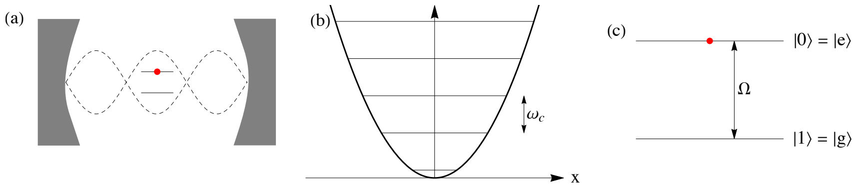

Figure 3.3: (a) Typical scenario for light-matter interaction: an atom, modeled as a two-level system, is placed inside a cavity in which there is only one cavity mode. The atom then absorbs and emits photons jumping up and down from the ground-state to the excited state. (b) The cavity field is represented by a harmonic oscillator of frequency ω_c. (c) The atom is represented as a two-level system (qubit) with energy gap Ω. When the atom Hamiltonian is $+\sigma_z$ then the ground-state will be $|1\rangle$ and the excited state will be $|0\rangle$.

where ϵ is the pump amplitude and is related to the laser power P according to $|\epsilon|^2 = \gamma P/\hbar\omega_p$ where γ is the cavity loss rate (the rate at which photons can go through the semi-transparent mirror). This Hamiltonian is very simple, but is time-dependent. Lucky for us, however, this time dependence can be eliminated using the concept of a rotating frame, as will be discussed below.

Jaynes-Cummings and Rabi models

Quantum information has always been intimately related with quantum optics and atomic physics, so *light-matter interaction* is an essential topic in the field. The two most important models in this sense are the Jaynes-Cummings and Rabi models, both of which describe the interaction of a single radiation mode with a single atom, approximated as a two-level system. The basic idea of both models is the exchange of quanta between the two systems; that is, sometimes the atom absorbs a photon and jumps to an excited state and sometimes it emits a photon and drops down to the ground-state. These effects of course take place on free space, but we are usually interested in controlled experiments performed inside optical cavities. The situation is then like that of

Fig. 3.3.

The Jaynes-Cummings model reads

$$H = \omega a^\dagger a + \frac{\Omega}{2}\sigma_z + \lambda(a\sigma_+ + a^\dagger \sigma_-). \tag{3.23}$$

The first two terms are the free Hamiltonians of the cavity field, with frequency ω_c, and the atom, with energy gap Ω. Whenever the atom Hamiltonian is written as $+\sigma_z$, the ground-state will be $|g\rangle = |1\rangle$ and the excited state will be $|e\rangle = |0\rangle$ [see Fig. 3.3(c)]. Finally, the last term in (3.23) is the light-atom coupling. The term $a\sigma_+$ describes the process where a photon is annihilated and the atom jumps to the excited state. Similarly, $a^\dagger\sigma_-$ describes the opposite process. The Hamiltonian must always be Hermitian so every time we include a certain type of process, we must also include its reverse.

The type of interaction in Eq. (3.23) introduces a special *symmetry* to the problem. Namely, it conserves the number of quanta in the system:

$$[H, a^\dagger a + \sigma_z] = 0. \tag{3.24}$$

This means that if you start the evolution with 7 photons and the atom in the ground-state, then at all times you will either have 7 photons + ground-state or 6 photons and the atom in the excited state. This is a very special symmetry and is the reason why the Jaynes-Cummings model turns out to be easy to deal with.

However, if we start with a physical derivation of the light-atom interaction, we will see that it is not exactly like the Jaynes-Cummings Hamiltonian (3.23). Instead, it looks more like the Rabi model

$$H = \omega a^\dagger a + \frac{\Omega}{2}\sigma_z + \lambda(a + a^\dagger)\sigma_x. \tag{3.25}$$

The difference is only in the last term. In fact, if we recall that $\sigma_x = \sigma_+ + \sigma_-$, we get

$$(a + a^\dagger)\sigma_x = (a\sigma_+ + a^\dagger\sigma_-) + (a^\dagger\sigma_+ + a\sigma_-).$$

The first term in parenthesis is exactly the Jaynes-Cummings interaction, so the new thing here is the term $(a^\dagger\sigma_+ + a\sigma_-)$. It describes a process where the atom jumps to the excited state *and* emits a photon, something which seems rather strange at first. Moreover, this new term destroys the pretty symmetry (3.24), making the Rabi model much more complicated to deal with, but also much richer from a physical point of view. Notwithstanding, as we will see below, if λ is small compared to ω_c, Ω this new term becomes negligible and the Rabi model approximately tends to the JC Hamiltonian.

3.3 Rotating frames and interaction picture

In this section I want to introduce the concept of *rotating frames*, which is a small generalization of the interaction and Heisenberg pictures that you may have learned in quantum mechanics. Consider a system with density matrix ρ evolving according to von Neumann's equation (we could do the same with Schrödinger's equation)

$$\frac{d\rho}{dt} = -i[H(t), \rho], \tag{3.26}$$

where $H(t)$ is a possibly time-dependent Hamiltonian. We can always move to a *rotating frame* by defning a new density matrix

$$\tilde{\rho}_t = S(t)\rho S^\dagger(t), \tag{3.27}$$

where $S(t)$ is an arbitrary unitary. I will leave to you as an exercise to show that $\tilde{\rho}$ will also obey a von Neumann equation

$$\frac{\mathrm{d}\tilde{\rho}}{\mathrm{d}t} = -i[\tilde{H}(t), \tilde{\rho}], \tag{3.28}$$

but with an effective Hamiltonian[2]

$$\boxed{\tilde{H}(t) = i\frac{\mathrm{d}S}{\mathrm{d}t}S^\dagger + SHS^\dagger.} \tag{3.29}$$

Thus, we see that in any rotating frame the system always obeys von Neumann's (or Schrödinger's) equation, but the Hamiltonian changes from $H(t)$ to $\tilde{H}(t)$. Note that this result is absolutely general and holds for any unitary $S(t)$. Of course, whether it is useful or not will depend on your smart choice for $S(t)$.

Before we move to applications, I need to mention that computing the first term in Eq (3.29) can be tricky. Usually we write unitaries as $S(t) = e^{iK(t)}$ where K is Hermitian. Then, one may easily verify the following BCH expansion

$$\boxed{\frac{\mathrm{d}e^{iK}}{\mathrm{d}t}e^{-iK} = i\frac{\mathrm{d}K}{\mathrm{d}t} + \frac{i^2}{2}[K, \frac{\mathrm{d}K}{\mathrm{d}t}] + \frac{i^3}{3!}[K,[K,\frac{\mathrm{d}K}{\mathrm{d}t}]] + \ldots.} \tag{3.30}$$

The important point here is whether or not K commutes with $\mathrm{d}K/\mathrm{d}t$. If that is the case then only the first term survives and things are easy and pretty. Otherwise, you may get an infinite series. I strongly recommend you always use this formula, because then you are always sure you will not get into trouble.

Eliminating time-dependences

A simple yet useful application of rotating frames is to eliminate the time-dependence of certain simple Hamiltonians, such as the pumped cavity (3.22). In this case the unitary that does the job is

$$S(t) = e^{i\omega_p t a^\dagger a}. \tag{3.31}$$

---

[2] To derive this equation it is necessary to use the following trick: since $SS^\dagger = 1$ then

$$0 = \frac{\mathrm{d}SS^\dagger}{\mathrm{d}t} = S\frac{\mathrm{d}S^\dagger}{\mathrm{d}t} + \frac{\mathrm{d}S}{\mathrm{d}t}S^\dagger \qquad \longrightarrow \qquad S\frac{\mathrm{d}S^\dagger}{\mathrm{d}t} = -\frac{\mathrm{d}S}{\mathrm{d}t}S^\dagger.$$

That is, we move to a frame that is rotating at the same frequency as the pump laser ω_p. Using the BCH expansion (1.70) one may show that

$$\boxed{e^{i\alpha a^\dagger a} a e^{-i\alpha a^\dagger a} = e^{-i\alpha} a, \qquad e^{i\alpha a^\dagger a} a^\dagger e^{-i\alpha a^\dagger a} = e^{i\alpha} a^\dagger,} \tag{3.32}$$

which are easy to remember: a goes with negative α and $a^\dagger$ with positive α. It then follows that

$$S(t)\Big[\epsilon a^\dagger e^{-i\omega_p t} + \epsilon a e^{i\omega_p t}\Big] S^\dagger(t) = \epsilon a^\dagger + \epsilon a,$$

while $S(t)$ has no effect on $a^\dagger a$. Moreover, this is one of those cases where only the first term in (3.30) contributes:

$$\frac{\mathrm{d}S}{\mathrm{d}t} S^\dagger = i\omega_p a^\dagger a.$$

Thus Eq. (3.29) becomes

$$\boxed{\tilde{H} = (\omega_c - \omega_p) a^\dagger a + \epsilon a^\dagger + \epsilon^* a.} \tag{3.33}$$

We therefore conclude that in this rotating frame the Hamiltonian is time-independent, but evolves according to the **detuned frequency** $\Delta = \omega_c - \omega_p$. This idea of *detuning* a frequency is extremely important in quantum optics applications since it is an easy way to change the parameters in the problem.

For more general bosonic Hamiltonians containing a pump term, the time-dependence can be eliminated by the same transformation, provided the remainder of the Hamiltonian conserves the number of quanta (i.e., when all operators have an equal number of as and $a^\dagger$s). This is due to the simple rule imposed by (3.32), which says that every a gets a term $e^{-i\omega_p t}$ while every $a^\dagger$ gets a $e^{i\omega_p t}$. Thus, a Hamiltonian such as

$$H = \omega_a^\dagger a + \frac{U}{2} a^\dagger a^\dagger a a + \epsilon a^\dagger e^{-i\omega_p t} + \epsilon^* a e^{i\omega_p t},$$

will lead to a rotating frame Hamiltonian

$$\tilde{H} = (\omega - \omega_p) a^\dagger a + \frac{U}{2} a^\dagger a^\dagger a a + \epsilon a^\dagger + \epsilon^* a.$$

Once you get the hang of it, it is quite easy: detune the frequency and get rid of the exponential. But be careful. This can only be done if the number of as and $a^\dagger$s is the same. For instance,

$$H = \omega_a^\dagger a + \chi (a + a^\dagger)^4 + \epsilon a^\dagger e^{-i\omega_p t} + \epsilon^* a e^{i\omega_p t},$$

would not have a time-independent rotating frame under the transformation (3.31) because if you expand $(a + a^\dagger)^4$ there will be terms with a unbalanced number of as and $a^\dagger$s.

A similar rotating frame transformation also works for qubit systems of the form

$$H = \frac{\Omega}{2}\sigma_z + \frac{\lambda}{2}(\sigma_+ e^{-i\omega_p t} + \sigma_- e^{i\omega_p t}) \tag{3.34}$$

$$= \frac{\Omega}{2}\sigma_z + \frac{\lambda}{2}[\sigma_x \cos(\omega_p t) + \sigma_y \sin(\omega_p t)]. \tag{3.35}$$

This Hamiltonian appears often in magnetic resonance because it represents a spin 1/2 particle subject to a constant field Ω in the z direction and a rotating field λ in the xy plane. Remarkably, the transformation here is almost exactly as in the bosonic case:

$$S(t) = e^{i\omega_p t \sigma_z/2}. \tag{3.36}$$

In this case the idea of a rotating frame becomes a bit more intuitive: the Hamiltonian is time-dependent because there is a field rotating in the xy plane. So to get rid of it, we go to a frame that is rotating around the z axis by an angle $\omega_p t$. I will leave for you to check that this $S(t)$ indeed does the job. One thing that is useful to know is that Eq. (3.32) is translated almost literally to the spin case:

$$e^{i\alpha\sigma_z/2}\sigma_- e^{-i\alpha\sigma_z/2} = e^{-i\alpha}\sigma_-, \qquad e^{i\alpha\sigma_z/2}\sigma_+ e^{-i\alpha\sigma_z/2} = e^{i\alpha}\sigma_+, \tag{3.37}$$

Interaction picture

Now let us consider another scenario. Suppose the Hamiltonian is time-independent but can be written in the standard perturbation-theory-style

$$H = H_0 + V, \tag{3.38}$$

where H_0 is easy to handle but V is not. Then choose

$$S(t) = e^{iH_0 t}. \tag{3.39}$$

Eq. (3.29) then becomes

$$\boxed{\tilde{H}(t) = S(t) V S^\dagger(t).} \tag{3.40}$$

This is the interaction picture: we eliminate the dependence on H_0 at the cost of transforming a time-independent Hamiltonian $H_0 + V$ into a time-dependent Hamiltonian $SVS^\dagger$.

The interaction picture is usually employed as the starting point of time-dependent perturbation theory. We will learn a bit more about this below. But to get a first glimpse, consider the Rabi Hamiltonian (3.25) and let us move to the interaction picture with respect to $H_0 = \omega a^\dagger a + \frac{\Omega}{2}\sigma_z$. Using Eqs. (3.32) and (3.37) we then find

$$\tilde{H}(t) = \lambda\Big[a\sigma_+ e^{i(\Omega-\omega_c)t} + a^\dagger\sigma_- e^{-i(\Omega-\omega_c)t}\Big] + \lambda\Big[a^\dagger\sigma_+ e^{i(\Omega+\omega_c)t} + a\sigma_- e^{-i(\Omega+\omega_c)t}\Big]. \tag{3.41}$$

In the interaction picture we see more clearly the difference between the two types of couplings. The first term, which is the Jaynes-Cummings coupling, oscillates in time with a frequency $\Omega - \omega_c$, which will be very small when Ω is close to ω_c. The second term, on the other hand, oscillates quickly with frequency $\omega_c + \Omega$, which is in general a much faster frequency that $\omega_c - \Omega$. We therefore see the appearance of two time scales, the JC term, which is slow, and the Rabi dude which give rise to fast oscillations.

Eq. (3.41) is frequently used as the starting point to justify why sometimes we can throw away the last term (and hence obtain the Jaynes-Cummings model (3.23) from the Rabi model). The idea is called the **rotating-wave approximation (RWA)** and is motivated by the fact that if $\Omega + \omega$ is very large, the last terms will oscillate rapidly around zero average and hence will have a small contribution to the dynamics. But this explanation is only partially convincing, so be careful. In the end of the day, the RWA is really an argument on time-dependent perturbation theory. Hence, it will only be good when λ is small compared to ω_c and Ω. Thus, the RWA is better stated as follows: *if* $\lambda \ll \omega_c, \Omega$ *and* $\omega_c \sim \Omega$*, it is reasonable to throw away the fast oscillating terms in the interaction picture*. For an interesting discussion connection with perturbation theory, see the Appendix in `arXiv 1601.07528`.

Heisenberg picture

In the interaction picture we started with a Hamiltonian $H = H_0 + V$ and went to a rotating frame with H_0. In the Heisenberg picture, we go all the way through. That is, we go to a rotating frame (3.29) with $S(t) = e^{iHt}$. For now I will assume H is time-independent, but the final result also holds in the time-dependent case. As a result we find

$$\tilde{H} = 0 \tag{3.42}$$

Consequently, the solution of the rotating frame Eq. (3.28) will be simply

$$\tilde{\rho}(t) = \tilde{\rho}(0) = \rho(0). \tag{3.43}$$

But by Eq. (3.27) we have $\tilde{\rho}(t) = S(t)\rho(t)S^\dagger(t)$ so we get

$$\rho(t) = S^\dagger(t)\rho(0)S(t) = e^{-iHt}\rho(0)e^{iHt}. \tag{3.44}$$

You may now be thinking "DUH! This is is just the solution of the of von Neumann's equation!". Yes, that's exactly the point. The solution of von Neumann's equation is exactly that special rotating frame where time stands still (like in the Rush song!).

In the Heisenberg picture we usually transfer the time-dependence to the operators, instead of the states. Recall that given an arbitrary operator A, its expectation value will be $\langle A\rangle = \text{tr}(A\rho)$. Using Eq. (3.44) we then get

$$\langle A\rangle = \text{tr}\Big\{Ae^{-iHt}\rho(0)e^{iHt}\Big\} = \text{tr}\Big\{e^{iHt}Ae^{iHt}\rho(0)\Big\}. \tag{3.45}$$

This formula summarizes well the Schrödinger vs. Heisenberg ambiguity. It provides two equivalent ways to compute $\langle A\rangle$. In the first, which is the usual Schrödinger picture approach, the state $\rho(t)$ evolves in time and A is time-independent. In the second, the state ρ is fixed at $\rho(0)$ and we transfer the time evolution to the operator. It is customary to define the *Heisenberg operator*

$$A_H(t) = A(t) = e^{iHt}Ae^{-iHt}. \tag{3.46}$$

Some people write $A_H(t)$ to emphasize that this is different from A What I usually do is just be careful to always write the time argument in $A(t)$.

By direct differentiation one may verify that the operator $A(t)$ satisfies the **Heisenberg equation**

$$\boxed{\frac{\mathrm{d}A(t)}{\mathrm{d}t} = i[H, A(t)].} \tag{3.47}$$

This is to be interpreted as an equation for the evolution of the operator $A(t)$. If what you are interested is instead the evolution of the expectation value $\langle A\rangle_t$, then it doesn't matter which picture you use. In the Heisenberg picture, Eq. (3.47) directly gives you

$$\boxed{\frac{\mathrm{d}\langle A\rangle}{\mathrm{d}t} = i\langle [H, A]\rangle.} \tag{3.48}$$

But you can also get the same equation in the Schrödinger picture using the von Neumann equation:

$$\frac{\mathrm{d}\langle A\rangle}{\mathrm{d}t} = \operatorname{tr}\left\{A\frac{\mathrm{d}\rho}{\mathrm{d}t}\right\} = -i\operatorname{tr}\left\{A[H,\rho]\right\} = i\operatorname{tr}\left\{[H,A]\rho\right\},$$

where, in the last line, all I did was rearrange the commutator using the cyclic property of the trace.

About time-dependent Hamiltonians

The solution of Schrödinger's or von Neumann's equation for time-independent Hamiltonians is very easy, being simply e^{-iHt}. However, when the Hamiltonian is time-dependent this solution no longer works. Let us then see how to write down the solution in this case. I will do so for the case of Schödinger's equation, simply because it looks a little bit cuter. It is straightforward to generalized to von Neumann's equation. Our starting point is thus the equation

$$\partial_t|\psi_t\rangle = -iH(t)|\psi_t\rangle. \tag{3.49}$$

In order to figure out what the solution will be in this case, we follow the maxim of Polish mathematician Marc Kac: **"be wise, discretize!"** That is, we assume that the Hamiltonian $H(t)$ is actually piecewise constant at intervals Δt, having the value $H(n\Delta t)$ during the interval between $n\Delta t$ and $(n+1)\Delta t$ (something like what is shown in Fig. 3.4, but for the operator $H(t)$). We can then solve Eq. (3.49) exactly for one interval:

$$|\psi((n+1)\Delta t)\rangle = e^{-i\Delta t H(n\Delta t)}|\psi(n\Delta t)\rangle. \tag{3.50}$$

From this we can proceed sequentially, using the solution for a given interval as the initial condition for the next. This allows us to glue together a solution between $t_0 = M\Delta t$ and $t = (N+1)\Delta t$ (with M, N integers and $N > M$):

$$|\psi_t\rangle = \left[e^{-i\Delta t H(N\Delta t)}e^{-i\Delta t H((N-1)\Delta t)}\dots e^{-i\Delta t H(M\Delta t)}\right]|\psi_{t_0}\rangle. \tag{3.51}$$

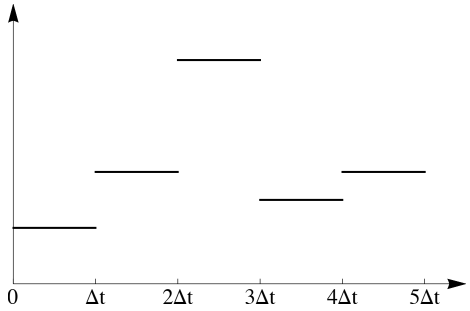

Figure 3.4: A silly example of a piecewise constant function.

Of course, this discretization is just a trick. We can now take $\Delta t \to 0$ and we will have solved for the most general time-dependent Hamiltonian.

If we define the time-evolution operator according to

$$|\psi_t\rangle = U(t, t_0)|\psi_{t_0}\rangle, \tag{3.52}$$

then we see that

$$\boxed{U(t, t_0) = e^{-i\Delta t H(N\Delta t)} e^{-i\Delta t H((N-1)\Delta t)} \ldots e^{-i\Delta t H(M\Delta t)}.} \tag{3.53}$$

Since this becomes exact when $\Delta t \to 0$, we conclude that this is *the* general solution of the time-dependent problem. Admittedly, this solution is still quite a mess and part of our effort below will be to clean it up a bit. But if you ever wonder "what is the solution with a time-dependent Hamiltonian?", I recommend you think about (3.53).

It is interesting to note that this operator $U(t, t_0)$ satisfies all properties of its time-independent cousin:

$$U(t_0, t_0) = 1, \tag{3.54}$$

$$U(t, t_1)U(t_1, t_0) = U(t, t_0), \qquad t_0 < t_1 < t, \tag{3.55}$$

$$U(t, t_0)U^\dagger(t, t_0) = 1, \tag{3.56}$$

$$U^\dagger(t, t_0) = U(t_0, t). \tag{3.57}$$

Eq. (3.55) is particularly important, because it shows that even in the time-dependent case the solution can still be broken down in pieces.

The important point that must be remembered concerning Eq. (3.53) is that in general you *cannot* recombine the exponentials since the Hamiltonian at different times may not commute:

$$\text{in general} \quad [H(t), H(t')] \neq 0. \tag{3.58}$$

If this happens to be the case, then the problem is very easy and Eq. (3.53) becomes

$$
\begin{aligned}
U(t,t_0) &= \exp\Big\{-i\Delta t\sum_{n=M}^{N} H(n\Delta t)\Big\}\\
&= \exp\Big\{-i\int_{t_0}^{t} H(t')\,\mathrm{d}t'\Big\},
\end{aligned}
$$

where, in the last line, I already took the limit $\Delta t \to 0$ and transformed the sum to an integral.

However, if $H(t)$ does not commute at different times, this solution is incorrect. Instead, we can use a trick to write down the solution in a way that looks formally similar. We define the *time-ordering* operator $\mathcal{T}$ such that, when acting on any set of time-dependent operators, it always puts later times to the left:

$$
\mathcal{T}A(t_1)A(t_2) = \begin{cases} A(t_1)A(t_2) & \text{if } t_1 > t_2 \\ A(t_2)A(t_1) & \text{if } t_2 > t_1 \end{cases} \tag{3.59}
$$

This time-ordering operator can now be used to combine exponentials. If we recall the Zassenhaus (BCH) formula (1.68):

$$
e^{t(A+B)} = e^{tA}e^{tB}e^{-\frac{t^2}{2}[A,B]}e^{\frac{t^3}{3!}(2[B,[A,B]]+[A,[A,B]])}\ldots, \tag{3.60}
$$

we see that the combination-recombination of exponentials involves only commutators. Now suppose $t_2 > t_1$. Then

$$
\mathcal{T}[A(t_2),B(t_1)] = \mathcal{T}\Big(A(t_2)B(t_1) - B(t_1)A(t_2)\Big) = A(t_2)B(t_1) - A(t_2)B(t_1) = 0.
$$

Consequently, if we expand $e^{A(t_2)+B(t_1)}$ and then apply $\mathcal{T}$, the only term that will survive will be $e^{A(t_2)}e^{B(t_1)}$. Hence,

$$
e^{A(t_2)}e^{B(t_1)} = \mathcal{T}e^{A(t_2)+B(t_1)}. \tag{3.61}
$$

Within the protection of the time-ordering operator, we can freely recombine exponentials.

Using this time-ordering trick we may now recombine all terms in the product (3.53), leading to

$$
\boxed{U(t,t_0) = \mathcal{T}\exp\Big\{-i\int_{t_0}^{t} H(t')\,\mathrm{d}t'\Big\},} \tag{3.62}
$$

where I already transformed this into an integral. This is the way we usually write the formal solution of a time-dependent problem. The time-ordering operator $\mathcal{T}$ is just a compact way to write down the solution in Eq. (3.53). If you are ever confused about how to operate with it, go back to Eq. (3.53). Finally, let me mention that Eq. (3.62) can also be viewed as the solution of the initial value problem

$$\frac{\mathrm{d}U(t,t_0)}{\mathrm{d}t} = -iH(t)U(t,t_0), \qquad U(t_0,t_0) = 1. \tag{3.63}$$

This may not be so evident from Eq. (3.62), but it is if we substitute Eq. (3.52) into (3.49).

Magnus expansion

We are now in a good point to discuss time-dependent perturbation theory. The scenario is as follows. We start with $H_0 + V$ and move to the interaction picture where the rotating frame Hamiltonian becomes the time-independent operator (3.40). We then try to solve the von Neumann equation for this operator. Or, what is equivalent, we try to find the time-evolution operator $\tilde{U}(t,t_0)$ which, as in (3.63), will be the solution of

$$\frac{\mathrm{d}\tilde{U}(t,t_0)}{\mathrm{d}t} = -i\tilde{H}(t)\tilde{U}(t,t_0), \qquad \tilde{U}(t_0,t_0) = 1. \tag{3.64}$$

There are many ways to do this. Sometimes the perturbation theory is done in terms of states and sometimes it is done in terms of operators (in which case it is called a **Dyson series**).

Here I will try to do it in a slightly different way, using something called a Magnus expansion. Parametrize the time evolution operator as

$$\tilde{U}(t,t_0) = e^{-i\Omega(t,t_0)}, \qquad \Omega(t_0,t_0) = 0, \tag{3.65}$$

where $\Omega(t,t_0)$ is an operator to be determined. To find an equation for it, we first multiply Eq. (3.64) bu $U^\dagger$ on the left, leading to

$$\frac{\mathrm{d}e^{-i\Omega}}{\mathrm{d}t}e^{i\Omega} = -i\tilde{H}(t).$$

Then we use Eq. (3.30) to find

$$\dot{\Omega} - \frac{i}{2}[\Omega,\dot{\Omega}] - \frac{1}{3!}[\Omega,[\Omega,\dot{\Omega}]] + \ldots = \tilde{H}(t), \tag{3.66}$$

which is a really weird equation for $\Omega(t,t_0)$.

We now write this in perturbation-theory-style by assuming that $\tilde{H}(t) \to \epsilon\tilde{H}(t)$ where ϵ is a small parameter. Moreover, we expand Ω as

$$\Omega = \epsilon\Omega_1 + \epsilon^2\Omega_2 + \epsilon^3\Omega_3 + \ldots. \tag{3.67}$$

Substituting in Eq. (3.66) and collecting terms of the same order in ϵ we are then led to a system of equations

$$\dot{\Omega}_1 = \tilde{H}(t), \tag{3.68}$$

$$\dot{\Omega}_2 = \frac{i}{2}[\Omega_1,\dot{\Omega}_1], \tag{3.69}$$

$$\dot{\Omega}_3 = \frac{i}{2}[\Omega_1,\dot{\Omega}_2] + \frac{i}{2}[\Omega_2,\dot{\Omega}_1] + \frac{1}{3!}[\Omega_1,[\Omega_1,\dot{\Omega}_1]]. \tag{3.70}$$

and so on. These can now be solved sequentially, leading to

$$\Omega_1(t) = \int_{t_0}^{t} \mathrm{d}t_1 \; \tilde{H}(t_1), \tag{3.71}$$

$$\Omega_2(t) = -\frac{i}{2}\int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \; [\tilde{H}(t_1), \tilde{H}(t_2)], \tag{3.72}$$

$$\Omega_3(t) = -\frac{1}{6}\int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \; \Big\{[\tilde{H}(t_1), [\tilde{H}(t_2), \tilde{H}(t_3)]] + [\tilde{H}(t_3), [\tilde{H}(t_2), \tilde{H}(t_1)]]\Big\}. \tag{3.73}$$

This is the Magnus expansion. Higher order terms become more and more cumbersome. From this one may obtain the Dyson series expanding Eq. (3.65) in a Taylor series.

It is also important to note that if the Hamiltonian commutes at different times, then the series truncates at the first term. If this were always the case, there would be no need for perturbation theory at all. The need for time-dependent perturbation theory is really a consequence of the non-commutativity of $\tilde{H}$ at different times.

Rotating wave approximation

Consider once again the interaction picture Rabi Hamiltonian (3.41) and let us compute the first order term in the Magnus expansion, Eq. (3.71). We get, assuming $t_0 = 0$,

$$\int_0^t \mathrm{d}t_1 \; \tilde{H}(t_1) = \frac{\lambda}{i(\Omega-\omega_c)}\Big[a\sigma_+(e^{i(\Omega-\omega_c)t}-1) - a^\dagger\sigma_-(e^{-i(\Omega-\omega_c)t}-1)\Big]$$

$$+\frac{\lambda}{i(\Omega+\omega_c)}\Big[a^\dagger\sigma_+(e^{i(\Omega+\omega_c)t}-1) - a\sigma_-(e^{-i(\Omega+\omega_c)t}-1)\Big].$$

The Rotating-wave approximation scenario is now apparent: when we do perturbation theory, the Jaynes-Cummings terms will multiply $\lambda/(\Omega-\omega_c)$ whereas the non-JC terms will contain $\lambda/(\Omega-\omega_c)$. If we are close to resonance ($\Omega \sim \omega_c$) and if λ is small the first term will be very large and the second very small. Consequently, the second term may be neglected.

3.4 Coherent states

Coherent states are a very special set of states which form the basis of continuous variables quantum information. In this section we will discuss some of its basic properties. If you ever need more advanced material, I recommend the paper by K. Cahill and R. Glauber in *Phys. Rev.* **177**, 1857-1881 (1969).

We begin by defining the **displacement operator**

$$\boxed{D(\alpha) = e^{\alpha a^\dagger - \alpha^* a}.} \tag{3.74}$$

where α is an arbitrary complex number and α^* is its complex conjugate. The reason why it is called a "displacement" operator will become clear soon. A coherent state is defined as the action of $D(\alpha)$ into the vacuum state:

$$\boxed{|\alpha\rangle = D(\alpha)|0\rangle.} \tag{3.75}$$

We sometimes say that **"a coherent state is a displaced vacuum"**. This sounds like a typical Star Trek sentence: "Oh no! He displaced the vacuum. Now the entire planet will be annihilated!"

$D(\alpha)$ displaces a and $a^\dagger$

Let us first try to understand why $D(\alpha)$ is called a displacement operator. First, one may verify directly from Eq. (3.74) that

$$D^\dagger(\alpha)D(\alpha) = D(\alpha)D^\dagger(\alpha) = 1 \qquad \text{(it is unitary)}, \tag{3.76}$$

$$D^\dagger(\alpha) = D(-\alpha). \tag{3.77}$$

This means that if you displace by a given α and then displace back by $-\alpha$, you return to where you started. Next I want to compute $D^\dagger(\alpha)aD(\alpha)$. To do that we use the BCH formula (1.70):

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \dots. \tag{3.78}$$

with $B = a$ and $A = \alpha^* a - \alpha a^\dagger$. Using the commutation relations $[a, a^\dagger] = 1$ we get

$$[\alpha^* a - \alpha a^\dagger, a] = \alpha.$$

But this is a c-number, so that all higher order commutators in the BCH expansion will be zero. We therefore conclude that

$$\boxed{D^\dagger(\alpha)aD(\alpha) = a + \alpha.} \tag{3.79}$$

This is why we call D the displacement operator: it displacements the operator by an amount α. Since $D^\dagger(\alpha) = D(-\alpha)$ it follows that

$$D(\alpha)aD^\dagger(\alpha) = a - \alpha. \tag{3.80}$$

The action on $a^\dagger$ is similar: you just need to take the adjoint: For instance

$$D^\dagger(\alpha)a^\dagger D(\alpha) = a^\dagger + \alpha^*. \tag{3.81}$$

The coherent state is an eigenstate of a

What I want to do now is apply a to the coherent state $|\alpha\rangle$ in Eq. (3.75). Start with Eq. (3.79) and multiply by $D(\alpha)$ on the left. Since D is unitary we get $aD(\alpha) = D(\alpha)(a+\alpha)$. Thus

$$a|\alpha\rangle = aD(\alpha)|0\rangle = D(\alpha)(a+\alpha)|0\rangle = D(\alpha)(\alpha)|0\rangle = \alpha|\alpha\rangle,$$

where I used the fact that $a|0\rangle = 0$. Hence we conclude that **the coherent state is the eigenvector of the annihilation operator**:

$$\boxed{a|\alpha\rangle = \alpha|\alpha\rangle.} \tag{3.82}$$

The annihilation operator is not Hermitian so its eigenvalues do not have to be real. In fact, this equation shows that the eigenvalues of a are all complex numbers.

Alternative way of writing D

It is possible to express D in a different way, which may be more convenient for some computations. Using the Zassenhaus formula (3.60) we see that, if it happens that $[A,B]$ commute with both A and B, then

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]}. \tag{3.83}$$

Since $[a,a^\dagger] = 1$, we may write

$$\boxed{D(\alpha) = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} e^{-\alpha^* a} = e^{|\alpha|^2/2} e^{-\alpha^* a} e^{\alpha a^\dagger}.} \tag{3.84}$$

This result is useful because now the exponentials of a and $a^\dagger$ are completely separated.

From this result it follows that

$$\boxed{D(\alpha)D(\beta) = e^{(\beta^*\alpha - \alpha^*\beta)/2} D(\alpha+\beta).} \tag{3.85}$$

This means that if you do two displacements in a sequence, it is almost the same as doing just a single displacement; the only thing you get is a phase factor (the quantity in the exponential is purely imaginary).

Poisson statistics

Let us use Eq. (3.84) to write the coherent state a little differently. Since $a|0\rangle = 0$ it follows that $e^{-\alpha a}|0\rangle = |0\rangle$. Hence we may also write Eq. (3.75) as

$$\boxed{|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger}|0\rangle.} \tag{3.86}$$

Now we may expand the exponential and use Eq. (3.14) to write $(a^\dagger)^n|0\rangle$ in terms of the number states. We get

$$|\alpha\rangle = e^{-|\alpha|^2/2}\sum_{n=0}^\infty \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \tag{3.87}$$

Thus we find that

$$\langle n|\alpha\rangle = e^{-|\alpha|^2/2}\frac{\alpha^n}{\sqrt{n!}}. \tag{3.88}$$

The probability of finding it in a given state $|n\rangle$, given that it is in a coherent state, is therefore

$$|\langle n|\alpha\rangle|^2 = e^{-|\alpha|^2}\frac{(|\alpha|^2)^n}{n!}. \tag{3.89}$$

This is a Poisson distribution with parameter $\lambda = |\alpha|^2$. The photons in a laser are usually in a coherent state and the Poisson statistics of photon counts can be measured experimentally. If you measure this statistics for thermal light you will find that it is not Poisson (usually it follows a geometric distribution). Hence, Poisson statistics is a signature of coherent states.

Orthogonality

Coherent states are not orthogonal. To figure out the overlap between two coherent states $|\alpha\rangle$ and $|\beta\rangle$ we use Eq. (3.86):

$$\langle\beta|\alpha\rangle = e^{-|\beta|^2/2}e^{-|\alpha|^2/2}\langle 0|e^{\beta^* a}e^{\alpha a^\dagger}|0\rangle.$$

We need to exchange the two operators because we know how a acts on $|0\rangle$ and how $a^\dagger$ acts on $\langle 0|$. To do that we use Eq. (3.83):

$$e^{\beta^* a}e^{\alpha a^\dagger} = e^{\alpha a^\dagger}e^{\beta^* a}e^{\beta^*\alpha}. \tag{3.90}$$

We therefore conclude that

$$\boxed{\langle\beta|\alpha\rangle = \exp\left\{\beta^*\alpha - \frac{|\beta|^2}{2} - \frac{|\alpha|^2}{2}\right\}.} \tag{3.91}$$

The overlap of the two states, squared, can be simplified to read:

$$\boxed{|\langle\beta|\alpha\rangle|^2 = \exp\left\{-|\alpha-\beta|^2\right\}.} \tag{3.92}$$

Hence, the overlap between two coherent states decays *exponentially* with their distance. For large α and β they therefore become approximately orthogonal. Also, as a sanity check, if $\beta = \alpha$ then

$$\langle\alpha|\alpha\rangle = 1, \tag{3.93}$$

which we already knew from Eq. (3.75) and the fact that D is unitary. Coherent states are therefore normalized, but they do *not* form an orthonormal basis. In fact, they form an overcomplete basis in the sense that there are more states than actually needed.

Completeness

Even though the coherent states do not form an orthonormal basis, we can still write down a completeness relation for them. However, it looks a little different:

$$\boxed{\int \frac{\mathrm{d}^2\alpha}{\pi}\, |\alpha\rangle\langle\alpha| = 1.} \tag{3.94}$$

This integral is over the entire complex plane. That is, if $\alpha = x + iy$ then $\mathrm{d}^2\alpha = \mathrm{d}x\,\mathrm{d}y$. This is, therefore, just your old-fashioned integral over two variables. The proof of Eq. (3.94) is a little bit cumbersome. You can find it in Gardiner and Zoller.

Trace of a displacement operator

Due to the orthogonality (3.94), you can also use the coherent state basis to compute traces:

$$\mathrm{tr}(O) = \int \frac{\mathrm{d}^2\alpha}{\pi}\, \langle\alpha|O|\alpha\rangle. \tag{3.95}$$

As an example, let us compute the trace of the displacement operator:

$$\mathrm{tr}\, D(\lambda) = \int \frac{\mathrm{d}^2\alpha}{\pi}\, \langle\alpha|D(\lambda)|\alpha\rangle = \int \frac{\mathrm{d}^2\alpha}{\pi}\, \langle 0|D^\dagger(\alpha)D(\lambda)D(\alpha)|0\rangle.$$

But since $D(\alpha)$ is unitary, it infiltrates everywhere:

$$D^\dagger(\alpha)D(\lambda)D(\alpha) = \exp\Big\{D^\dagger(\alpha)(\lambda a^\dagger - \lambda^* a)D(\alpha)\Big\} = e^{\lambda\alpha^* - \lambda^*\alpha} D(\lambda).$$

Thus we get

$$\mathrm{tr}\, D(\lambda) = \int \frac{\mathrm{d}^2\alpha}{\pi} \;= e^{\lambda\alpha^* - \lambda^*\alpha}\langle 0|D(\lambda)|0\rangle = e^{-|\lambda|^2/2} \int \frac{\mathrm{d}^2\alpha}{\pi}\, e^{\lambda\alpha^* - \lambda^*\alpha} \tag{3.96}$$

where I used the fact that $\langle 0|D(\lambda)|0\rangle = \langle 0|\lambda\rangle = e^{-|\lambda|^2/2}$ [Eq. (3.88)].

The remaining integral is actually an important one. Let us write $\alpha = x + iy$ and $\lambda = u + iv$. Then

$$\lambda\alpha^* - \lambda^*\alpha = 2ixv - 2iuy.$$

Thus

$$\int \frac{\mathrm{d}^2\alpha}{\pi}\, e^{\lambda\alpha^* - \lambda^*\alpha} = \int \mathrm{d}x e^{2ixv} \int \mathrm{d}y e^{-2iuy}$$

But each one is now a Dirac delta

$$\int_{-\infty}^{\infty} \mathrm{d}x e^{ixk} = 2\pi\delta(k).$$

Whence

$$\boxed{\int \frac{\mathrm{d}^2\alpha}{\pi}\, e^{\lambda\alpha^* - \lambda^*\alpha} = \pi\delta(\lambda).} \tag{3.97}$$

where $\delta(\lambda) = \delta(\mathrm{Re}(\lambda))\delta(\mathrm{Im}(\lambda))$. This integral is therefore nothing but the two-dimensional Fourier transform in terms of the complex variable α.

Substituting this in Eq. (3.96) we finally conclude that

$$\boxed{\mathrm{tr}\, D(\lambda) = \pi\ \delta(\lambda),} \tag{3.98}$$

where I omitted the factor of $e^{-|\lambda|^2/2}$ since the Dirac delta make it irrelevant. Using this and Eq. (3.85) also allows us to write the neat formula

$$\mathrm{tr}\Big[D(\alpha)D^\dagger(\beta)\Big] = \pi\delta(\alpha - \beta). \tag{3.99}$$

This is a sort of orthogonality relation, but between operators.

$D(\alpha)$ as a basis for operators

Due to Eqs. (3.98) and (3.99), it turns out that the displacement operators form a basis for the Hilbert space, in the sense that any operator F may be decomposed as

$$\boxed{F = \int \frac{\mathrm{d}^2\alpha}{\pi}\, f(\alpha)D^\dagger(\alpha)} \tag{3.100}$$

where

$$f(\alpha) := \mathrm{tr}\Big[F D(\alpha)\Big]. \tag{3.101}$$

This is just like decomposing a state in a basis, but we are actually decomposing an operator.

3.5 The Husimi-Q function

A big part of dealing with continuous variables systems is the idea of *quantum phase space*, similarly to the classical coordinate-momentum phase space in classical mechanics. There are many ways to represent continuous variables in phase space. The three most important are the Husimi-Q function, the Wigner function and the Glauber-Sudarshan P function. Each has its own advantages and disadvantages. Since this chapter is meant to be a first look into this topic, we will focus here on the simplest one of them, the Q function.

The Husimi-Q function is defined as the expectation value of the density matrix in a coherent state

$$\boxed{Q(\alpha^*, \alpha) = \frac{1}{\pi}\langle\alpha|\rho|\alpha\rangle.} \tag{3.102}$$

Here α and α^* are to be interpreted as independent variables. If that confuses you, define $\alpha = x + iy$ and interpret Q as a function of x and y. In fact, following the transformation between $a, a^\dagger$ and the quadrature operators q, p in Eq. (3.3), $x/\sqrt{2}$ represents the position in phase space, whereas $y/\sqrt{2}$ represents the momentum.

Using Eq. (3.95) for the trace in the coherent state basis, we get

$$1 = \operatorname{tr}\rho = \int \frac{\mathrm{d}^2\alpha}{\pi}\langle\alpha|\rho|\alpha\rangle.$$

Thus, we conclude that the Husimi Q function is normalized as

$$\int \mathrm{d}^2\alpha \; Q(\alpha^*, \alpha) = 1 \tag{3.103}$$

which resembles the normalization of a probability distribution.

If we know Q we can also use it to compute the expectation value of operators. For instance, since $a|\alpha\rangle = \alpha|\alpha\rangle$ it follows that

$$\langle a\rangle = \operatorname{tr}(\rho a) = \int \frac{\mathrm{d}^2\alpha}{\pi}\,\langle\alpha|\rho a|\alpha\rangle = \int \mathrm{d}^2\alpha \; Q(\alpha, \alpha^*)\alpha,$$

which is intuitive. As another example, recalling that $\langle\alpha|a^\dagger = \langle\alpha|\alpha^*$, we get

$$\langle aa^\dagger\rangle = \operatorname{tr}(a^\dagger\rho a) = \int \frac{\mathrm{d}^2\alpha}{\pi}\,\langle\alpha|a^\dagger\rho a|\alpha\rangle = \int \mathrm{d}^2\alpha \; Q(\alpha, \alpha^*)|\alpha|^2.$$

It is interesting to see here how the ordering of operators play a role. Suppose you want to compute $\langle a^\dagger a\rangle$. Then you should first reorder it as $\langle a^\dagger a\rangle = \langle aa^\dagger\rangle - 1$ and then use the above result for $\langle aa^\dagger\rangle$.

More generally, we may obtain a rule for computing the expectation values of *anti-normally ordered* operators. That is, operators which have all $a^\dagger$s to the right. If this is the case then we can easily write

$$\langle a^k(a^\dagger)^\ell\rangle = \int \mathrm{d}^2\alpha \;\; \alpha^k(\alpha^*)^\ell Q(\alpha^*, \alpha). \tag{3.104}$$

Thus, to compute the expectation value of an arbitrary operator, we should first use the commutation relations to put it in anti-normal order and then use this result.

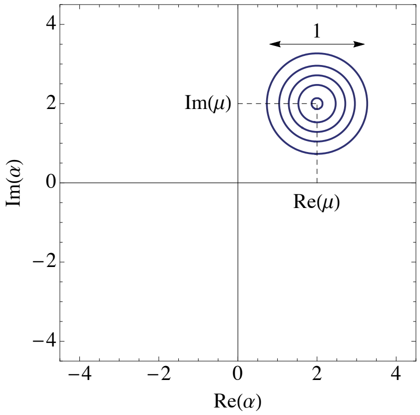

Figure 3.5: Example of the Husimi function (3.106) for $\mu = 2 + 2i$.

The Q function is always non-negative. But not all Q functions correspond to valid states. For instance, $\delta(\alpha)$ is not a valid Husimi function since it would lead to

$$\langle aa^\dagger \rangle = \int \frac{d^2\alpha}{\pi} |\alpha|^2 \delta^2(\alpha) = 0, \tag{3.105}$$

which is impossible since $\langle aa^\dagger \rangle = \langle a^\dagger a \rangle + 1$ and $\langle a^\dagger a \rangle \geq 0$.

Let us now turn to some examples of Q functions.

Example: coherent state

If the state is a coherent state $|\mu\rangle$, then $\rho = |\mu\rangle\langle\mu|$ and we get from (3.92) and (3.102):

$$Q(\alpha^*, \alpha) = \frac{1}{\pi}\langle\alpha|\mu\rangle\langle\mu|\alpha\rangle = \frac{1}{\pi}\exp\Big\{ - |\alpha - \mu|^2 \Big\} \tag{3.106}$$

This is a *Gaussian distribution in the complex plane*, centered around μ and with unit variance (see Fig. 3.5). The ground-state of the harmonic oscillator is also a coherent state, but with $\mu = 0$. It will therefore also be a unit-variance Gaussian, but centered at zero. This is why we say *the coherent state is a displaced vacuum*: it has the same distribution, but simply displaced in the complex plane by μ.

Example: Schrödinger cat state

In the context of continuous variables, we sometimes call the superposition

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|\mu\rangle + |-\mu\rangle\Big), \tag{3.107}$$

a Schrödinger cat state. Using Eq. (3.91) we then get

$$Q(\alpha, \alpha^*) = \frac{1}{\pi} e^{-|\alpha-\mu|^2}\Big\{ 1 + \frac{e^{-2\mu^*\alpha} + e^{-2\mu\alpha^*}}{2} \Big\}. \tag{3.108}$$

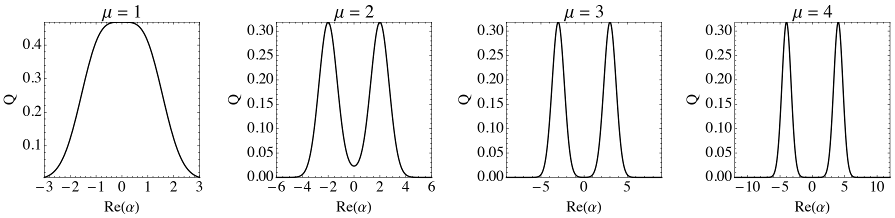

Figure 3.6: Example of the Husimi function (3.108) for a Schrödinger cat state (3.107), assuming μ real. The plots correspond to a cut at $\mathrm{Im}(\alpha) = 0$.

An example of this function is shown in Fig. 3.6. It corresponds to roughly two Gaussians superposed. If μ is small then the two peaks merge into one, but as μ increases they become more distinguishable.

Example: thermal state

Next let us consider a thermal Gibbs state

$$\rho_{\text{th}} = \frac{e^{-\beta\omega a^\dagger a}}{Z}, \tag{3.109}$$

where

$$Z = \mathrm{tr}(e^{-\beta\omega a^\dagger a}) = (1 - e^{-\beta\omega})^{-1}, \tag{3.110}$$

is the partition function. The Husimi function will be

$$Q(\alpha^*, \alpha) = \frac{(1 - e^{-\beta\omega})}{\pi} \sum_{n=0}^{\infty} e^{-\beta\omega n} \langle\alpha|n\rangle\langle n|\alpha\rangle.$$

This is a straightforward and fun calculation, which I will leave for you as an exercise. All you need is the overlap formula (3.88). The result is

$$Q(\alpha^*, \alpha) = \frac{1}{\pi(\bar{n}+1)} \exp\left\{ -\frac{|\alpha|^2}{\bar{n}+1} \right\}, \tag{3.111}$$

where

$$\bar{n} = \frac{1}{e^{\beta\omega} - 1}, \tag{3.112}$$

is the Bose-Einstein thermal occupation of the harmonic oscillator. Thus, we see that the thermal state is also a Gaussian distribution, centered at zero but with a variance proportional to $\bar{n} + 1$. At zero temperature we get $\bar{n} = 0$ and we recover the Q function for the vacuum $\rho = |0\rangle\langle 0|$. The width of the Gaussian distribution can be taken as a measure of the fluctuations in the system. At high temperatures $\bar{n}$ becomes large and so does the fluctuations. Thus, in the classical limit we get a big fat Gaussian. But even at $T = 0$ there is still a finite width, which is a consequence of quantum fluctuations.

The two examples above motivate us to consider a **displaced thermal state**. It is defined in terms of the displacement operator (3.74) as

$$\rho = D(\mu)\frac{e^{-\beta\omega a^\dagger a}}{Z}D^\dagger(\mu). \tag{3.113}$$

The corresponding Q function, as you can probably expect, is

$$Q(\alpha^*,\alpha) = \frac{1}{\pi(\bar{n}+1)}\exp\bigg\{-\frac{|\alpha-\mu|^2}{\bar{n}+1}\bigg\}, \tag{3.114}$$

which is sort of a mixture of Eqs. (3.106) and (3.111): it represents a thermal Gaussian displaced in the complex plane by an amount μ.

Heterodyne measurements

The Husimi-Q function allows for an interesting interpretation in terms of measurements in the coherent state basis $|\alpha\rangle$, which is called heterodyne measurements. Recall that the basis $|\alpha\rangle$ is not orthonormal and therefore such a measurement is not a projective measurement. Instead, it is a generalized measurement in the same spirit of Sec. 2.10. In particular, please recall Eqs. (2.166)-(2.168). In our case, the set of measurement operators are

$$M_\alpha = \frac{1}{\sqrt{\pi}}|\alpha\rangle\langle\alpha|. \tag{3.115}$$

They are appropriately normalized as

$$\int d^2\alpha\; M_\alpha^\dagger M_\alpha = \int \frac{d^2\alpha}{\pi}\;|\alpha\rangle\langle\alpha| = 1,$$

which is nothing but the completeness relation (3.94).

If outcome α is obtained, then the state after the measurement will collapse to $|\alpha\rangle\langle\alpha|$. And the probability of obtaining outcome α is, by Eq. (2.167),

$$\boxed{p_\alpha = \operatorname{tr} M_\alpha \rho M_\alpha^\dagger = \frac{1}{\pi}\langle\alpha|\rho|\alpha\rangle = Q(\alpha,\alpha^*).} \tag{3.116}$$

Thus, we see that the Husimi-Q function is nothing but the probability outcome if we were to perform a heterodyne measurement. This gives a nice interpretation to Q: whenever you see a plot of $Q(\alpha,\alpha^*)$ you can imagine "that is what I would get if I were to measure in the coherent state basis".

3.6 von Neumann's measurement model

In this section I want to use what we learned about continuous variables to discuss a more realistic measurement model. The calculations we are going to do here are a variation of an original proposal given by von Neumann. Suppose we have a system S that has been prepared in some state $|\psi\rangle$ and we wish to measure some observable K in this state. We write the eigenstuff of K as

$$K = \sum_k k|k\rangle\langle k|. \tag{3.117}$$

In order to measure this observable, what we are going to do is couple the system to an ancilla, consisting of a single continuous variable bosonic mode a, according to the interaction Hamiltonian

$$H = igK(a^\dagger - a). \tag{3.118}$$

This Hamiltonian represents a displacement of the bosonic mode which is proportional to the operator K. We could also do the same with $(a + a^\dagger)$ which looks more like a coordinate q. But doing it for $i(a^\dagger - a)$ turns out to be a bit simpler.

We assume the ancila starts in the vacuum so the initial state is

$$|\Phi(0)\rangle_{SA} = |\psi\rangle_S \otimes |0\rangle_A. \tag{3.119}$$

We then compute the time evolution of S+A under the interaction Hamiltonian (3.118). We will not worry here about the free part of the Hamiltonian. Including it would complicate the analysis, but will not lead to any new physics. Our goal then is to compute the state at time t

$$|\Phi(t)\rangle_{SA} = e^{-iHt}|\Phi(0)\rangle_{SA}. \tag{3.120}$$

To evaluate the matrix exponential we expand it in a Taylor series

$$e^{-iHt} = 1 - iHt + \frac{(-i)^2}{2}H^2t^2 + \dots$$

We now note that, using the eigenstuff (3.117), we can write (being a bit sloppy with the $\otimes$):

$$\begin{aligned}
H &= \sum_k |k\rangle\langle k|(igk)(a + a^\dagger),\\
H^2 &= \sum_k |k\rangle\langle k|(igk)^2(a + a^\dagger)^2,\\
&\vdots\\
H^n &= \sum_k |k\rangle\langle k|(igk)^n(a + a^\dagger)^n.
\end{aligned}$$

Thus we may write

$$e^{-iHt} = \sum_k |k\rangle\langle k| e^{gtk(a+a^\dagger)} = \sum_k |k\rangle\langle k| \otimes D(gtk), \tag{3.121}$$

where I introduced here displacement operator $D(\alpha_k) = e^{\alpha_k a^\dagger - \alpha_k^* a}$ [Eq. (3.74)].

It is now easy to apply the evolution operator to the initial state, as in Eq. (3.120). We simply get

$$|\Phi(t)\rangle_{SA} = \sum_k \Big(|k\rangle\langle k| \otimes D(gtk) \Big)\Big(|\psi\rangle_S \otimes |0\rangle_A \Big),$$

or

$$\boxed{|\Phi(t)\rangle_{SA} = \sum_k \big[\langle k|\psi\rangle\big]\; |k\rangle_S \otimes |gtk\rangle_A,} \tag{3.122}$$

where $|gtk\rangle_A = D(gtk)|0\rangle_A$ is the coherent state at position $\alpha = gtk$. This result is quite important. It says that after a time t the combined S+A system will be in an entangled state, corresponding to a superposition of the system being in $|k\rangle$ and the ancilla being in $|gtk\rangle$.

Reduced density matrix of the ancilla

Since the states $|k\rangle$ form an orthonormal basis, the reduced density matrix of the ancilla will be simply

$$\boxed{\rho_A(t) = \text{tr}_S\, |\Phi(t)\rangle\langle\Phi(t)| = \sum_k |\langle k|\psi\rangle|^2 |gtk\rangle\langle gtk|.} \tag{3.123}$$

This is just an incoherent combination of coherent states, with the coherent state $|gtk\rangle$ occurring with probability

$$p_k = |\langle k|\psi\rangle|^2. \tag{3.124}$$

The corresponding Q function will then be simply a sum of terms of the form (3.106):

$$\boxed{Q(\alpha,\alpha^*) = \frac{1}{\pi}\sum_k p_k\, e^{-|\alpha - gtk|^2}.} \tag{3.125}$$

To give an example, suppose our system is a spin 2 particle with dimension $d = 5$ and suppose that the eigenvalues k in Eq. (3.117) are some spin component which can take on the values $k = 2, 1, 0, -1, -2$ [there is nothing special about this example; I'm just trying to give an example that is not based on qubits!]. Suppose also that the state of the system was prepared in

$$|\psi\rangle = \frac{1}{2}\Big\{ |2\rangle - |1\rangle - |-1\rangle + |-2\rangle \Big\}, \tag{3.126}$$

where the states here refer to the basis $|k\rangle$ in (3.117). Some examples of the Q function for this state and different values of gt are shown in Fig. 3.7. Remember that the Q function represents a heterodyne detection on the ancilla. These examples show that

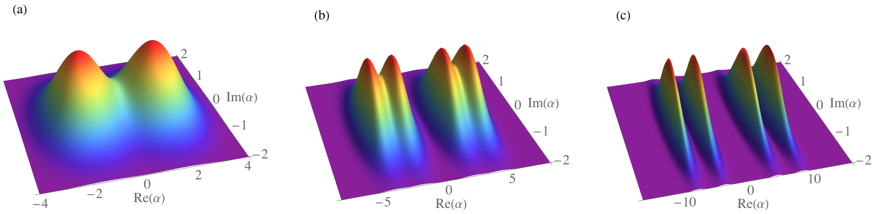

Figure 3.7: Example of the Q function (3.125) computed for the example state (3.126) for different values of gt. Namely (a) 1, (b) 2 and (c) 4.

if gt is small then the different peaks become blurred so such a measurement would not be able to appropriately distinguish between the different peaks. Conversely, as gt gets larger (which means a longer interaction time or a stronger interaction) the peak separation becomes clearer. Thus, the more S and A interact (or, what is equivalent, the more entangled they are) the larger is the amount of information that you can learn about S by performing a heterodyne detection on A.

Reduced density matrix of the system

Next let us compute the reduced density matrix of the system, staring with the composite state (3.122). We get

$$\rho_S(t) = \mathrm{tr}_A\,|\Phi(t)\rangle\langle\Phi(t)| = \sum_{k,k'}\Big(\langle k|\psi\rangle\langle\psi|k'\rangle\langle gtk|gtk'\rangle\Big)|k\rangle\langle k'|.$$

We can simplify this using the orthogonality relation between coherent states, Eq. (3.91), which gives

$$\langle gtk|gtk'\rangle = \exp\left\{-\frac{(gt)^2}{2}(k-k')^2\right\}.$$

Thus, the reduced density matrix of S becomes

$$\rho_S(t) = \sum_{k,k'}\rho_{k,k'}(t)|k\rangle\langle k'|, \tag{3.127}$$

where

$$\boxed{\rho_{k,k'}(t) = \langle k|\psi\rangle\langle\psi|k'\rangle\exp\left\{-\frac{(gt)^2}{2}(k-k')^2\right\}.} \tag{3.128}$$

Just as a sanity check, at $t = 0$ we recover the pure state $\rho_S(0) = |\psi\rangle\langle\psi|$.

What is really interesting about Eq. (3.128) is that the diagonal entries of ρ_S in the basis $|k\rangle$ are not effected:

$$\rho_{kk}(t) = \langle k|\psi\rangle\langle\psi|k\rangle = \rho_{k,k}(0). \tag{3.129}$$

Conversely, the off-diagonal coherences are exponentially damped and if we never turn off the S+A interaction we will eventually end up with

$$\lim_{t\to\infty} \rho_{k,k'}(t) = 0, \qquad k' \neq k. \tag{3.130}$$

Thus, the system initially started in a state $|\psi\rangle$ which was a superposition of the states $|k\rangle$. But, if we allow the system and ancilla to interact for a really long time, the system will end up in a incoherent mixture of states. It is also cool to note how the damping of the coherences is stronger for k and k' which are farther apart.

This analysis shows the emergence of a **preferred basis**. Before we turned on the S+A interaction, the system had no preferred basis. But once that interaction was turned on, the basis of the operator K, which is the operator we chose to couple to the ancila in Eq. (3.118), becomes a preferred basis, in the sense that populations and coherences behave differently in this basis.

Our model also allows us to interpolate between *weak measurements* and *strong measurements*. If gt is small then we perturb the system very little but we also don't learn a lot about it by measuring A. Conversely, if gt is large then we can learn a great deal more, but we also damage the system way more.

Conditional state given measurement outcome

Finally, let us analyze what happens if at time t we perform an actual heterodyne measurement with the operator set M_α in Eq. (3.115). Then if outcome α is obtained, the composite state of S+A will collapse so

$$|\Phi(t)\rangle\langle\Phi(t)| \to \frac{M_\alpha|\Phi(t)\rangle\langle\Phi(t)|M_\alpha^\dagger}{Q(\alpha,\alpha^*)}, \tag{3.131}$$

where I already used Eq. (3.116) to relate the outcome probability p_α with the Husimi function. After the measurement the ancilla will collapse to the coherent state $|\alpha\rangle\langle\alpha|$. Taking the partial trace of Eq. (3.131) over A we then get the reduced density matrix of S, given that the measurement outcome was α. I will leave the details of this calculation to you. The result is

$$\rho_{S|\alpha}(t) = \sum_{k,k'} \rho_{k,k'|\alpha}(t)|k\rangle\langle k'|, \tag{3.132}$$

where

$$\rho_{k,k'|\mu} = \frac{1}{\pi Q(\alpha,\alpha^*)}\langle k|\psi\rangle\langle\psi|k'\rangle\langle\alpha|gtk\rangle\langle gtk'|\alpha\rangle. \tag{3.133}$$

In particular, we can look at the diagonal elements $\rho_{k,k|\alpha}$

$$\rho_{k|\alpha}(t) = \frac{p_k e^{-|\alpha-gtk|^2}}{\sum\limits_{k'} p_{k'} e^{-|\alpha-gtk'|^2}}. \tag{3.134}$$

These quantities represent *the populations in the* $|k\rangle$ *basis, given that the measurement outcome was* α.

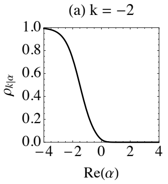

Figure 3.8: The conditional populations in Eq. (3.134) for the example state (3.126) and $gt = 1$.

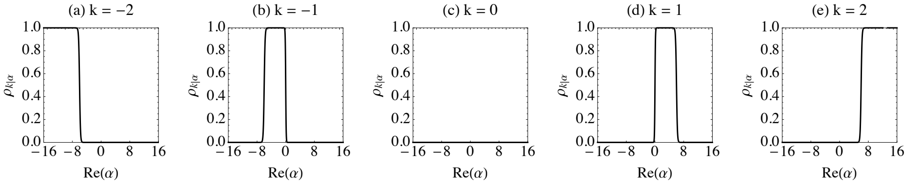

Figure 3.9: Same as Fig. 3.8 but for $gt = 4$.

An example of these conditional populations is shown in Fig. 3.8, which represent $\rho_{k|\alpha}$ for different values of k as a function of Re(α) for the example state (3.126). We can read this as follows. Consider Fig. 3.8(a), which represents $\rho_{-2|\alpha}$. What we see is that if Re(α) $\ll -2$ then it is very likely that the system is found in $k = -2$. Similarly, if Re(α) is around -2, as in Fig. 3.8(b), there is a large probability that the system is found in $k = -1$.

The results in Fig. 3.8 correspond to $gt = 1$ and therefore are not strong measurements. Conversely, in Fig. 3.9) we present the results for $gt = 4$. Now one can see a much shaper distinction of the probabilities. For instance, if Re(α) = 5 then it is almost certain that the system is in $k = 1$, as in Fig. 3.9(d).

3.7 Lindblad dynamics for the quantum harmonic oscillator

We already briefly touched upon the idea of a Lindblad master equation in Sec. 2.2, particularly in Eq. (2.22). The Lindblad master equation is a modification of von Neumann's equation to model *open quantum systems*. That is, the contact of the system with an external bath. Next chapter will be dedicated solely to open quantum systems. But here, I want to take another quick look at this problem, focusing on continuous variables. What I propose is to just show you what is the most widely used Lindblad equation in this case. Then we can just play with it a bit and get a feeling of what it means. The *derivation* of this master equation, together with a deeper discussion of what it means, will be done in the next chapter.

We return to the pumped cavity model described in Fig. 3.2. We assume the optical cavity contains only a single mode of radiation a, of frequency ω_c, which is pumped externally by a laser at a frequency ω_p. The Hamiltonian describing this system is given by Eq. (3.22):

$$H = \omega_c a^\dagger a + \epsilon a^\dagger e^{-i\omega_p t} + \epsilon^* a e^{i\omega_p t}. \tag{3.135}$$

In addition to this, we now include also the loss of photons through the semi-transparent mirror. This is modeled by the following master equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho] + D(\rho), \tag{3.136}$$

where $D(\rho)$ is called the **Lindblad dissipator** and is given by

$$D(\rho) = \gamma\Big[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\Big]. \tag{3.137}$$

Here $\gamma > 0$ is a constant which quantifies the loss rate of the cavity. Recall that the pump term ϵ in Eq. (3.135) was related to the laser power P by $|\epsilon|^2 = \gamma P/\hbar\omega_p$, which therefore depends on γ. This is related to the fact that the mechanism allowing for the photons to get in is the same that allows them to get out, which is the semi-transparent mirror. I should also mention that sometimes Eq. (3.137) is written instead with another constant, $\gamma = 2\kappa$. There is a sort of unspoken rule that if Eq. (3.137) has a 2 in front, the constant should be named κ. If there is no factor of 2, it should be named γ. If you ever want to be mean to a referee, try changing that order.

For qubits the dimension of the Hilbert space is finite so we can describe the master equation by simply solving for the density matrix. Here things are not so easy. Finding a general solution for any density matrix is a more difficult task. Instead, we need to learn alternative ways of dealing with (and understanding) this type of equation.

Before we do anything else, it is important to understand the meaning of the structure of the dissipator, in particular the meaning of a term such as $a\rho a^\dagger$. Suppose at $t = 0$ we prepare the system with certainty in a number state so $\rho(0) = |n\rangle\langle n|$. Then

$$D(|n\rangle\langle n|) = \gamma n\Big\{|n-1\rangle\langle n-1| - |n\rangle\langle n|\Big\}.$$

The first term, which comes from $a\rho a^\dagger$, represents a state with one photon less. This is precisely the idea of a *loss process*. But this process must also preserve probability, which is why we also have another term to compensate. The structure of the dissipator (3.137) represents a very finely tuned equation, where the system looses photons, but does so in such a way that the density matrix remains positive and normalized at all times. We also see from this result that

$$D(|0\rangle\langle 0|) = 0. \tag{3.138}$$

Thus, if you start with zero photons, nothing happens with the dissipator term . We say that the the vacuum is a **fixed point** of the dissipator (it is not necessarily a fixed point of the unitary evolution).

The case of zero pump, $\epsilon = 0$

Let us consider the case $\epsilon = 0$, so that the Hamiltonian (3.135) becomes simply $H = \omega_c a^\dagger a$. This means the photons can never be injected, but only lost. As a consequence, if our intuition is correct, the system should eventually relax to the vacuum. That is, we should expect that

$$\lim_{t\to\infty} \rho(t) = |0\rangle\langle 0|. \tag{3.139}$$

We are going to try to verify this in several ways. The easiest way is to simply verify that if $\rho^* = |0\rangle\langle 0|$ then

$$-i\omega_c[a^\dagger a, \rho^*] + D(\rho^*) = 0,$$

so the vacuum is indeed a steady-state of the equation. If it is unique (it is) and if the system will always converge to it (it will), that is another question.

Next let us look at the populations in the Fock basis

$$p_n = \langle n|\rho|n\rangle. \tag{3.140}$$

They represent the probability of finding the system in the Fock state $|n\rangle$. We can find an equation for $p_n(t)$ by sandwiching Eq. (3.136) in $\langle n|\ldots|n\rangle$. The unitary part turns out to give zero since $|n\rangle$ is an eigenstate of $H = \omega_c a^\dagger a$. As for $\langle n|D(\rho)|n\rangle$, I will leave for you to check that we get

$$\frac{\mathrm{d}p_n}{\mathrm{d}t} = \gamma\Big[(n+1)p_{n+1} - np_n\Big]. \tag{3.141}$$

This is called a **Pauli master equation** and is nothing but a **rate equation**, specifying how the population $p_n(t)$ changes with time. Positive terms increase p_n and negative terms decrease it. So the first term in Eq. (3.141) describes the increase in p_n due to populations coming from p_{n+1}. This represents the decays from higher levels. Similarly, the second term in Eq. (3.141) is negative and so describes how p_n decreases due to populations at p_n that are falling down to p_{n-1}.

The steady-state of Eq. (3.141) is obtained by setting $\mathrm{d}p_n/\mathrm{d}t = 0$, which gives

$$p_{n+1} = \frac{n}{n+1} p_n, \tag{3.142}$$

In particular, if $n = 0$ we get $p_1 = 0$. Then plugging this in $n = 1$ gives $p_2 = 0$ and so on. Thus, the steady-state correspond to all $p_n = 0$. The only exception is p_0 which, by normalization, must then be $p_0 = 1$.

Evolution of observables

Another useful thing to study is the evolution of observables, such as $\langle a\rangle$, $\langle a^\dagger a\rangle$, etc. Starting from the master equation (3.136), the expectation value of any observables is

$$\frac{\mathrm{d}\langle O\rangle}{\mathrm{d}t} = \mathrm{tr}\Big\{O\frac{\mathrm{d}\rho}{\mathrm{d}t}\Big\} = -i\,\mathrm{tr}\Big\{O[H,\rho]\Big\} + \mathrm{tr}\Big\{OD(\rho)\Big\}.$$

Rearranging the first term we may write this as

$$\frac{\mathrm{d}O}{\mathrm{d}t} = i\langle[H,O]\rangle + \mathrm{tr}\Big\{OD(\rho)\Big\}. \tag{3.143}$$

The first term is simply Heisenberg's equation (3.48) for the unitary part. What is new is the second term. It is convenient to write this as the trace of ρ times "something", so that we can write this as an expectation value. We can do this using the cyclic property of the trace:

$$\operatorname{tr}\left\{O\left[a\rho a^\dagger - \frac{1}{2}a^\dagger a\rho - \frac{1}{2}\rho a^\dagger a\right]\right\} = \langle a^\dagger O a - \frac{1}{2}a^\dagger a O - \frac{1}{2}O a^\dagger a\rangle. \tag{3.144}$$

Using this result for $O = a$ and $O = a^\dagger a$ gives, playing with the algebra a bit,

$$\operatorname{tr}\left\{a\mathcal{D}(\rho)\right\} = -\frac{\gamma}{2}\langle a\rangle, \qquad \operatorname{tr}\left\{a^\dagger a\mathcal{D}(\rho)\right\} = -\gamma\langle a^\dagger a\rangle. \tag{3.145}$$

Using these results in Eq. (3.143) then gives

$$\frac{\mathrm{d}\langle a\rangle}{\mathrm{d}t} = -(i\omega + \gamma/2)\langle a\rangle, \tag{3.146}$$

$$\frac{\mathrm{d}\langle a^\dagger a\rangle}{\mathrm{d}t} = -\gamma\langle a^\dagger a\rangle. \tag{3.147}$$

Thus, both the first and the second moments will relax exponentially with a rate γ, except that $\langle a\rangle$ will also oscillate:

$$\langle a\rangle_t = e^{-(i\omega+\gamma/2)t}\langle a\rangle_0, \tag{3.148}$$

$$\langle a^\dagger a\rangle_t = e^{-\gamma t}\langle a^\dagger a\rangle_0 \tag{3.149}$$

As $t \to \infty$ the average number of photons $\langle a^\dagger a\rangle$ tends to zero, no matter which state you begin at. Looking at a handful of observables is a powerful way to have an idea about what the density matrix is doing.

Evolution in the presence of a pump

Let us now go back to the full master Eq. (3.136). We can move to the interaction picture exactly as was done in Eq. (3.31), defining

$$\tilde{\rho}_t = S(t)\rho S^\dagger(t), \qquad S(t) = e^{i\omega_p t a^\dagger a}.$$

This transforms the Hamiltonian (3.135) into the detuned time-independent Hamiltonian (3.33):

$$\boxed{\tilde{H} = \Delta a^\dagger a + \epsilon a^\dagger + \epsilon^* a,} \tag{3.150}$$

where $\Delta = \omega_c - \omega_p$ is the detuning. Moreover, I will leave for you as an exercise to check that this does not change in any way the dissipative term. Thus, $\tilde{\rho}$ will evolve according to

$$\frac{\mathrm{d}\tilde{\rho}}{\mathrm{d}t} = -i[\tilde{H}, \tilde{\rho}] + D(\tilde{\rho}). \tag{3.151}$$

To get a feeling of what is going on, let us use Eq. (3.143) to compute the evolution of $\langle a\rangle$. Everything is identical, except for the new pump term that appears. As a result we get

$$\frac{\mathrm{d}\langle a\rangle}{\mathrm{d}t} = -(i\Delta + \gamma/2)\langle a\rangle - i\epsilon. \tag{3.152}$$

As before, $\langle a\rangle$ will evolve as a damped oscillation. However, now it will not tend to zero in the long-time limit, but instead will tend to

$$\langle a\rangle_{\mathrm{ss}} = -\frac{i\epsilon}{i\Delta + \gamma/2}. \tag{3.153}$$

I think this summarizes well the idea of a *pumped cavity*: the steady-state is a competition of how much we pump (unitary term) and how much we drain (the dissipator). Interestingly, the detuning Δ also affects this competition, so for a given ϵ and γ, we get more photons in the cavity if we are at resonance, $\Delta = 0$.

We can also try to ask the more difficult question of what is the density matrix ρ^* in the steady-state. It turns out it is a coherent state set exactly at the value of $\langle a\rangle$:

$$\tilde{\rho}^* = |\alpha\rangle\langle\alpha|, \qquad \alpha = -\frac{i\epsilon}{i\Delta + \gamma/2}. \tag{3.154}$$

One way to check this is to take the coherent state as an ansatz and then try to find what is the value of α which solves Eq. (3.151). The average number of photons will then be

$$\langle a^\dagger a\rangle = |\alpha|^2 = \frac{\epsilon^2}{\Delta^2 + \gamma^2/4}. \tag{3.155}$$

The purpose of this section was to show you a practical use of master equations and open quantum systems. This "cavity loss" dissipator is present in literally every quantum optics setup which involves a cavity. In fact, I know of several papers which sometimes even forget to tell that this dissipator is there, but it always is. We will now turn to a more detailed study of open quantum systems.

Chapter 4

Open quantum systems

4.1 Quantum operations

Let's go back for a second to the basic postulates of quantum mechanics. Recall that when we first establish the theory, we begin by postulating that a system can be represented by an abstract state $|\psi\rangle$. Then we also postulate that the time evolution of $|\psi\rangle$ must be given by a **map** which is (i) linear and (ii) preserves probability, $\langle\psi_t|\psi_t\rangle =$ const. This is the entry point for the **unitaries**: any evolution in quantum mechanics can be represented by a unitary operator

$$|\psi\rangle \to |\psi'\rangle = U|\psi\rangle. \tag{4.1}$$

However, after a while we realized that the state $|\psi\rangle$ is not the most general state of a system. Instead, the general state is the density matrix ρ.

We can then rethink the evolution postulate: *what is the most general evolution which is (i) linear and (ii) maps density matrices into density matrices?* We already saw that unitary evolutions are translated to density matrices as maps of the form

$$\rho \to \rho' = U\rho U^\dagger. \tag{4.2}$$

This is certainly a linear map and if ρ is a valid density matrix, then so will ρ'. But is it the most general kind of map satisfying these properties? The answer is no. The most general map is actually called a **quantum operation**, $\mathcal{E}(\rho)$, and has the form:

$$\boxed{\rho \to \rho' = \mathcal{E}(\rho) = \sum_k M_k \rho M_k^\dagger, \qquad \text{with} \qquad \sum_k M_k^\dagger M_k = 1.} \tag{4.3}$$

This way of representing the map $\mathcal{E}(\rho)$ in terms of a set of operators M_k is called the **operator-sum representation**. If there is only one M_k then it must be unitary and we recover (4.2). A set of operators $\{M_k\}$ satisfying $\sum_k M_k^\dagger M_k = 1$ are called **Kraus operators**.

The take-home message I want you to keep is that quantum operations are *the* most general evolution map a density matrix can have. This chapter will be all about quantum operations and their ramifications, so we will have quite a lot to discuss about this. But for now let us start slow. In this section we will do two things: first I will show you that quantum operations are the natural language for describing *open quantum systems*. Any evolution of a system connected to an external environment can be written as a quantum operation. Second, we will prove the claim surrounding Eq. (4.3); that is, that any linear map which takes density matrices into density matrices can be written in the form (4.3).

Example: amplitude damping

Consider a qubit system and let

$$M_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\lambda} \end{pmatrix}, \qquad M_1 = \begin{pmatrix} 0 & \sqrt{\lambda} \\ 0 & 0 \end{pmatrix}, \tag{4.4}$$

with $\lambda \in [0,1]$. This is a valid set of Kraus operators since $M_0^\dagger M_0 + M_1^\dagger M_1 = 1$. Its action on a general qubit density matrix reads:

$$\rho = \begin{pmatrix} p & q \\ q^* & 1-p \end{pmatrix} \to \rho' = \begin{pmatrix} \lambda + p(1-\lambda) & q\sqrt{1-\lambda} \\ q^*\sqrt{1-\lambda} & (1-\lambda)(1-p) \end{pmatrix}. \tag{4.5}$$

If $\lambda = 0$ nothing happens, $\rho' = \rho$. Conversely, if $\lambda = 1$ then

$$\rho \to \rho' = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{4.6}$$

This is why this is called an **amplitude damping**: no matter where you start, the map tries to push the system towards $|0\rangle$. It does so by destroying coherences, $q \to q\sqrt{1-\lambda}$, and by affecting the populations, $p \to \lambda + p(1-\lambda)$. The larger the value of λ, the stronger is the effect.

Amplitude damping from a master equation

Consider a quantum master equation of the form

$$\frac{d\rho}{dt} = \gamma\Big[\sigma_+\rho\sigma_- - \frac{1}{2}\{\sigma_+\sigma_-, \rho\}\Big]. \tag{4.7}$$

We have briefly touched upon this type of equation in Secs. 2.2 and 3.7. And we will have a lot more to say about it below. Applying this equation to a general density matrix yields the pair of equations

$$\frac{dp}{dt} = \gamma(1-p) \qquad \to \qquad p(t) = p_0 e^{-\gamma t} + (1 - e^{-\gamma t}),$$

$$\frac{dq}{dt} = -\frac{\gamma q}{2} \qquad \to \qquad q(t) = q_0 e^{-\gamma t/2}.$$

Comparing this with Eq. (4.5) we see that the solution of the differential Eq. (4.7) can be viewed, at any given time t, as a map

$$\rho(t) = \sum_k M_k \rho(0) M_k^\dagger, \tag{4.8}$$

with the same Kraus operators (4.4) and

$$\lambda = 1 - e^{-\gamma t}. \tag{4.9}$$

If $t = 0$ then $\lambda = 0$ and nothing happens. If $t \to \infty$ then $\lambda \to 1$ and the system collapses completely towards $|0\rangle$, as in Eq. (4.6).

Amplitude damping from system-environment interactions

Let us now label our system S and suppose it interacts with an *environment ancilla* E by means of the Hamiltonian

$$H = g(\sigma_+^S \sigma_-^E + \sigma_-^S \sigma_+^E), \tag{4.10}$$

where g is some parameter. The corresponding unitary evolution matrix will be

$$U = e^{-iHt} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos gt & -i\sin gt & 0 \\ 0 & -i\sin gt & \cos gt & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{4.11}$$

Suppose that the ancila starts in the state $|0\rangle_E$ whereas the system starts in an arbitrary state ρ_S. Then we compute

$$\rho'_{SE} = U\Big[\rho_S \otimes |0\rangle_E\langle 0|\Big]U^\dagger,$$

and finally take the partial trace over E to obtain $\rho'_S = \mathrm{tr}_E\, \rho'_{SE}$. I will leave this task for you as an exercise. The result is

$$\rho'_S = \begin{pmatrix} p + (1-p)\sin^2(gt) & q\cos(gt) \\ q^*\cos(gt) & (1-p)\cos^2(gt) \end{pmatrix}. \tag{4.12}$$

Comparing this with the amplitude damping result (4.5) we see that this is also a quantum operation, again with the same Kraus operators (4.4), but with

$$\lambda = \sin^2(gt). \tag{4.13}$$

Thus, the evolution of two qubits, when viewed from the perspective of only one of them, will behave like a quantum operation. But unlike in the master equation example above, here the amplitude damping parameter λ will not increase monotonically, but will rather oscillate in time. If you happen to interrupt the evolution when gt is an integer multiple of π then it will look like a complete damping. But if we wait a bit longer it will seem that less damping occurred. This is what happens when the environment is small (in this case it is only one qubit). If your environment had 10^{23} qubits, which is what Eq. (4.7) tries to model, you would not observe these revivals.

Amplitude damping and spontaneous emission

The amplitude damping process is also what happens if you have an atom in the excited state interacting with the electromagnetic vacuum. In this case, the atom may fall down to the ground-state and emit a photon, a process we call spontaneous emission. To have a toy model to describe this, suppose that the atom only interacts with one mode of the electromagnetic field, whose frequency ω matches that of the atom Ω. In that case the Hamiltonian reduces to the resonant Jaynes-Cummings model [cf. Eq. (3.23)].

$$H = \Omega a^\dagger a + \frac{\Omega}{2}\sigma_z + g(a^\dagger\sigma_- + a\sigma_+). \tag{4.14}$$

In the resonant case we can move to the interaction picture and still get a time-independent Hamiltonian

$$\tilde{H} = g(a^\dagger\sigma_- + a\sigma_+). \tag{4.15}$$

Suppose now that the electromagnetic mode starts in the vacuum, $|0\rangle_E$, whereas the atom starts in an arbitrary state ρ_S. In principle, this Hamiltonian will act on the full Hilbert space, which is spanned by $|0,n\rangle_{SE}$ and $|1,n\rangle_{SE}$, where $n = 0, 1, 2, \ldots$ is the number of photons in the mode a. But since the Jaynes-Cummings Hamiltonian preserves the total number of quanta [Eq. (3.24)] and since the electromagnetic mode started in the vacuum, at any time there will be either 0 or 1 photons in the mode. Thus, the only basis elements that will matter to us are $|0,0\rangle_{SE}$, $|0,1\rangle_{SE}$ and $|1,0\rangle_{SE}$.

The matrix elements of $\tilde{H}$ in these states are

$$\tilde{H} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & g \\ 0 & g & 0 \end{pmatrix}.$$

Hence, the time-evolution operator will be

$$U = e^{-i\tilde{H}t} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(gt) & -i\sin(gt) \\ 0 & -i\sin(gt) & \cos(gt) \end{pmatrix}. \tag{4.16}$$

I wrote down this result just so you could have a look at it. But the truth is we don't need it. Since we are restricting the dynamics to this sub-space, the problem is exactly identical to that generated by the Hamiltonian (4.10) (except for a phase factor, which makes no difference). Indeed, if you now repeat the steps of computing ρ_{SE}' and then ρ_S', you will find as a result *exactly* the state (4.12).

This example serves to show that many Hamiltonians may lead to the same quantum operation. The quantum operation describes a dynamical evolution from the perspective of the system's density matrix and has *no information* on what exactly generated that evolution. It could have been one qubit, one electromagnetic mode, 10^{23} water molecules in a bucket of water or a swarm of killer bees armed with machine guns. From the perspective of the *map*, they may all lead to the same result.

The above paragraph is a common source of confusion. You may immediately protest and say "How can a one qubit environment lead to the same evolution as a 10^{23}-atom environment?". They don't! They lead to the same *map*, not the same evolution. That's the point. If we analyze the evolution as a function of time, both will be completely different. But if we are only interested in the map that takes you from one state to another, then this map can be engineered by a single qubit or by 10^{23} of them.

Proof of the operator-sum representation

After this warm-up, we are now ready to prove Eq. (4.3). But let us be very precise on what we want to prove. We define $\mathcal{E}(\rho)$ as a map satisfying

1. Linearity: $\mathcal{E}(\alpha\rho_1 + \beta\rho_2) = \alpha\mathcal{E}(\rho_1) + \beta\mathcal{E}(\rho_2)$.
2. Trace preserving: $\text{tr}[\mathcal{E}(\rho)] = \text{tr}(\rho)$.
3. Completely positive: if $\rho \geq 0$ then $\mathcal{E}(\rho) \geq 0$.

There is a subtle difference between a map that is positive and a map that is *completely* positive. Completely positive means $\mathcal{E}(\rho) \geq 0$ even if ρ is a density matrix living in a larger space than the one $\mathcal{E}$ acts on. For instance, suppose $\mathcal{E}$ acts on the space of a qubit. But the ρ it is acting on could mean the density matrix of 2 entangled qubits, even though the map acts on only one of them. If even in this case the resulting ρ' is positive semi-definite, we say it is completely positive.[1] A map satisfying properties 1, 2 and 3 above is called a **Completely Positive Trace Preserving (CPTP) map**.

Our goal is now to show that any CPTP map can be written as an operator-sum representation [Eq. (4.3)] for some set of operators $\{M_k\}$. The proof of this claim is usually based on a powerful, yet abstract, idea related to what is called the *Choi isomorphism*. Let S denote the space where our map $\mathcal{E}$ acts and define an auxiliary space R which is an exact copy of S. Define also the (unnormalized) Bell state

$$|\Omega\rangle = \sum_i |i\rangle_R \otimes |i\rangle_S, \tag{4.17}$$

where $|i\rangle$ is an arbitrary basis and from now on I will always write the R space in the left and the S space in the right. We now construct the following operator:

$$\boxed{\Lambda_{\mathcal{E}} = (\mathcal{I}_R \otimes \mathcal{E}_S)(|\Omega\rangle\langle\Omega|).} \tag{4.18}$$

This is called the **Choi matrix** of the map $\mathcal{E}$. Note how it is like a density operator. It is the outcome of applying the map $\mathcal{E}_S$ on one side of the maximally entangled Bell state of R+S.

The most surprising thing about the Choi matrix is that it completely determines the map $\mathcal{E}$. That is, if we somehow learn how our map $\mathcal{E}$ acts on $|\Omega\rangle\langle\Omega|$ we have completely determined how it will act on *any* other density matrix. This is summarized by the following formula:

$$\mathcal{E}(\rho) = \text{tr}_R\Big\{(\rho^{\text{T}} \otimes I_S)\Lambda_{\mathcal{E}}\Big\}. \tag{4.19}$$

---

[1] There aren't many examples of maps that are positive but not completely positive. The only example I know is the partial trace (see, for instance, Box 8.2 of Nielsen and Chuang).

I know what you are thinking: this is really weird! Yes, it is. But it is true. Note that here ρ^{T} is placed on the auxiliary space R in which the trace is being taken. Consequently, the result on the left-hand side is still an operator living on S. To verify that Eq. (4.19) is true we first rewrite (4.18) as

$$\Lambda_E = \sum_{i,j} |i\rangle_R\langle j| \otimes \mathcal{E}(|i\rangle\langle j|). \tag{4.20}$$

Then we get

$$\begin{aligned}
\mathrm{tr}_R\Big\{(\rho^{\mathrm{T}} \otimes I_S)\Lambda_{\mathcal{E}}\Big\} &= \sum_{i,j} \mathrm{tr}_R\Big\{(\rho^{\mathrm{T}} \otimes I_S)\Big[|i\rangle\langle j| \otimes \mathcal{E}(|i\rangle\langle j|)\Big]\Big\} \\
&= \sum_{i,j} \langle j|\rho^{\mathrm{T}}|i\rangle \mathcal{E}(|i\rangle\langle j|) \\
&= \mathcal{E}\Big(\sum_{i,j} \rho_{i,j}|i\rangle\langle j|\Big) \\
&= \mathcal{E}(\rho).
\end{aligned}$$

Here I used the fact that $\langle j|\rho^{\mathrm{T}}|i\rangle = \langle i|\rho|j\rangle = \rho_{i,j}$. Moreover, I used our assumption that $\mathcal{E}$ is a linear map.

We are now in the position to prove our claim. As I mentioned, the Choi matrix looks like a density matrix on R+S. In fact, we are assuming that our map $\mathcal{E}$ is CPTP. Thus, since $|\Omega\rangle\langle\Omega|$ is a positive semi-definite operator, then so will $\Lambda_{\mathcal{E}}$ (although it will not be normalized). We may then diagonalize $\Lambda_{\mathcal{E}}$ as

$$\Lambda_{\mathcal{E}} = \sum_k \lambda_k |\lambda_k\rangle\langle\lambda_k|,$$

where $|\lambda_k\rangle$ are vectors living in the big R+S space and $\lambda_k \geq 0$. For the purpose of what we are going to do next, it is convenient to absorb the eigenvalues into the eigenvectors (which will no longer be normalized) and define

$$\Lambda_{\mathcal{E}} = \sum_k |m_k\rangle\langle m_k|, \qquad |m_k\rangle = \sqrt{\lambda_k}|\lambda_k\rangle, \tag{4.21}$$

Note that here CPTP is crucial because it implies that $\lambda_k \geq 0$ so that $\langle m_k| = \langle\lambda_k|\sqrt{\lambda_k}$. To finish the proof we insert this into Eq. (4.19) to get

$$\mathcal{E}(\rho) = \sum_k \mathrm{tr}_R\Big\{(\rho^{\mathrm{T}} \otimes I_S)|m_k\rangle\langle m_k|\Big\}. \tag{4.22}$$

The right-hand side will still be an operator living in S, since we only traced over R. All we are left to do is convince ourselves that this will have the shape of the operator-sum representation in Eq. (4.3).

To do that things will get a little nasty. The trick is to connect the states $|m_k\rangle$ of the Choi matrix $\Lambda_{\mathcal{E}}$ with the Kraus operators M_k appearing in the operator-sum representation (4.3):

$$\mathcal{E}(\rho) = \sum_k M_k\rho M_k^\dagger.$$

This is done by noting that since $|m_k\rangle$ lives on the R+S space, it can be decomposed as

$$|m_k\rangle = \sum_{i,j} (M_k)_{j,i} |i\rangle_R \otimes |j\rangle_S, \tag{4.23}$$

where $(M_k)_{j,i}$ are a set of coefficients which we can interpret as a matrix M_k. To establish this connection we first manipulate (4.22) to read

$$\mathcal{E}(\rho) = \sum_k \sum_{i,j} {}_R\langle i|\rho^{\mathrm{T}}|j\rangle_R \, {}_R\langle j|m_k\rangle\langle m_k|i\rangle_R.$$

Then we insert Eq. (4.23) to find

$$\begin{aligned}\mathcal{E}(\rho) &= \sum_k \sum_{i,j} \sum_{i',j'} \rho_{j,i} (M_k)_{j',j} (M_k^*)_{i',i} |j'\rangle\langle i'| \\ &= \sum_k \sum_{i,j} \sum_{i',j'} |j'\rangle\langle j'|M_k|j\rangle\langle j|\rho|i\rangle\langle i|M_k^\dagger|i'\rangle\langle i'|. \\ &= \sum_k M_k \rho M_k^\dagger,\end{aligned}$$

and voilá!

In conclusion, we have seen that any map which is linear and CPTP can be described by an operator-sum representation, Eq. (4.3). I like this a lot because we are not asking for much: linearity and CPTP is just the *basic* things we expect from a physical map. Linearity should be there because everything in quantum mechanics is linear and CPTP must be there because the evolution must map a physical state into a physical state. When we first arrived at the idea of a unitary, we were also very relaxed because all we required was the conservation of ket probabilities. The spirit here is the same. For this reason, the quantum operation is really just a very natural and simplistic generalization of the evolution of quantum systems, using density matrices instead of kets.

4.2 Stinespring dilations

In the previous section we defined quantum operations based on the idea of a general map that takes density matrices to density matrices. We also showed that these maps may arise in different circumstances, such as from a master equation or from the unitary interaction of a qubit with a one-qubit environment. This last idea is very powerful and is related to the concept of a **dilation**. That is, the representation of a quantum operation as larger unitary between our system and some environment, as illustrated in Fig. 4.1. It turns out that this dilation idea is always possible and it works in both ways:

- Given a S+E unitary, the corresponding map in terms of S will be given by a quantum operation.

- Given a quantum operation, we can always find a global S+E unitary representing it (in fact, there is an infinite number of such unitaries, as we will see).

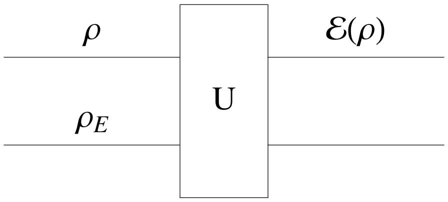

Figure 4.1: Idea behind a Stinespring dilation: a quantum operation $\mathcal{E}(\rho)$ can always be constructed by evolving the system together with an environment, with a global unitary U, and then discarding the environment.

More precisely, a dilation is described as follows. Our quantum system, with density matrix ρ, is put to interact via a global unitary U with an environment (which can be of any size) having an initial density matrix ρ_E. After the interaction we throw away the environment. The result, from the perspective of the system, is a quantum operation. This can be summarized by the expression:

$$\boxed{\mathcal{E}(\rho) = \text{tr}_E \Big\{ U(\rho \otimes \rho_E) U^\dagger \Big\}.} \tag{4.24}$$

We will now demonstrate that this is indeed a quantum operation.

Top-down, easy case

Let $|e_k\rangle$ denote a basis for the enviroment. To warm up assume the initial state of the environment is pure, $\rho_E = |e_0\rangle\langle e_0|$. Then Eq. (4.24) becomes

$$\mathcal{E}(\rho) = \sum_k \langle e_k|U\rho|e_0\rangle\langle e_0|U^\dagger|e_k\rangle,$$

which is similar to a calculation we did in Sec. 2.10. Since ρ and $|e_0\rangle$ live on different Hilbert spaces, we may define[2]

$$\boxed{M_k = \langle e_k|U|e_0\rangle,} \tag{4.25}$$

with which we arrive at the usual formula for a quantum operation.

$$\mathcal{E}(\rho) = \sum_k M_k \rho M_k^\dagger. \tag{4.26}$$

---

[2] Remember that what this formula really means is

$$M_k = \Big[1_S \otimes \langle e_k|\Big] U \Big[1_S \otimes |e_0\rangle\Big].$$

We can also check that the M_k in Eq. (4.25) form a valid set of Kraus operators:

$$\sum_k M_k^\dagger M_k = \sum_k \langle e_0|U^\dagger|e_k\rangle\langle e_k|U^\dagger|e_0\rangle = 1$$

Each term in this sum cancelled sequentially: first a completeness relation of the $|e_k\rangle$, then the unitarity of U, then $\langle e_0|e_0\rangle = 1$. The result is still an identity on the space of S.

Top-down, general case

It turns out that the assumption that the environment started in a pure state is not at all restrictive. After all, we can always *purify* the mixed state ρ_E. That is, we can always say the environment actually lives on a larger Hilbert space in which its state is pure. Notwithstanding, it is still useful, from a practical point of view, to generalize (4.25) for general mixed states. In this case the trick is to choose the environment basis $|e_k\rangle$ as the eigenbasis of ρ_E. That is,

$$\rho_E = \sum_k p_k|e_k\rangle\langle e_k|.$$

We now write Eq. (4.24) as

$$\mathcal{E}(\rho) = \sum_{k,q}\langle e_k|U\rho p_q|e_q\rangle\langle e_q|U^\dagger|e_k\rangle.$$

And, instead of (4.25), we define the Kraus operators as

$$M_{k,q} = \sqrt{p_q}\langle e_k|U|e_q\rangle. \tag{4.27}$$

Then the map becomes

$$\mathcal{E}(\rho) = \sum_{k,q} M_{k,q}\rho M_{k,q}^\dagger. \tag{4.28}$$

At first it seems we are cheating a bit because we have two indices. But if we think about (k, q) as a collective index α, then we go back to the usual structure of the quantum operation.

Bottom-up

Now let's go the other way around. Suppose we are given a quantum operation of the form (4.26), with a given set of Kraus operators $\{M_k\}$. We then ask how to construct a global S+E unitary with some environment E, such as to reproduce this quantum operation. That turns out to be quite simple.

First let us ask what should be the dimension of the environment. If we had a vector of dimension d, we all now that the most general linear operation would be given by a $d \times d$ matrix. In our case our system has dimensions d, but we want operations on a density matrix, which is already a $d \times d$ matrix. However, recall that matrices also form a vector space, so the quantum operation can be thought of as an operation on a vector with d^2 entries. The only point is that this vector is displaced like a matrix, so things become messy because we have to multiply it on both sides. Notwithstanding, we can infer from this argument that we need at most d^2 Kraus operators M_k in order to fully describe a quantum operation. But we have already seen from Eq. (4.25) that the number of k values is related to the number of basis elements $|e_k\rangle$ of the environment. Hence, we conclude that *any quantum operation on a d-dimensional system may be reproduced by a dilation with an environment of dimension* d^2. This fact is quite remarkable. In many cases we are interested in what happens when a system S interacts with a very large environment E. But this argument shows that, as far as the map is concerned, we can always reproduce it with an environment that is only d^2.

Suppose now that the environment starts in some state $|e_0\rangle$. We then construct a unitary U such as to obtain the Kraus operators in Eq. (4.25). This unitary is more easily mocked up if we consider the Hilbert space structure $\mathcal{H}_E \otimes \mathcal{H}_S$ (that is, the environment on the left). Then the unitary that does the job can be written in Block form as

$$U = \begin{pmatrix} M_0 & \dots & \dots & \dots \\ M_1 & \dots & \dots & \dots \\ M_2 & \dots & \dots & \dots \\ \vdots & \dots & \dots & \dots \\ M_{d^2-1} & \dots & \dots & \dots \end{pmatrix}. \tag{4.29}$$

where the remainder of the matrix should be filled with whatever it needs to make U an actual unitary. The reason why this works is actually related all the way back to the matrix definition of the Kronecker product, Eq. (2.43). The operator M_k is just the matrix element $U_{k,0}$ in the basis of the environment.

As an example, consider the unitary in the two-qubit example (4.11). In this case the left blocks are

$$M_0 = \begin{pmatrix} 1 & 0 \\ 0 & \cos(gt) \end{pmatrix}, \qquad M_1 = \begin{pmatrix} 0 & -i\sin(gt) \\ 0 & 0 \end{pmatrix}.$$

This is the same as the amplitude damping Kraus operators in Eq. (4.4), with $\lambda = \sin^2(gt)$ [Eq. (4.13)]. There is an extra weird factor of i, but that doesn't matter because it vanishes when we do $M_1\rho M_1^\dagger$.

Interpretation in terms of measurements

There is a nice way to picture a quantum operation within this Stinespring dilation setting. You of course noticed that what we are doing here is somewhat similar to the generalized measurement scenario discussed in Sec. 2.10. In fact, there we said that a generalized measurement was also described by a set of Kraus operators $\{M_k\}$ and was such that the probability of obtaining measurement outcome k was

$$p_k = \operatorname{tr}(M_k\rho M_k^\dagger).$$

Moreover, if outcome k was obtained, the state would collapse to

$$\rho \to \rho_k = \frac{M_k\rho M_k^\dagger}{p_k}.$$

We can therefore interpret a quantum operation of the form (4.26) as

$$\mathcal{E}(\rho) = \sum_k M_k \rho M_k^\dagger = \sum_k p_k \rho_k.$$

That is, we can view it as just a random sampling of states ρ_k with probability p_k. The total effect of the quantum operation is a convex combinations of the possible outcomes with different probability weights. Of course, we don't really need to do a measurement. Is just how the system behaves from the eyes of S.

Freedom in the operator-sum representation

There is a reason why we distinguish between the terms "quantum operation" and "operator-sum representation". As the name of the latter implies, when we write a quantum operation in terms of the Kraus operators, like in Eq. (4.26), we are really introducing a *representation* for the map. And the point I wish to make now is that this representation is not unique: there is a freedom in how we choose the Kraus operators which lead to the same quantum operation. The same happens for unitaries: two unitaries U and $U' = e^{i\theta} U$ are physically equivalent so multiplying by a global phase changes nothing. For quantum operations the freedom is even larger.

Let $\{M_k\}$ be a set of Kraus operators and consider the quantum operation (4.26). Now define a new set of Kraus operators $\{N_\alpha\}$ as

$$\boxed{N_\alpha = \sum_k V_{\alpha,k} M_k, \qquad M_k = \sum_\alpha V^*_{\alpha,k} N_\alpha,} \tag{4.30}$$

where V is a unitary matrix.[3] Substituting (4.30) in (4.26) we find

$$\mathcal{E}(\rho) = \sum_{k,\alpha,\beta} V^*_{\alpha,k} V_{\beta,k} N_\alpha \rho N_\beta^\dagger.$$

The trick now is to do the sum over k first. Since V is unitary

$$\sum_k V^*_{\alpha,k} V_{\beta,k} = \sum_k V_{\beta,k} (V^\dagger)_{k,\alpha} = \delta_{\beta,\alpha}.$$

Hence we conclude that

$$\mathcal{E}(\rho) = \sum_k M_k \rho M_k^\dagger = \sum_\alpha N_\alpha \rho N_\alpha^\dagger. \tag{4.31}$$

Thus, *two sets of Kraus operators connected by a unitary transformation lead to the same quantum operation.* It is cool that this even works when the two sets have a

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[3] I know this can sound strange at first. Here M_k are operators (maybe there are 7 of them). But we can arrange them to form a list. What we are doing is writing each element in this list as a linear combination of another set of operators N_α. However, we are choosing the coefficients of this linear combinations $V_{k,\alpha}$ to form a unitary matrix, $VV^\dagger = V^\dagger V = 1$.

different number of elements. For instance, suppose $\{M_k\}$ has 5 elements, $M_0, \ldots, M_4$, and $\{N_\alpha\}$ has 3 elements, $N_0, \ldots, N_2$. Then we can add to the list $\{N_\alpha\}$ two zero elements $N_3 = 0$ and $N_4 = 0$. Now both have the same number of elements and we can construct a unitary connecting the two sets.

The next interesting question is what is the origin of this freedom. It turns out it is related to local operations on the environment. Recall that, as shown in Eq. (4.25), $M_k = \langle e_k|U|e_0\rangle$. Now suppose that before we finish the evolution, we perform a unitary $V_E \otimes 1_S$ on the environment. Then the new set of Kraus operators will be

$$N_\alpha = \langle e_\alpha|(V\otimes 1)U|e_0\rangle = \sum_k \langle e_\alpha|V|e_k\rangle\langle e_k|U|e_0\rangle = \sum_k V_{\alpha,k}M_k,$$

which is exactly Eq. (4.30). Thus, we can view this freedom of choice as a sort of "post-processing" on the environment, which has no effect on the system.

Partial trace as a quantum operation

So far we have considered quantum operations that map a given Hilbert space to the same space. However, the entire framework generalizes naturally to maps taking a density matrix in a given subspace $\mathcal{H}_1$ to another subspace $\mathcal{H}_2$. In this case all that changes is that the condition on Kraus operators become

$$\sum_k M_k^\dagger M_k = I_1 \tag{4.32}$$

That is, with the identity being on the space $\mathcal{H}_1$. An example of such an operation is the partial trace. Suppose our system S is actually a bipartite system AB. The partial trace over B is written, as we know, as

$$\mathrm{tr}_B(\rho) = \sum_k \langle b_k|\rho|b_k\rangle = \sum_k (1_A\otimes\langle b_k|)\rho(1_A\otimes|b_k\rangle). \tag{4.33}$$

If we define the Kraus operators

$$\boxed{M_k = 1_A\otimes\langle b_k|,} \tag{4.34}$$

then the partial trace can be identified with the quantum operation

$$\mathrm{tr}_B(\rho) = \sum_k M_k\rho M_k^\dagger. \tag{4.35}$$

Moreover we see that

$$\sum_k M_k^\dagger M_k = \sum_k 1_A\otimes|b_k\rangle\langle b_k| = 1_{AB}.$$

That is, the identity on the original space.

We can also do the opposite. That is, we can define a quantum operation which *adds* a state to the system. For instance, suppose we have a system S and we want to add an environment ancilla E in a state $|e_0\rangle$. Then we can define the Kraus operators

$$M_0 = 1_S \otimes |e_0\rangle_E. \tag{4.36}$$

The corresponding quantum operation will then be

$$M_0 \rho M_0^\dagger = \rho \otimes |e_0\rangle\langle e_0|. \tag{4.37}$$

Moreover,

$$M_0^\dagger M_0 = 1_S\,.$$

Of course, if we want to add an ancilla in a more general state, all we need to do is construct a larger set of Kraus operators. With these ideas we can actually cover all types of quantum operations. That is, any map can always be described by quantum operations mapping the same Hilbert space, combined with partial traces and adding ancillas.

4.3 Lindblad master equations

We have seen that a quantum operation is the most general map taking density matrices to density matrices. But sometimes maps are not so useful and it is better to have a differential equation for $\rho(t)$. That is, something like

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \mathcal{L}(\rho), \tag{4.38}$$

where $\mathcal{L}(\rho)$ is some linear superoperator (a superoperator is just an operator acting on an operator). It is also customary to call $\mathcal{L}(\rho)$ the **Liouvillian** because of the analogy between Eq. (4.38) and the Liouville equation appearing in classical mechanics. An equation of the form (4.38) is also historically known as a **master equation**, a name which was first introduced in a completely different problem,[4] but is supposed to mean an equation from which all other properties can be derived from.

We may then ask the following question: *"Given an initial genuine density matrix* $\rho(0)$*, what is the general structure a Liouvillian* $\mathcal{L}$ *must have in order to ensure that the solution* $\rho(t)$ *of Eq. (4.38) will also be a genuine density matrix at all times* t*?"* Putting it differently, suppose we happen to solve Eq. (4.38). Then the solution will be given by some linear map of the form

$$\rho(t) = \mathcal{V}_t(\rho(0)). \tag{4.39}$$

where $\mathcal{V}_t$ is some superoperator. What we then really want is for $\mathcal{V}_t$ to be a quantum operation at all times t. If that is the case we say the master equation is CPTP (because the map it generates is CPTP).

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[4] A. Nordsieck, W. E. Lamb and G. T. Uhlenbeck, *Physica*, **7**, 344 (1940).

Eq. (4.38) has the form of a linear equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = Ax. \tag{4.40}$$

Equations of this form always have the property of being *divisible*. That is, the solution from $t = 0$ to $t = t_2$ can always be split into a solution from $t = 0$ to $t = t_1$ and then a solution from $t = t_1$ to $t = t_2$. Consequently, this implies that $\mathcal{V}_t$ must satisfy the *semigroup property*:[5]

$$\mathcal{V}_{t_2}\mathcal{V}_{t_1} = \mathcal{V}_{t_2+t_1}. \tag{4.41}$$

Semigroup is therefore implied by the structure of Eq. (4.38). We can then ask, when can a semigroup map be CPTP? Quite remarkably, just by imposing these two properties one can determine a very specific structure for the Liouvillian ρ. This is the content of **Lindblad's theorem**:[6] *The generator of any quantum operation satisfying the semigroup property must have the form:*

$$\boxed{\mathcal{L}(\rho) = -i[H,\rho] + \sum_k \gamma_k\Big[L_k\rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k,\rho\}\Big],} \tag{4.42}$$

where H is a Hermitian operator, L_k are arbitrary operators and $\gamma_k \geq 0$. Master equations having this structure are then called Linbdlad equations or, more generally, Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) equations. If you have any equation satisfying this structure, then the corresponding evolution is guaranteed to be CPTP (i.e., physical). Conversely, any CPTP and divisible map is guaranteed to have to this form. Of course, this does not say anything about how to *derive* such an equation. That is a hard question, which we will start to tackle in the next section. But this result gives us an idea of what kind of structure we should look for and that is already remarkably useful.

Now here is our battle plan for this section: first, we will discuss some examples. Then we will prove Lindblad's theorem. Finally I will show you some tricks of the trade for dealing with these equations, specially from a numerical point of view.

Amplitude damping at finite temperature

We have already discussed the amplitude damping master equation in Sec. 4.1. But in that case the equation described a zero temperature effect. For instance, as illustrated in Eq. (4.6), the steady-state of the equation was the pure state $|0\rangle\langle 0|$. The generalization to finite temperatures is captured by a dissipator of the form

$$\mathcal{D}(\rho) = \gamma(1-f)\Big[\sigma_-\rho\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-,\rho\}\Big] + \gamma f\Big[\sigma_+\rho\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+,\rho\}\Big], \tag{4.43}$$

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[5] It is a semigroup because this looks like the composition property of a group, but the inverse is not necessarily a member of the group.

[6] G. Lindblad, *Comm. Math. Phys*, **48**, 119 (1976).

where $\gamma > 0$ and $f \in [0,1]$. After a while we get tired of writing these equations explicitly, so it is more convenient to break them in blocks. Define

$$\boxed{D[L] = L\rho L^\dagger - \frac{1}{2}\{L^\dagger L, \rho\}.} \tag{4.44}$$

Then we can rewrite Eq. (4.43) as

$$\boxed{\mathcal{D}(\rho) = \gamma(1-f)D[\sigma_-] + \gamma f D[\sigma_+].} \tag{4.45}$$

To know what a dissipator such as this is doing, we look at the fixed points. That is, the density matrix satisfying $\mathcal{D}(\rho^*) = 0$. Of course, we also need to include the Hamiltonian part, which we will do so below. But for now let's just forget about H for a second. In this case you can check that the steady-state of $\mathcal{D}$ is

$$\rho^* = \begin{pmatrix} f & 0 \\ 0 & 1-f \end{pmatrix}. \tag{4.46}$$

Thus, the constant f appearing in (4.45) represent the populations in the computational basis. If $f = 1$ the system will relax all the way to the north pole $|0\rangle$. If $f = 0$ it will relax to the south pole $|1\rangle$. For intermediate f, it will relax somewhere in the middle of the z axis, having $\langle\sigma_z\rangle_* = 2f - 1$.

After looking at the steady-sate, the next nice thing is to look at the relaxation towards the steady-state. In this case, if we let $p = \langle 0|\rho|0\rangle$ be the population in the north pole and $q = \langle 0|\rho|1\rangle$, then the evolution under Eq. (4.45) will lead to the equations

$$\frac{\mathrm{d}p}{\mathrm{d}t} = \gamma(f - p), \tag{4.47}$$

$$\frac{\mathrm{d}q}{\mathrm{d}t} = -\frac{\gamma}{2} q. \tag{4.48}$$

The solutions are simply

$$p(t) = p(0)e^{-\gamma t} + f(1 - e^{-\gamma t}), \tag{4.49}$$

$$q(t) = q(0)e^{-\gamma t/2}. \tag{4.50}$$

Thus, the population $p(t)$ will relax exponentially towards the "bath-imposed" population f, whereas the coherence will relax towards zero. It is interesting to note that $q(t)$ always relaxes to zero, irrespective of what is the value of f.

Competition

I like to view master equations such as (4.42) as a competition between different terms. Each ingredient in the equation is trying to push the system toward some direction and the steady-state will be a kind of compromise between the relative strengths of each term. This is already clear in the dissipator (4.44): the first term pushes to the south pole and the second term to the north pole. As a result, the system eventually settles down in the state (4.46), which is somewhere in the middle.

Unitary terms also contribute to the competition and this mixture of unitary and dissipative elements lead to interesting effects. To have an idea of what can happen, consider the Liouvillian

$$\mathcal{L}(\rho) = -i\frac{\Omega}{2}[\sigma_z, \rho] + \gamma(1-f)D[\sigma_-] + \gamma f D[\sigma_+]. \tag{4.51}$$

This is just like Eq. (4.45), except that now we added a Hamiltonian term corresponding to a qubit in the σ_z basis. The action of this unitary term turns out to be quite simple. All it will do is change the evolution of $q(t)$ to $q(t) = q(0)e^{-(i\Omega+\gamma/2)t}$. Thus, $q(t)$ will also oscillate a bit while relaxing. However, the steady-state remains the same, being given simply by Eq. (4.46).

Now let's consider a tiny variation of Eq. (4.51), where the Hamiltonian is modified from σ_z to σ_x:

$$\mathcal{L}(\rho) = -i\frac{\Omega}{2}[\sigma_x, \rho] + \gamma(1-f)D[\sigma_-] + \gamma f D[\sigma_+]. \tag{4.52}$$

The steady-state of this equation is now completely different, being given by

$$p^* = \frac{f\gamma^2 + \Omega^2}{\gamma^2 + 2\Omega^2}, \tag{4.53}$$

$$q^* = i(2f-1)\frac{\gamma\Omega}{\gamma^2 + 2\Omega^2} \tag{4.54}$$

This is now a weird mixed state lying somewhere in the yz plane. If $\gamma \gg \Omega$ then we recover back the state (4.46). However, if $\Omega \gg \gamma$ then the state actually tends to the maximally mixed state $\rho^* = \mathbb{I}/2$. This is interesting because we could naively think the system would tend to the x axis. But it doesn't because unitary and dissipative contributions behave differently. Dissipative terms push you to places, whereas unitaries like to oscillate around.

A harmonic oscillator subject to a finite temperature bath

In Sec. 3.7 we discussed the idea of a lossy cavity, which is described by a Lindblad dissipator that pumps energy away from the system. A similar idea applies to a continuous variable mode subject to a finite temperature bath. But in this case energy is not only drained out, but some may also come in. The dissipator describing this type of process is

$$\begin{aligned}\mathcal{D}(\rho) &= \gamma(\bar{n}+1)\Big[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\Big] + \gamma\bar{n}\Big[a^\dagger\rho a - \frac{1}{2}\{aa^\dagger, \rho\}\Big] \\ &= \gamma(\bar{n}+1)D[a] + \gamma\bar{n}D[a^\dagger],\end{aligned} \tag{4.55}$$

where $\gamma > 0$ and $\bar{n}$ is the Bose-Einstein distribution

$$\bar{n} = \frac{1}{e^{\beta\omega} - 1}, \tag{4.56}$$

with ω being the oscillator's frequency and $\beta = 1/T$ the inverse temperature. If $T = 0$ then $\bar{n} = 0$ and we recover the lossy cavity dissipator of Sec. 3.7.

Let us first ask what is the steady-state of (4.55). A honest guess would be a thermal state at temperature β. Indeed, I will leave for you the exercise of verifying that

$$\mathcal{D}(e^{-\beta\omega a^\dagger a}) = 0, \tag{4.57}$$

which works *only* if the β here is the same β appearing in Eq. (4.56). Thus, the steady-state is a thermal state with the same temperature as that imposed by the bath.

Dealing with these infinite dimensional master equations can sometimes be cumbersome. What I usually do is to always look first at expectation values of operators. And in this case it is useful to generalize a bit some of the tricks discussed in Sec. 3.7. Let us write our master equation as

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho] + \mathcal{D}(\rho). \tag{4.58}$$

Now we compute the expectation value of some operator O, which reads

$$\frac{\mathrm{d}\langle O\rangle}{\mathrm{d}t} = i\langle[H,O]\rangle + \mathrm{tr}\Big\{O\mathcal{D}(\rho)\Big\}. \tag{4.59}$$

The first term is simply the Heisenberg equation. It is useful to write down the second term in a similar way, as the expectation value of something on the state ρ.

Suppose we have a dissipator of the form $D[L]$ in Eq. (4.44). Then, using the cyclic property of the trace, we can write

$$\mathrm{tr}\Big\{O\Big[L\rho L^\dagger - \frac{1}{2}\{L^\dagger L,\rho\}\Big]\Big\} = \langle L^\dagger O L - \frac{1}{2}\{L^\dagger L, O\}\rangle. \tag{4.60}$$

This motivates us to define the **adjoint dissipator**

$$\bar{D}[L](O) = L^\dagger O L - \frac{1}{2}\{L^\dagger L, O\}. \tag{4.61}$$

which is a superoperator acting on observables O, instead of density matrices. It is nice to have a look at the structure of $\bar{D}$. In the original dissipator (4.44) the first term has $L \bullet L^\dagger$ but the second term has $L^\dagger L$. In the adjoint dissipator, on the other hand, everything is in the same order, with $L^\dagger$ always in the left. What is more, because of this more symmetric structure, we can actually factor the adjoint dissipator as

$$\boxed{\bar{D}[L](O) = \frac{1}{2}L^\dagger[O,L] + \frac{1}{2}[L^\dagger, O]L.} \tag{4.62}$$

With this structure it is now extremely easy to compute expectation values of observables since it amounts only to the computation of a commutator. And just to summarize, can now write Eq. (4.59) as

$$\boxed{\frac{\mathrm{d}\langle O\rangle}{\mathrm{d}t} = i\langle[H,O]\rangle + \langle\bar{\mathcal{D}}(O)\rangle.} \tag{4.63}$$

Going back to the harmonic oscillator dissipator (4.55), the corresponding adjoint dissipator will be

$$\begin{aligned}\bar{\mathcal{D}}(O) &= \gamma(\bar{n}+1)\Big[a^\dagger O a - \frac{1}{2}\{a^\dagger a, O\}\Big] + \gamma\bar{n}\Big[aOa^\dagger - \frac{1}{2}\{aa^\dagger, O\}\Big] \\ &= \frac{\gamma}{2}(\bar{n}+1)\Big\{a^\dagger[O,a] + [a^\dagger,O]a\Big\} + \frac{\gamma}{2}\bar{n}\Big\{a[O,a^\dagger] + [a,O]a^\dagger\Big\}.\end{aligned} \tag{4.64}$$

Please take a second to notice what I did. In the first line I just used the shape of the original dissipator (4.55) and changed the order $L\rho L^\dagger \to L^\dagger O L$. In the second line I just used the structure of Eq. (4.62) to rewrite this in terms of commutators.

Let us now look at some examples, starting with $O = a$. Inserting this in Eq. (4.64) leads to

$$\bar{\mathcal{D}}(a) = \gamma(\bar{n}+1)\Big\{-\frac{a}{2}\Big\} + \gamma\bar{n}\Big\{\frac{a}{2}\Big\} = -\frac{\gamma a}{2}. \tag{4.65}$$

For concreteness, let us also suppose $H = \omega a^\dagger a$. Then the equation for $\langle a\rangle$ will be simply

$$\frac{\mathrm{d}a}{\mathrm{d}t} = -(i\omega + \gamma/2)\langle a\rangle. \tag{4.66}$$

Interestingly, this is the same equation as for the zero temperature case. Thus, thermal fluctuations turn out not to affect the first moment $\langle a\rangle$.

Next we turn to $O = a^\dagger a$. Eq. (4.64) then gives

$$\bar{\mathcal{D}}(a^\dagger a) = \gamma(\bar{n}+1)\Big\{-a^\dagger a\Big\} + \gamma\bar{n}\Big\{aa^\dagger\Big\} = -\gamma a^\dagger a + \gamma\bar{n} \tag{4.67}$$

The evolution of $\langle a^\dagger a\rangle$ will then be given by

$$\frac{\mathrm{d}\langle a^\dagger a\rangle}{\mathrm{d}t} = \gamma(\bar{n} - \langle a^\dagger a\rangle). \tag{4.68}$$

This will therefore be an exponential relaxation, from the initial occupation $\langle a^\dagger a\rangle_0$ to the bath-imposed occupation $\bar{n}$. It is interesting to note how the right-hand side of Eq. (4.68) can be viewed as the **current of quanta**, in the sense of a *continuity equation*:

$$\frac{\mathrm{d}\langle a^\dagger a\rangle}{\mathrm{d}t} := J. \tag{4.69}$$

That is, the rate at which the number of quanta changes is related to the *flux* of quanta from the system to the environment. If at any given time $\langle a^\dagger a\rangle > \bar{n}$ then the current will be negative, meaning quanta is flowing from the system to the environment. Conversely, if $\langle a^\dagger a\rangle < \bar{n}$ the current becomes positive, meaning that quanta is flowing from the environment to the system.

Proof of Lindblad's theorem

Let us now prove Lindblad's theorem. That is, we will show that any quantum operation which also satisfies the semigroup property can be written in the Lindblad form (4.42). If the dynamics is to satisfy the semigroup property (i.e., if it is divisible) then we must be able to write the evolution over an infinitesimal time Δt as

$$\rho(t+\Delta t) = \sum_k M_k(\Delta t)\rho(t)M_k^\dagger(\Delta t), \tag{4.70}$$

where the Kraus operators $M_k(\Delta t)$ cannot depend on the time t. Let us then ask what we want for the $M_k(\Delta t)$. We are after a differential equation for $\rho(t)$, of the form (4.38). This means that for small Δt we want something like

$$\rho(t+\Delta t) \simeq \rho(t) + \Delta t \mathcal{L}(\rho(t)). \tag{4.71}$$

In general, since the first correction is of the order Δt, we will then need to have $M_k(\Delta t) = \sqrt{\Delta t} L_k$, where L_k is some operator. This is so because then $M_k \rho M_k^\dagger \sim \Delta t$. But we also have the additional property that, if $\Delta t = 0$, then nothing should happen: $\sum_k M_k(0)\rho M_k(0) = \rho$. One way to introduce this would be to take one Kraus operator, for instance $k = 0$, to be $M_k = I$. However, as we will see, this will give us trouble with the normalization of the Kraus operators.

The correct way to fix it is by defining

$$\boxed{M_0 = I + G\Delta t, \qquad M_k = \sqrt{\Delta t} L_k, \qquad k \neq 0} \tag{4.72}$$

where G and L_k are arbitrary operators. The normalization condition for the Kraus operators then leads to

$$\begin{aligned} 1 = \sum_k M_k^\dagger M_k &= M_0^\dagger M_0 + \sum_{k\neq 0} M_k^\dagger M_k \\ &= (I + G^\dagger \Delta t)(I + G\Delta t) + \Delta t \sum_{k\neq 0} L_k^\dagger L_k \\ &= I + (G + G^\dagger)\Delta t + \Delta t \sum_{k\neq 0} L_k^\dagger L_k + \mathbb{O}(\Delta t^2). \end{aligned}$$

This shows why we need this G guy. Otherwise, we would never be able to normalize the Kraus operators. Since G is arbitrary, we may parametrize it as

$$G = K - iH, \tag{4.73}$$

where K and H are both Hermitian. It then follows from the normalization condition that

$$K = -\frac{1}{2}\sum_{k\neq 0} L_k^\dagger L_k, \tag{4.74}$$

whereas nothing can be said about H.

With this at hand, we can finally substitute our results in Eq. (4.70). We then get

$$\begin{aligned}\rho(t+\Delta t) &= (I+G\Delta t)\rho(I+G^\dagger\Delta t) + \Delta t\sum_{k\neq 0} L_k\rho L_k^\dagger \\ &= \rho(t) + \Delta t(G\rho+\rho G^\dagger) + \Delta t\sum_{k\neq 0} L_k\rho L_k^\dagger \\ &= \rho(t) - i\Delta t[H,\rho] + \Delta t\sum_{k\neq 0}\Big[L_k\rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k,\rho\}\Big]\end{aligned}$$

Rearranging and taking the limit $\Delta t \to 0$ we then finally obtain

$$\frac{\rho(t+\Delta t)-\rho(t)}{\Delta t} \simeq \frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho] + \sum_{k\neq 0}\Big[L_k\rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k,\rho\}\Big], \tag{4.75}$$

which is Lindblad's equation (4.42). Woo-hoo! We did it! The only tiny difference is that in Eq. (4.42) there are also some coefficients γ_k. But you can just think that we redefine $\sqrt{\gamma_k}L_k \to L_k$, so they are both really the same thing.

In summary, we have seen that if we combine the semigroup property and the structure of a quantum operation, the corresponding differential equation must have Lindblad's form. As I mentioned before, we still have no idea of what the operators H and L_k should be. That will be the topic of next section. But it is great that we can already tell what the general structure should be.

Vectorization/Choi-Jamiolkowski isomorphism

Master equations and quantum operations can be annoying because we always have to multiply ρ on both sides. But if you remember your linear algebra course, you will recall that matrices also form a vector space. Hence, we can think of superoperators (such as the Liouvillian) as just a big matrices multiplying a big vector ρ. This idea can be made more formal using the Choi-Jamiolkowski isomorphism, or vectorization. It is neatly captured by the following relation:

$$\boxed{|i\rangle\langle j| \to |j\rangle\otimes|i\rangle.} \tag{4.76}$$

That is, we can think about an outer product (which has two indices) as being just a vector (with one index) in a doubled dimension. In this way, when we have an arbitrary density matrix

$$\rho = \sum_{i,j}\rho_{i,j}|i\rangle\langle j|, \tag{4.77}$$

we can write its vectorized form as

$$\mathrm{vec}(\rho) = \sum_{i,j}\rho_{i,j}|j\rangle\otimes|i\rangle. \tag{4.78}$$

From a matrix point of view, this operation is the same as *stacking columns of a matrix*

$$\boxed{\text{vec}\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a \\ c \\ b \\ d \end{pmatrix}.} \tag{4.79}$$

This vectorization trick is very useful, in particular due to two main properties. The first is related to the *Hilbert-Schmidt inner product*, defined as

$$(A, B) := \text{tr}(A^\dagger B). \tag{4.80}$$

This quantity satisfies all properties of an inner product and is therefore the operator analog of $\langle\psi|\phi\rangle$. And, in terms of the vectorized operators (4.79), it becomes exactly what one would intuitively guess:

$$\boxed{\text{tr}(A^\dagger B) = \text{vec}(A)^\dagger \text{vec}(B).} \tag{4.81}$$

That is, just the inner product between the two vectors.

A particularly important state in this sense is the vectorized version of the identity operator:

$$I = \sum_i |i\rangle\langle i| \qquad \to \qquad \text{vec}(I) = \sum_i |i\rangle \otimes |i\rangle. \tag{4.82}$$

We therefore see that the identity vectorizes to the (unnormalized) maximally entangled Bell state. One of the reasons why the identity is so important is in connection with the normalization of a density matrix:

$$\text{tr}(\rho) = \text{vec}(I)^\dagger \text{vec}(\rho) = 1. \tag{4.83}$$

The second useful property of the vectorization is as follows. Suppose we vectorize the product of three matrices ABC. It then turns out that

$$\boxed{\text{vec}(ABC) = (C^{\text{T}} \otimes A)\text{vec}(B).} \tag{4.84}$$

(Please note that what appears here is not the dagger, but the transpose). This is certainly not an intuitive property. The best way I know of convincing ourselves that it works is to simply write it out in the ugliest way possible:

$$ABC = \sum_{i,j,k,\ell,m,n} (A_{i,j}|i\rangle\langle j|)(B_{k,\ell}|k\rangle\langle \ell|)(C_{m,n}|m\rangle\langle n|) = \sum_{i,j,m,n} A_{i,j}B_{j,m}C_{m,n}|i\rangle\langle n|.$$

Then

$$\text{vec}(ABC) = \sum_{i,j,m,n} A_{i,j}B_{j,m}C_{m,m}|n\rangle \otimes |i\rangle.$$

On the other hand

$$(C^{\mathrm{T}}\otimes A)\mathrm{vec}(B) = \Big(\sum_{m,n,i,j} C_{m,n} A_{i,j} |n\rangle\langle m|\otimes|i\rangle\langle j|\Big)\sum_{k,\ell} B_{k,\ell}|\ell\rangle\otimes|k\rangle = \sum_{m,n,i,j} C_{m,n}A_{i,j}B_{j,m}|n\rangle\otimes|i\rangle,$$

which is the same thing.

The usefulness of Eq. (4.84) lies in the fact that it provides us with a recipe to write superoperator products such as $A\rho C$ in the form of a big matrix times $\mathrm{vec}(\rho)$:

$$\mathrm{vec}(A\rho C) = (C^{\mathrm{T}}\otimes A)\mathrm{vec}(\rho).$$

This also works for terms like

$$\mathrm{vec}(H\rho) = \mathrm{vec}(H\rho I) = (I\otimes H)\mathrm{vec}(\rho).$$

In this way we can write the full Liouvillian as just a big big matrix:

$$\mathrm{vec}\Big(-i[H,\rho]\Big) = -i\Big[I\otimes H - H^{\mathrm{T}}\otimes I\Big]\mathrm{vec}(\rho), \tag{4.85}$$

$$\mathrm{vec}\Big(L\rho L^\dagger - \frac{1}{2}\{L^\dagger L,\rho\}\Big) = \Big[L^*\otimes L - \frac{1}{2}I\otimes L^\dagger L - \frac{1}{2}(L^\dagger L)^{\mathrm{T}}\otimes I\Big]\mathrm{vec}(\rho) \tag{4.86}$$

Taking the vec of the original master equation (4.38), we can now rewrite it as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{vec}(\rho) = \hat{\mathcal{L}}\,\mathrm{vec}(\rho), \tag{4.87}$$

where $\hat{\mathcal{L}}$ is now a matrix (which is why I put a hat on it). For the general Liouvillian structure such as (4.42), this matrix will then read

$$\boxed{\hat{\mathcal{L}} = -i(I\otimes H - H^{\mathrm{T}}\otimes I) + \sum_k \gamma_k\Big[L_k^*\otimes L_k - \frac{1}{2}I\otimes L_k^\dagger L_k - \frac{1}{2}(L_k^\dagger L_k)^{\mathrm{T}}\otimes I\Big]} \tag{4.88}$$

Eq. (4.87) then nothing but a simple matrix-vector equation so that its properties can all be deduced from the properties of the matrix $\mathcal{L}$.

As an example of Eq. (4.88), the vectorized version of the amplitude damping dissipator (4.43) is

$$\hat{\mathcal{D}} = \begin{pmatrix} -\gamma(1-f) & 0 & 0 & \gamma f \\ 0 & -\gamma/2 & 0 & 0 \\ 0 & 0 & -\gamma/2 & 0 \\ \gamma(1-f) & 0 & 0 & -\gamma f \end{pmatrix}. \tag{4.89}$$

The matrix is not Hermitian. Notwithstanding, we will now see that it does satisfy a series of special properties.

Spectral properties of $\mathcal{L}$

As you may know from the theory of ordinary differential equations, the solution of Eq. (4.87) is simply

$$\text{vec}(\rho(t)) = e^{\hat{\mathcal{L}}t}\,\text{vec}(\rho(0)). \tag{4.90}$$

Hence, all properties of the solution are determined by this matrix exponential and hence by the spectral properties of $\hat{\mathcal{L}}$. In principle $\hat{\mathcal{L}}$ may not be diagonalizable. But let's assume it is. However, since it is not Hermitian, it will in general have different left and right eigenvectors

$$\hat{\mathcal{L}}\,\boldsymbol{x}_\alpha = \lambda_\alpha \boldsymbol{x}_\alpha, \tag{4.91}$$

$$\boldsymbol{y}_\alpha^\dagger \hat{\mathcal{L}} = \lambda_\alpha \boldsymbol{y}_\alpha^\dagger. \tag{4.92}$$

where λ_α are the eigenvalues and $\boldsymbol{x}_\alpha$ and $\boldsymbol{y}_\alpha$ are the corresponding right and left eigenvectors (they are both column vectors so $\boldsymbol{y}_\alpha^\dagger$ is a row vector). The diagonal decomposition of $\hat{\mathcal{L}}$ will then read

$$\hat{\mathcal{L}} = S\Lambda S^{-1}. \tag{4.93}$$

where $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots)$ is the diagonal matrix containing the eigenvalues and S is the matrix whose columns are the right eigenvectors $\boldsymbol{x}_\alpha$, whereas S^{-1} is a matrix whose rows are $\boldsymbol{y}_\alpha^\dagger$. Hence we may also write the diagonal decomposition as

$$\hat{\mathcal{L}} = \sum_\alpha \lambda_\alpha \boldsymbol{x}_\alpha \boldsymbol{y}_\alpha^\dagger, \tag{4.94}$$

These decompositions are useful when we want to write the matrix exponential, which simply becomes

$$e^{\hat{\mathcal{L}}t} = S\,e^{\Lambda t} S^{-1} = \sum_\alpha e^{\lambda_\alpha t} \boldsymbol{x}_\alpha \boldsymbol{y}_\alpha^\dagger. \tag{4.95}$$

With this form, we can now finally ask what should the properties of the eigenvalues and eigenvectors be in order for the dynamics to be physically consistent.

First we look at the trace preserving property (4.83). Multiplying Eq. (4.87) by $\text{vec}(I)^\dagger$ we get

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}\text{vec}(I)^\dagger \text{vec}(\rho) = \text{vec}(I)^\dagger \hat{\mathcal{L}} \text{vec}(\rho).$$

But this must be true for all density matrices. Hence, we must have

$$\text{vec}(I)^\dagger \hat{\mathcal{L}} = 0. \tag{4.96}$$

Comparing this with Eq. (4.92), we then conclude that the identity must *always* be a left eigenstate of $\hat{\mathcal{L}}$ with eigenvalue 0. Let us label this eigenvector $\alpha = 0$. Then $\lambda_0 = 0$ and $\boldsymbol{y}_0 = \text{vec}(I)$. But what about $\boldsymbol{x}_0$? Well, if we think about it, this will be nothing but the *steady-state* of the Liouvillian. That is,

$$\boxed{\boldsymbol{x}_0 = \text{vec}(\rho^*) \qquad \text{where} \qquad \mathcal{L}(\rho^*) = 0.} \tag{4.97}$$

This is a really powerful result: *any trace-preserving Liouvillian must have a zero eigenvalue. Its right eigenvector will be the steady-state of the equation, whereas the left eigenvector will be the identity.* Of course, a more subtle question is whether this steady-state is unique. That is, whether the eigenvalue 0 is degenerate or not. I would say quite often the steady-state is unique, but unfortunately this really depends on the problem in question.

Let us now return to the general solution (4.90). Using the diagonal decomposition (4.95) we get

$$\rho(t) = \sum_\alpha e^{\lambda_\alpha t}\, \boldsymbol{x}_\alpha \Big[\boldsymbol{y}_\alpha^\dagger \text{vec}(\rho(0))\Big] = \sum_\alpha c_\alpha\, e^{\lambda_\alpha t}\, \boldsymbol{x}_\alpha, \tag{4.98}$$

where $c_\alpha = \boldsymbol{y}_\alpha^\dagger \text{vec}(\rho(0))$ are just coefficients related to the initial conditions (you may see a similarity here with the usual solution of Schrödinger's equation). From this result we also arrive at another important property of Liouvillians: *the eigenvalues must always have a non-positive real part*. That is to say, either $\lambda_\alpha = 0$ or $\text{Re}(\lambda_\alpha) < 0$. Otherwise, the exponentials would blow up, which would be unphysical.

As an example, the Liouvillian in Eq. (4.89) has eigenvalues

$$\text{eigs}(\hat{\mathcal{D}}) = \Big\{ -\gamma, -\frac{\gamma}{2}, -\frac{\gamma}{2}, 0\Big\}. \tag{4.99}$$

In this case they turn out to be real. But if we also add a unitary term, then they will in general be complex. Notwithstanding their real part will always be non-positive.

Assume now that the zero eigenstate is unique. Then we can write Eq. (4.98) as

$$\rho(t) = c_0 \boldsymbol{x}_0 + \sum_{\alpha\neq 0} c_\alpha\, e^{\lambda_\alpha t}\, \boldsymbol{x}_\alpha. \tag{4.100}$$

I really like this result. First, note that in the first term $c_0 = \boldsymbol{y}_0^\dagger \text{vec}(\rho(0)) = 1$ by normalization. Secondly, in the second term all eigenvalues have negative real part so that, in the long-time limit, they will relax to zero. Consequently, we see that

$$\lim_{t\to\infty} \rho(t) = \boldsymbol{x}_0. \tag{4.101}$$

which, as expected, is the steady-state (4.97). Thus, we conclude that if the steady-state is unique, no matter where you start, the system will always eventually relax towards the steady-sate. The real part of the eigenvalues λ_α therefore tell you about the *relaxation rate* of the different terms. That is, they give you information on the time-scale with which the relaxation will occur.

4.4 Microscopic derivation of the Lindblad equation

In this section we will begin our discussion concerning microscopic derivations of quantum master equations. The idea is quite simple: we start with a system S interacting with an environment E through some coupling Hamiltonian V. We then assume E is enormous, chaotic, filthy and ugly, so that we can try to trace it out and obtain an equation just for S. Our hope is that despite all the approximations, our final equations will have Lindblad's form [Eq. (4.42)]. But reality is not so kind, so you may get a bit frustrated as we go along.

This is due to two main reasons. First, we will have to do several approximations which are hard to justify. They are hard because they involve assumptions about a macroscopically large and highly chaotic bath, for which it is really hard to do any calculations. Secondly, these derivations are highly model dependent. I will try to give you a general recipe, but we will see examples where this recipe is either insanely hard to implement or, what is worse, leads to unphysical results.

The derivation of microscopic equations for quantum systems is a century old topic. And for many decades this did not advance much. The reason is precisely because these derivations are model dependent. In classical stochastic processes that is not the case and you can write down quite general results. In fact, you can even write them down without microscopic derivations, using only phenomenological ingredients. For instance, Langevin augmented Newton's equation with a random force and then *later* deduced what the properties of this force had to be, using equilibrium statistical mechanics. Langevin's equation works great! It describes a ton of experiments in the most wide variety of situations, from particles in a fluid to noise in electrical circuits. In the quantum realm, unfortunately, that is simply not the case. It is impossible to write down general equations using only phenomenology. And everything *has* to be model-dependent because operators don't commute, so if add a new ingredient to the Hamiltonian, it will not necessarily commute with what was there before.

Setting up the problem

Ok. Sorry about the bla-bla-bla. Let's get down to business. Here is the deal: we have a composite S+E system evolving according to a Hamiltonian

$$H = H_S + H_E + V, \tag{4.102}$$

where H_S and H_E live on the separate Hilbert spaces of S and E, whereas V connects the two. We now consider their unitary evolution according to von Neumann's equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho], \tag{4.103}$$

where ρ is the total density matrix of S+E. What we want is to take the partial trace of Eq. (4.103) and try to write down an equation involving only $\rho_S = \mathrm{tr}_E\,\rho$.

Everything is done in the interaction picture with respect to $H_0 = H_S + H_E$ [see Sec. 3.3]: That is, we define $\tilde{\rho} = e^{iH_0t}\rho e^{-iH_0t}$. Then $\tilde{\rho}$ will also satisfy a von Neumann equation, but with an effective Hamiltonian $\tilde{V}(t) = e^{iH_0t}Ve^{-iH_0t}$. In order not to clutter the notation I will henceforth drop the tilde and write this equation simply as

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[V(t),\rho], \qquad V(t) = e^{iH_0t}Ve^{-iH_0t}. \tag{4.104}$$

I know this seems sloppy, but you will thank me later, as these tilde's make everything so much uglier. Just please remember that this ρ is not the same as the ρ appearing in

Eq. (4.103). In considering the evolution of Eq. (4.104), we will also assume that at $t = 0$ the system and the environment were uncorrelated, so that

$$\rho(0) = \rho_S(0) \otimes \rho_E(0) = \rho_S(0)\rho_E(0). \tag{4.105}$$

The initial state of S can be anything, whereas the initial state of $\rho_E(0)$ is usually assumed to be a thermal state,

$$\rho_E(0) = \frac{e^{-\beta H_E}}{Z}, \qquad Z = \text{tr}(e^{-\beta H_E}), \tag{4.106}$$

although other variations may also be used.

The result I want to derive does not depend on the model we choose for the environment. However, in 99.99% of the cases, one chooses the bath to be composed of a (usually infinite) set of harmonic oscillators. That is, the Hamiltonian H_E in Eq. (4.102) is usually chosen to be

$$H_E = \sum_k \Omega_k b_k^\dagger b_k, \tag{4.107}$$

where the b_k are a set of independent bosonic operators[7] and Ω_k are some frequencies. Usually it is assumed that the Ω_k varies almost continuously with k. The logic behind the assumption (4.107) is based on the fact that the two most widely used baths in practice are the electromagnetic field and the phonons in a crystal, both of which are bosonic in nature.

As for the system-environment interaction, it is usually assumed that this is *linear* in the bosonic operators b_k. So V would look something like

$$V = \sum_{\alpha,k} \Big\{ g_{\alpha k} M_\alpha b_k^\dagger + g_{\alpha k}^* A_\alpha^\dagger b_k \Big\}, \tag{4.108}$$

where M_α are system operators and $g_{\alpha k}$ are numbers. The justification for this kind of coupling is two-fold. First, it turns out there are many system in the literature where this type of coupling naturally appears; and second because this is one of the few types of couplings for which we can actually do the calculations! An important property of the a coupling such as (4.108) and a thermal state such as (4.106) is that, since $\langle b_k \rangle_{\text{th}} = 0$, it follows that

$$\text{tr}_E \Big[V \rho_E(0) \Big] = 0. \tag{4.109}$$

This property will greatly simplify the calculations we shall do next.[8]

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[7] Whenever we say "independent set" we mean they all commute. Thus, the bosonic algebra may be written as

$$[b_k, b_q^\dagger] = \delta_{k,q}, \qquad [b_k, b_q] = 0.$$

[8] Pro-tip: If you ever encounter a model where for which (4.109) is not true, redefine the system Hamiltonian and the interaction potential to read

$$V' = V - \text{tr}_E(V\rho_E(0)), \qquad H_S = H_S + \text{tr}_E(V\rho_E(0)).$$

This of course doesn't change the total Hamiltonian. But now $\text{tr}_E(V'\rho_E(0)) = 0$. But please note that this only works when $[\rho_E(0), H_E] = 0$.

The Nakajima-Zwanzig method

We are now ready to introduce the main method that we will use to trace out the environment. There are many ways to do this. I will use here one introduced by Nakajima and Zwanzig[9] because, even though it is not the easiest one, it is (i) the one with the highest degree of control and (ii) useful in other contexts. The method is based on a *projection superoperator* defined as

$$\mathcal{P}\rho(t) = \rho_S(t)\rho_E(0) = \text{tr}_E(\rho(t))\rho_E(0). \tag{4.110}$$

Yeah, I know: this looks weird. The idea is that $\mathcal{P}$ almost looks like a *marginalizator* (I just came up with that name!): that is, if in the right-hand side we had $\rho_E(t)$ instead of $\rho_E(0)$, this $\mathcal{P}$ would be projecting a general (possibly entangled) state $\rho(t)$ into its marginal states $\rho_S(t) \otimes \rho_E(t)$. This is like projecting onto a uncorrelated subspace of the full Hilbert space. But $\mathcal{P}$ does a bit more than that. It projects onto a state where E didn't really move. This is motivated by the idea that the bath is insanely large so that as the system evolves, it practically doesn't change.

For the purpose of simplicity, I will henceforth write $\rho_E(0)$ as simply ρ_E. So let us then check that $\mathcal{P}$ is indeed a projection operator. To do that we project twice:

$$\mathcal{P}^2\rho(t) = \mathcal{P}\Big[\rho_S(t)\rho_E\Big] = \text{tr}_E(\rho_S(t)\rho_E)\rho_E = \rho_S(t)\rho_E,$$

which is the same as just projecting once. Since this is a projection operator, we are naturally led to define its complement $\mathcal{Q} = 1 - \mathcal{P}$, which projects onto the remaining subspace. It then follows that $\mathcal{Q}^2 = \mathcal{Q}$ and $\mathcal{QP} = \mathcal{PQ} = 0$. To summarize, $\mathcal{P}$ and $\mathcal{Q}$ are projection superoperators satisfying

$$\mathcal{P}^2 = \mathcal{P}, \qquad \mathcal{Q}^2 = \mathcal{Q}, \qquad \mathcal{QP} = \mathcal{PQ} = 0. \tag{4.111}$$

If you ever want to write down a specific formula for this $\mathcal{P}$ operator, it is actually a quantum operation defined as

$$\mathcal{P}(\rho) = \sum_{k,q} p_k (I_S \otimes |k\rangle\langle q|)\rho(I_S \otimes |q\rangle\langle k|), \tag{4.112}$$

where $|q\rangle$ is an arbitrary basis of the environment, whereas $|k\rangle$ is the eigenbasis of $\rho_E = \rho_E(0)$ with eigenvalue p_k [i.e., $\rho_E|k\rangle = p_k|k\rangle$]. I don't think this formula is very useful, but it is nice to know that you can write down a more concrete expression for it. If we happen to know $\mathcal{P}\rho$, then it is easy to compute $\rho_S(t)$ because, due to Eq. (4.110),

$$\rho_S(t) = \text{tr}_E\Big\{\mathcal{P}\rho(t)\Big\}. \tag{4.113}$$

We will also need one last silly change of notation. We define a superoperator

$$\mathcal{V}_t(\rho) = -i[V(t), \rho], \tag{4.114}$$

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[9] S. Nakajima, *Progr. Theor. Phys.* **20**, 984 (1958) and R. Zwanzig, *J. Chem. Phys.* **33**, 1338 (1960).

so that Eq. (4.104) becomes

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \mathcal{V}_t\rho. \tag{4.115}$$

We are now ready for applying the Nakajima-Zwanzig projection method.

We begin by multiplying Eq. (4.114) by $\mathcal{P}$ and then $\mathcal{Q}$ on both sides, to obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho = \mathcal{P}\mathcal{V}_t\rho,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{Q}\rho = \mathcal{Q}\mathcal{V}_t\rho.$$

Next we insert a $1 = \mathcal{P} + \mathcal{Q}$ on the right-hand side, leading to

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho = \mathcal{P}\mathcal{V}_t\mathcal{P}\rho + \mathcal{P}\mathcal{V}_t\mathcal{Q}\rho, \tag{4.116}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{Q}\rho = \mathcal{Q}\mathcal{V}_t\mathcal{P}\rho + \mathcal{Q}\mathcal{V}_t\mathcal{Q}\rho. \tag{4.117}$$

The main point is that now this looks like a system of equations of the form

$$\frac{\mathrm{d}x}{\mathrm{d}t} = A(t)x + A(t)y, \tag{4.118}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = B(t)x + B(t)y, \tag{4.119}$$

where $x = \mathcal{P}\rho$ and $y = \mathcal{Q}\rho$ are just "vectors", whereas $A(t) = \mathcal{P}\mathcal{V}_t$ and $B(t) = \mathcal{Q}\mathcal{V}_t$ are just "matrices" (superoperators). What we want in the end is $x(t)$, whereas $y(t)$ is the guy we want to eliminate.

One way to do that is to formally solve for y treating $B(t)x(t)$ as just some time-dependent function, and then insert the result in the equation for x. The formal solution for y is

$$y(t) = G(t,0)y(0) + \int_0^t G(t,t')B(t')x(t'), \tag{4.120}$$

where $G(t,t')$ is the Green's function for the y equation,

$$G(t,t') = \mathcal{T}\exp\left\{\int_{t'}^t \mathrm{d}s B(s)\right\} = \mathcal{T}\exp\left\{\int_{t'}^t \mathrm{d}s\mathcal{Q}\mathcal{V}_s\right\} \tag{4.121}$$

Here I had to use the time-ordering operator $\mathcal{T}$ to write down the solution, exactly as we did when we had to deal with time-dependent Hamiltonians [c.f. Eq. (3.62)].

One lucky simplification we get is that the first term in Eq. (4.120) turns out to be zero. The reason is that $y = \mathcal{Q}\rho$ so $y(0) = \mathcal{Q}\rho(0)$. But initially the system and the bath start uncorrelated so $\mathcal{P}\rho(0) = \rho(0)$. Consequently, $\mathcal{Q}\rho(0) = 0$ since $\mathcal{Q} = 1 - \mathcal{P}$. Inserting Eq. (4.120) into Eq. (4.118) then yields

$$\frac{\mathrm{d}x}{\mathrm{d}t} = A(t)x + A(t)\int_0^t \mathrm{d}t'\; G(t,t')B(t')x(t'). \tag{4.122}$$

This is not bad! We have succeed in eliminating completely $y(t)$ and write down an equation for $x(t)$ only. The downside is that this equation is not local in time, with the derivative of x depending on its entire history from time 0 to time t.

Here Eq. (4.109) starts to become useful. To see why, let us rewrite the first term $A(t)x$:

$$A(t)x = \mathcal{P}\mathcal{V}_t\mathcal{P}\rho = \mathcal{P}\mathcal{V}_t\rho_S\rho_E$$

We further expand this recalling Eq. (4.114):

$$A(t)x = -i\mathcal{P}[V(t), \rho_S\rho_E] = -i\,\mathrm{tr}_E\Big\{[V(t), \rho_S\rho_E]\Big\}\rho_E.$$

But the guy inside is zero because of Eq. (4.109) and this must be true for any ρ_S. Hence, we conclude that

$$\mathrm{tr}_E\Big\{V(t)\rho_E\Big\} = 0 \quad\rightarrow\quad \mathcal{P}\mathcal{V}_t\mathcal{P} = 0. \tag{4.123}$$

This, in turn, implies that $A(t)x = 0$, so only the last term in Eq. (4.124) survives:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \int\limits_0^t \mathrm{d}t'\; A(t)G(t,t')B(t')x(t'). \tag{4.124}$$

Going back to our original notation we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho = \int\limits_0^t \mathrm{d}t'\; \mathcal{P}\mathcal{V}_t G(t,t')\mathcal{Q}\mathcal{V}_{t'}\mathcal{P}\rho(t').$$

A final naughty trick is to write $\mathcal{Q} = 1 - \mathcal{P}$. Then there will be a term which is again $\mathcal{P}\mathcal{V}_t\mathcal{P} = 0$. Hence we finally get

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho = \int\limits_0^t \mathrm{d}t'\; \mathcal{P}\mathcal{V}_t G(t,t')\mathcal{V}_{t'}\mathcal{P}\rho(t').} \tag{4.125}$$

This is the Nakajima-Zwanzig equation. It is a reduced equation for $\mathcal{P}\rho(t)$ after integrating out the environment. And, what is coolest, this equation is *exact*. Think about it: we didn't do a single approximation so far. We did use some assumptions, in particular Eqs. (4.105) and (4.109). But these are not really restrictive. This is what I like about this Nakajima-Zwanzig method: it gives us, as a starting point, an exact equation for the reduced dynamics of the system. The fact that this equation is non-local in time is then rather obvious. After all, our environment could very well be a single qubit.

The next step is then to start doing a bunch of approximations on top of it, which will be true when the environment is large and nasty.

Approximations! Approximations everywhere!

Now we have to start doing some approximations in order to get an equation of the Lindblad form. Justifying these approximations will not be easy and, unfortunately, their validity is usually just verified *a posteriori*. But essentially they are usually related to the fact that the bath is macroscopically large and usually, highly complex. Here is a quick dictionary of all the approximations that are usually done:

- **Born (or weak-coupling) approximation**: assume that the system-environment interaction is weak so that the state of the bath is barely affected.
- **Markov approximation**: assume bath correlation functions decay quickly. That is, bath-related stuff are fast, whereas system stuff are slow. This is similar in spirit to classical Brownian motion, where your big grain of pollen moves slowly through a bunch of rapidly moving and highly chaotic molecules (chaos helps the excitations die out fast).
- **Rotating-wave (secular) approximation**: like when the CIA tries to kill Jason Bourne to clean up the mess they created.

We will now go through these approximations step by step, starting with Born/weak coupling. In this case it is useful to rescale the potential by a parameter $V \to \epsilon V$ where ϵ is assumed to be small (in the end we can reabsorb ϵ inside V). In this case the same will be true for the superoperator $\mathcal{V}_t$ in Eq. (4.114). Hence, Eq. (4.125) is already an equation of order ϵ^2. We will then neglect terms of higher order in ϵ. These terms actually appear in the Green's function $G(t, t')$, which we defined in Eq. (4.121). Since now the exponential is of order ϵ, if we expand it in a Taylor series we will get

$$G(t,t') = 1 + \epsilon \mathcal{T} \int_{t'}^{t} \mathrm{d}s \mathcal{Q}\mathcal{V}_s + O(\epsilon)^2.$$

Thus, if we restrict to an equation of order ϵ^2, it suffices to approximate $G(t, t') \simeq 1$ in Eq. (4.125). This is essentially a statement on the fact that the bath state practically does not change. We then get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = \int_0^t \mathrm{d}t'\ \mathcal{P}\mathcal{V}_t\mathcal{V}_{t'}\mathcal{P}\rho(t'), \tag{4.126}$$

where I already reabsorbed ϵ inside $\mathcal{V}$, since we won't need it anymore.

Next we talk about the Markov approximation. You should always associate the name Markov with *memory*. A Markovian system is one which has a very poor memory (like fish!). In this case memory is related to how information about the system is dispersed in the environment. The idea is that if the environment is macroscopically large and chaotic, when you shake the system a little bit, the excitations will just diffuse away through the environment and will never come back. So the state of the system at a given time will not really influence it back at some later time by some excitations that bounced back.

To impose this on Eq. (4.126) we do two things. First we assume that $\rho(t')$ in the right-hand side can be replaced with $\rho(t)$. This makes the equation time-local in $\rho(t)$. We then get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = \int_0^t \mathrm{d}t'\, \mathcal{P}\mathcal{V}_t\mathcal{V}_{t'}\mathcal{P}\rho(t).$$

Next, change integration variables to $s = t - t'$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = \int_0^t \mathrm{d}s\, \mathcal{P}\mathcal{V}_t\mathcal{V}_{t-s}\mathcal{P}\rho(t).$$

This guy still depends on information occurring at $t = 0$. To eliminate that we set the upper limit of integration to $+\infty$ (then then term $\mathcal{V}_{t-s}$ will sweep all the way from $-\infty$ to t). We then get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = \int_0^\infty \mathrm{d}s\, \mathcal{P}\mathcal{V}_t\mathcal{V}_{t-s}\mathcal{P}\rho(t). \tag{4.127}$$

This equation is now the starting point for writing down actual master equations.

It is convenient to rewrite it in a more human-friendly format. Expanding the superoperators, we get

$$\begin{aligned}\mathcal{P}\mathcal{V}_t\mathcal{V}_{t-s}\mathcal{P}\rho(t) &= \mathcal{P}\mathcal{V}_t\mathcal{V}_{t-s}\rho_S(t)\rho_E \\ &= (-i)^2\mathcal{P}[V(t),[V(t-s),\rho_S(t)\rho_E]] \\ &= -\operatorname{tr}_E\Big\{[V(t),[V(t-s),\rho_S(t)\rho_E]]\Big\}\rho_E\end{aligned}$$

Thus Eq. (4.127) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_S(t)\rho_E = -\int_0^\infty \mathrm{d}s\;\operatorname{tr}_E\Big\{[V(t),[V(t-s),\rho_S(t)\rho_E]]\Big\}\rho_E.$$

Taking the trace over E is now trivial and thus gives

$$\boxed{\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = -\int_0^\infty \mathrm{d}s\;\operatorname{tr}_E\Big\{[V(t),[V(t-s),\rho_S(t)\rho_E]]\Big\}.} \tag{4.128}$$

This is now starting to look like a recipe. All we need to do is plug in a choice for $V(t)$ and then carry out the commutations, then the E-traces and finally an integral. The result will be an equation for $\rho_S(t)$. Once we are done, we just need to remember that we are still in the interaction picture, so we may want to go back to the Shcrödinger picture. For practical purposes it is also convenient to open the commutators and rearrange this as follows:

$$\boxed{\frac{\mathrm{d}\rho_S}{\mathrm{d}t} = \int\limits_0^\infty \mathrm{d}s \;\operatorname{tr}_E \Big\{V(t)\rho_S(t)\rho_E V(t-s) - \rho_S(t)\rho_E V(t-s)V(t)\Big\} + \text{h.c.},} \tag{4.129}$$

where h.c. stands for Hermitian Conjugate and simply means we should add the dagger of whatever we find in the first term. This is convenient because then out of the four terms, we only need to compute two.

As we will see below, it turns out that sometimes Eq. (4.129) is still not in Lindblad form. In these cases we will have to make a third approximation, which is the rotating-wave approximation (RWA) we discussed in the context of the Rabi model (Sec. 3.3). That is, *every now and then we will have to throw away some rapidly oscillatory terms*. The reason why this may be necessary is related to an argument about *time-scales and coarse graining*. The point worth remembering is that **bath-stuff are fast and system-stuff are slow**. This is again similar to classical Brownian motion: if the bath is a bear, trying to score some honey, then the bath is a swarm of bees desperately fighting to save their home.[10] During the time scale over which the bear takes a few steps, the bees have already lived half their lifetime. Due to this reason, a master equation is only *resolved* over time-scales much larger than the bath scales. If we ever encounter rapidly oscillatory terms, then they mean we are trying to model something in a time scale which we are not resolved. That is why it is justified to throw them away. So, in a sense, the RWA here is us trying to fix up the mess we ourselves created.

4.5 Open quantum harmonic oscillator

Now that we have a general recipe for finding Lindblad equations, we need to learn how to apply it. Let's do that in the context of a quantum harmonic oscillator coupled to a bath of harmonic oscillators. The total Hamiltonian $H = H_S + H_E + V$, Eq. (4.102), will be taken to be

$$H = \omega a^\dagger a + \sum_k \Omega_k b_k^\dagger b_k + \sum_k \lambda_k (a^\dagger b_k + b_k^\dagger a). \tag{4.130}$$

This is the simplest model possible of an open quantum system. Just so you can have an idea of where we want to arrive at, the dissipator that will come out of all of this is

$$D(\rho_S) = \gamma(\bar{n}+1)\Big[a\rho_S a^\dagger - \frac{1}{2}\{a^\dagger a, \rho_S\}\Big] + \gamma\bar{n}\Big[a^\dagger \rho_S a - \frac{1}{2}\{a a^\dagger, \rho_S\}\Big], \tag{4.131}$$

where $\gamma > 0$ and $\bar{n} = (e^{\beta\omega} - 1)^{-1}$ is the Bose-Einstein distribution with $\beta = 1/T$ and T being the bath temperature (I always set the Boltzmann constant to $k_B = 1$). I should

---

[10] A. A. Milne, *Winnie-the-Pooh*. New York, NY: Penguin Group, 1954.

also mention that this model can be solved exactly, which we will in fact do later on. Doing so is a nice way of checking the validity of all approximations we did in deriving the master equation.

Another quite similar model is that of a qubit interacting with a bath of oscillators. In this case the Hamiltonian is almost identical, we just replace a with σ_-:

$$H = \frac{\omega}{2}\sigma_z + \sum_k \Omega_k b_k^\dagger b_k + \sum_k \lambda_k(\sigma_+ b_k + b_k^\dagger \sigma_-). \tag{4.132}$$

Here we will work with Eq. (4.130) and I will leave it for you to repeat the steps for the Hamiltonian (4.132).

What we need to do is essentially apply Eq. (4.129). And this involves three steps:

1. Compute $V(t)$.
2. Compute the trace over E.
3. Compute the s integral.

For the first step, using Eq. (3.32) we get

$$V(t) = e^{iH_0t}Ve^{-iH_0t} = \sum_k \lambda_k \Big\{ e^{i\Delta_k t}a^\dagger b_k + e^{-i\Delta_k t} b_k^\dagger a\Big\}, \tag{4.133}$$

where $\Delta_k = \omega - \Omega_k$ is the detuning between the system oscillator and each bath mode. Now we plug this into the first term in Eq. (4.129). This gives a messy combination of four term:

$$\begin{aligned} V(t)\rho_S\rho_E V(t-s) = \sum_{k,q} \lambda_k\lambda_q \Big\{ & e^{i(\Delta_k+\Delta_q)t}e^{-i\Delta_q s}\; a^\dagger b_k \rho_S\rho_E a^\dagger b_q \\ & + e^{i(\Delta_k-\Delta_q)t}e^{i\Delta_q s}\; a^\dagger b_k\rho_S\rho_E a b_q^\dagger \\ & + e^{-i(\Delta_k-\Delta_q)t}e^{-i\Delta_q s}\; a b_k^\dagger \rho_S\rho_E a^\dagger b_q \\ & + e^{-i(\Delta_k+\Delta_q)t}e^{i\Delta_q s}\; a b_k^\dagger\rho_S\rho_E a b_q^\dagger \Big\}. \end{aligned}$$

This is still just the first term Eq. (4.129). However, once we learn how to deal with it, it will be easy to repeat the procedure for the other terms.

Next we take the trace over the environment. This is a nice exercise on how to move things around. For instance,

$$\text{tr}_E\left\{a^\dagger b_k \rho_S\rho_E a b_q^\dagger\right\} = a^\dagger\rho_S\, a\, \text{tr}_E\left\{b_k\rho_E b_q^\dagger\right\} = a^\dagger\rho_S a\langle b_q^\dagger b_k\rangle.$$

Thus, we get

$$\begin{aligned}\mathrm{tr}_E\Big\{V(t)\rho_S\rho_E V(t-s)\Big\} = \sum_{k,q}\lambda_k\lambda_q\Big\{&e^{i(\Delta_k+\Delta_q)t}e^{-i\Delta_q s}\; a^\dagger\rho_S a^\dagger\langle b_q b_k\rangle\\ &+e^{i(\Delta_k-\Delta_q)t}e^{i\Delta_q s}\; a^\dagger\rho_S a\langle b_q^\dagger b_k\rangle\\ &+e^{-i(\Delta_k-\Delta_q)t}e^{-i\Delta_q s}\; a\rho_S a^\dagger\langle b_q b_k^\dagger\rangle\\ &+e^{-i(\Delta_k+\Delta_q)t}e^{i\Delta_q s}\; a\rho_S a\langle b_q^\dagger b_k^\dagger\rangle\Big\}. \end{aligned} \tag{4.134}$$

So far nothing has been said about the initial state of the bath. But from now on some assumption must be made in order to compute the bath correlation functions $\langle b_q^\dagger b_k\rangle$ and $\langle b_q b_k\rangle$. If we assume that the bath is in the thermal Gibbs state (4.106), we get

$$\langle b_q b_k\rangle = 0, \tag{4.135}$$

$$\langle b_q^\dagger b_k\rangle = \delta_{q,k}\bar{n}(\Omega_k), \tag{4.136}$$

$$\langle b_k b_q^\dagger\rangle = \langle b_q^\dagger b_k\rangle + \delta_{k,q} = \delta_{k,q}(\bar{n}(\Omega_k)+1), \tag{4.137}$$

where

$$\bar{n}(x) = \frac{1}{e^{\beta x}-1}. \tag{4.138}$$

Plugging everything together we then get

$$\mathrm{tr}_E\Big\{V(t)\rho_S\rho_E V(t-s)\Big\} = \sum_k \lambda_k^2\Big\{e^{i(\omega-\Omega_k)s}\;\bar{n}(\Omega_k)\; a^\dagger\rho_S a + e^{-i(\omega-\Omega_k)s}[\bar{n}(\Omega_k)+1]\; a\rho_S a^\dagger\Big\}. \tag{4.139}$$

Note how the Lindblad structure of Eq. (4.131) is starting to appear.

This is now a good point to introduce an important quantity known as the **spectral density of the bath**. It is defined as

$$J(\Omega) = 2\pi\sum_k \lambda_k^2\;\delta(\Omega-\Omega_k). \tag{4.140}$$

This is a function of a continuous variable Ω and, in general, this function will look like a series of delta-peaks whenever Ω equals one of the Ω_k. However, for a macroscopically large bath, the frequencies Ω_k will change smoothly with k and therefore $J(\Omega)$ will become a smooth function. In terms of the spectral density, Eq. (4.139) can be written as an integral

$$\mathrm{tr}_E\Big\{V(t)\rho_S\rho_E V(t-s)\Big\} = \int_0^\infty \frac{\mathrm{d}\Omega}{2\pi}\; J(\Omega)\Big\{e^{i(\omega-\Omega)s}\bar{n}(\Omega)a^\dagger\rho_S a + e^{-i(\omega-\Omega)s}(\bar{n}(\Omega)+1)a\rho_S a^\dagger\Big\}. \tag{4.141}$$

Here we are also implicitly assuming that the frequencies Ω_k vary smoothly between 0 and ∞ (they cannot be negative since a mode with negative frequency would be unstable). It is really nice to notice that all properties of the system-bath interaction are summarized in the spectral density $J(\Omega)$. This means that the tiny details of λ_k do not matter. All that matter is their combined effect.

Finally, still with Eq. (4.129) in mind, we compute the integral in s:

$$\int_0^\infty \mathrm{d}s\,\mathrm{tr}_E\Big\{V(t)\rho_S\rho_E V(t-s)\Big\} = \int_0^\infty \mathrm{d}s \int_0^\infty \frac{\mathrm{d}\Omega}{2\pi}\, J(\Omega)\Big\{e^{i(\omega-\Omega)s}\bar{n}(\Omega)a^\dagger\rho_S a + e^{-i(\omega-\Omega)s}(\bar{n}(\Omega)+1)a\rho_S a^\dagger\Big\}. \tag{4.142}$$

To continue, the best thing to do is to take the s integral first. And, of course, what we would love to do is use the delta-function identity

$$\int_{-\infty}^\infty \frac{\mathrm{d}s}{2\pi}\, e^{i(\omega-\Omega)s} = \delta(\omega-\Omega). \tag{4.143}$$

But there is one tiny problem: in Eq. (4.142) the lower limit of integration is 0 instead of $-\infty$. The correct identity is then

$$\int_0^\infty \frac{\mathrm{d}s}{2\pi}\, e^{i(\omega-\Omega)s} = \frac{1}{2}\delta(\omega-\Omega) - \frac{i}{2}P\frac{1}{\omega-\Omega}, \tag{4.144}$$

where P denotes the Cauchy principal value. It can be shown that this last term only causes a tiny rescaling of the oscillator frequency ω called a **Lamb shift**. (i.e., it leads to a unitary contribution, instead of a dissipative one). Computing the Lamb shift is actually a difficult task. However, since in practice all it does is rescale ω, we can simply pretend it doesn't exist and focus only on the first term.

Neglecting the lamb-shift we then get

$$\begin{aligned}\int_0^\infty \mathrm{d}s\,\mathrm{tr}_E\Big\{V(t)\rho_S\rho_E V(t-s)\Big\} &= \int_0^\infty \mathrm{d}\Omega\, \frac{J(\Omega)}{2}\delta(\omega-\Omega)\Big\{\bar{n}(\Omega)a^\dagger\rho_S a + (\bar{n}(\Omega)+1)a\rho_S a^\dagger\Big\} \\ &= \frac{J(\omega)}{2}\Big\{\bar{n}(\omega)a^\dagger\rho_S a + (\bar{n}(\omega)+1)a\rho_S a^\dagger\Big\}.\end{aligned} \tag{4.145}$$

We did it! We started all the way with Eq. (4.129) and we computed the first term!

Computing the second term is now quite easy: Going back to Eq. (4.134), we now compute

$$\begin{aligned}\mathrm{tr}_E\Big\{\rho_S\rho_E V(t-s)V(t)\Big\} = \sum_{k,q}\lambda_k\lambda_q\Big\{&e^{i(\Delta_k+\Delta_q)t}e^{-i\Delta_q s}\;\rho_S a^\dagger a^\dagger\langle b_q b_k\rangle \\ &+e^{i(\Delta_k-\Delta_q)t}e^{i\Delta_q s}\;aa^\dagger\rho_S\langle b_q^\dagger b_k\rangle \\ &+e^{-i(\Delta_k-\Delta_q)t}e^{-i\Delta_q s}\;\rho_S a^\dagger a\langle b_q b_k^\dagger\rangle \\ &+e^{-i(\Delta_k+\Delta_q)t}e^{i\Delta_q s}\;\rho_S aa\langle b_q^\dagger b_k^\dagger\rangle\Big\}.\end{aligned} \tag{4.146}$$

And we are done! If you just think about this for a second you will notice that this has the *exact* same structure as (4.134), except that the order of the operators is exchanged. For instance, in the second line of (4.134) we had $a^\dagger \rho_S a^\dagger$. Now we have $\rho_S a a^\dagger$.

The entire procedure we did for the first term is now repeated identically for this new guy, so in the end we will arrive at the same form as (4.145), but with the operators exchanged:

$$\mathrm{tr}_E \Big\{ \rho_S \rho_E V(t-s) V(t) \Big\} = \frac{J(\omega)}{2} \Big\{ \bar{n}(\omega) \rho_S a a^\dagger + (\bar{n}(\omega)+1) \rho_S a^\dagger a \Big\}. \tag{4.147}$$

For simplicity, I will now change notations to

$$J(\omega) := \gamma, \qquad \bar{n}(\omega) := \bar{n} = \frac{1}{e^{\beta\omega}-1}. \tag{4.148}$$

Then, combining (4.145) and (4.147) into Eq. (4.129) we get

$$\frac{d\rho_S}{dt} = \frac{\gamma}{2}\bar{n}\Big\{ a^\dagger \rho_S a - a a^\dagger \rho_S \Big\} + \frac{\gamma}{2}(\bar{n}+1)\Big\{ a \rho_S a^\dagger - a^\dagger a \rho_S \Big\} + \text{h.c.}.$$

We cannot forget the h.c. Plugging it back, we then finally get

$$\boxed{\frac{d\rho_S}{dt} = \gamma\bar{n}\Big[a^\dagger \rho_S a - \frac{1}{2}\{a a^\dagger, \rho_S\} \Big] + \gamma(\bar{n}+1)\Big[a \rho_S a^\dagger - \frac{1}{2}\{a^\dagger a, \rho_S\} \Big],} \tag{4.149}$$

which is Eq. (4.131) and we are done.

What is cool about this is that not only can we derive a Lindblad master equation from a microscopic theory of system-environment interactions, but we can also attribute a clear physical meaning to the damping rate γ: it is simply given by the spectral density $J(\Omega)$ evaluated at the system's frequency ω. The spectral density is defined in Eq. (4.140) and represents the intensity of the S-E interaction λ_k^2. The damping rate γ is therefore found to be related to the coupling strength between the system and those oscillators whose frequency Ω_k are in the vicinity of ω; i.e., this is a resonant effect.

We should also never forget that we are working in the interaction picture so that ρ_S in Eq. (4.149) is actually $\tilde{\rho}_S$, which was defined as

$$\tilde{\rho}_S(t) = e^{iH_S t} \rho_S e^{-iH_S t}.$$

Going back turns out to be quite easy however because the dissipative part (4.149) is invariant under the rotating frame transformation. The reason is that $a \to a e^{i\omega t}$ and $a^\dagger \to a^\dagger e^{-i\omega t}$. But since a and $a^\dagger$ always appear in pairs in the dissipator, these exponentials cancel. For this reason, going back to the Schrödinger picture amounts to simply reintroducing the system Hamiltonian H_S:

$$\frac{d\rho_S}{dt} = -i[H_S, \rho] + D(\rho). \tag{4.150}$$

And voilá, we are done.

Non-RWA interaction

Before we move on to another model, I want to quickly explore what happens if we use, instead of the initial Hamiltonian (4.130), a Hamiltonian of the form

$$H = \omega a^\dagger a + \sum_k \Omega_k b_k^\dagger b_k + \sum_k \lambda_k (a^\dagger + a)(b_k^\dagger + b_k). \tag{4.151}$$

The difference is only in the last term. This is the same idea as in the Jaynes-Cummings vs. Rabi discussion. Such a term no longer preserves the number of quanta in the system, making everything more complicated. But we study it because it appears often in nature. One context in which it appears is in the dissipative properties of mechanical systems.

Consider a mechanical harmonic oscillator with coordinate and momenta q and p, coupled to an infinite number of harmonic oscillators modeled by coordinate and momenta Q_k and P_k. The total Hamiltonian may look like

$$H = \left(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2\right) + \left(\sum_k \frac{P_k^2}{2M_k} + \frac{1}{2} M_k \Omega_k^2 Q_k^2\right) + \frac{1}{2}\sum_k c_k (q - Q_k)^2. \tag{4.152}$$

This is the typical *harmonic coupling*: the interaction potential depends on the relative displacement $(q - Q_k)^2$. If we now expand the square in the last term we get $q^2 + Q_k^2 - 2qQ_k$. The first two terms can actually be reabsorbed into renormalized system and bath frequencies:

$$\frac{1}{2} m\omega^2 q^2 + \frac{1}{2}\sum_k c_k q^2 := \frac{1}{2} m\tilde{\omega}^2 q^2,$$

$$\frac{1}{2} M_k \Omega_k^2 Q_k^2 + \frac{c_k}{2} Q_k^2 := \frac{1}{2} M_k \tilde{\Omega}_k Q_k^2$$

We now define creation and annihilation operators for the system and bath as

$$q = \sqrt{\frac{\hbar}{m\tilde{\omega}}}(a + a^\dagger), \qquad Q_k = \sqrt{\frac{\hbar}{M_k \tilde{\Omega}_k}}(b_k + b_k^\dagger).$$

With these choices (and similar definitions for p and P_k) the mechanical Hamiltonian (4.152) becomes

$$H = \tilde{\omega} a^\dagger a + \sum_k \tilde{\Omega}_k b_k^\dagger b_k - \sum_k \frac{\hbar c_k}{\sqrt{m\tilde{\omega} M_k \tilde{\Omega}_k}} (a + a^\dagger)(b_k + b_k^\dagger), \tag{4.153}$$

which is of the form of Eq. (4.151) with a certain redefinition of the λ_k.

To analyze a Hamiltonian such as (4.151), the recipe we developed may not be the most ideal. It all depends on whether the coupling strength λ_k are much smaller than the frequency ω or not. If they are, then we will see that a rotating-wave approximation will give us the same Lindblad equation as in (4.149). This is usually the case in quantum optical systems. But it is often violated in the case of mechanical vibrations, for which a more detailed theory must be developed. This theory is usually called

Quantum Brownian Motion. Two papers which I particularly like about QBM are `arXiv 0904.0950` (theory) and `arXiv 1305.6942` (experiment).

Let's then see what happens if we apply our recipe to the Hamiltonian (4.151). First we compute the interaction picture potential

$$
\begin{aligned}
V(t) &= \sum_k \lambda_k (a^\dagger e^{i\omega t} + a e^{-i\omega t})(b_k^\dagger e^{i\Omega_k t} + b_k e^{-i\Omega_k t}) \\
&= \sum_k \lambda_k \Big\{ a^\dagger b_k e^{i\Delta_k t} + a b_k^\dagger e^{-i\Delta_k t} + a^\dagger b_k^\dagger e^{i(\omega+\Omega_k)t} + a b_k e^{-i(\omega+\Omega_k)t} \Big\}.
\end{aligned}
$$

Next we use this to compute terms such as $V(t)\rho_S\rho_E V(t-s)$. As you can probably see, this will become quite a mess. I will spare you the sordid details. All I want to focus on is the following result:

$$
\begin{aligned}
\int_0^\infty \mathrm{d}s\, \mathrm{tr}_E \Big\{ V(t)\rho_S(t)\rho_E V(t-s) \Big\} = \frac{J(\omega)}{2} \Big\{ & \bar{n}(\omega) a^\dagger \rho_S a + (\bar{n}(\omega)+1) a \rho_S a^\dagger \\
& + \bar{n}(\omega) a \rho_S a\, e^{-2i\omega t} + (\bar{n}(\omega)+1) a^\dagger \rho_S a^\dagger\; e^{2i\omega t} \Big\}.
\end{aligned}
$$

The first line is exactly what we had before, Eq. (4.145). But now we see the appearance of two new terms in the second line. These terms are fundamentally different in the sense that they are rapidly oscillatory terms, even thought we are in the interaction picture, where things should oscillate less. Moreover, we see that this is not yet in Lindblad's form. This is where the rotating-wave approximation applies. If $\omega \gg \gamma J(\omega)$ then these new terms will induce fast oscillations on top of a slowly changing evolution. In this case it is therefore reasonable to neglect them. Otherwise, one must resort to quantum Brownian motion.

4.6 The spin-boson model

The name spin-boson refers to a single qubit interacting with an infinite number of bosonic modes. Just like with the British royal family, when we talk about this model, there is a good boy and a bad boy. They are:

$$
H = \frac{\omega}{2}\sigma_z + \sum_k \Omega_k b_k^\dagger b_k + \sum_k \lambda_k\, \sigma_z (b_k + b_k^\dagger), \qquad \text{(good boy)}, \tag{4.154}
$$

$$
H = \frac{\omega}{2}\sigma_z + \sum_k \Omega_k b_k^\dagger b_k + \sum_k \lambda_k\, \sigma_x (b_k + b_k^\dagger), \qquad \text{(bad boy)}. \tag{4.155}
$$

The fundamental difference between the two models is that in the first the operator appearing in the S-E interaction (σ_z) is the same as the operator in H_S. Consequently, the model (4.154) cannot generate transitions between energy levels (population changes) and, consequently, the most that can happen is environment-induced decoherence. In Eq. (4.155), on the other hand, the operator σ_x is the spin flip and therefore causes population changes. Consequently, it will give rise to an amplitude damping-type of dynamics.

In this section we will talk about the good-boy spin-boson model, Eq. (4.154). First we will try to find a master equation for the qubit, by simply plugging it into our recipe, Eq. (4.129). Then we will discuss an *exact* solution of it, which as we will see, has a much richer physics.

Approximate derivation of the master equation

In this section we follow once again the steps in our recipe (4.129). In the interaction picture the S-E interaction of Eq. (4.154) becomes

$$V(t) = \sum_k \lambda_k \, \sigma_z (b_k e^{-i\Omega_k t} + b_k^\dagger e^{i\Omega_k t}). \tag{4.156}$$

Then

$$V(t)\rho_S\rho_E V(t-s) = \sum_{k,q} \lambda_k\lambda_q(\sigma_z\rho_S\sigma_z)(b_k e^{-i\Omega_k t} + b_k^\dagger e^{i\Omega_k t})\rho_E(b_q e^{-i\Omega_q(t-s)} + b_q^\dagger e^{i\Omega_q(t-s)}),$$

where I already moved things around a bit in order to separate system operators and bath operators. Next:

$$\begin{aligned}\mathrm{tr}_E\Big\{V(t)\rho_S\rho_E V(t-s)\Big\} &= \sum_k \lambda_k^2 \, \sigma_z\rho_S\sigma_z\Big\{\bar{n}(\Omega_k)e^{-i\Omega_k s} + (\bar{n}(\Omega_k)+1)e^{i\Omega_k s}\Big\}\\ &= \int\limits_0^\infty \frac{\mathrm{d}\Omega}{2\pi} \, J(\Omega) \, \sigma_z\rho_S\sigma_z\Big\{\bar{n}(\Omega)e^{-i\Omega s} + (\bar{n}(\Omega)+1)e^{i\Omega s}\Big\}.\end{aligned}$$

And finally,

$$\int\limits_0^\infty \mathrm{d}s \, \mathrm{tr}_E\Big\{V(t)\rho_S\rho_E V(t-s)\Big\} = \int\limits_0^\infty \frac{\mathrm{d}\Omega}{2\pi} \, J(\Omega) \, (2\bar{n}(\Omega)+1)\delta(\Omega) \, \sigma_z\rho_S\sigma_z.$$

We now reach a somewhat awkward place because the Dirac delta will push $J(\Omega)$ towards $J(0)$ and $\bar{n}(\Omega)$ towards $\bar{n}(0)$. But in this limit $\bar{n}(\Omega) = (e^{\beta\Omega}-1)^{-1}$ diverges, whereas $J(\Omega)$ tends to zero. This is one of those buggy features of trying to apply a general recipe for all types of open-system problems. Below when we compute the exact solution, no problem of this sort will appear.

If we want to continue, the best we can do is to assume that even though one diverges and the other tends to zero, their product tends to a finite value, which we define, just for convenience, as

$$\lim_{\Omega\to 0} J(\Omega)(2\bar{n}(\Omega)+1) := \frac{\lambda}{4} \tag{4.157}$$

Then we get

$$\int\limits_0^\infty \mathrm{d}s \, \mathrm{tr}_E\Big\{V(t)\rho_S\rho_E V(t-s)\Big\} = \frac{\lambda}{4}\sigma_z\rho_S\sigma_z.$$

The other term in Eq. (4.129) is identical, except that the order of the operators changes to $\rho_S \sigma_z \sigma_z = \rho_S$. Thus we get, considering also the Hermitian conjugate (which in this case is the same as the operator)

$$D(\rho_S) = \frac{\lambda}{2}(\sigma_z \rho_S \sigma_z - \rho_S). \tag{4.158}$$

This is the dephasing dissipator that we studied all the way back in Eq. (2.22). There we saw that such a dissipator does not induce any changes in population, but only causes the coherence $q(t) = \langle 0|\rho_S(t)|1\rangle$ to decay exponentially as

$$q(t) = q(0)e^{-\lambda t}. \tag{4.159}$$

Exact solution

Now let's find the *exact* solution for $\rho_S(t)$. This is one of the few models for which exact solutions are available, so enjoy it! The starting point is von Neumann's equation (in the Schrödinger picture) for the total density matrix of S+E:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H, \rho], \tag{4.160}$$

where H is the total Hamiltonian (4.154). This is subject to the initial condition

$$\rho(0) = \rho_S(0)\rho_E(0), \qquad \rho_E(0) = \frac{e^{-\beta H_E}}{Z_E}. \tag{4.161}$$

However, now we are interested in exact dynamics so the bath will also evolve in time and the system and bath will become correlated (no Born and no Markov approximations).

The solution of Eq. (4.160) is

$$\rho(t) = e^{-iHt}\rho_S(0)\rho_E(0)e^{iHt}.$$

What we want is the partial trace over the environment

$$\rho_S(t) = \mathrm{tr}_E\left\{e^{-iHt}\rho_S(0)\rho_E(0)e^{iHt}\right\}.$$

Let us now divide the total Hamiltonian H as

$$H = H_S + H_0,$$

where $H_S = \frac{\omega}{2}\sigma_z$ and

$$H_0 = \sum_k \Omega_k b_k^\dagger b_k + \sum_k \lambda_k \sigma_z (b_k + b_k^\dagger)$$

The Hamiltonian H_S lives on the qubit space and therefore can be taken out of the partial trace:

$$\rho_S(t) = e^{-iH_S t}\,\mathrm{tr}_E\left\{e^{-iH_0 t}\rho_S(0)\rho_E(0)e^{iH_0 t}\right\}e^{iH_S t}.$$

In this way, we have separated the local unitary dynamics, described by H_S, to the dissipative dynamics described by everything inside the trace. In fact, if you think about it, this whole partial trace is a quantum operation in the spirit of Stinespring's theorem. So for now let us focus on this dissipative part defined by the map

$$\tilde{\rho}_S(t) = \mathrm{tr}_E\left\{e^{-iH_0t}\rho_S(0)\rho_E(0)e^{iH_0t}\right\}.$$

The easiest way to proceed from here is to actually look at the matrix elements of this map in the computational basis. The reason why this is useful is because H_0 is already diagonal in the qubit sector. In fact, we can define

$$H_0|0\rangle = H_0^+|0\rangle, \qquad H_0|1\rangle = H_0^-|1\rangle,$$

where

$$H_0^\pm = \sum_k \Omega_k b_k^\dagger b_k \pm \sum_k \lambda_k(b_k + b_k^\dagger)$$

We then have, for instance

$$\begin{aligned}\langle 0|\tilde{\rho}_S(t)|0\rangle &= \langle 0|\,\mathrm{tr}_E\left\{e^{-iH_0t}\rho_S(0)\rho_E(0)e^{iH_0t}\right\}|0\rangle\\
&= \mathrm{tr}_E\left\{\langle 0|e^{-iH_0t}\rho_S(0)\rho_E(0)e^{iH_0t}|0\rangle\right\}\\
&= \mathrm{tr}_E\left\{e^{-iH_0^+t}\langle 0|\rho_S(0)|0\rangle\rho_E(0)e^{iH_0^+t}\right\}\\
&= \langle 0|\rho_S(0)|0\rangle\,\mathrm{tr}_E\left\{e^{-iH_0^+t}\rho_E(0)e^{iH_0^+t}\right\}\end{aligned}$$

This set of steps is important and a bit confusing, so make sure you understand what I am doing. I push the system bra and ket $|0\rangle$ inside the partial trace. But then I know how H_0 acts on it. And after it has acted, H_0^+ will no longer have any components on the qubit space, so we can move $|0\rangle$ through it at will. Finally, when $\langle 0|$ and $|0\rangle$ encounter $\rho_S(0)$, they form a number, which can then be taken outside the partial trace.

But now comes the magic trick: $H_0^\pm$ is an operator that lives only on the environment's Hilbert space. Hence, we are now allowed to use the cyclic property of the trace. This is a useful trick to remember: *if an operator lives on a larger space, cyclic property is forbidden. But if acts only over the space you are tracing, then it becomes allowed again.* And if we do that the two exponentials cancel and we are left with

$$\langle 0|\tilde{\rho}_S(t)|0\rangle = \mathrm{tr}_E\left\{\langle 0|\rho_S(0)|0\rangle\rho_E(0)\right\} = \langle 0|\rho_S(0)|0\rangle. \tag{4.162}$$

Thus, as anticipated, we see that the action of the bath does not change the populations (diagonal elements) of ρ_S. A similar argument can of course be used for $\langle 1|\tilde{\rho}_S(t)|1\rangle$ but we don't need to do it because, if $\langle 0|\tilde{\rho}_S(t)|0\rangle$ doesn't change, then $\langle 1|\tilde{\rho}_S(t)|1\rangle$ cannot change also due to normalization.

Next we look at the off-diagonal element

$$\langle 0|\tilde{\rho}_S(t)|1\rangle = \langle 0|\rho_S(0)|1\rangle\,\mathrm{tr}_E\left\{e^{-iH_0^+t}\rho_E(0)e^{iH_0^-t}\right\}. \tag{4.163}$$

We see now that the exponentials do not cancel, so the result of the trace will not be just $\text{tr}_E\, \rho_E(0) = 1$. In fact, motivated by Eq. (4.159), let us define a general dephasing rate as

$$\boxed{e^{-\Lambda(t)} = \text{tr}_E \left\{ e^{-iH_0^+ t} \rho_E(0) e^{iH_0^- t} \right\}.} \tag{4.164}$$

Then Eq. (4.163) acquires the more familiar form

$$\langle 0|\tilde{\rho}_S(t)|1\rangle = \langle 0|\rho_S(0)|1\rangle e^{-\Lambda(t)t}. \tag{4.165}$$

Our task has now been reduced to the calculation of the decoherence rate $\Lambda(t)$.

Explicit calculation of the decoherence rate

To compute the trace in Eq. (4.164) we being by noticing that the calculation factors into a product of traces, one for each mode of the environment:

$$\begin{aligned} e^{-\Lambda(t)} &= \prod_k \text{tr} \left\{ e^{-it\left[\Omega_k b_k^\dagger b_k + \lambda_k (b_k + b_k^\dagger)\right]} \rho_k e^{it\left[\Omega_k b_k^\dagger b_k - \lambda_k (b_k + b_k^\dagger)\right]} \right\} \\ &= \langle e^{it\left[\Omega_k b_k^\dagger b_k - \lambda_k (b_k + b_k^\dagger)\right]} e^{-it\left[\Omega_k b_k^\dagger b_k + \lambda_k (b_k + b_k^\dagger)\right]} \rangle. \end{aligned}$$

where ρ_k is the initial state of mode k of the environment. If we assume the environment is in a thermal state then

$$\rho_k = (1 - e^{-\beta\Omega_k}) e^{-\beta\Omega_k b_k^\dagger b_k}.$$

Since the calculations for all modes are equivalent, let us clean up the notation a bit and focus on the quantity

$$B = \langle e^{it\left[\Omega b^\dagger b - \lambda(b+b^\dagger)\right]} e^{-it\left[\Omega b^\dagger b + \lambda(b+b^\dagger)\right]} \rangle \tag{4.166}$$

Computing this is a good exercise on operator algebra.

We will need to recall some definitions of displacement operators $D(\alpha) = e^{\alpha b^\dagger - \alpha^* b}$, discussed in Sec. 3.4. Recall that $D^\dagger(\alpha) b D(\alpha) = b + \alpha$. We can then use this to write

$$\Omega b^\dagger b \pm \lambda(b + b^\dagger) = \Omega\, D^\dagger({\pm\lambda}/{\Omega})(b^\dagger b) D({\pm\lambda}/{\Omega}) - \frac{\lambda^2}{\Omega}. \tag{4.167}$$

But the displacement operator is unitary, so it can enter or leave exponentials at will. Consequently

$$e^{-it\left[\Omega b^\dagger b + \lambda(b+b^\dagger)\right]} = e^{-it\lambda^2/\Omega} D^\dagger({\lambda}/{\Omega}) e^{-i\Omega t b^\dagger b} D({\lambda}/{\Omega}),$$

with a similar result for the other exponential. Eq. (4.166) then becomes

$$\begin{aligned} B &= \langle D^\dagger({-\lambda}/{\Omega}) e^{i\Omega t b^\dagger b} D({-\lambda}/{\Omega}) D^\dagger({\lambda}/{\Omega}) e^{-i\Omega t b^\dagger b} D({\lambda}/{\Omega}) \rangle \\ &= \langle D({\lambda}/{\Omega}) e^{i\Omega t b^\dagger b} D^\dagger({2\lambda}/{\Omega}) e^{-i\Omega t b^\dagger b} D({\lambda}/{\Omega}) \rangle, \end{aligned}$$

where I used the fact that $D(-\alpha) = D^\dagger(\alpha)$ and that $D(\alpha)D(\alpha) = D(2\alpha)$ (all these properties are described in Sec. 3.4).

In the middle term we infiltrate the exponential inside $D^\dagger({}^{2\lambda}/_{\Omega})$:

$$\begin{aligned}
e^{i\Omega t b^\dagger b} D^\dagger({}^{2\lambda}/_{\Omega}) e^{-i\Omega t b^\dagger b} &= \exp\bigg\{ -\frac{2\lambda}{\Omega} e^{i\Omega t b^\dagger b}(b^\dagger - b) e^{-i\Omega t b^\dagger b}\bigg\} \\
&= \exp\bigg\{ -\frac{2\lambda}{\Omega}(b^\dagger e^{i\Omega t} - b e^{-i\Omega t})\bigg\} \\
&= D^\dagger({}^{2\lambda e^{i\Omega t}}/_{\Omega})
\end{aligned}$$

We then arrive at the simpler result:

$$B = \langle D({}^{\lambda}/_{\Omega}) D^\dagger({}^{2\lambda e^{i\Omega t}}/_{\Omega}) D({}^{\lambda}/_{\Omega})\rangle$$

Finally, we combine the three displacement operators using $D(\alpha)D(\beta) = e^{(\beta^*\alpha - \alpha^*\beta)/2} D(\alpha + \beta)$ [c.f. Eq. (3.85)]. We then finally arrive at

$$\boxed{B = \langle D(\alpha_t)\rangle, \qquad \alpha_t := \frac{2\lambda}{\Omega}(1 - e^{i\Omega t}).} \tag{4.168}$$

This result is somewhat general since it holds for an arbitrary bath initial state.

Next let us specialize it for the case of a thermal state. In this case, it turns out that the trace of a displacement operator in a thermal state is:[11]

$$\boxed{B = \langle D(\alpha_t)\rangle = \exp\bigg\{ -|\alpha_t|^2(\bar{n} + {}^1/_2)\bigg\}, \qquad \text{when } \rho = (1 - e^{-\beta\Omega})e^{-\beta\Omega b^\dagger b},} \tag{4.169}$$

where $\bar{n} = (e^{\beta\Omega} - 1)^{-1}$.

Analysis of the decoherence rate

Going back now to Eq. (4.164) and reintroducing an index k everywhere, we get

$$e^{-\Lambda(t)} = \prod_k \exp\bigg\{ -|\alpha_{k,t}|^2(\bar{n}(\Omega_k) + {}^1/_2)\bigg\}.$$

---

[11] One way to derive this result is to write it as

$$\langle D(\alpha)\rangle = (1 - e^{-\beta\Omega}) \sum_{n=0}^{\infty} e^{-\beta\Omega n}\langle n|D(\alpha)|n\rangle.$$

In K. Cahill and R. Glauber in *Phys. Rev.* **177**, 1857-1881 (1969), they show that $\langle n|D(\alpha)|n\rangle = e^{-|\alpha|^2/2} L_n(|\alpha|^2)$ where $L_n(x)$ are the Laguerre polynomials. The sum in n may then be related to the generating function of Laguerre polynomials:

$$\sum_{n=0}^{\infty} x^n L_n(y) = \frac{1}{1-x}\exp\bigg\{ -\frac{yx}{1-x}\bigg\}.$$

Using this yields, after some simplifications, the result in Eq. (4.169).

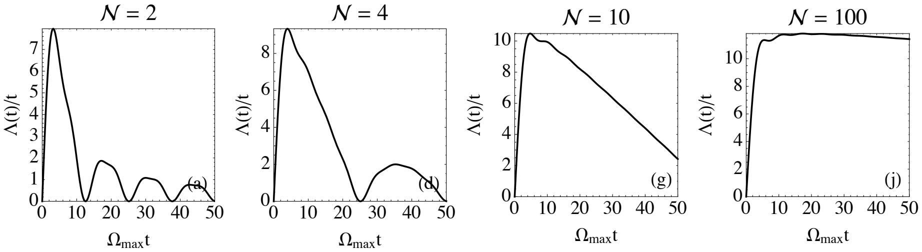

Figure 4.2: The decoherence rate $\Lambda(t)/t$ defined in Eq. (4.170) for different numbers of bath modes N. The parameters Ω_k and λ_k were chosen as in Eqs. (4.171) and (4.172). The temperature was fixed at $T/\Omega_c = 1$.

Or, taking the log on both sides,

$$\Lambda(t) = \sum_k \frac{4\lambda_k^2}{\Omega_k^2}[1 - \cos(\Omega_k t)] \coth\left(\frac{\Omega_k}{2T}\right), \tag{4.170}$$

where I used the fact that $2\bar{n}(x) + 1 = \coth(x/2T)$ and $|\alpha_t|^2 = \frac{8\lambda^2}{\Omega^2}(1 - \cos\Omega t)$. I think Eq. (4.170) is pretty cool. It is an exact result and therefore holds for an *arbitrary* number of bath modes. This is therefore a good opportunity for us to try to visualize the transition between non-Markovian and Markovian behavior as the number of bath oscillators increases.

For concreteness let us make some assumptions about Ω_k and λ_k. Let us assume that Ω_k varies linearly between 0 and a maximum *cut-off* value Ω_c. That is, if we take a bath of N modes, then we define

$$\Omega_k = \frac{k}{N}\Omega_c, \qquad k = 1, 2, \ldots, N. \tag{4.171}$$

Moreover, let us assume that the coupling constants vary as

$$\lambda_k = \sqrt{\frac{\Omega_k}{N}}. \tag{4.172}$$

The logic behind this will be explained below, but essentially it is the condition to obtain what is called an **Ohmic bath**. We also rescale the λ_k with the number of modes since this allows us to compare different values of N.

We present some results for different values of N in Fig. 4.2. As can be seen, if $N = 2$ is small the damping rate is first positive but then goes back all the way to zero at certain points. Having $\Lambda(t) = 0$ means the system didn't dephase at all. This is a signature of non-Markovian behavior. For initial times there is some dephasing. But then information backflows towards the system and it can eventually get back exactly to its initial state when $\Lambda(t) = 0$. As we increase N these backflows start to become more seldom and also occur at larger and larger times. Then, as $N \to \infty$ information never flows back and the dynamics becomes Markovian.

On the other hand, for large N we see that at large times $\Lambda(t)/t$ tends to a constant. This means that the decoherence behaves as $q(t) = q_0 e^{-\Lambda_0 t}$, which is the Lindblad result (4.159). But we also see, for instance in the curve with $N = 100$, that for small times there is an adjustment period in which $\Lambda(t)/t$ is not constant. So this means that for very short times there is always some weird stuff going on, even if the bath is infinitely large. The microscopic derivations of master equations don't capture this type of effect because they only take into account a coarse-graining dynamics at large times.

In fact, the complicated behavior of $\Lambda(t)$ can be clarified if we assume that the number of modes is infinite. In this case we can introduce the spectral density of the bath [Eq. (4.140)]

$$J(\Omega) = 2\pi \sum_k \lambda_k^2 \, \delta(\Omega - \Omega_k),$$

so that Eq. (4.170) becomes

$$\Lambda(t) = \frac{2}{\pi} \int_0^\infty \mathrm{d}\Omega \; \frac{J(\Omega)}{\Omega^2}(1 - \cos\Omega t)\coth\left(\frac{\Omega}{2T}\right). \tag{4.173}$$

We continue to assume Eqs. (4.171) and (4.172) for Ω_k and λ_k. Since $\lambda_k \sim \sqrt{\Omega_k}$ and $J(\Omega) \sim \lambda_k^2$, we see that these assumptions imply an Ohmic spectral density $J(\Omega) \sim \Omega$. As for the cut-off, we have two choices. One is to assume $J(\Omega) = 0$ when $\Omega > \Omega_c$ (a *hard* cut-off) and the other is to assume that $J(\Omega) \sim e^{-\Omega/\Omega_c}$ (a *soft* cut-off). We shall take the latter. That is, we shall assume that

$$J(\Omega) = A\Omega e^{-\Omega/\Omega_c}, \tag{4.174}$$

where A is some positive dimensionless pre-factor, which we will henceforth set to $A = 1$.

The calculation of the decoherence rate (4.173) now reduces to the following integral:

$$\Lambda(t) = \gamma \int_0^\infty \mathrm{d}\Omega \; \frac{e^{-\Omega/\Omega_c}}{\Omega}(1 - \cos\Omega t)\coth\left(\frac{\Omega}{2T}\right). \tag{4.175}$$

This integral can actually be played with analytically. You will find this analysis on Sec. 4.2 of Breuer and Petruccione. The result is:

$$\Lambda(t) \simeq \begin{cases} \frac{\Omega_c^2 t^2}{2} & t \ll \Omega_c^{-1} \\ \ln \Omega t & \Omega_c^{-1} \ll t \ll \frac{1}{\pi T} \\ \pi t T & \frac{1}{\pi T} \ll t \end{cases} \tag{4.176}$$

Here Ω_c^{-1} and $1/(\pi T)$ represent characteristic time scales of the problem. The first is a very small time scale (because the cut-off is usually insanely large) and describes the behavior at very short times. Conversely, $1/(\pi T)$ dominates the behavior of the system at the short time scales.

It is interesting to note, from all of this, that led us to Eq. (4.158) using the approximate method, turn out to be not so bad after all. What is this. Have a look back at

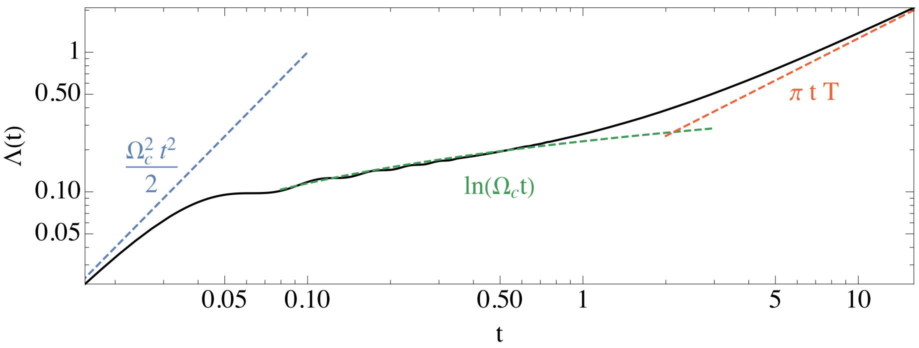

Figure 4.3: The three regimes of the decoherence rate, Eq. (4.176), compared with numerical simulations for $N = 10^4$ bath modes. The other parameters were $\Omega_c = 100$ and $T = 1$.

Eq. (4.157). If we now use Eq. (4.174) for $J(\Omega)$ then, in the limit of $\Omega \to 0$ we get (forgetting about any constants for now):

$$\lim_{\Omega\to 0} \Omega \coth\left(\frac{\Omega}{2T}\right) \sim T$$

Thus, according to the microscopic derivation, the decoherence rate should be proportional to T. That is exactly what we find in Eq. (4.176) for the larger time scale. Thus, we see that the microscopic derivation method of Sec. (4.4) cannot resolve the details at very short times. But for larger times it can, giving the correct type of prediction (here large times means in comparison with $1/(\pi T)$).

Chapter 5

Applications of open quantum systems

5.1 A crash course on Gaussian systems

In Sec. 3.5 we introduced the Husimi-Q function $Q(\alpha, \alpha^*) = \langle\alpha|\rho|\alpha\rangle/\pi$, describing the quantum phase space of continuous variable systems. In that context, a quantum state is called **Gaussian** if its Husimi-Q function is a Gaussian function of the coherent state variables. For instance, the thermal state of a bosonic mode [Eq. (3.111)]

$$Q(\alpha^*, \alpha) = \frac{1}{\pi(\bar{n}+1)} \exp\bigg\{ -\frac{|\alpha|^2}{\bar{n}+1} \bigg\},$$

is Gaussian. On the other hand,the Schrödinger cat state [Eq. (3.108)]

$$Q(\alpha, \alpha^*) = \frac{1}{\pi} e^{-|\alpha-\mu|^2} \bigg\{ 1 + \frac{e^{-2\mu^*\alpha} + e^{-2\mu\alpha^*}}{2} \bigg\},$$

is not.

A **Gaussian preserving map**, on the other hand, is a map that takes Gaussian states to Gaussian states. For a system of an arbitrary number of bosonic modes a_i, the most general such map corresponds to:

- The Hamiltonian being at most *quadratic* in the a_i and $a_i^\dagger$. Thus, the most general Gaussian preserving Hamiltonian has the form

$$H = \sum_{i,j} \bigg\{ A_{ij} a_i^\dagger a_j + \frac{1}{2}(B_{ij} a_i^\dagger a_j^\dagger + B_{ij}^* a_i a_j) \bigg\} + \sum_i (f_i a_i^\dagger + f_j a_j^\dagger),$$

  where A_{ij}, B_{ij} and f_i are coefficients (the factor of 1/2 is placed only for convenience). In order for H to be Hermitian we must have $A^\dagger = A$ and $B^{\mathrm{T}} = B$.

- The Lindblad generators L_α of a master equation being at most *linear* in the a_i and $a_i^\dagger$. Thus, the thermal bath generator

  $$D(\rho) = \gamma\bar{n}\Big[a^\dagger \rho a - \frac{1}{2}\{aa^\dagger, \rho\}\Big] + \gamma(\bar{n}+1)\Big[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\Big],$$

  is Gaussian preserving, whereas the bosonic dephasing model

  $$D(\rho) = \lambda\Big[a^\dagger a \rho a^\dagger a - \frac{1}{2}\{(a^\dagger a)^2, \rho\}\Big],$$

  is not.

Gaussian states and Gaussian preserving maps are extremely useful since they simplify dramatically a potentially unsolvable problem. When dealing with continuous variables it is common to encounter models that have no analytical solutions. For instance, adding a term such as $a^\dagger a^\dagger aa$ to a Hamiltonian usually makes it unsolvable. If your problem involves only a single bosonic mode, than you can probably still deal with it numerically. But if you have a multi-mode system with these kinds of terms, then not even numerics will save you. Gaussian maps, on the other hand, can *always* be dealt with analytically, irrespective of the number of modes we have.

The reason is that for a Gaussian map the equations for the first and second moments are closed. By first moments I mean averages such as $\langle a_i\rangle$, whereas by second moments I mean covariances such as $\langle a_i^\dagger a_j\rangle - \langle a_i^\dagger\rangle\langle a_j\rangle$. In the non-Gaussian scenario, the equation for these guys will depend also on higher order moments, leading to an infinite hierarchy of coupled equations. But for Gaussian maps the equations are closed so that first moments only depend on first moments and second moments only depend on second moments. In the same spirit, just like in classical probability theory, a Gaussian state is fully determined by the first and second moments. So we don't ever need to work with ρ directly; it suffices to work with the moments. We therefore reduce the problem of dealing with an infinite dimensional Hilbert space, to that of only a few expectation values.

Gaussian systems play an important role in quantum information. One of the reasons is that many physical implementations involving quantum optics, mechanical vibrations and even collective atomic excitations, can be described in terms of Gaussian states. Unfortunately, however, Gaussian states cannot be used for universal quantum computing: even though most basic circuit operations can be implemented using Gaussian gates, for some operations non-Gaussian gates are necessary.

If you are interested in a more detailed source of information, I recommend the excellent book by Alessio Serafini entitled "Quantum Continuous Variables".

Algebraic structure

Consider a system of N bosonic modes $a_1, \ldots, a_N$ satisfying the usual algebra

$$[a_i, a_j^\dagger] = \delta_{i,j}, \qquad [a_i, a_j] = 0. \tag{5.1}$$

Alternatively, we may prefer to work with *quadratures*

$$q_i = \frac{1}{\sqrt{2}}(a_i^\dagger + a_i), \qquad p_i = \frac{i}{\sqrt{2}}(a_i^\dagger - a_i). \tag{5.2}$$

These are then Hermitian and satisfy the algebra

$$[q_i, p_j] = i\delta_{i,j}, \qquad [q_i, q_j] = [p_i, p_j] = 0. \tag{5.3}$$

Next define a vector of operators

$$\boldsymbol{X} = (a_1, a_1^\dagger, \ldots, a_N, a_N^\dagger), \qquad \boldsymbol{Y} = (q_1, p_1, \ldots, q_N, p_N). \tag{5.4}$$

In terms of these vectors, the algebras (5.1) and (5.3) become:

$$[X_i, X_j^\dagger] = \Sigma_{i,j}, \qquad [Y_i, Y_j] = i\Omega_{i,j}, \tag{5.5}$$

where Σ and Ω are called **symplectic forms** and are defined as

$$\Sigma = \bigoplus_{i=1}^{N} \sigma_z, \qquad \Omega = \bigoplus_{i=1}^{N} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \bigoplus_{i=1}^{N} (i\sigma_y). \tag{5.6}$$

The symbol $\oplus$ here means *direct sum* and stands for the block-wise composition of matrices. For instance, if we have $N = 2$ then the matrix Ω would read

$$\Omega = (i\sigma_y) \oplus (i\sigma_y) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix},$$

which is just two blocks joined together.

Eq. (5.5) is somewhat important because it establishes the algebra of the group of operators. All other properties follow from this algebra. It turns out that there is a deep connection between this algebraic structure and the so-called **symplectic group** in classical mechanics. If you are interested in this topic, I recommend the papers by R. Simon (e.g. `arXiv:quant-ph/9509002v3`).

I should also mention that the two vectors $\boldsymbol{X}$ and $\boldsymbol{Y}$ are connected by

$$\boldsymbol{Y} = \Lambda \boldsymbol{X}, \qquad \Lambda = \bigoplus_{i=1}^{N} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -i/\sqrt{2} & i/\sqrt{2} \end{pmatrix}, \tag{5.7}$$

which is simply a different way of writing the linear transformation (5.3). The matrix Λ is unitary so the inverse transformation is simply

$$\boldsymbol{X} = \Lambda^\dagger \boldsymbol{Y}, \qquad \Lambda^\dagger = \bigoplus_{i=1}^{N} \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ 1/\sqrt{2} & -i/\sqrt{2} \end{pmatrix}.$$

Covariance matrix

Given now the vector of operators, either $\boldsymbol{X}$ or $\boldsymbol{Y}$, we define their first moments as simply $x_i = \langle X_i \rangle$ and $y_i \langle Y_i \rangle$, which we shall sometimes also group to form a vector $\boldsymbol{x}$

(or $\boldsymbol{y}$). More interestingly, we define the **covariance matrix** (CM) as[1]

$$\Theta = \frac{1}{2}\langle\{X_i, X_j^\dagger\}\rangle - \langle X_i\rangle\langle X_j^\dagger\rangle = \frac{1}{2}\langle\{\delta X_i, \delta X_j^\dagger\}\rangle, \tag{5.8}$$

$$\sigma = \frac{1}{2}\langle\{Y_i, Y_j\}\rangle - \langle Y_i\rangle\langle Y_j\rangle = \frac{1}{2}\langle\{\delta Y_i, \delta Y_j\}\rangle. \tag{5.9}$$

In the second equality on each line I defined an operator $\delta X_i = X_i - \langle X_i\rangle$. This is the fluctuation operator, which means only the quantum fluctuations around the average value. I will leave for you as an exercise to check that the definition using δX_i coincides with the other one.

The covariance matrices are constructed in this way in order to have nice properties. In particular, we always use the symmetrized version $\{X_i, X_j^\dagger\} = X_i X_j^\dagger + X_j^\dagger X_i$. Consequently, by construction we have that Θ is Hermitian, $\Theta^\dagger = \Theta$, whereas σ is real and symmetric, $\sigma^{\mathrm{T}} = \sigma$. For example, if $N = 1$ we have

$$\Theta = \begin{pmatrix} \langle\delta a^\dagger \delta a\rangle + 1/2 & \langle\delta a \delta a\rangle \\ \langle\delta a^\dagger \delta a^\dagger\rangle & \langle\delta a^\dagger \delta a\rangle + 1/2 \end{pmatrix}, \qquad \sigma = \begin{pmatrix} \langle\delta q^2\rangle & \frac{1}{2}\langle\{\delta q, \delta p\}\rangle \\ \frac{1}{2}\langle\{\delta q, \delta p\}\rangle & \langle\delta p^2\rangle \end{pmatrix}.$$

Let me also show you how they look like for $N = 2$. In this case, in order to make things clearer I will assume $\langle a_i\rangle = 0$ so that we don't need to distinguish between δa_i and a_i. But please remember that in general there should be δ's everywhere. For $N = 2$ the CMs look like:

$$\Theta = \begin{pmatrix} \langle a_1^\dagger a_1\rangle + 1/2 & \langle a_1 a_1\rangle & \langle a_1 a_2^\dagger\rangle & \langle a_1 a_2\rangle \\ \langle a_1^\dagger a_1^\dagger\rangle & \langle a_1^\dagger a_1\rangle + 1/2 & \langle a_1^\dagger a_2^\dagger\rangle & \langle a_1^\dagger a_2\rangle \\ \langle a_1^\dagger a_2\rangle & \langle a_1 a_2\rangle & \langle a_2^\dagger a_2\rangle + 1/2 & \langle a_2 a_2\rangle \\ \langle a_1^\dagger a_2^\dagger\rangle & \langle a_1 a_2^\dagger\rangle & \langle a_2^\dagger a_2^\dagger\rangle & \langle a_2^\dagger a_2\rangle + 1/2 \end{pmatrix},$$

and

$$\sigma = \begin{pmatrix} \langle q_1^2\rangle & \frac{1}{2}\langle\{q_1, p_1\}\rangle & \langle q_1 q_2\rangle & \langle q_1 p_2\rangle \\ \frac{1}{2}\langle\{q_1, p_1\}\rangle & \langle p_1^2\rangle & \langle p_1 q_2\rangle & \langle p_1 p_2\rangle \\ \langle q_2 q_1\rangle & \langle q_2 p_1\rangle & \langle q_2^2\rangle & \frac{1}{2}\langle\{q_2, p_2\}\rangle \\ \langle p_2 q_1\rangle & \langle p_2 p_1\rangle & \frac{1}{2}\langle\{q_2, p_2\}\rangle & \langle p_2^2\rangle \end{pmatrix}$$

Notice how the matrix is structured in blocks. The diagonal parts represent the CMs of modes 1 and 2, whereas the off-diagonal blocks represent their *correlations*. From one CM we can obtain the other using the same transformation as Eq. (5.7). Namely,

$$\sigma = \Lambda\Theta\Lambda^\dagger. \tag{5.10}$$

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[1] Some authors define σ with a 2 in front, so that their covariance matrix is twice as ours. Please be careful!.

For instance, if $N = 1$ this is essentially a compact form of writing

$$\begin{aligned} q^2 &= \frac{1}{2}(2a^\dagger a + 1 + aa + a^\dagger a^\dagger), \\ p^2 &= \frac{1}{2}(2a^\dagger a + 1 - aa - a^\dagger a^\dagger), \\ \frac{1}{2}\{q, p\} &= \frac{i}{2}(a^\dagger a^\dagger - aa) \end{aligned} \tag{5.11}$$

Generalized uncertainty relations

Consider the operator

$$Z = \sum_{i=1}^{N} \delta X_i \, z_i,$$

where z_i are arbitrary complex numbers. It then follows by construction that $\langle ZZ^\dagger \rangle \geq 0$ since $ZZ^\dagger$ is a positive semi-definite operator. However, we also have that

$$\langle ZZ^\dagger \rangle = \sum_{i,j} z_i z_j^* \langle \delta X_i \delta X_j^\dagger \rangle.$$

But using the general algebraic structure in Eq. (5.5), which also holds for the fluctuation operators δX_i, we get

$$\{\delta X_i, \delta X_j^\dagger\} = 2\delta X_i \delta X_j^\dagger - \Sigma_{i,j}.$$

Thus,

$$\langle ZZ^\dagger \rangle = \sum_{i,j} z_i z_j^* \Big[\Theta_{i,j} + \Sigma_{i,j}/2\Big] \geq 0.$$

This sum is now a quadratic form with respect to the matrix $\Theta + \Sigma/2$. It is a general theorem in linear algebra that the condition for a quadratic form to be non-negative, for any choice of numbers z_i, is that the matrix in question must be positive semi-definite. Hence, we conclude that the covariance matrix must satisfy what is usually called a *bona fide* (in good faith) relation:

$$\boxed{\Theta + \frac{\Sigma}{2} \geq 0, \qquad \sigma + \frac{i\Omega}{2} \geq 0.} \tag{5.12}$$

Here I also included the same result for σ, which is obtained by simply applying Eq. (5.10) to the first equation.

Eq. (5.12) is actually a stronger statement, or a type of generalization, of Heisenberg's uncertainty relation. To see that, take as an example a single mode. Then

$$\sigma + \frac{i\Omega}{2} = \begin{pmatrix} \langle \delta q^2 \rangle & \frac{1}{2}\langle\{\delta q, \delta p\}\rangle + i/2 \\ \frac{1}{2}\langle\{\delta q, \delta p\}\rangle - i/2 & \langle \delta p^2 \rangle \end{pmatrix}.$$

For this matrix to be positive semi-definite both of its eigenvalues must be non-negative. Or, what is equivalent, both its trace and determinant must be non-negative. The trace is clearly non-negative. As for the determinant, we get

$$|\sigma + \frac{i\Omega}{2}| = \langle \delta q^2 \rangle \langle \delta p^2 \rangle - \frac{1}{4} - \frac{1}{4} \langle \{\delta q, \delta p\} \rangle^2 \geq 0$$

This therefore leads to

$$\boxed{\langle \delta q^2 \rangle \langle \delta p^2 \rangle \geq \frac{1}{4} + \frac{1}{4} \langle \{\delta q, \delta p\} \rangle^2,} \tag{5.13}$$

In the literature this is usually called the **Robertson-Schrödinger uncertainty relation**. Note how it is stronger than the usual Heisenberg relation, which is contained only in the first term.

Another way in which I like to think about Eq. (5.12) is in comparison to classical probability theory. In this case, the condition on the covariance matrix of a classical Gaussian distribution is simply $\sigma \geq 0$ or $\Theta \geq 0$. Thus, a term like $\Sigma/2$ in Eq. (5.12) represents a *quantum correction*, which imposes a stronger bound due to quantum fluctuations. In fact, the uncertainty bound is found for the vacuum state, for which

$$\Theta = \sigma = \frac{\mathbb{I}_2}{2}.$$

Thus, we see that *the covariance matrix is never zero*. Even in the vacuum some fluctuations remain. That is in stark contrast with classical probability theory where zero fluctuations are perfectly allowed (the variables are then deterministic). On the other hand, if your fluctuations are really really large than the extra terms in Eq. (5.12) don't really matter so that $\Theta + \Sigma/2 \geq 0$ is practically the same as $\Theta \geq 0$.

Example: single-mode squeezing

To give a non-trivial example, consider a single-mode system prepared in the **squeezed thermal state**:

$$\rho = S_z \frac{e^{-\beta\omega a^\dagger a}}{Z} S_z^\dagger, \qquad S_z = \exp\left\{\frac{1}{2}(z a^\dagger a^\dagger - z^* a a)\right\}, \tag{5.14}$$

where $Z = (1 - e^{-\beta\omega})$ and z is a complex number that we parametrize as $z = re^{i\theta}$. This contemplates, as particular cases, the thermal state ($z = 0$) and the **squeezed vacuum**,

$$\rho = S_z |0\rangle\langle 0| S_z^\dagger,$$

which is obtained by taking $T = (1/\beta) \to 0$. In the squeezed thermal state the first moments are zero, whereas the second moments are given by

$$\Theta = \begin{pmatrix} \langle \delta a^\dagger \delta a \rangle + 1/2 & \langle \delta a \delta a \rangle \\ \langle \delta a^\dagger \delta a^\dagger \rangle & \langle \delta a^\dagger \delta a \rangle + 1/2 \end{pmatrix} = \begin{pmatrix} (\bar{n} + 1/2)\cosh(2r) & (\bar{n} + 1/2)e^{i\theta}\sinh(2r) \\ (\bar{n} + 1/2)e^{-i\theta}\sinh(2r) & (\bar{n} + 1/2)\cosh(2r) \end{pmatrix} \tag{5.15}$$

where $\bar{n} = (e^{\beta\omega} - 1)^{-1}$ is the Bose-Einstein thermal occupation.

In terms of the quadratures, using Eq. (5.11) we get

$$\langle \delta q^2 \rangle = (\bar{n} + 1/2)\Big[\cosh(2r) + \sinh(2r)\cos(\theta)\Big],$$

$$\langle \delta p^2 \rangle = (\bar{n} + 1/2)\Big[\cosh(2r) - \sinh(2r)\cos(\theta)\Big],$$

$$\frac{1}{2}\langle \{\delta q, \delta p\} \rangle = (\bar{n} + 1/2)\sinh(2r)\sin(\theta).$$

From these results it becomes easier to understand the physical meaning of $\bar{n}$, r and θ. First, suppose that $\theta = 0$. Then these simplify to

$$\langle \delta q^2 \rangle = (\bar{n} + 1/2)e^{2r},$$

$$\langle \delta p^2 \rangle = (\bar{n} + 1/2)e^{-2r},$$

$$\frac{1}{2}\langle \{\delta q, \delta p\} \rangle = 0.$$

Thus, $\bar{n}$ gives the overall width of the position and momentum fluctuations, whereas r (as the name already implies) gives the degree of *squeezing* of each quadrature. We see that if we squeeze in one direction, we must expand in the other. Notwithstanding, the uncertainty product (5.13) continues to be dictated by the thermal fluctuations

$$\langle \delta q^2 \rangle \langle \delta p^2 \rangle = (\bar{n} + 1/2)^2 \geq \frac{1}{4}.$$

This attributes a clear meaning to $\bar{n}$ vs. $1/2$. The former represents the overall width of the distribution, whereas the latter represents the width of the quantum fluctuations. At high temperatures $\bar{n} + 1/2 \simeq \bar{n}$ and we recover a classical harmonic oscillator.

But we also see that one quadrature may also go below the uncertainty bound, at the expense of the other going up. That will happen when $(\bar{n} + 1/2)e^{-2r} \leq 1/2$. This therefore defines a critical squeezing

$$r_c = \frac{1}{2}\ln(2\bar{n} + 1). \tag{5.16}$$

If $r > r_c$ then one quadrature has surpassed the uncertainty bound. This is also related to a concept known as **P representability** introduced by C. T. Lee in *PRA* **41** 2775 (1991), which is a famous paper in the quantum optics community. Essentially, the argument behind **P representability** is that if $r > r_c$ then the state cannot be represented as being simply a superposition of coherent states.

Husimi-Q function of a single-mode Gaussian state

The most general Gaussian state of a single mode turns out to be displaced squeezed thermal state

$$\rho = D(\alpha)S_z \frac{e^{-\beta\omega a^\dagger a}}{Z} S_z^\dagger D^\dagger(\alpha), \qquad S_z = \exp\left\{\frac{1}{2}(z a^\dagger a^\dagger - z^* aa)\right\},$$

where $D(\alpha) = e^{\alpha a^\dagger - \alpha^* a}$. This state has $\langle a \rangle = \alpha$ and a covariance matrix Θ whose entries are exactly (5.15). Although I will not demonstrate this here, I wanted to write down the Husimi-Q function for this state. It reads

$$Q(\alpha, \alpha^*) = \frac{1}{\pi \sqrt{|\tilde{\Theta}|}} \exp\left\{ -\frac{1}{2} \boldsymbol{\alpha}^\dagger \tilde{\Theta}^{-1} \boldsymbol{\alpha} \right\}, \qquad \tilde{\Theta} = \Theta + \mathbb{I}_2/2. \tag{5.17}$$

That is, what appears in the argument is a quadratic form over the vector $\boldsymbol{\alpha} = (\alpha, \alpha^*)$, but not with the covariance matrix itself, but rather $\Theta + \mathbb{I}_2/2$.

As I probably mentioned before, the Husimi-Q function is not the only way of representing quantum phase space. Notably, two other important representations are the Wigner function and the Glauber-Sudarshan P function. Both have a similar structure for Gaussian states. In the Wigner function the quadratic form is with Θ itself, whereas in the P function it is with $\Theta - \mathbb{I}_2/2$.

Dynamics of Gaussian systems: the Lyapunov equation

We now turn to the dynamical evolution of Gaussian systems subject to a Lindblad master equation of the form

$$\frac{d\rho}{dt} = -i[H, \rho] + D(\rho), \tag{5.18}$$

where H is some Gaussian Hamiltonian and $D(\rho)$ is a Gaussian preserving Lindblad dissipator (in the spirit of what was discussed in the beginning of the section). As already mentioned, in this case the equations describing the evolution of the averages and the covariance matrix will be completely decoupled from each other. Here I want to convince you that these equations have the following form. First, the vector of averages $\boldsymbol{x} = \langle \boldsymbol{X} \rangle$ will evolve according to

$$\frac{d\boldsymbol{x}}{dt} = W\boldsymbol{x} - \boldsymbol{f}, \tag{5.19}$$

where the matrix W and the vector $\boldsymbol{f}$ depend on the choice of Hamiltonian and dissipators. Second, the covariance matrix Θ evolves according to the **Lyapunov equation**

$$\boxed{\frac{d\Theta}{dt} = W\Theta + \Theta W^\dagger + F,} \tag{5.20}$$

where F is a matrix that depends only on the dissipators, whereas the matrix W that appears here is *the same* as the one appearing in Eq. (5.19).

I will not try to convince you of this in the general case, but we will focus only on a single mode and then I will show you how this could be extended to multi-modes. Recall from Sec. 4.3 that given a master equation of the form (5.18), the evolution of any observable could be written as in Eq. (4.63):

$$\frac{d\langle O \rangle}{dt} = i\langle [H, O] \rangle + \langle \bar{\mathcal{D}}(O) \rangle, \tag{5.21}$$

where $\bar{D}$ is the adjoint dissipator, defined in Eq. (4.62). Here we assume to have a single mode subject to the Hamiltonian

$$H = \omega a^\dagger a + \frac{1}{2}(\lambda a^\dagger a^\dagger + \lambda^* aa) + (f a^\dagger + f^* a),$$

and the thermal dissipator

$$D(\rho) = \gamma\bar{n}\Big[a^\dagger\rho a - \frac{1}{2}\{aa^\dagger, \rho\}\Big] + \gamma(\bar{n}+1)\Big[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\Big].$$

First moments: we have

$$i[H, a] = -i\omega a - i\lambda a^\dagger - if$$

and, as already discussed in Sec. 4.3,

$$\langle\bar{D}(a)\rangle = -\frac{\gamma}{2}\langle a\rangle,$$

Hence, the equation for $x = \langle a\rangle$ will be

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -i\omega x - i\lambda x^* - \frac{\gamma}{2}x - if. \tag{5.22}$$

This can now be cast in the form (5.19) for the vector $\boldsymbol{x} = (x, x^*)$. We simply need to identify:

$$W = -i\begin{pmatrix} \omega & \lambda \\ -\lambda^* & -\omega \end{pmatrix} - \frac{\gamma}{2}\mathbb{I}_2, \qquad \boldsymbol{f} = -i\begin{pmatrix} f \\ -f^* \end{pmatrix}, \tag{5.23}$$

which is the desired result.

Second moments: we have

$$i[H, a^\dagger a] = -i\lambda a^\dagger a^\dagger + i\lambda^* aa - if a^\dagger + if^* a,$$

$$i[H, aa] = -2i\omega aa - 2i\lambda(a^\dagger a + 1/2) - 2ifa$$

and, again as found in Sec. 4.3,,

$$\langle\bar{D}(a^\dagger a)\rangle = \gamma(\bar{n} - \langle a^\dagger a\rangle), \qquad \langle\bar{D}(aa)\rangle = -\gamma\langle aa\rangle.$$

Hence

$$\frac{\mathrm{d}\langle a^\dagger a\rangle}{\mathrm{d}t} = \gamma(\bar{n} - \langle a^\dagger a\rangle) - i\lambda\langle a^\dagger a^\dagger\rangle + i\lambda^*\langle aa\rangle - if\langle a^\dagger\rangle + if^*\langle a\rangle.$$

$$\frac{\mathrm{d}\langle aa\rangle}{\mathrm{d}t} = -(\gamma + 2i\omega)\langle aa\rangle) - 2i\lambda(\langle a^\dagger a\rangle + 1/2) - 2if\langle a\rangle.$$

As can be seen, not only are the equations a bit messy, but they also mix second moments with the first moments. However, we must never forget that the covariance matrix depends on the fluctuation operators, so we should actually look for an equation for $\langle \delta a^\dagger \delta a\rangle + 1/2$ and $\langle \delta a \delta a\rangle$. Thus we have, for instance,

$$\frac{\mathrm{d}\Theta_{11}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}(\langle \delta a^\dagger \delta a\rangle + 1/2) = \frac{\mathrm{d}\langle \delta a^\dagger \delta a\rangle}{\mathrm{d}t} = \frac{\mathrm{d}\langle a^\dagger a\rangle}{\mathrm{d}t} - \frac{\mathrm{d}\langle a^\dagger\rangle}{\mathrm{d}t}\langle a\rangle - \langle a^\dagger\rangle\frac{\mathrm{d}\langle a\rangle}{\mathrm{d}t}$$

Substituting the equations for $\langle a^\dagger a\rangle$, $\langle a\rangle$ and $\langle a^\dagger\rangle$ we then get

$$\begin{aligned}\frac{\mathrm{d}\Theta_{11}}{\mathrm{d}t} &= \gamma(\bar{n} - \langle \delta a^\dagger \delta a\rangle) - i\lambda\langle \delta a^\dagger \delta a^\dagger\rangle + i\lambda^*\langle \delta a \delta a\rangle \\ &= \gamma(\bar{n} + 1/2 - \Theta_{11}) - i\lambda\Theta_{21} + i\lambda^*\Theta_{12}.\end{aligned}$$

Similarly, the equation for $\langle \delta a \delta a\rangle$ is

$$\frac{\mathrm{d}\Theta_{12}}{\mathrm{d}t} = -(\gamma + 2i\omega)\Theta_{12} - 2i\lambda\Theta_{11}.$$

What I want you to remember about this result is that the terms depending on f vanish identically, whereas all other remain completely intact. Hence, the second moments become fully decoupled from the first moments.

Now that we have these equations for the entries of Θ, we just need to play around with them a bit in order to write them in a more organized way. I will therefore leave for you to check that they can be written in the Lypaunov form (5.20), with the same matrix W as in Eq. (5.23) and a matrix F which reads

$$F = \gamma\begin{pmatrix}\bar{n} + 1/2 & 0 \\ 0 & \bar{n} + 1/2\end{pmatrix}. \tag{5.24}$$

This is what we wanted to show.

A popular thing to study, in the context of Lyapunov equations, is the steady-state, which is the solution of

$$W\Theta + \Theta W^\dagger = -F. \tag{5.25}$$

This represents the state that the system will relax to in the long-time limit. Solving this by hand can become nasty quickly, but all numerical libraries have routines to do so. In Mathematica it is called `LyapunovSolve[W,-F]` and in Matlab it is called `lyap(W,-F)`.

For the problem in question, with W given in Eq. (5.23) and F in Eq. (5.25), we get (assuming $\lambda \in \mathbb{R}$ for simplicity)

$$\Theta = \frac{\bar{n} + 1/2}{\gamma^2 + 4(\omega^2 - \lambda^2)}\begin{pmatrix}\gamma^2 + 4\omega^2 & -2i\lambda(\gamma - 2i\omega) \\ 2i\lambda(\gamma + 2i\omega) & \gamma^2 + 4\omega^2\end{pmatrix}.$$

If $\lambda = 0$ we get a thermal state, $\Theta = (\bar{n} + 1/2)\mathbb{I}_2$. But for $\lambda \neq 0$ we get a competition between the dissipative and the squeezing terms, which end up pushing the system towards a squeezed thermal state.

Application: transport of heat in a bosonic chain

In the next section we will start discussing some real applications of these techniques, in particular to optomechanics and optical parametric oscillators. For now, let me give you a simpler example. Suppose we have two bosonic modes, a_1 and a_2, each connected to a Lindblad thermal dissipator having its own coupling constant γ_i and its own temperature $\bar{n}_i$. That is, we take the total dissipator to have the form

$$D(\rho) = D_1(\rho) + D_2(\rho),$$

where

$$D_i(\rho) = \gamma_i \bar{n}_i \Big[a_i^\dagger \rho a_i - \frac{1}{2}\{a_i a_i^\dagger, \rho\}\Big] + \gamma_i(\bar{n}_i + 1)\Big[a_i \rho a_i^\dagger - \frac{1}{2}\{a_i^\dagger a_i, \rho\}\Big].$$

Moreover, suppose they interact according to the Hamiltonian

$$H = \omega_1 a_1^\dagger a_1 + \omega_2 a_2^\dagger a_2 + g a_1^\dagger a_2 + g^* a_1 a_2^\dagger, \tag{5.26}$$

(I leave the parameters quite general so that we can keep track of them as we move along; in the end you can set $\omega_1 = \omega_2$, $g = g^*$ and so on).

To treat this problem let us start with the unitary part. We try to write an equation for the vector $\boldsymbol{x} = (\langle a_1\rangle, \langle a_1^\dagger\rangle, \langle a_2\rangle, \langle a_2^\dagger\rangle)$. We therefore list the commutators appearing in Eq. (5.21):

$$i[H, a_1] = -i\omega_1 a_1 - iga_2$$

$$i[H, a_1^\dagger] = -i\omega_1 a_1^\dagger + ig^* a_2^\dagger$$

$$i[H, a_2] = -i\omega_1 a_2 - ig^* a_1$$

$$i[H, a_2^\dagger] = -i\omega_1 a_2^\dagger iga_1^\dagger$$

From this we can already read off the unitary contribution of the matrix W in Eq. (5.19):

$$W\Big|_{\text{unitary}} = \begin{pmatrix} -i\omega_1 & 0 & -ig & 0 \\ 0 & i\omega_1 & 0 & ig^* \\ -ig^* & 0 & -i\omega_2 & 0 \\ 0 & ig & 0 & i\omega_2 \end{pmatrix} \tag{5.27}$$

The point I want to emphasize is that, now that we have found this matrix for the first moments, it will also be the matrix appearing in the Lyapunov equation, so that we don't have to find it again.

Next, the dissipative part is also really easy because the dissipators act separately on each mode. Thus, their contributions will always appear in block form:

$$W\Big|_{\text{dissipative}} = \begin{pmatrix} -\frac{\gamma_1}{2}\mathbb{I}_2 & 0 \\ 0 & -\frac{\gamma_2}{2}\mathbb{I}_2 \end{pmatrix},$$

and

$$F = \begin{pmatrix} \gamma_1(\bar{n}_1 + 1/2)\mathbb{I}_2 & 0 \\ 0 & \gamma_2(\bar{n}_2 + 1/2)\mathbb{I}_2 \end{pmatrix}.$$

With these matrices, we now have all the ingredients to study the first and second moments. Since there is no pump term, the first moments will evolve according to

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = W\boldsymbol{x}.$$

The matrix W definitely has eigenvalues with a negative real part, so that the first moments will simply relax towards zero, $\boldsymbol{x}(t \to \infty) \to 0$.

Next we turn to the second moments and the Lyapunov equation (5.20). In particular, we focus on the steady-state, which is the solution of Eq. (5.25). For simplicity I will now assume that $\gamma_1 = \gamma_2 = \gamma$, $\omega_1 = \omega_2 = \omega$ and $g^* = g$. Dr. Mathematica then tells us that the solution is

$$\Theta = \begin{pmatrix} \langle a_1^\dagger a_1\rangle + 1/2 & 0 & \langle a_1 a_2^\dagger\rangle & 0 \\ 0 & \langle a_1^\dagger a_1\rangle + 1/2 & 0 & \langle a_1^\dagger a_2\rangle \\ \langle a_1^\dagger a_2\rangle & 0 & \langle a_2^\dagger a_2\rangle + 1/2 & 0 \\ 0 & \langle a_1 a_2^\dagger\rangle & 0 & \langle a_2^\dagger a_2\rangle + 1/2 \end{pmatrix},$$

where

$$\begin{aligned} \langle a_1^\dagger a_1\rangle &= \bar{n}_1 + \frac{2g^2}{4g^2+\gamma^2}(\bar{n}_2 - \bar{n}_1), \\ \langle a_2^\dagger a_2\rangle &= \bar{n}_2 - \frac{2g^2}{4g^2+\gamma^2}(\bar{n}_2 - \bar{n}_1), \\ \langle a_1^\dagger a_2\rangle &= \frac{ig\gamma}{4g^2+\gamma^2}(\bar{n}_2 - \bar{n}_1). \end{aligned} \tag{5.28}$$

I think these results are quite interesting. First we see that the populations of 1 and 2 are not exactly $\bar{n}_1$ and $\bar{n}_2$, which is what the Lindblad dissipators would want. Instead, it is modified by a term proportional to the interaction g between them. However, this term only exists if there is a "temperature gradient" between the two modes; that is, if $\bar{n}_1 \neq \bar{n}_2$. In fact, we also see that this gradient generates *correlation* between the two modes $\langle a_1^\dagger a_2\rangle$.

To understand the meaning of a term such as $\langle a_1^\dagger a_2\rangle$, it is helpful to look at the **current of quanta** between the two modes. First we write down the equation for $\langle a_1^\dagger a_1\rangle$:

$$\frac{\mathrm{d}\langle a_1^\dagger a_1\rangle}{\mathrm{d}t} = \gamma(\bar{n}_1 - \langle a_1^\dagger a_1\rangle) - ig(\langle a_1^\dagger a_2\rangle - \langle a_1 a_2^\dagger\rangle). \tag{5.29}$$

This can now be viewed as a *continuity equation*. It essentially says that the rate at which the number of quanta in mode 1 changes is due to a current of quanta entering from the bath (the first term) and the current of quanta leaving towards mode 2. In the steady-state $\mathrm{d}\langle a_1^\dagger a_1\rangle/\,\mathrm{d}t = 0$ and the two currents therefore coincide:

$$\gamma(\bar{n}_1 - \langle a_1^\dagger a_1\rangle) = ig(\langle a_1^\dagger a_2\rangle - \langle a_1 a_2^\dagger\rangle) := J \tag{5.30}$$

We therefore see that the imaginary part of $\langle a_1^\dagger a_2\rangle$ is actually related to the current of quanta. This means that for energy to flow, the two modes must be correlated, which makes sense since a current implies that information is being transferred from one mode to the other.

The explicit formula for J is found using the results in Eq. (5.28) and reads:

$$J = \frac{2g^2\gamma}{4g^2+\gamma^2}(\bar{n}_2 - \bar{n}_1). \tag{5.31}$$

This result makes sense: the current is zero if $g = 0$ (we break the link between 1 and 2) or if $\gamma = 0$ (we break the link between 1,2 and their baths). Moreover, the current increases with the temperature gradient $\bar{n}_2 - \bar{n}_1$ and its *sign* depends on whether 1 is warmer than 2 or vive-versa. Thus, as intuitively expected, current always flows from hot to cold.

Of course, these ideas can be extended in an infinite number of ways and, in fact, that is a line of research which I really like. But in order for us to not get off track, I will stop with this for now.

Gaussian quantum information

Finally, I want to discuss some tricks for dealing with information-theoretic quantities of Gaussian states, such as measures of purity and correlations. The literature on this subject is quite vast. But here I would like to focus on the particularly recent result of `arXiv 1203.5116`, which bases the entire analysis on the Rényi-2 entropy.

In Sec. 2.9, when we talked about entropy, I mentioned the so-called *strong subadditivity inequality* of the von Neumann entropy: given an arbitrary tri-partite system, it reads

$$S(AB) + S(BC) \geq S(ABC) - S(B). \tag{5.32}$$

The strong subadditivity is, in a sense, an "approval seal" that an entropy should have in order to be employed as an information-theoretic quantity. And, in general, strong subadditivity is a unique feature of von Neumann's entropy and does not hold for the Rényi-α entropies. It is for this reason that in most of quantum information, the von Neumann reigns supreme, as the ultimate entropic quantifier.

The key result of `arXiv 1203.5116` was to show that, **for Gaussian states, strong subadditivity holds for the Rényi-2**. And this is extremely useful because the Rényi-2 is very easy to compute since it is simply related to the purity of the state:

$$S_2(\rho) = -\ln \mathrm{tr}(\rho^2). \tag{5.33}$$

What is even more remarkable, for Gaussian states the purity actually turns out to be

$$\mathrm{tr}(\rho^2) = \frac{1}{2^N\sqrt{|\Theta|}}, \tag{5.34}$$

where N is the number of modes in question.[2] I will leave the demonstration of this result for you as an exercise (see problem set). Consequently, we find that the Rényi-2 entropy of a Gaussian state is

$$\boxed{S_2(\Theta) = \frac{1}{2}\ln|\Theta| + N\ln 2.} \tag{5.35}$$

Maybe I should have written $S_2(\rho)$, but I like to write it as $S_2(\Theta)$ to emphasize that for a Gaussian state all that matters is the CM. As far as Gaussian states are concerned, the Rényi-2 entropy (5.35) is therefore a perfectly valid entropic measure, so that everything that can be done with von Neumann's, can also be done with Rényi-2.

An obvious reason why Eq. (5.35) is easy to deal with is because computing a determinant is easy. But another, perhaps even stronger reason, is that given a density matrix of a multi-partite system, finding the **partial trace** is *trivial*. Suppose you have two modes, A and B. The joint covariance matrix of the two modes can then be written in block form as

$$\Theta_{AB} = \begin{pmatrix} \Theta_A & S_{AB} \\ S_{AB}^\dagger & \Theta_B \end{pmatrix}, \tag{5.36}$$

where Θ_A and Θ_B are the covariance matrices of A and B individually and S_{AB} represents their correlation. If we now wish to take the partial trace over B, for instance, then the reduced state of A will still be a Gaussian state. Consequently, it is fully characterized by its covariance matrix Θ_A. Hence, taking the partial trace over a system simply means throwing away the lines and columns in the matrix that you don't want anymore.

For instance, suppose we have a tripartite system ABC with a CM

$$\Theta_{ABC} = \begin{pmatrix} \Theta_A & S_{AB} & S_{AC} \\ S_{AB}^\dagger & \Theta_B & S_{BC} \\ S_{AC}^\dagger & S_{BC}^\dagger & \Theta_C \end{pmatrix}. \tag{5.37}$$

Now suppose we wish to take the partial trace over B. The reduced density matrix of AC will then still be a Gaussian state, with a CM:

$$\Theta_{AC} = \begin{pmatrix} \Theta_A & S_{AC} \\ S_{AC}^\dagger & \Theta_C \end{pmatrix}.$$

You see what I did there? I simply threw away the lines and columns corresponding to system B.

As a first application, consider a bipartite system AB and let us compute the mutual information

$$\boxed{\mathcal{I}_{AB} = S_A + S_B - S_{AB} = \frac{1}{2}\ln\left\{\frac{|\Theta_A||\Theta_B|}{|\Theta_{AB}|}\right\}.} \tag{5.38}$$

---

[2] Sanity check: for the vacuum state of N modes, $\Theta = \mathbb{I}_{2N}/2$ so that $|\Theta| = (1/2)^{2N}$ and hence $2^N\sqrt{|\Theta|} = 1$, so that the system is in a pure state, $\text{tr}(\rho^2) = 1$.

Recall that the mutual information is a quantifier of the *total* correlations between two systems, irrespective of whether these correlations are quantum or classical. The proof that this quantity is non-negative (which is the as proving the sub-additivity inequality) can be done using something called the **Hadamard-Fisher inequality**.

Let M denote a positive semi-definite Hermitian matrix of size K and let α, β denote index sets of $\{1, \ldots, K\}$. For instance, $\alpha = \{1, 2, 3\}$ and $\beta = \{1, 5, 20\}$, or whatever. Moreover, given an index set α, let M_α denote the matrix M chopped up to contain only the rows and columns of the index set α . The Hadamard-Fisher inequality then says that

$$|M_{\alpha\cup\beta}||M_{\alpha\cap\beta}| \leq |M_\alpha||M_\beta|, \tag{5.39}$$

with the proviso that $|M_\varnothing| = 1$. In the case of Eq. (5.38) we take α to refer to the index set of modes A and β to refer to the index set of modes B, which then gives $|\Theta_{AB}| \leq |\Theta_A||\Theta_B|$. Hence $\mathcal{I}_{AB} \geq 0$.

If the composite AB system is in a pure state then all correlation must be entanglement. In this case we know that $S_{AB} = 0$. Moreover, as we have seen when we discussed the Schmidt decomposition in Sec. 2.8, we also have $S_A = S_B$. Hence

$$\mathcal{I}_{AB} = 2S(\Theta_A) = 2S(\Theta_B), \qquad \text{For a pure state AB.} \tag{5.40}$$

In this case the mutual information gives twice the entanglement entropy between the two sub-systems.

The inequality appearing in the strong subadditivity inequality (5.32) can be used to define a **conditional mutual information**

$$\boxed{\mathcal{I}(A:C|B) := S_{AB} + S_{BC} - S_{ABC} - S_C = \frac{1}{2}\ln\left\{\frac{|\Theta_{AB}||\Theta_{BC}|}{|\Theta_{ABC}||\Theta_C|}\right\}.} \tag{5.41}$$

This represents the amount of information shared between A and C, intermediated by B. The positivity of this quantity is again demonstrated using the Hadamard-Fisher inequality (5.39). One need only take α to denote the index set of AB and β to denote the index set of BC.

We can go further and also define measures of Rényi-2 entanglement and Rényi-2 quantum discord. I will not go through these guys right now, since they take some time to discuss. If you are interested, please have a look at `arXiv 1203.5116`.

Duan-Duan

To finish this section, I want to briefly discuss a criteria for determining whether two continuous variables are entangled or not when they are in a *mixed* state. If the state is pure, then correlation = entanglement. But if the state is mixed, part of the correlations may be quantum and part may be classical (recall that, by classical, we mean a correlation related to our lack of knowledge about the system). We haven't discussed a lot about this quantum-classical separation (sorry about that!) but I will try to compensate this a bit now. The main point is that this separation is not sharp, meaning there is no universal criteria for separating quantum and classical correlations.

Essentially, what one would hope is to be able to divide the the mutual information as $\mathcal{I} = \mathcal{I}_C + \mathcal{I}_Q$, where $\mathcal{I}_C$ quantifies the classical correlations and $\mathcal{I}_Q$ quantifies the quantum correlations. This is the approach of the so-called **quantum discord**, introduced by Henderson and Vedral in `arXiv quant-ph/0105028` and simultaneously by Ollivier and Zurek in `arXiv quant-ph/0105072`. But discord is not perfect and there are heated debates in the literature about it. Some people love it. Some people hate it. (As for me, I'm just too stupid to have a strong opinion about it).

What we *do* have, however, is some idea of when a state contains quantum features and when it does not. And this can lead us to the criteria of **separability**. It is fair to assume that a state such as $\rho_A \otimes \rho_B$ does not have any quantum correlations between A and B. Of course, inside ρ_A and ρ_B there can still be a bunch of quantum features. But as far as AB correlations are concerned, such a product state has none. Motivated by this, we define a **separable** state as a state of the form

$$\rho_{AB} = \sum_i p_i\, \rho_{A,i} \otimes \rho_{B,i}, \qquad p_i \in [0,1], \qquad \sum_i p_i = 1. \tag{5.42}$$

The logic here is that such a state is just a classical probabilistic combination of product states and, therefore, any correlations cannot come from entanglement, but must come from the classical probabilities p_i. For this reason, we can say that a separable state is not entangled.

Instead of trying to quantify the degree of entanglement, we can now take on a more soft approach and simply ask whether a certain state is separable or not. If it is separable than all correlations must be of classical origin, whereas if it is not separable, than some degree of quantum correlation is present (exactly how much we cannot know). A large number of criteria are available for both discrete and continuous variables. A comprehensive review can be found in a famous review by the Horodecki clan (`arXiv quant-ph/0702225`). Here I will focus on continuous variables and discuss a criteria developed in `arXiv quant-ph/9908056` by Duan, Giedke, Cirac and Zoller. For some reason, people forget about the other authors and simply call it the **Duan criteria**. The idea is as follows. Consider two bosonic modes with operators a_1 and a_2. Define the quadrature for the first, as usual:

$$q_1 = \frac{1}{\sqrt{2}}(a_1^\dagger + a_1), \qquad p_1 = \frac{i}{\sqrt{2}}(a_1^\dagger - a_1).$$

But for the second, define rotated quadrature operators

$$q_2 = \frac{1}{\sqrt{2}}(e^{i\phi}a_2^\dagger + e^{-i\phi}a_2), \qquad p_2 = \frac{i}{\sqrt{2}}(e^{i\phi}a_2^\dagger - e^{-i\phi}a_2),$$

where ϕ is an arbitrary angle. Note that we still have $[q_2, p_2] = i$. Finally, define

$$Q_+ = \frac{q_1 + q_2}{\sqrt{2}}, \qquad P_- = \frac{p_1 - p_2}{\sqrt{2}}. \tag{5.43}$$

According to Duan, Giedke, Cirac and Zoller, a sufficient criteria for a state to be separable is

$$\boxed{\langle \delta Q_+^2 \rangle + \langle \delta P_-^2 \rangle \geq 1,} \tag{5.44}$$

for all ϕ. This criteria holds even for non-Gaussian states. However, for Gaussian states, it turns out it is both sufficient *and* necessary. Thus, within the context of Gaussian states, if you find a angle ϕ such that $\langle \delta Q_+^2 \rangle + \langle \delta P_-^2 \rangle < 1$, then the state is definitely not separable.

5.2 Optomechanics

The name optomechanics refers, as you probably guessed, to the combined interaction of an optical mode and mechanical vibrations. The two most typical configurations are shown in Fig. 5.1. For simplicity, the problem is usually approximated to that of a single radiation mode interacting with a single harmonic oscillator. However, the interaction between the two is either cubic or quartic, so that Gaussianity is not preserved. Much of our mathematical work will then be on an approximation method which is used to re-Gaussianize the theory.

The radiation mode is a standing mode of a cavity, of frequency ω_c, which is pumped by a laser at frequency ω_p through a semi-transparent mirror. In the configuration of Fig. 5.1(a) the other mirror is allowed to vibrate slightly from its equilibrium position and this vibration is modeled as a harmonic oscillator. In (b), on the other hand, both mirrors are fixed, but a semi-transparent membrane is placed inside the cavity and allowed to vibrate.

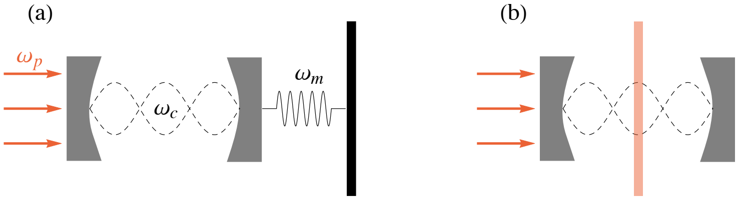

Figure 5.1: Schematic representation of the two most widely used optomechanical configurations. In both cases an optical cavity of frequency ω_c is pumped with a laser at frequency ω_p through a semi-transparent mirror. In (a) one of the mirrors is allowed to vibrate with a frequency ω_m. In (b), on the other hand, the mechanical vibration is that of a semi-transparent membrane placed inside the cavity.

When dealing with physical implementations, such as this one, it is always recommended that you start by establishing the Hamiltonian and the dissipation channels. I will call this **awesome advice # 1**. In the end, we want to start with a master equation of the form

$$\frac{d\rho}{dt} = -i[H, \rho] + D(\rho),$$

for some Hamiltonian H and some dissipator $D(\rho)$. Let us start with the cavity mode, which we associate with an annihilation operator a. Its Hamiltonian was discussed in Sec. 3.2 and reads

$$H_c = \hbar\omega_c a^\dagger a + \hbar\epsilon a^\dagger e^{-i\omega_p t} + \hbar\epsilon^* a e^{i\omega_p t}. \tag{5.45}$$

I have reintroduced $\hbar$ for now, just for completeness. But I will get rid of it very soon. Recall also that ϵ is the pump intensity and can be written as $|\epsilon|^2 = 2\kappa P/\hbar\omega_p$ where κ is the loss rate [that also appears in $D(\rho)$] and P is the laser pump power. Moreover, the loss of photons through the cavity is described by the dissipator

$$D_c(\rho) = 2\kappa\Big[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\Big], \tag{5.46}$$

which, as I probably mentioned before, is absolutely standard in all descriptions of lossy cavities.

Next we turn to the mechanical mode. We assume it is a single harmonic oscillator with position Q and momentum P satisfying $[Q, P] = i\hbar$. Its free Hamiltonian will then be

$$H_m = \frac{P^2}{2m} + \frac{1}{2}m\omega_m^2 Q^2 = \hbar\omega_m(b^\dagger b + 1/2), \tag{5.47}$$

where m is the mass, ω_m is the mechanical frequency and

$$b = \frac{1}{\sqrt{2}}\bigg\{\sqrt{\frac{m\omega_m}{\hbar}}Q + \frac{iP}{\sqrt{m\hbar\omega_m}}\bigg\}, \tag{5.48}$$

is the annihilation operator for the mechanical mode.

A much harder question concerns the choice of dissipator for the mechanical mode. The mechanical mode is of course dissipative because it is connected to your sample so the bath in this case are the phonons; i.e., the mechanical vibrations of the material which makes up both the vibrating mirror and its surroundings. Consequently, they will cause the oscillator to thermalize at the temperature of your experimental setup. But is not well modeled by a Lindblad equation, since Lindblad assumes a rotating-wave approximation, which is usually not good for mechanical frequencies. In fact, more than that, as shown recently in `arXiv 1305.6942`, the dynamics can actually be highly non-Markovian, so not even that is guaranteed. Traditionally, one normally uses quantum Brownian motion, in which the degree of non-Markovianity can be taken into account. However, this makes the entire treatment quite difficult.

So we now arrive at **awesome advice # 2**: *never* start with very realistic descriptions of your model. Realistic descriptions are always too complicated and always contain an enormous number of parameters whose values you usually don't know very well. This will then completely mask the physics of the problem. Instead, the advice is to always start with the simplest description possible, containing only a small amount of parameters. *Even if that description is not very good.* Then, after your learned everything you can from this simplified picture, you start to add ingredients and see how they affect your toy-model results. Even though this may at first seem like extra work, it turns out it is not: if you start with a complicated realistic model, it will take you forever to obtain answers. But if you start with a simple model, then each ingredient you add will only change the calculations by a small bit and therefore they will not be so hard.

Concerning the dissipative channel of the mechanical mode, the simplification I will adopt is to use a Lindblad equation to model $D_m(\rho)$. This is definitely a rough approximation, but will allow us to extract the physics more clearly. Thus, we will assume that

$$D_m(\rho) = \gamma(\bar{n}+1)\Big[b\rho b^\dagger - \frac{1}{2}\{b^\dagger b, \rho\}\Big] + \gamma\bar{n}\Big[b^\dagger\rho b - \frac{1}{2}\{bb^\dagger, \rho\}\Big]. \tag{5.49}$$

where γ is the coupling constant of the mechanical mode to its bath and $\bar{n} = (e^{\omega_m/T} - 1)^{-1}$ is the Bose-Einstein distribution, with T being the temperature of the mechanical mode.

Finally, we reach que most important question, which concerns the **optomechanical interaction**. Here we shall focus on the setup in Fig. 5.1(a). In this case the coupling comes from the fact that the cavity frequency ω_c actually depends on the position of the mirror. In fact, from electromagnetism[3] one can show that the dependence is of the form $\omega_c(L) = A/L$ where L is the size of the cavity and A is a constant. When the mirror is allowed to vibrate we should then replace L by $L + Q$. Assuming that Q is small compared to L we can then get

$$\omega_c(L+Q) \simeq \frac{A}{L}\Big(1 - \frac{Q}{L}\Big) = \omega_c - \frac{\omega_c}{L}Q,$$

where $\omega_c = \omega_c(L)$ is the equilibrium frequency of the cavity. Consequently, we see that the Hamiltonian $\omega_c a^\dagger a$ is to be transformed into

$$\omega_c a^\dagger a \to \omega_c a^\dagger a - \frac{\omega_c}{L} a^\dagger a Q.$$

We therefore now have a coupling between $a^\dagger a$ and Q. This is called the **radiation pressure** coupling. And if you think about it, it makes all the sense in the world: A term such as $-fQ$ in a Hamiltonian means a force f pushing the coordinate Q. This is exactly what we have here, except that now the force actually depends on the number of photons $a^\dagger a$ inside the cavity. The more photons we have, the more we push the mirror. Makes sense!

Collecting everything, our Hamiltonian can then be written as

$$H = \hbar\omega_c a^\dagger a + \hbar\omega_m b^\dagger b - \frac{\hbar\omega_c}{L} a^\dagger a Q + \hbar\epsilon a^\dagger e^{-i\omega_p t} + \hbar\epsilon^* a e^{i\omega_p t}.$$

To make it a little bit cleaner, we substitute $Q = \sqrt{\frac{\hbar}{2m\omega_m}}(b + b^\dagger)$ and then write this as

$$\boxed{H = \hbar\omega_c a^\dagger a + \hbar\omega_m b^\dagger b - \hbar g_0 a^\dagger a (b + b^\dagger) + \hbar\epsilon a^\dagger e^{-i\omega_p t} + \hbar\epsilon^* a e^{i\omega_p t},} \qquad (5.50)$$

where $g_0 = \frac{\omega_c}{L}\sqrt{\frac{\hbar}{2m\omega_m}}$. This is the so-called *radiation pressure optomechanical coupling*. You will find it in most papers on optomechanics. Note also that this is *not* a Gaussian Hamiltonian since the interaction term is cubic in the creation and annihilation operators. Thus, it cannot be solved exactly and we will therefore have to resort to some approximations.

To summarize, the model in Fig. 5.1(a) can be described, to a first approximation, as

$$\boxed{\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho] + D_c(\rho) + D_m(\rho),} \qquad (5.51)$$

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[3] The standard reference on this is C. Law, *Phys. Rev. A.*, **51**, 2537-2541 (1995).

Table 5.1: Typical parameters for an optomechanical setup, all given in Hz. Based on arXiv 1602.06958. Typical temperatures are of the order of 1 K, which give $\bar{n} = (e^{\hbar\omega_m/k_BT} - 1)^{-1} \sim 10^3$.

Parameter	ω_c	ω_m	κ	γ	g_0	ϵ
Order of magnitude (Hz)	10^{14}	10^6	10^7	10	10^3	10^{12}

where H is given in (5.50), $D_c(\rho)$ is given in (5.46) and $D_m(\rho)$ is given in (5.49). As discussed above, the weakest link here is the choice of D_m, which is in general a bit drastic. All other ingredients are, in general, quite well justified. Typical values of the parameters for an experiment that I participated a few years ago (`arXiv 1602.06958`) are shown in Table 5.1. But, of course, part of the experimental game is to really have flexibility in changing these parameters.

Before we delve deeper into Eq. (5.51), let me comment on the configuration in Fig. 5.1(b). I will not try to derive the Hamiltonian in this case. But I want to simply point out that it *definitely* cannot be the same as (5.50) due to its symmetry. The Hamiltonian (5.50) is linear in Q precisely because it pushes the mirror in one specific direction. In the case of Fig. 5.1(b) there is no preferred direction. Thus, from such an argument we expect that the radiation pressure interaction in this case should, to lowest order in Q, be *quadratic*. That is, something like

$$g_0^{(2)} a^\dagger a (b + b^\dagger)^2,$$

for some constant $g_0^{(2)}$. Indeed, that is what is found from a more careful derivation.

Pump it up!

The first step in dealing with the Hamiltonian (5.50) is to move to a rotating frame with respect to the pump frequency, exactly as was done in Sec. 3.3. That is, the unitary transformation is taken to be $e^{i\omega_p t a^\dagger a}$, while nothing is done on the mechanical part. The dissipative part does not change, whereas the Hamiltonian simplifies to

$$H = \Delta' a^\dagger a + \omega_m b^\dagger b - g_0 a^\dagger a (b + b^\dagger) + \epsilon a^\dagger + \epsilon^* a, \tag{5.52}$$

where $\Delta' = \omega_c - \omega_p$ is the cavity detuning (I'm using Δ' instead of Δ because below we will come across another quantity that I will want to call Δ). As promised, here I already set $\hbar = 1$.

This Hamiltonian is still non-linear (higher than quadratic) and therefore cannot be solved analytically. However, in this case, and in many other problems involving cavities, there is a trick to obtain very good approximations, which is related to the pump intensity. Roughly speaking $\langle a \rangle$ will try to follow the intensity ϵ. So if the pump is sufficiently large the first moments $\langle a \rangle$ and $\langle b \rangle$ will tend to be much larger than the fluctuations (i.e., the second moments such as $\langle \delta a^\dagger \delta a \rangle$). This then allows us to *linearize* our equations and Hamiltonians and therefore obtain solvable models. I call this the **pump trick**. In statistical mechanics they would call it a mean-field approximation.

To see how it works, let us consider the evolution equations for the first moments $\alpha = \langle a \rangle$ and $\beta = \langle b \rangle$. Following the usual procedure, they read

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = -(\kappa + i\Delta')\alpha - i\epsilon + ig_0\langle a(b + b^\dagger)\rangle,$$

$$\frac{\mathrm{d}\beta}{\mathrm{d}t} = -(\frac{\gamma}{2} + i\omega_m)\beta + ig_0\langle a^\dagger a\rangle.$$

Thus, as promised, since the Hamiltonian is non-Gaussian, the evolution of the first moments actually depend on second moments. And if we were to try to compute the evolution of the second moments, they would depend on third moments and so on.

The pump trick is now to write $a = \alpha + \delta a$ and $b = \beta + \delta b$. Exploiting the fact that $\langle \delta a \rangle = \langle \delta b \rangle = 0$, by construction, we can then write, for instance,

$$\langle ab \rangle = \langle (\alpha + \delta a)(\beta + \delta b) \rangle = \alpha\beta + \langle \delta a \delta b \rangle.$$

So far this is exact. The approximation is now to assume that the second term is much smaller than the first, so that it may be neglected. A similar idea holds for all other terms.

With this trick the equations for α and β become *closed, but non-linear*:

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = -(\kappa + i\Delta')\alpha - i\epsilon + ig_0\alpha(\beta + \beta^*), \tag{5.53}$$

$$\frac{\mathrm{d}\beta}{\mathrm{d}t} = -(\frac{\gamma}{2} + i\omega_m)\beta + ig_0|\alpha|^2. \tag{5.54}$$

We are interested in the steady-states of these equations, obtained by setting $\mathrm{d}\alpha/\mathrm{d}t = \mathrm{d}\beta/\mathrm{d}t = 0$. From the second equation we get

$$\beta = \frac{ig_0|\alpha|^2}{\gamma/2 + i\omega_m}. \tag{5.55}$$

This result highlights some of the weirdness of using a Lindblad description for the mechanical mode. What we are talking about here is really the *equilibrium configuration* of the mirror and $\mathrm{Re}(\beta)$ is proportional the displacement $\langle Q \rangle$, whereas $\mathrm{Im}(\beta)$ is related to $\langle P \rangle$. Of course, since we are talking about a mechanical dude, equilibrium should mean $\langle P \rangle = 0$, but this is not what happens in Eq. (5.55). So Lindblad predicts an equilibrium with a finite momentum, which doesn't make much sense. As I said, in this case the rotating wave approximation is a bit rough. However, lucky for us, the value of γ is usually really small (see Table 5.1) so that this imaginary part is almost negligible. In fact, if we discard it we get something that makes quite some sense, which is a displacement $\langle Q \rangle = \mathrm{Re}(\beta)$ proportional to the number of photons $|\alpha|^2$.

Substituting (5.55) into (5.53) then yields the equation

$$\left\{\kappa + i\Delta' - \frac{2ig_0^2\omega_m|\alpha|^2}{\frac{\gamma^2}{4} + \omega_m^2}\right\}\alpha = -i\epsilon.$$

This is now a non-linear equation for α, which has to be solved numerically. It is convenient to define an effective detuning

$$\Delta = \Delta' - g_0(\beta + \beta^*) = \Delta' - \frac{2g_0^2\omega_m|\alpha|^2}{\frac{\gamma^2}{4} + \omega_m^2}, \tag{5.56}$$

so that we can rewrite the equation above as

$$\alpha = \frac{-i\epsilon}{\kappa + i\Delta}. \tag{5.57}$$

Of course, Δ is still a function α so this is an implicit equation. But we can just assume that we have solved this equation numerically and therefore found the numerical value of Δ.

Another useful trick is to adjust the relative phase of ϵ in order to make α real. The phase of the pump is arbitrary so we can also tune it in this way. And, of course, the final result will not depend on this, so it is just a way to make the calculations a bit simpler. Hence, from now on we will assume that $\alpha \in \mathbb{R}$.

Fluctuations around the average

The next step is to rewrite the master equation (5.51) in terms of the fluctuation operators $\delta a = a - \alpha$ and $\delta b = b - \beta$. Note that these are still bosonic operators, the only difference is that they now have zero mean and therefore describe only fluctuations around the average. We start with the Hamiltonian (5.50) and then express each term as something like:

$$a^\dagger a = |\alpha|^2 + \alpha\delta a^\dagger + \alpha^*\delta a + \delta a^\dagger \delta a.$$

Doing this for every term allow us to write

$$H = \text{const} + H_1 + H_2 + H_3,$$

where "const" refers to a unimportant constant and

$$H_1 = \Delta'(\alpha\delta a^\dagger + \alpha^*\delta a) + \omega_m(\beta\delta b^\dagger + \beta^*\delta b) + \epsilon\delta a^\dagger + \epsilon^*\delta a \tag{5.58}$$

$$-g_0\Big\{|\alpha|^2(\delta b + \delta b^\dagger) + (\beta + \beta^*)(\alpha\delta a^\dagger + \alpha^*\delta a)\Big\}, \tag{5.59}$$

$$H_2 = \Delta'\delta a^\dagger\delta a + \omega_m\delta b^\dagger\delta b - g_0(\alpha\delta a^\dagger + \alpha^*\delta a)(\delta b + \delta b^\dagger) \tag{5.60}$$

$$-g_0(\beta + \beta^*)\delta a^\dagger\delta a, \tag{5.61}$$

$$H_3 = -g_0\delta a^\dagger\delta(\delta b + \delta b^\dagger). \tag{5.62}$$

Yeah. I know its messy. But don't panic. There is nothing conceptually difficult. It is just a large number of terms that we have to be patiently organized.

The key difficulty lies with the term H_3, which is cubic in the creation and annihilation operators. But note also that this is the *only* term which is not multiplied by either α or β. This is the spirit behind the pump trick: we are assume the pump is large so α and β are large. Consequently, the cubic term H_3 will be much smaller than the other terms and we may then neglect it. If we do so, the resulting theory is quadratic and therefore Gaussianity is restored.

Next let us do the same expansion for the dissipators. It is useful to write down the following formulas, which I will leave for you as an exercise to check:

$$D[a] = -\frac{1}{2}[\alpha\delta a^\dagger - \alpha^*\delta a, \rho] + D[\delta a], \tag{5.63}$$

$$D[a^\dagger] = \frac{1}{2}[\alpha\delta a^\dagger - \alpha^*\delta a, \rho] + D[\delta a^\dagger] \tag{5.64}$$

It is interesting to realize that the linear contribution in this expansion actually looks like a unitary term. Of course, these formulas hold for any operator a, or b, expanded around its average. Thus, for instance, the dissipator $D_m(\rho)$ of the mechanical part, Eq. (5.49), becomes

$$D_m(\rho) = -\frac{\gamma}{2}[\beta\delta b^\dagger - \beta^*\delta b, \rho] + \gamma(\bar{n}+1)D[\delta b] + \gamma\bar{n}D[\delta b^\dagger].$$

If we now plug all these results into the master equation (5.51) we shall get, already neglecting H_3,

$$\begin{aligned}\frac{\mathrm{d}\rho}{\mathrm{d}t} &= -i[H_1 - i\kappa(\alpha\delta a^\dagger - \alpha^*\delta a) - i\frac{\gamma}{2}(\beta\delta b^\dagger - \beta^*\delta b), \rho] \\ &\quad -i[H_2, \rho] + 2\kappa D[\delta a] + \gamma(\bar{n}+1)D[\delta b] + \gamma\bar{n}D[\delta b^\dagger].\end{aligned}$$

The first line in this expression contains only linear terms, whereas the second line contains quadratic terms. Let me call the term inside the commutator in the first line as $H_{1,\text{eff}}$. Organizing it a bit, we may write it as

$$\begin{aligned}H_{1,\text{eff}} &= i\delta a^\dagger\Big\{ - (\kappa + i\Delta')\alpha + ig_0\alpha(\beta+\beta^*) - i\epsilon\Big\} \\ &\quad + i\delta b^\dagger\Big\{ - (\frac{\gamma}{2} + i\omega_m)\beta + ig_0|\alpha|^2\Big\} + \text{h.c.}.\end{aligned}$$

I wrote it in this clever/naughty way because I already have Eqs. (5.53) and (5.54) in mind: the terms multiplying each operator are just the steady-state of these equations. Thus, if we are only interested in the fluctuations around the average, then $H_{1,\text{eff}} = 0$. It should be noted, however, that in practice we don't actually need to worry about this. When a Hamiltonian is Gaussian, the linear terms do not interfere with the evolution of the covariance matrix. So we don't even need to care about the linear terms. All that is going to matter for us is the quadratic part.

But, in any case, summarizing, we find that after *linearizing* the system around the fluctuations, we end up with the master equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H_2, \rho] + 2\kappa D[\delta a] + \gamma(\bar{n}+1)D[\delta b] + \gamma\bar{n}D[\delta b^\dagger]. \tag{5.65}$$

which is now a quadratic and Gaussian equation for the new operators δa and δb. Let us also work a bit more on H_2 in Eq. (5.60). The term multiplying $\delta a^\dagger \delta a$ is actually $\Delta' - g_0(\beta + \beta^*)$, which is nothing but the quantity Δ in Eq. (5.56). Thus,

$$H_2 = \Delta \delta a^\dagger \delta a + \omega_m \delta b^\dagger \delta b - g_0(\alpha \delta a^\dagger + \alpha^* \delta a)(\delta b + \delta b^\dagger).$$

This Hamiltonian is Gaussian so we could in principle just keep going. However, the final result will appear rather ugly, so it is convenient to do here another approximation. Namely, we shall do a rotating-wave approximation and neglect the counter-rotating terms $\delta a \delta b$ and $\delta a^\dagger \delta b^\dagger$. With this approximation our Gaussian Hamiltonian simplifies further to

$$H_2 = \Delta \delta a^\dagger \delta a + \omega_m \delta b^\dagger \delta b - g(\delta a^\dagger \delta b + \delta a \delta b^\dagger), \tag{5.66}$$

where $g = g_0 \alpha$ and only now did I assume that α was real. After we are done, it is a good idea to come back and redo the calculations without the RWA, which I will leave for you as an exercise.

Lyapunov equation

We are now ready to set up our Lyapunov equation for the covariance matrix using the tools we developed in the previous section. In this case the covariance matrix Θ, defined in Eq. (5.8), has the form

$$\Theta = \begin{pmatrix} \langle \delta a^\dagger \delta a \rangle + 1/2 & \langle \delta a \delta a \rangle & \langle \delta a \delta b^\dagger \rangle & \langle \delta a \delta b \rangle \\ \langle \delta a^\dagger \delta a^\dagger \rangle & \langle \delta a^\dagger \delta a \rangle + 1/2 & \langle \delta a^\dagger \delta b^\dagger \rangle & \langle \delta a^\dagger \delta b \rangle \\ \langle \delta a^\dagger \delta b \rangle & \langle \delta a \delta b \rangle & \langle \delta b^\dagger \delta b \rangle + 1/2 & \langle \delta b \delta b \rangle \\ \langle \delta a^\dagger \delta b^\dagger \rangle & \langle \delta a \delta b^\dagger \rangle & \langle \delta b^\dagger \delta b^\dagger \rangle & \langle \delta b^\dagger \delta b \rangle + 1/2 \end{pmatrix},$$

and it will satisfy the Lyapunov equation (5.20):

$$\frac{\mathrm{d}\Theta}{\mathrm{d}t} = W\Theta + \Theta W^\dagger + F.$$

The matrices W and F can be found using the tricks discussed in the previous section. I will simply state the result. The matrix F has two diagonal blocks containing the contributions from each dissipative channel:

$$F = \begin{pmatrix} \kappa\, \mathbb{I}_2 & 0 \\ 0 & \gamma(\bar{n} + 1/2)\, \mathbb{I}_2 \end{pmatrix}.$$

The matrix W, on the other hand, has both a dissipative and a unitary contribution. In fact, the unitary contribution is identical to Eq. (5.27) since our final Hamiltonian H_2 in Eq. (5.66) is structurally identical to the Hamiltonian (5.26). Thus,

$$W = \begin{pmatrix} -i\Delta - \kappa & 0 & ig & 0 \\ 0 & i\Delta - \kappa & 0 & -ig \\ ig & 0 & -i\omega_m - \gamma/2 & 0 \\ 0 & -ig & 0 & i\omega_m - \gamma/2 \end{pmatrix}.$$

It is now a matter of asking the friendly electrons living in our computer to solve for the steady-state:

$$W\Theta + \Theta W^\dagger = -F.$$

As a result we find a CM with the following structure

$$\Theta = \begin{pmatrix} \langle \delta a^\dagger \delta a \rangle + 1/2 & 0 & \langle \delta a \delta b^\dagger \rangle & 0 \\ 0 & \langle \delta a^\dagger \delta a \rangle + 1/2 & 0 & \langle \delta a^\dagger \delta b \rangle \\ \langle \delta a^\dagger \delta b \rangle & 0 & \langle \delta b^\dagger \delta b \rangle + 1/2 & 0 \\ 0 & \langle \delta a \delta b^\dagger \rangle & 0 & \langle \delta b^\dagger \delta b \rangle + 1/2 \end{pmatrix},$$

where

$$\langle \delta a^\dagger \delta a \rangle = \frac{2g^2\gamma\bar{n}(\gamma + 2\kappa)}{2g^2(\gamma+2\kappa)^2 + \gamma\kappa[(\gamma+2\kappa)^2 + 4(\Delta-\omega_m)^2]},$$

$$\langle \delta b^\dagger \delta b \rangle = \bar{n} - \frac{4g^2\kappa\bar{n}(\gamma + 2\kappa)}{2g^2(\gamma+2\kappa)^2 + \gamma\kappa[(\gamma+2\kappa)^2 + 4(\Delta-\omega_m)^2]},$$

$$\langle \delta a^\dagger \delta b \rangle = \frac{2g\gamma\kappa\bar{n}[2(\Delta-\omega_m) - i(\gamma+2\kappa)]}{2g^2(\gamma+2\kappa)^2 + \gamma\kappa[(\gamma+2\kappa)^2 + 4(\Delta-\omega_m)^2]}.$$

You see, even though we already did a bunch of approximations, we still end up with a rather ugly result.

To clarify the physics, it is useful to assume (as is often the case) that $\gamma \ll \kappa$. In this case the results are more neatly expressed in terms of a quantity called the **cooperativity**:

$$C = \frac{2g^2}{\kappa\gamma}. \tag{5.67}$$

We then get

$$\langle \delta a^\dagger \delta a \rangle = \frac{g^2\bar{n}}{\kappa^2(1+C) + (\Delta-\omega_m)^2}. \tag{5.68}$$

$$\langle \delta b^\dagger \delta b \rangle = \bar{n} - \frac{\bar{n}\kappa^2 C}{(1+C)\kappa^2 + (\Delta-\omega_m)^2}, \tag{5.69}$$

$$\langle \delta a^\dagger \delta b \rangle = \frac{g\bar{n}(\Delta-\omega_m - i\kappa)}{(1+C)\kappa^2 + (\Delta-\omega_m)^2}. \tag{5.70}$$

Now things are starting to look much better.

So let us extra the physics from Eqs. (5.68)-(5.70). We first look at a phenomenon called **sideband cooling**. Namely, we look at the thermal fluctuations of the mechanical mode, Eq. (5.69). As can seen, $\langle \delta b^\dagger \delta b \rangle$ is always *lower* than the sample temperature $\bar{n}$. And we can lower it more by two different paths. The first is by increasing the cooperativity C in Eq. (5.67). This makes sense since C is a type of competition between the coupling g and the damping mechanisms κ and γ. So the higher is the value of C

the more strongly coupled are the optical and mechanical modes. Hence, by making the coupling stronger, we can cool the mechanical mode more.

However, making C large is not always an easy task. Instead, another efficient way to make the cooling effect stronger is by playing with $\Delta - \omega_m$. This is something that can be done rather easily since the Detuning Δ is something one usually has great control over. Thus, we see that cooling is maximized in the so-called **side-band cooling condition** $\Delta = \omega_m$. In this case Eqs. (5.68)-(5.70) can be simplified even further to

$$\langle \delta a^\dagger \delta a \rangle = \frac{g^2 \bar{n}}{\kappa^2 (1 + C)}. \tag{5.71}$$

$$\langle \delta b^\dagger \delta b \rangle = \frac{\bar{n}}{1 + C}, \tag{5.72}$$

$$\langle \delta a^\dagger \delta b \rangle = -\frac{i g \bar{n}}{\kappa (1 + C)}. \tag{5.73}$$

Another result that is also more transparent in this case is the fact that the steady-state photon fluctuations are proportional to $\bar{n}$. If the cavity was not coupled to the mechanical mode, the electromagnetic mode would be in a coherent state, which has $\langle \delta a^\dagger \delta a \rangle = 0$. Instead, due to the contact with the mechanical vibration, the occupation increases a bit by a term proportional to both the coupling strength, g^2 and the thermal fluctuations $\bar{n}$.