International Master
Physics of Complex Systems

Dynamics of Quantum Systems

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1 Introduction (1h)

1.1 Closed and open systems in equilibrium

1.1.1 Classical

In *classical Hamiltonian mechanics*, the state of a *closed* system at a given instant corresponds to a point in phase space, with generalised coordinates $\{\vec{p}_i, \vec{x}_i\}$. Here i is the label that identifies the particles/individuals, $i = 1, \ldots, N$, $\vec{x}_i$ is the position of the ith particle in a d dimensional space, and $\vec{p}_i$ the associated momentum. The physical quantities characterising the system are functions of these coordinates and possibly also time, $f(\{\vec{p}_i, \vec{x}_i\}, t)$. Through Hamilton's equations, one can then deduce – at least in principle – the evolution of the system from the initial conditions and predict its state at any future instant.

Classical mechanics usually deals with the evolution of a system of a few particles, possibly in interaction and under the effect of some external potential. Imagine though that the system is made of $N \to \infty$ elements. We then enter the realm of *Statistical Physics*. In cases in which one focuses on a (small) part of the whole isolated system and treats the (large) rest as an environment, the selected system is now *open* and its dynamics become *dissipative and noisy*, described by, a Langevin or master equation, the Fokker-Planck formalism.

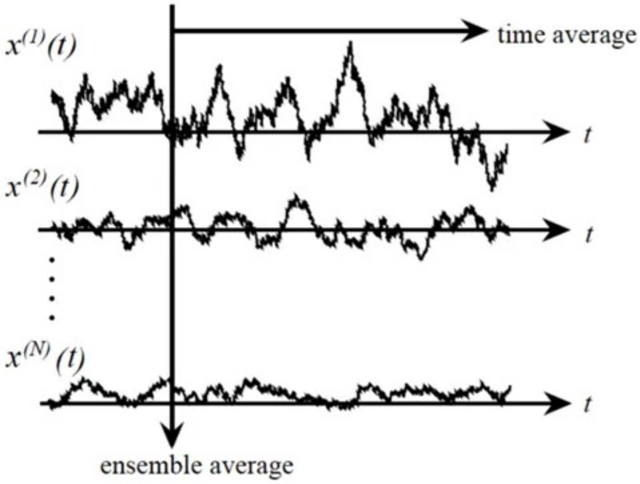


Figure 1.1: Ergodicity in classical systems

Under equilibrium conditions, *ergodicity* states that *temporal averages* of (non pathological) observables which depend on time only through the phase space variables, which are performed over a sufficiently long time interval after a sufficiently long equilibration time, coincide with *statistical averages* calculated as an average of the observable weighted with a static distribution of the phase space variables, $P(\{\vec{p}_i, \vec{x}_i\})$. The Gibbs-Boltzmann equilibrium theory tells us which is the form of this probability depending on whether the system is closed (microcanonical) or open (canonical, grand-canonical).

In practice, what this means is that an experimentalist can take two routes. On the one hand, let a single system evolve in time and calculate from the trajectory the time average of the desired observable. On the other had, take many copies of the same system, let them evolve independently, and calculate, at a chosen time, the statistical average of the observable over all those copies.

It is usually very difficult to prove ergodicity. It can only be assumed, used and the consequences checked. Of course, there are many cases of great interest where it is clear that it does not hold. This is the subject of classical out of equilibrium dynamics.

When the number of constituents of the system of interest diverges, that is, in the *thermodynamic limit* - be it isolated or in contact with an environment - collective effects can emerge and lead to *phase transitions* and other unexpected behaviors like *non-equilibrium slow dynamics* and the impossibility of reaching equilibrium in reasonable experimental times. This is the content of the expression “More is different” coined by P. W. Anderson to motivate the study of complex systems in general. This is what we are interested in.

1.1.2 Quantum

Do these consideration apply/vary quantum mechanically?

In *quantum mechanics*, when the state of a closed system is perfectly known, it is represented by a state vector in a Hilbert space from which one can extract the expectation values of operators which are related to the physical observables that characterise the system.

In other cases, the state of the system is not perfectly known. One then adopts a *statistical description*, based on the idea of copying the system many times. The equilibrium hypothesis forces the density operator (similar to the probability distribution of the classical problem) to be of the special Gibbs-Boltzmann form. The study of quantum many-body problems at or very close to (linear response) equilibrium has concentrated most analytic and experimental studies until a decade ago or so. *Quantum phase transitions*, taking place at strictly zero temperature and driven by another control parameter that basically measures the strength of the quantum fluctuations have been predicted and measured both experimentally and numerically.

Since fully isolating a quantum system is extremely difficult, many relevant experimental situations concern open quantum systems rather than isolated quantum systems. It is therefore necessary to build models of *environments* and *couplings* between the system of interest and its surroundings. This is non-trivial and brings about many interesting features.

Out of equilibrium quantum systems also exist and they are the focus of very active research nowadays.

1.2 Being out of equilibrium

Equilibrium is the exception rather than the rule in physical situations. Certainly, there is only one way of being in equilibrium which is compatible with the conservation laws. For instance, a fully isolated system is in the microcanonical ensemble, one that exchanges energy with a thermal environment in the canonical one, and so on.

There are many ways to be out of equilibrium. Some, realizable in the classical limit as well as under quantum fluctuations, are the following.

- Take a system in equilibrium and weakly perturb it so as to take it away from equilibrium but not much. To treat these cases, *linear response theory* was built. This is a very well established theory that captures correctly these weakly out of equilibrium situations.
- Take an isolated system in (microcanonical) equilibrium and suddenly (or with some time-dependent protocol) change a parameter of its Hamiltonian. The time evolution under the new Hamiltonian will occur out of equilibrium and reaching (or not) new equilibrium conditions may take very long. These procedures are called *quenches* and they have mostly been studied in quantum settings, where they are called quantum quenches. The putative stationary conditions reached could be the standard equilibrium ones (as expected for interacting non-integrable many body systems) or could take new forms, of Generalized Gibbs Ensemble form, for integrable systems.
- Take an open system in (canonical) equilibrium and suddenly (or with some time-dependent protocol) change a control parameter of the bath, be it temperature, pressure, etc. The time evolution under the new conditions will take place out of equilibrium. Reaching (or not) new equilibrium conditions may take very long. These procedures are also called *quenches* for the instantaneous ones or *annealing* for the time-dependent ones. They have been studied at length in classical statistical physics, for example, in coarsening/domain growth problems, or in the context of glassy systems.
- Strongly perturb an otherwise closed system with an external, for instance, a periodic time-dependent, force. These protocols can be performed on classical and quantum systems as well. They have been fashionable in the quantum setting recently and are associated with the name *Floquet theory*.
- Strongly perturb an open dissipative system with an external drive. These setting arise in classical cases, for example, the physics of granular matter, and in quantum cases like what is studied with quantum optics platforms. A question typically asked in these setting is whether a *non-equilibrium steady state* is reached, how long does it take to reach it if it is possible, and which are its characteristics.

1.3 Classical examples

There are many classical system which evolve out of equilibrium.

The well-known phenomenon of *Brownian motion* or just *diffusion* is out of equilibrium. Why so? Because the mean-square displacement of the Brownian particle grows with no limit. The description of generic Brownian motion is typically done with a Langevin equation where a model of the environment is assumed and a choice of friction and thermal noise is made. The simplest one corresponds to a Markov process with memory-less friction and white noise. Non-Markovian classical baths also exist. The deterministic force can include quenched random effects in the form of a quenched random potential or a random force (in both cases the values are taken from a probability distribution and held fixed during evolution). In normal diffusion the growth is linear in time. In sub or super diffusion the power is smaller or larger than one. The main point is that in none of these cases a saturation limit is reached.

The simplest macroscopic example is the growth of order when a system is taken across a second order phase transition. This can be done by changing abruptly a parameter in the Hamiltonian of the system (e.g. in a simulation) or the temperature of the bath (e.g. in an experiment). It is a quench. The standard example is the case of a magnetic system, taken from a paramagnetic state to conditions under which it should magnetise. How does it do it? By *growing domains* of the competing possible orderings. In an Ising model in two or more dimensions, these are two oppositely magnetised equivalent low temperature states. Locally the system choses one or the other and in the course of time it grows these regions, ones at the expense of the other ones but in a symmetric way. Eventually, after a time that diverges as a function of system size, the spontaneous symmetry breaking mechanism takes place and one of the two equilibrium states is selected. But during this very long term evolution the system remains far from equilibrium with vanishing averaged magnetisation density. The description of this process can be done at a microscopic level, with Monte Carlo simulations, for example. Analytically, one proposes a time-dependent Ginzburg-Landau equation which is a Langevin equation on a field, the coarse-grained magnetisation. A model for the environment is also necessary, to decide the functional form of the friction and noise terms. Usually, a Markov choice is made.

Phase separation is also an out of equilibrium process. The difference with the magnetic domain growth explained in the previous paragraph is that the order parameter of phase separation is conserved. For example, if you consider a mixture of oil and water, the mass of each of the phases remains constant in time since oil cannot be transformed into water or vice versa. This imposes a conservation law and the microscopic dynamics or mesoscopic Langevin equation have to respect it.

Glassy systems are ensembles of spins, atoms, molecules, polymers, or other constituents with astronomically long relaxation times at low temperatures/high pressures. Examples are spin-glasses, window glasses, plastics, etc. They do not reach their ideal ordered (e.g. crystalline) equilibrium states in experimentally relevant time-scales. For these samples/models, there is no clear growth of local order developing in the course of time and in this sense they are different (and more complex) than coarsening systems. The slow relaxation is due to metastability, due to complex free-energy landscapes. Glasses obviously exist in contact with surroundings.

Externally driven systems, as can be *sheared liquids* or *periodically shaken granular matter* can reach non-equilibrium steady states that are, though, different from Gibbs-Boltzmann equilibrium. Active matter is kept away from equilibrium thanks to the constant injection of energy that is typically done on their borders.

Active matter is a very timely example of driven-dissipative out of equilibrium many-body systems. The peculiarity of these "materials" is that the injection of energy is done at the microscopic constituent level. They exist at very different scales, from the microscopic to the macroscopic. Examples are bacteria colonies and flocks of birds on the natural side and groups Janus particles or asymmetric grains on the artificial one. In usual cases they reach a non-equilibrium steady state with peculiar properties. Several lectures in this program discuss this problem in great detail.

1.4 Why quantum?

Strong experimental activity in condensed matter and atomic physics has relaunched the interest in developing formalism for, and obtaining results on, out of equilibrium situations in which quantum fluctuations pay a role.

Let us explore parallel examples to the ones presented in the previous Section, now in their quantum realisation.

Consider a trapped cold atom system. For example, the atoms can be trapped in a long (compared to the atomic scale) linear tube (approximately one dimensional space) or on a finite sector of the plane. A few atoms of a given species can be inserted in these spaces and be surrounded by many atoms of another species that act as a bath with respect to the less numerous ones. This setting reproduces the classical Brownian motion one, now under quantum fluctuations. The nature of the bath is more complex than the classical one for which a Markov assumption is usually acceptable. Such *quantum Brownian motion* has been realised by several experimental groups. Quenched random potentials can also be at least approximately realised with light.

Quantum phase separation can also be studied in cold atom platforms by starting the system in a, say, uniform mixture of two species which repulsive interaction between different atoms. Magnets at very low temperatures undergo *quantum domain growth*.

Quantum spin-glasses and *quantum glasses* also exist and have similar slow relaxations to classical ones. The former ones are systems of quantum spins placed at fixed random positions in a host material. The quenched randomness in the distances between the magnetic moments translates into quenched random interactions since the latter depend on the former. In the case of quantum glasses, there are no quenched random couplings but the atoms or molecules, which follow quantum mechanical rules, also display slow out of equilibrium dynamics.

In atomic physics *cold atom* platforms as the one sketched in Fig. 1.2(b) have allowed one to study quantum systems with many (though not infinite) atoms in almost perfect isolation. Light beams are used to generate periodic potentials that trap the atoms in lattice structures. The magic of these systems is that the parameters (interaction, hopping) can be tuned in real-time [16]. Questions about the equilibration of the samples are posed. Periodic modulation of hopping ("shaking") or the interactions can also be controlled in these cases.

In analog quantum simulators, such as ultracold atom platforms, arrays of atoms with long-range interactions, and trapped atomic ions, one can exert control over constituent degrees of freedom by tuning the Hamiltonian governing their interactions. The possibility of highly coherent and controllable Hamiltonian dynamics has led to important questions about *universality* in the approach to thermal equilibrium.

Digital quantum simulators, formed by, e.g. formed of superconducting qubits, could afford an even greater degree of control. Their time evolution would take place in *discrete-time* through the application of unitary operations, measurements, and feedback. Successful implementation of these operations is a stepping-stone towards the goal of building a fault-tolerant quantum computer. Researchers are asking in this context which collective quantum phenomena, or dynamical phases of matter, could emerge in such *quantum circuits*?

In the quantum realm, another possible out of equilibrium situation is the so-called *many-body localisation*. It is the extension of Anderson localisation to problems with many interacting electrons in a medium with quenched randomness. Though the existence of these systems is still debated, the idea is that they would have neither diffusion nor transport and quenched disorder could arrest thermalisation entirely. These localisation properties would not resist coupling to an environment.

In condensed matter physics many *pump-probe* experiments as the one sketched in Fig. 1.2(a) are being conducted to try to understand the behaviour of samples. Periodic perturbation induced by strong (classical) light fields, with tuneable frequency and amplitude, have also been used. The typical question is 'How rapidly (and radically) can we change the property of a material with light?'

Both in condensed matter systems and atomic physics the idea to use non-equilibrium perturbations as a new knob to control/stabilize/create new quantum phases of matter is intensively being studied. This is called *Floquet engineering*. One can note that a similar question was fashionable in the context of granular matter around 20 years ago.

The idea to use *quantum* mechanics to *compute* in a more efficient way than with classical rules was put forward by Feynman in 1981. Concomitantly, it became necessary to understand how to process *quantum information*.

The difficulty of *factoring* large integers into products of prime numbers is at the basis of schemes for public key cryptography. The solutions of factoring can be easily verified, once found. However, they are hard to find: if p and q are large prime numbers, the product $n = pq$ can be computed quickly (the number of elementary bit operations required is about $\log_2 p \log_2 q$). The the time needed to give an answer to the reversed question "given n, find the factors p and q" in the worst case is supposed (not proven)

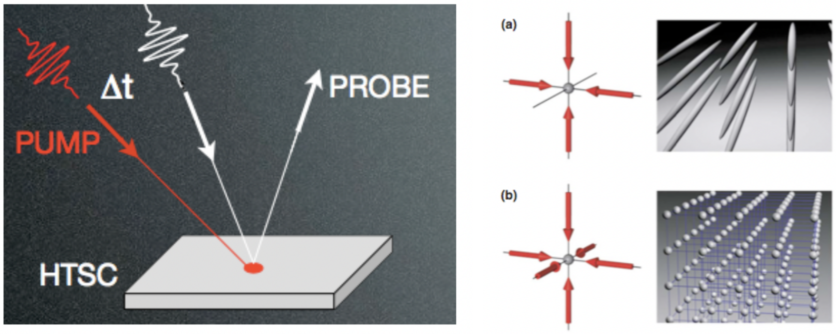


Figure 1.2: (a) Pump-probe experiments: electrons in solids under ultrafast optical fields. (b) Neutral atoms trapped in optical lattices.

to grow faster than any power of n. Indeed, the faster algorithm known to date uses $\exp[c(\ln n)^{1/3}(\ln\ln n)^{2/3}]$ with $c = (64/9)^{1/3} \sim 1.9$. Estimates are such that factoring a 400 digit number would take about 10^{10} years.

Shor proved in 1994 that a quantum computer can factor a large number efficiently, in polynomial time $O[(\ln n)^3]$. Shor's algorithm could factor a 400 digit number in less than 3 years.

Leaving aside the extensive experimental efforts to build controllable large-scale quantum devices, many theoretical questions are posed in the context of quantum computation and information. The following list is a selection of the ones given in the MIT Physics Department website:

- *Quantum algorithms and complexity.* If a perfectly functioning quantum computer were built, which problems could it solve faster than conventional computers, and which problems do not admit any speedup?
- *Quantum information theory.* Meaning and limits of communicating classical and quantum information over quantum channels How can we store, transfer, or manipulate quantum information in the presence of noise? How can we efficiently communicate and compute in the presence of errors? What are the basic properties of quantum entanglement and information?
- *Measurement and control.* How can we efficiently manipulate and characterize quantum devices?
- *Applications and connections.* How can ideas from quantum information science contribute to other research areas as diverse as convex optimizations, black holes, and exotic quantum phases of matter? Is there a unified framework to efficiently describe quantum entanglement and information in complex systems?

1.5 Aim of these lectures

These lectures are an introduction to some methods used in the study of many-body quantum systems in and out of equilibrium.

We will start reviewing the formalism of quantum mechanics in Sec. 2 and some generic properties of correlation and linear response functions in Sec. 3. The classical limits of these properties are important and will be discussed. While discussing quantum mechanical concepts we will pay special attention to the essential property of entanglement. Open classical and quantum systems will be dealt with in Sec. 4 (e.g. Langevin equations in the classical case, Lindblad formalism in the quantum). The path integral formalism, useful to establish perturbative expansions, renormalisation group analysis and self-consistent approximations both in and out of equilibrium will be explained in Sec. 5. Finally, we will study some elements of quantum chaos, and Anderson and Many-Body Localisation, in Sec. 6.

1.6 General references

Several books describe part of the formalism that we will discuss in these lectures [1–5]. Review articles are more specific and touch upon more modern issues [6–9].

Interestingly enough, and not always known to everyone, the questions asked, formalisms used, and results obtained for quantum and classical many-body systems can be very similar. We will stress these coincidences in these lectures. Of course, some aspects are specific to quantum mechanics.

2 Quantum mechanics

In this Section we introduce a bit of notation, and we recall concepts and postulates of quantum physics [10,11]. We present them with the aim of giving a very basic introduction to quantum information and quantum computation, following in part the presentation in [12]. In Preskill's words *information* is something encoded in the state of a physical system and *computation* is something that can be carried out on an actual physically realizable device. Both belong to the area of physics, theoretical and experimental.

2.1 Concepts and notation

2.1.1 Hilbert space, pure states and linear superposition

A pure quantum state is a mathematical entity, a vector with norm one in a Hilbert space, that embodies knowledge of a quantum system. A Hilbert space is a (finite or infinite dimensional) vector space equipped with an inner product that induces a distance function.

Symbol	Name, object, property
$\mathcal{H}$	Hilbert **space** (a complex vector space with a scalar product)
$\vert\psi\rangle$	A vector - a ket - in $\mathcal{H}$
$c\vert\psi\rangle + d\vert\phi\rangle$ with $c, d \in \mathbb{C}$	A linear combination, also in $\mathcal{H}$
$c^*\langle\psi\vert + d^*\langle\phi\vert$	Bra dual to $c\vert\psi\rangle + d\vert\phi\rangle$
$\langle\psi\vert\phi\rangle \in \mathbb{C}$	Inner product
$\langle\phi\vert\psi\rangle = \langle\psi\vert\phi\rangle^*$	Complex conjugate
$\langle\eta\vert(c\vert\psi\rangle + d\vert\phi\rangle) = c\langle\eta\vert\psi\rangle + d\langle\eta\vert\phi\rangle$	Associativity
$\langle\phi\vert\phi\rangle \geq 0$	Postulate of definite metric
$\langle\phi\vert\phi\rangle^{1/2}$	Norm of $\vert\phi\rangle$
$\langle\psi\vert\phi\rangle = 0$	Orthogonality
$\{\vert\psi_n\rangle\}$ with $\langle\psi_n\vert\psi_m\rangle = \delta_{nm}$	Orthonormal basis of finite dim $\mathcal{H}$
$\vert\psi\rangle = \sum_n c_n\vert\psi_n\rangle$ with $c_n = \langle\psi_n\vert\psi\rangle \in \mathbb{C}$	Representation of $\vert\psi\rangle$ in the basis $\{\vert\psi_n\rangle\}$

Imagine that you have a classical system which has K energy levels (for simplicity, suppose the spectrum is discrete). Classically it can be in one of these levels and one can identify its state from the value of the index k which runs from 1 to K. In quantum mechanics the *linear superposition principle* states that the system is placed in a linear superposition of these K states with complex coefficients. Concretely, if the K staes are the orthonormal states $|\psi_1\rangle, \ldots, |\psi_K\rangle$, a generic *pure state* of the system is

$$|\psi\rangle = c_1|\psi_1\rangle + \cdots + c_K|\psi_K\rangle \tag{2.1}$$

with $c_k \in \mathbb{C}$ and $\sum_{k=1}^{K} |c_k|^2 = 1$. This is a linear superposition of the basis states $\{|\psi_k\rangle\}$.

An informal way to think about the meaning of this statement is that the system has not made its mind about which situation $\{|\psi_k\rangle\}$ it is in (until it is measured).

One can define the dual of the ket $|\psi\rangle$, called the bra, $\langle\psi|$:

$$\langle\psi| = c_1^*\langle\psi_1| + \cdots + c_K^*\langle\psi_K| \tag{2.2}$$

The squared modulus of the vector $|\psi\rangle$ is then

$$\langle\psi|\psi\rangle = (c_1^*\langle\psi_1| + \cdots + c_K^*\langle\psi_K|)(c_1|\psi_1\rangle + \cdots + c_K|\psi_K\rangle) = \sum_{k=1}^{K} |c_k|^2 = 1 \tag{2.3}$$

Example

Take as an example a qubit or two state system, $k = 1, K = 2$. Classically, the qubit has two possible configurations, 0 and 1. Quantum mechanically it is a vector in a two-dimensional complex vector (Hilbert) space with inner product. A basis of this Hilbert space is

$$|\psi_1\rangle = |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |\psi_2\rangle = |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{2.4}$$

which are eigenvectors of the operator $\hat{\sigma}^z$ with eigenvalue 1 and -1, respectively. The definition and properties of the spin operators and Pauli matrices are recalled in App. A.

The duals of the kets above are

$$\langle\psi_1| = \langle 0| = \begin{bmatrix} 1 & 0 \end{bmatrix} \qquad \langle\psi_2| = \langle 1| = \begin{bmatrix} 0 & 1 \end{bmatrix} \tag{2.5}$$

The two states are orthogonal $\langle 0|1\rangle = \langle 1|0\rangle = 0$ and normalized to one $\langle 0|0\rangle = \langle 1|1\rangle = 1$. For such a system, a generic pure state with norm one is $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$, with $|c_0|^2 + |c_1|^2 = 1$.

From a *quantum information* viewpoint, a quantum system can carry continuous information about the relative balance of each of the states in which it can be. For a qubit, one can argue that the system has information about the relative balance of $|0\rangle$ and $|1\rangle$, through the coefficients c_0 and c_1. Quantum algorithms can sometimes use this fact to run more efficiently than their classical counterparts. Quantum information is also *not deterministic*. When someone takes a look at a classical bit, it simply is a 0 or a 1, as it was beforehand and as it will be afterward, apart from the possibility of error. This is not so with qubits, the result of the measurement has a probabilistic meaning and the state is affected by the measurement.

A pure state can be described by a single vector. A *mixed state* is a statistical ensemble of pure states. Mixed states arise in two different situations: first, when the preparation of the system is not fully known, and one must deal with a statistical ensemble of possible preparations; second, when one wants to describe a physical system which is entangled with another, as its state cannot be described by a pure state. States can be described by density operators, with the pure ones taking a very simple form. We will come back to the description of mixed states and the meaning of entanglement in Sec. 2.2.3.

2.1.2 Operators

Given vectors and dual vectors we can define operators of the form

$$\hat{O} = |\psi\rangle\langle\phi| \tag{2.6}$$

$\hat{O}$ acts on a vector in $\mathcal{H}$ and produces as result another vector in $\mathcal{H}$.

The Hermitian conjugate is

$$\hat{O}^\dagger = |\phi\rangle\langle\psi| \tag{2.7}$$

with the combined operation of transposition and complex conjugation which are easy to visualise in the matrix representation of operators.

An operator is Hermitian if $\hat{O}^\dagger = \hat{O}$. A special case is the *projector*

$$\hat{P}^\dagger = |\psi\rangle\langle\psi| \tag{2.8}$$

which satisfies $\hat{P}^\dagger = \hat{P}$ and $\hat{P}^2 = \hat{P}$.

Given the orthonormal basis of a finite dimensional Hilbert space $\mathcal{H}$, $\{|\psi_n\rangle\}$ with $\langle\psi_n|\psi_m\rangle = \delta_{nm}$, one has the *closure* relation

$$\sum_n |\psi_n\rangle\langle\psi_n| = \mathbb{I} \tag{2.9}$$

2.1.3 Measurement

It is postulated that a measurable physical quantity of a physical system is represented by a linear *Hermitian operator*, termed an *observable*, that acts on vectors of the Hilbert space representing the physical system.

The process of measuring an observable $\hat{A}$ in a state $|\psi\rangle$ goes as follows.

– First, one needs to express the observable $\hat{A}$ in terms of its eigen-basis. For that, one needs to determine its eigenstates $\{|a_n\rangle\}$ and eigenvalues $\{a_n\}$. The eigenstates satisfy:

$$\hat{A}|a_n\rangle = a_n|a_n\rangle.$$

The eigenvalues a_n are the possible outcomes of the measurement, and the eigenstates $|a_n\rangle$ form another basis for the Hilbert space.

Symbol	Name, object, property
$\hat{A}$	Observable - **Operator**
$\hat{A}\lvert\psi\rangle = \lvert\psi'\rangle$	Action on a vector in $\mathcal{H}$
$\hat{A}(c\lvert\psi\rangle + d\lvert\phi\rangle) = c\hat{A}\lvert\psi\rangle + d\hat{A}\lvert\phi\rangle$	Linearity
$\langle\psi\rvert\hat{A}^\dagger$ with $\hat{A}^\dagger$ the adjoint of $\hat{A}$	bra associated to the ket $\hat{A}\lvert\psi\rangle$
$\hat{A} = \hat{A}^\dagger$	Hermitian
$\langle\phi\rvert\hat{A}\lvert\psi\rangle = \langle\psi\rvert\hat{A}^\dagger\lvert\phi\rangle^*$	Self-adjoint
$\hat{A}^\dagger\hat{A} = \hat{A}\hat{A}^\dagger = \mathbb{I}$	Unitary
$\hat{A}\hat{B} \neq \hat{B}\hat{A}$	Non commutative (but associative)
$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$	Hermitian
$\lvert\psi\rangle\langle\phi\rvert$	Outer product: an operator
$\hat{A}\lvert a_n\rangle = a_n\lvert a_n\rangle$ with $a_n \in \mathbb{C}$	Eigenstate $\lvert a_n\rangle$ with eigenvalue a_n
$\hat{A} = \hat{A}^\dagger \implies a_n \in \mathbb{R} \quad \forall n$	real eigenvalues
$\{\lvert a_n\rangle\}$ with $a_n \neq a_m$	Orthonormal basis of $\mathcal{H}$
$\lvert\psi\rangle = \sum\limits_n c_n\lvert a_n\rangle$ with $c_n \in \mathbb{C}$	ket written in the basis $\{\lvert a_n\rangle\}$
$\langle a_n\rvert\hat{A}\lvert a_m\rangle = \langle a_m\rvert\hat{A}^\dagger\lvert a_n\rangle^*$	Matrix representation of $\hat{A}$ Hermitian = transpose & conjugate
$\mathrm{Tr}\hat{A} = \sum\limits_n \langle a_n\rvert\hat{A}\lvert a_n\rangle$	Trace of $\hat{A}$
$\hat{A} = \sum\limits_n a_n\lvert a_n\rangle\langle a_n\rvert$	Representation of $\hat{A}$
If $[\hat{A},\hat{B}] = 0$ then $\langle a_n\rvert\hat{B}\lvert a_m\rangle = \delta_{nm}$	Compatible operators, diagonal in same basis same eigenkets
$\langle(\Delta\hat{A})^2\rangle\langle(\Delta\hat{B})^2\rangle \geq \frac{1}{4}\lvert\langle[\hat{A},\hat{B}]^2\rangle\rvert^2$	Uncertainty relation
$\{\lvert\psi_n\rangle\}$ with $\langle\psi_n\vert\psi_m\rangle = \delta_{nm}$	Orthonormal basis of finite dim $\mathcal{H}$
$\sum\limits_n \lvert\psi_n\rangle\langle\psi_n\rvert = \mathbb{I}$	Closure

- Next, express the system's state $|\psi\rangle$ in terms of the eigenstates $\{|a_n\rangle\}$ of A:

$$|\psi\rangle = \sum_n c_n|a_n\rangle \ ,$$

  where $c_n = \langle a_n|\psi\rangle$ are the expansion coefficients, which represent the projection of $|\psi\rangle$ onto the eigenstate $|a_n\rangle$.
- The *Born rule* states that when one measures the observable $\hat{A}$, the system collapses into one of its eigenstates $|a_n\rangle$, and the corresponding eigenvalue a_n will be the measurement result. The probability $P(a_n)$ of measuring the eigenvalue a_n is given

by the squared modulus of the projection of $|\psi\rangle$ onto $|a_n\rangle$:

$$P(a_n) = |\langle a_n|\psi\rangle|^2 = |c_n|^2 \, .$$

It tells how likely it is to observe the outcome a_n when measuring $\hat{A}$ in the state $|\psi\rangle$. The outcome of a measurement is not deterministic, there is a probability element to it. Note that $|c_n|^2$ are positive real values and $\sum_n |c_n|^2 = 1$. One cannot access the phase of the coefficients c_n in this way.

Note that it is assumed that the measurement of an observable somehow *instantaneously* changes the quantum state of the system into one of the eigenstates of that operator.

There is, however, a way to access the phases of the coefficients c_k by working in another basis. Let us see how it works with an example.

Example

Take the two-level system, $k = 1, K = 2$ and consider the quantum state

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i\theta}}{\sqrt{2}}|1\rangle \tag{2.10}$$

The standard measurement would yield $|0\rangle$ with probability $p_0 = 1/2$ or $|1\rangle$ also with probability $p_1 = 1/2$.

Let us change basis to

$$|+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \qquad |-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) \tag{2.11}$$

eigenstates of σ^x with eigenvalues 1 and -1, respectively, which implies

$$|0\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle + |-\rangle\right) \qquad |1\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle - |-\rangle\right) \tag{2.12}$$

and use these expressions to rewrite $|\psi\rangle$ in this new basis:

$$\begin{aligned} |\psi\rangle &= \frac{1}{2}\left(|+\rangle + |-\rangle\right) + \frac{e^{i\theta}}{2}\left(|+\rangle - |-\rangle\right) = \frac{1}{2}\left(1 + e^{i\theta}\right)|+\rangle + \frac{1}{2}\left(1 - e^{i\theta}\right)|-\rangle \\ &= \frac{1}{2}\left(1 + \cos\theta + i\sin\theta\right)|+\rangle + \frac{1}{2}\left(1 - \cos\theta - i\sin\theta\right)|-\rangle \end{aligned} \tag{2.13}$$

Therefore, the probabilities of measuring $|+\rangle$ and $|-\rangle$ are

$$p_+ = \frac{1}{4}|\left(1 + \cos\theta + i\sin\theta\right)|^2 = \frac{1}{4}(1 + \cos\theta)^2 + (\sin\theta)^2 = \frac{1}{2}\left[1 + \cos\theta\right] = \cos^2\frac{\theta}{2} \tag{2.14}$$

$$p_- = \frac{1}{4}|\left(1 - \cos\theta - i\sin\theta\right)|^2 = \frac{1}{4}(1 - \cos\theta)^2 + (-\sin\theta)^2 = \frac{1}{2}\left[1 - \cos\theta\right] = \sin^2\frac{\theta}{2} \tag{2.15}$$

and one can thus measure θ.

A special operator is the Hamiltonian, which is restricted by two postulates of quantum mechanics:

- The Hamiltonian must be a Hermitian operator so that its eigenvalues (energy levels) are real.
- The spectrum must be bounded from below so as to have a finite ground state energy.

After a measurement, the quantum state collapses to an eigenstate of the operator measured. Other aspects of the state may be unknown. Repeating the same measurement will not alter the state which is already an eigenstate of the operator. In some cases, compatible measurements can further refine the state, causing it to be an eigenstate corresponding to all these measurements. A full set of compatible measurements produces a *pure state*.

Because of the *uncertainty principle*, *non-commuting observables* cannot simultaneously have precisely defined values. Performing a measurement of one observable $\hat{A}$ will necessarily influence the outcome of a subsequent measurement of an observable $\hat{B}$, if $\hat{A}$ and $\hat{B}$ do not commute. This is another way to see that the act of acquiring information about a physical system inevitably disturbs its state. This does not happen in classical physics.

Quantum information cannot be copied with perfect fidelity (no cloning principle, see Sec. 2.3.6) and one cannot use the trick of measuring on a copy without disturbing the original system in this way.

These are bad news when it comes to use quantum mechanics to build a quantum computer: reading the output of a quantum computer - making a measurement - would destroy most of the information it stores. Where once there was a superposition, the measurement takes the measured qu-bit to be in one of its two states. There are ways to avoid this problem, by introducing *ancilla qubits*, which are extra qubits added to implement irreversible logical operations on them.

The *spectrum* of the operators which correspond to observables are the values that these can take in a measurement. Since measurements should take real values, the operators associated to observables should be self-adjoint, $\hat{A} = \hat{A}^\dagger$ and have the same domain, thus be Hermitian. The eigenvalues of a Hermitian operator are real and the eigenvectors associated to different eigenvalues are orthogonal. The first statement reads as follows.

$$\text{For} \quad \hat{H} = \hat{H}^\dagger, \qquad \hat{H}|\psi_n\rangle = E_n|\psi_n\rangle \quad \text{with} \quad E_n \in \mathbb{R} \,. \tag{2.16}$$

Exercise 2.1 Prove the statement above.

> Proof. Take the inner product of this expression with $\langle\psi_m|$, and use the orthonormality of the eigenvectors to get $\langle\psi_n|\hat{H}|\psi_n\rangle = E_n$. Now, rewrite the left-hand-side as lhs$=\langle\psi_n|\hat{H}^\dagger|\psi_n\rangle^*$ and use the fact that $\hat{H} = \hat{H}^\dagger$, to get lhs$=\langle\psi_n|\hat{H}|\psi_n\rangle^* = E_n^*$. Equating to the right-hand-side, $E_n = E_n^*$.

Haydock and Kelly stated in 1975 that, while the Hermitian condition was sufficient to ensure real eigenvalues, it was not necessary. Attempts have been made to relax the Hermiticity condition, and work with non-Hermitian Hamiltonians (still with PT parity-time reversal symmetry) which have only real eigenvalues. Many such non-Hermitian

Hamiltonians were constructed and studied. This gave rise to the field of *non-Hermitian quantum mechanics* which is quite fashionable nowadays.

Symbol	Measurement
$\hat{A}\|\psi\rangle = a_n\|\psi\rangle$ iff $\|\psi\rangle = \|a_n\rangle$	Action on an eigenvector
$\|\psi\rangle \longrightarrow \|a_n\rangle$ an eigenvector of $\hat{A}$	Measurement of $\hat{A}$
	System projected on $\|a_n\rangle$
$\|\langle a_n\|\psi\rangle\|^2$	Probability of collapse on $\|a_n\rangle$ ($\|\psi\rangle$ normalized)
$\langle A\rangle_\psi = \langle\psi\|\hat{A}\|\psi\rangle$	Expectation value of $\hat{A}$ in the state
$= \sum_n a_n \, \|\langle a_n\|\psi\rangle\|^2$	$\|\psi\rangle = \sum_n c_n\|a_n\rangle = \sum_n \langle a_n\|\psi\rangle\|a_n\rangle$
$\{\|\psi\rangle\}$ Copies of the state	Pure ensemble

2.1.4 Expectation values

The expectation value represents the average value of a measurement over many trials for the given state. For a quantum state $|\psi\rangle = \sum_n c_n|a_n\rangle$ the expectation value of an operator $\hat{A}$ is given by:

$$\langle\hat{A}\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle = \sum_n a_n|\langle a_n|\psi\rangle|^2 = \sum_n a_n|c_n|^2 \; . \tag{2.17}$$

The expectation value is a single number (real if $\hat{A}$ is Hermitian because all a_n are real). It represents an average over many measurements, not a single measurement outcome. The process of calculating the expectation value does not alter the quantum state $|\psi\rangle\langle\psi|$ contrary to a measurement. The expectation value calculation is a theoretical computation.

Example

Consider the state $|\psi\rangle = |0\rangle$ (spin up). The expected value of the operator $\hat{\sigma}^z$ is $\langle 0|\hat{\sigma}^z|0\rangle = \langle 0|0\rangle = 1$. instead, if the state is a superposition of up and down $|\psi\rangle = a|0\rangle + b|1\rangle$, then $\langle\psi|\hat{\sigma}^z|\psi\rangle = (a^*\langle 0| + b^*\langle 1|)\;\hat{\sigma}^z\;(a|0\rangle + b|1\rangle) = (a^*\langle 0| + b^*\langle 1|)\;(a|0\rangle - b|1\rangle) = (|a|^2\langle 0|0\rangle - a^*b\langle 0|1\rangle + b^*a\langle 1|0\rangle - |b|^2\langle 1|1\rangle = |a^2| - |b|^2$. This means that the probability of measuring spin-up along the z axis is $|a|^2$ while the one of measuring spin-down along the same axis is $|b|^2$.

2.1.5 Unitary operators

Unitary operators are specially important since the time-evolution operator has to be unitary to ensure conservation of probability.

A unitary transformation is a rigid body rotation (or reflection) of the Hilbert space, which results in a transformation of the state vector that does not change its length.

Quantum gates

Take a qu-bit. A unitary operator can be represented by a two by two matrix with complex entries U with complex transpose $U^\dagger$:

$$U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \qquad U^\dagger = \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix} \tag{2.18}$$

with the condition $UU^\dagger = U^\dagger U = \mathbb{I}$.

There are a number of well-known operations, called *gates* in the quantum computational context:

- *Hadamard Gate.* Can be viewed as a reflection around $\pi/8$, or a rotation around $\pi/4$ followed by a reflection.

  $$\mathbb{H} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{2.19}$$

  $\mathbb{H}^2 = \mathbb{I}$ and $\mathbb{H}^\dagger \mathbb{H}$.
  The Hadamard gate acts as

  $$\mathbb{H}|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \left(\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right) = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \tag{2.20}$$

  and

  $$\mathbb{H}|1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}} \left(\begin{bmatrix} 1 \\ 0 \end{bmatrix} - \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right) = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \tag{2.21}$$

  that is, it transforms the eigenstates of $\hat{\sigma}^z$ in eigenstates of $\hat{\sigma}^x$.
- *Rotation Gate.* It rotates the plane by θ:

  $$\mathbb{R} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{2.22}$$

- *NOT Gate.* Flips the bit from $|0\rangle$ to $|1\rangle$ and vice versa

  $$\mathbb{NOT} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{2.23}$$

- *Phase flip.*

  $$\mathbb{Z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{2.24}$$

  This gate is a NOT gate acting on the $|+\rangle = 1/\sqrt{2}\,(|0\rangle + |1\rangle)$, $|-\rangle = 1/\sqrt{2}\,(|0\rangle - |1\rangle)$ basis, Eq. (2.11): $\mathbb{Z}|+\rangle = |-\rangle$ and $\mathbb{Z}|-\rangle = |+\rangle$.

  Proof.

  $$\mathbb{Z}|\pm\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} (|0\rangle \pm |1\rangle) = \frac{1}{\sqrt{2}} (|0\rangle \pm (-1)|1]\rangle) = |\mp\rangle \tag{2.25}$$

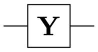
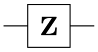
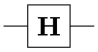
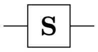
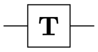
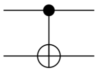
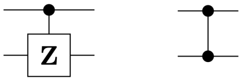
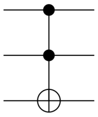
Operator	Gate(s)	Matrix
Pauli-X (X)		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)		$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$

Figure 2.1: Notation used to represent various gates. Source: Wikipedia.

2.1.6 Density operator

It is postulated that to each physical state it is associated a single linear operator, the *density operator*, $\hat{\rho}$, such that the expectation value of any observable is given by a trace of the operator in question times the density operator:

$$\langle \hat{O} \rangle = \mathrm{Tr}(\hat{\rho}\hat{O}) \tag{2.26}$$

The expectation value $\langle \hat{O} \rangle$ represents the average or mean value of the observable $\hat{O}$ over many measurements of the quantum system. Specifically, it gives the *average outcome* if one were to perform many measurements of $\hat{O}$ on identically prepared systems in the state with density operator s$\hat{\rho}$.

If $\hat{O}$ is a *diagonalizable operator*, its eigenvalues represent possible outcomes of a measurement, and $\langle\hat{O}\rangle$ is a weighted average of those outcomes, weighted by the corresponding probabilities.

For *non-diagonal operators*, $\langle\hat{O}\rangle$ might still be a real number, but it does not directly correspond to the probability of obtaining a particular outcome. Instead, it is a kind of average over all possible measurement outcomes, rather than a probability for a specific outcome.

In certain special cases the expectation value of an operator can be interpreted as a probability:

- If $\hat{O} = |o_n\rangle\langle o_n|$ is a projection operator, then $\langle\hat{O}\rangle = \mathrm{Tr}(\hat{\rho}|o_n\rangle\langle o_n|)$ gives the probability of collapsing the system on the state $|o_n\rangle$ and measuring the associated value.
- If $\hat{O}$ corresponds to an observable that is specifically designed to represent the probability of a particular outcome (like a measurement), then $\langle\hat{O}\rangle$ can be interpreted as a probability.

This is Born's rule as applied to mixed states. It provides the bridge between the abstract quantum formalism and the actual physical outcomes observed in experiments.

Example

The average of the operator $\hat{P}_0 = |0\rangle\langle 0|$ in the state with density operator $\hat{\rho}$ is, in the case of a projector, equal to the probability of obtaining the outcome corresponding to $|0\rangle$. The Born rule states:

$$p(0) = \mathrm{Tr}(\hat{\rho}\,|0\rangle\langle 0|).$$

For a general density matrix,

$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix},$$

the probability becomes

$$p(0) = \mathrm{Tr}\begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \rho_{00}$$

which is indeed real and in $[0, 1]$. Similarly, the probability of measuring 1, is $p(1) = \mathrm{Tr}(\hat{\rho}|1\rangle\langle 1|) = \rho_{11}$, and $\rho_{00}+\rho_{11} = 1$ ensure the conservation of probability. After the measurement, if the outcome associated with $|0\rangle$ is obtained, the state of the system collapses to the normalized projection of $\hat{\rho}$ onto $|0\rangle$

$$\hat{\rho}_{\mathrm{post}} = \frac{\hat{P}_0\hat{\rho}\hat{P}_0}{p(0)}$$

Substituting $\hat{P}_0$, $\hat{P}_0\hat{\rho}\hat{P}_0 = |0\rangle\langle 0|\hat{\rho}|0\rangle\langle 0| = \rho_{00}|0\rangle\langle 0|$. Therefore,

$$\hat{\rho}_{\mathrm{post}} = \frac{\rho_{00}|0\rangle\langle 0|}{\rho_{00}} = |0\rangle\langle 0|.$$

It is particularly important to use the density operator in the quantum theory of open systems, where a quantum system interacts with an external system whose evolution is unknown, and in the quantum theory of measurement and information.

Having said so, the dimension of the density matrix of the system is the square of that of the system's Hilbert space. This requirement may make their numerical solution prohibitively expensive, even for moderately sized quantum systems.

Pure states

The density operator of a pure state $|\psi\rangle$ takes the form

$$\hat{\rho} = |\psi\rangle\langle\psi| \tag{2.27}$$

The pure state $|\psi\rangle$ can be expanded in a basis $|\psi_n\rangle$ of the Hilbert space, $|\psi\rangle = \sum_n c_n|\psi_n\rangle$ and then

$$\hat{\rho} = \sum_{nm} c_n c_m^* \, |\psi_n\rangle\langle\psi_m| \tag{2.28}$$

In this same basis, the density matrix has elements

$$\rho_{nm} = \langle\psi_n| \sum_{kl} c_k c_l^* \, |\psi_k\rangle\langle\psi_l|\psi_m\rangle = \sum_{kl} c_k c_l^* \, \delta_{kn}\delta_{lm} = c_n c_m^* \tag{2.29}$$

The physical content of the density operator is more apparent when we compute the elements of the *density matrix* with respect to a complete, orthonormal basis. The diagonal elements are real numbers and they are referred to as *populations*, give the measurement probability of the system in each of the states, and add up to one. The off-diagonal elements are complex conjugates of each other and they are referred to as *coherences*; they give information about the relative phase of different components of the superposition. For example, if we write the state vector as a superposition with explicit phases, $c_n = |c_n|e^{i\phi_n}$,

$$\rho_{nm} = |c_n||c_m|e^{i(\phi_n - \phi_m)} \tag{2.30}$$

In another basis, say $\{|\phi_n\rangle\}$, the elements will be different. The state $|\psi\rangle$ will have different coefficients d_n when expanded in this new basis, $|\psi\rangle = \sum_n d_n|\phi_n\rangle$. Then,

$$\rho_{nm} = \langle\phi_n| \sum_{kl} d_k d_l^* \, |\phi_k\rangle\langle\phi_l|\phi_m\rangle = \sum_{kl} d_k d_l^* \, \langle\phi_n|\phi_k\rangle \, \langle\phi_l|\phi_m\rangle = d_n d_m^* \tag{2.31}$$

and $d_n d_m^* \neq c_n c_m^*$.

Example

Let us consider a pure state $|\psi\rangle$ of a two-level system, a particle with spin up or down, in a superposition,

$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle \tag{2.32}$$

The density operator is

$$\begin{aligned}\hat{\rho} = |\psi\rangle\langle\psi| &= c_0^* c_0 |0\rangle\langle 0| + c_0^* c_1 |0\rangle\langle 1| + c_1^* c_0 |1\rangle\langle 0| + c_1^* c_1 |1\rangle\langle 1| \\ &= |c_0|^2 |0\rangle\langle 0| + |c_1|^2 |1\rangle\langle 1| + \underbrace{c_0^* c_1 |0\rangle\langle 1| + c_1^* c_0 |1\rangle\langle 0|}_{\text{interference}} \end{aligned} \tag{2.33}$$

In the $|0\rangle, |1\rangle$ basis the density matrix is

$$\begin{bmatrix} |c_0|^2 & c_0^* c_1 \\ c_1^* c_0 & |c_1|^2 \end{bmatrix} \tag{2.34}$$

The trace of this matrix is $\mathrm{Tr}\hat{\rho} = |c_0|^2 + |c_1|^2 = 1$ by normalization. The interference terms are the off-diagonal ones in the matrix. *Decoherence* usually refers to the destruction of the interference terms or the off-diagonal elements in the matrix, leaving just the diagonal elements. Note however that whether or not there is any interference (non-zero off-diagonal elements in ρ) depends on our choice of basis. Just because a density matrix is diagonal in some basis does not mean the system is behaving classically. In this simple problem ρ is diagonal only if $|c_0|^2 = 0$ or $|c_1|^2 = 0$.

Use now the basis of eigenstates of the operator $\hat{\sigma}^x$, $|+\rangle \equiv (|0\rangle + |1\rangle)/\sqrt{2}$ with eigenvalue 1 and $|-\rangle \equiv (|0\rangle - |1\rangle)/\sqrt{2}$ with eigenvalue -1, and rewrite $\hat{\rho}$ in this basis. One has the new elements $\overline{\rho}_{11}, \overline{\rho}_{12}, \overline{\rho}_{21}, \overline{\rho}_{22}$. They read

$$\begin{aligned} 2\overline{\rho}_{11} &= (\langle 0| + \langle 1|)\,(c_0^* c_0 |0\rangle\langle 0| + c_0^* c_1 |0\rangle\langle 1| + c_1^* c_0 |1\rangle\langle 0| + c_1^* c_1 |1\rangle\langle 1|)\,(|0\rangle + |1\rangle) \\ &= c_0^* c_0 + c_0^* c_1 + c_1^* c_0 + c_1^* c_1 \end{aligned} \tag{2.35}$$

$$\begin{aligned} 2\overline{\rho}_{12} &= (\langle 0| + \langle 1|)\,(c_0^* c_0 |0\rangle\langle 0| + c_0^* c_1 |0\rangle\langle 1| + c_1^* c_0 |1\rangle\langle 0| + c_1^* c_1 |1\rangle\langle 1|)\,(|0\rangle - |1\rangle) \\ &= c_0^* c_0 - c_0^* c_1 + c_1^* c_0 - c_1^* c_1 \end{aligned} \tag{2.36}$$

$$\begin{aligned} 2\overline{\rho}_{21} &= (\langle 0| - \langle 1|)\,(c_0^* c_0 |0\rangle\langle 0| + c_0^* c_1 |0\rangle\langle 1| + c_1^* c_0 |1\rangle\langle 0| + c_1^* c_1 |1\rangle\langle 1|)\,(|0\rangle + |1\rangle) \\ &= c_0^* c_0 + c_0^* c_1 - c_1^* c_0 - c_1^* c_1 \end{aligned} \tag{2.37}$$

$$\begin{aligned} 2\overline{\rho}_{22} &= (\langle 0| - \langle 1|)\,(c_0^* c_0 |0\rangle\langle 0| + c_0^* c_1 |0\rangle\langle 1| - c_1^* c_0 |1\rangle\langle 0| - c_1^* c_1 |1\rangle\langle 1|)\,(|0\rangle - |1\rangle) \\ &= c_0^* c_0 - c_0^* c_1 - c_1^* c_0 + c_1^* c_1 \end{aligned} \tag{2.38}$$

The trace of this matrix is $2\mathrm{Tr}\overline{\rho} = [c_0^* c_0 + \cancel{c_0^* c_1} + \cancel{c_1^* c_0} + c_1^* c_1] + [c_0^* c_0 - \cancel{c_0^* c_1} - \cancel{c_1^* c_0} + c_1^* c_1] = 2|c_0|^2 + 2|c_1|^2 = 2$ and $\mathrm{Tr}\rho = \mathrm{Tr}\overline{\rho} = 1$. Can we choose the coefficients c_0, c_1 so as to make this matrix diagonal while keeping ρ non diagonal? The requirement $\overline{\rho}_{12} = \overline{\rho}_{21} = 0$ implies

$$c_0^* c_1 = c_1^* c_0 \qquad \text{and} \qquad |c_0|^2 = 0 \quad \text{or} \quad |c_1|^2 = 0 \tag{2.39}$$

so, it is not possible in this case. But this is not general.

One could have proceeded differently, that is, writing $|\psi\rangle$ in the $|+\rangle$, $|-\rangle$ basis. For that, we write

$$|0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) \qquad\qquad |1\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle) \tag{2.40}$$

and then

$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle = \frac{c_0}{\sqrt{2}}(|+\rangle + |-\rangle) + \frac{c_1}{\sqrt{2}}(|+\rangle - |-\rangle) = \frac{c_0 + c_1}{\sqrt{2}}|+\rangle + \frac{c_0 - c_1}{\sqrt{2}}|-\rangle \tag{2.41}$$

We now construct the elements of the $\overline{\rho}$ matrix,

$$\begin{aligned} \overline{\rho}_{11} &= \langle +|\psi\rangle\langle\psi|+\rangle = \Big(\langle +|\frac{c_0 + c_1}{\sqrt{2}}|+\rangle + \cancel{\langle +|\frac{c_0 - c_1}{\sqrt{2}}|-\rangle}\Big)\Big(\frac{c_0^* + c_1^*}{\sqrt{2}}\langle +|+\rangle + \cancel{\frac{c_0^* - c_1^*}{\sqrt{2}}\langle -|+\rangle}\Big) \\ &= \frac{c_0 + c_1}{\sqrt{2}}\frac{c_0^* + c_1^*}{\sqrt{2}} = \frac{1}{2}(|c_0|^2 + |c_1|^2 + c_0 c_1^* + c_0^* c_1) \end{aligned} \tag{2.42}$$

which is the same expression we found above. Similarly for the other components.

The density operator is Hermitian: $\hat{\rho}^\dagger = \hat{\rho}$. The proof is simple.

Let us first have a look at the elements of ρ in the original basis. According to (2.29) they are $\rho_{nm} = c_n^* c_m$. The elements of the matrix of the operator $\hat{\rho}^\dagger$ in the same basis are $(\rho^\dagger)_{nm} = (\underbrace{c_n^* c_m}_{n \leftrightarrow m})^* = (c_m^* c_n)^* = c_m c_n^* = \rho_{nm}$.

To get fully convinced that Hermiticity holds for all ways of writing the density operator, we now write $|\psi\rangle$ in the basis $\{|\psi_n\rangle\}$ and we sandwich the operator with respect to the basis $\{|\phi_n\rangle\}$. Taking the complex conjugate of those elements:

$$\begin{aligned} \rho_{mn}^* &= \sum_{kl} c_k c_l^* \langle \phi_m|\psi_k\rangle^* \langle \psi_l|\phi_n\rangle^* = \sum_{kl} c_k c_l^* \langle \phi_k|\psi_m\rangle \langle \psi_n|\phi_l\rangle \\ &= \sum_{kl} c_l c_k^* \langle \psi_n|\phi_l\rangle \langle \phi_k|\psi_m\rangle = \rho_{nm} \end{aligned} \tag{2.43}$$

The diagonal elements ρ_{nn} represent probabilities associated with the quantum state's measurement outcomes. Since probabilities must be real and non-negative, this aligns with the fact that the diagonal elements are real and non-negative.

The density operator has *unit trace*, $\text{Tr}\hat{\rho} = 1 = \sum_n \langle \phi_n|\hat{\rho}|\phi_n\rangle$ where $\{|\phi_n\rangle\}$ is a generic complete orthonormal set of vectors, a basis of the Hilbert space.

Although the density matrix depends on the basis in which it is calculated, its trace is independent of the basis chosen, since its diagonal elements represent the probabilities of getting the different outcomes (eigenvalues) of a particular observable whose eigenstates make up that particular basis. Their sum must add up to 1.

The density operator is *positive semi-definite* $\langle \psi|\hat{\rho}|\psi\rangle \geq 0$ for an arbitrary vector $|\psi\rangle$, and all eigenvalues are non-negative. (See Ex. 2.4 for a general proof.)

The fact that we could not have a diagonal density matrix in the basis of eigenvectors of $\hat{\sigma}^z$ and a non-diagonal one in the basis of eigenvectors of $\hat{\sigma}^x$ in the example is not general. One can have a diagonal ρ in a basis $\{|\psi_n\rangle\}$ that becomes non diagonal en the basis $\{|\phi_n\rangle\}$ In the new basis, the vectors $\{|\phi_n\rangle\}$ can be superpositions of the original basis vectors $\{|\psi_n\rangle\}$. When expressed in the new basis, the off-diagonal terms may appear, representing quantum coherences between the different states in that basis.

The expectation value of a generic observable $\hat{A}$ in a state $|\psi\rangle$ equals

$$\langle \hat{A} \rangle_\psi = \text{Tr}(\hat{A}\hat{\rho}) \tag{2.44}$$

where $\hat{\rho} = |\psi\rangle\langle\psi|$.

Exercise 2.2 Prove the statement above.

Proof. Consider $|\psi\rangle = \sum_n c_n |a_n\rangle$ with $|a_n\rangle$ the eigenvectors of the operator $\hat{A}$. The rhs of

(2.44) is

$$\begin{aligned}
\mathrm{Tr}(\hat{A}\hat{\rho}) &= \sum_n \langle a_n|\hat{A}\hat{\rho}|a_n\rangle = \sum_n \langle a_n|\hat{A}|\psi\rangle\langle\psi|a_n\rangle = \sum_n \langle a_n|\hat{A}\sum_m c_m|a_m\rangle \sum_r c_r^*\langle a_r|a_n\rangle \\
&= \sum_m c_m a_m \sum_n \langle a_n|a_m\rangle \sum_r c_r^*\delta_{rn} = \sum_m c_m a_m \sum_n \delta_{nm} c_n^* \\
&= \sum_n c_n a_n c_n^* = \sum_n a_n |c_n|^2 = \langle\psi|\hat{A}|\psi\rangle \qquad (2.45)
\end{aligned}$$

Mixed states

Consider a system that is prepared in a pure state (i.e. one that is described by a single wave function), but we do not know what this pure state is. It might be $|\psi_1\rangle$ or $|\psi_2\rangle$ with (let us assume) equal probability (where the probability reflects our ignorance rather than a property of the system itself). We express this ignorance as a *mixed state density matrix*:

$$\hat{\rho} = \frac{1}{2}\left(|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|\right) \qquad (2.46)$$

where the factors of $\frac{1}{2}$ are classical probabilities.

Example

An example would be the one of a spin which has been previously measured by a detector (prepared) along the z-axis. It is thus in a pure state of either $|0\rangle$ or $|1\rangle$ but, if we do not know which of the states it is in because, for example, we could not access the result of the measurement, we must describe it by a mixed state, with density operator $\hat{\rho} = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$, and equal probability 1/2 of being in $|0\rangle$ or $|1\rangle$. The components in the basis $|0\rangle, |1\rangle$ are $\rho_{11} = \rho_{22} = 1/2$ and $\rho_{12} = \rho_{21} = 0$, so the matrix is diagonal. The trace of the operator is $\mathrm{Tr}\hat{\rho} = 1$. Instead the matrix squared has elements $\rho_{11}^2 = \rho_{22}^2 = 1/4$ and $\rho_{12}^2 = \rho_{21}^2 = 0$ and its trace is $\mathrm{Tr}\rho^2 = 1/2 < 1$.

Note that this density operator is not the one of a pure state $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$, since for such the coefficients c_0 and c_1 are complex numbers with $|c_0|^2 + |c_1|^2 = 1$ and this implues $\mathrm{Tr}\rho^2 = \mathrm{Tr}(|\psi\rangle\langle\psi|)^2 = 1$. This density operator can also be expressed as $\hat{\rho} = \frac{1}{2}(|+\rangle\langle+| + |-\rangle\langle-|)$ with $|\pm\rangle$ the eigenstates of $\hat{\sigma}^x$ with eigenvalue ± 1, respectively. The same results apply, of course.

We can also use it to describe an *ensemble of systems* and the density operator describing a mixed state takes the form

$$\hat{\rho} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| \qquad (2.47)$$

where $0 \leq p_\alpha \leq 1 \in \mathcal{R}$ is the fraction of the ensemble in each pure state $|\psi_\alpha\rangle$. They satisfy $\sum_\alpha p_\alpha = 1$. The density matrix can be thought of as a way of using the one-particle formalism to describe the behavior of many similar particles by giving a probability distribution (or ensemble) of states that these particles can be found in.

The density operator of a mixed state is still Hermitian, $\hat{\rho}^\dagger = \hat{\rho}$ as obvious from its definition and the fact that $p_\alpha \in \mathcal{R}$.

Exercise 2.3 Prove that the trace of a mixed state also equals one $\mathrm{Tr}\hat{\rho} = 1$.

Proof. The trace density operator of a mixed state is $\mathrm{Tr}\hat{\rho} = \sum_n \left(\sum_\alpha \langle\psi_n| \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|\right) \psi_n\rangle$ where $\{|\psi_n\rangle\}$ is a basis of the Hilbert space. One has $\mathrm{Tr}\hat{\rho} = \sum_\alpha p_\alpha \sum_n |\langle\psi_n|\psi_\alpha\rangle|^2$. Each of the $|\psi_\alpha\rangle$ can be expanded in the basis $\{|\psi_n\}$: $|\psi_\alpha\rangle = \sum_m c_\alpha^m |\psi_m\rangle$ with $\sum_m |c_\alpha^m|^2 = 1$. Then, $|\langle\psi_n|\psi_\alpha\rangle|^2 = |\langle\psi_n| \sum_m c_\alpha^m \psi_m\rangle|^2 = |\sum_m c_\alpha^m \delta_{nm}|^2 = |c_\alpha^n|^2$. We can now replace tis result in the above expression for $\mathrm{Tr}\hat{\rho}$ and find $\mathrm{Tr}\hat{\rho} = \sum_\alpha p_\alpha \sum_n |c_\alpha^n|^2 = \sum_\alpha p_\alpha = 1$.
Another and shorter way of proving the same result is to write $\mathrm{Tr}\hat{\rho} = \mathrm{Tr} \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| = \sum_\alpha p_\alpha \mathrm{Tr}|\psi_\alpha\rangle\langle\psi_\alpha| = \sum_\alpha p_\alpha = 1$, which uses the fact that the trace of the density operator of a pure state equals one.

The density operator of a mixed state is still positive definite, $\langle\psi|\hat{\rho}|\psi\rangle \geq 0$ for an arbitrary vector $|\psi\rangle$.

Exercise 2.4 Prove this statement.

Proof. One must show that $\langle\psi|\hat{\rho}|\psi\rangle \geq 0$ for all states $|\psi\rangle$. The density operator is $\hat{\rho} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$, with $|\psi_\alpha\rangle$ normalized pure states ($\langle\psi_\alpha|\psi_\alpha\rangle = 1$), and $p_\alpha \geq 0$ probabilities with $\sum_\alpha p_\alpha = 1$. For any normalized state $|\psi\rangle$, consider the expectation value

$$\langle\psi|\hat{\rho}|\psi\rangle = \langle\psi| \left(\sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|\right) |\psi\rangle = \sum_\alpha p_\alpha \langle\psi|\psi_\alpha\rangle\langle\psi_\alpha|\psi\rangle$$

Since $\langle\psi|\psi_\alpha\rangle\langle\psi_\alpha|\psi\rangle = |\langle\psi|\psi_\alpha\rangle|^2 \geq 0$ and $p_\alpha \geq 0$, the expectation value is a weighted sum of non-negative terms:

$$\langle\psi|\hat{\rho}|\psi\rangle = \sum_\alpha p_\alpha |\langle\psi|\psi_\alpha\rangle|^2 \geq 0.$$

Thus, $\hat{\rho}$ is semi-positive definite.

Since the density matrix is Hermitian and semi-positive definite, its eigenvalues are real and non-negative. Therefore, all physical density operators meet the semi-positive definiteness criterion.

While the trace of the square of the density operator of a pure system still equals one, the trace of the square of a mixed system is smaller than one.

Exercise 2.5 Prove $\mathrm{Tr}(\hat{\rho})^2 = 1$ if $\hat{\rho} = \hat{\rho}_{\mathrm{pure}}$ is the one of a pure system and $\mathrm{Tr}(\hat{\rho})^2 < 1$ if $\hat{\rho} = \hat{\rho}_{\mathrm{mixed}}$ is the one of a mixed system.

Proof. If $\hat{\rho}$ is the one of a pure system $\hat{\rho}_{\mathrm{pure}} = |\psi\rangle\langle\psi|$ is a projector and the square of a projector is equal to itself, $(\hat{\rho}_{\mathrm{pure}})^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi|$. Then $\mathrm{Tr}(\hat{\rho}_{\mathrm{pure}})^2 = 1$.
Instead, if $\hat{\rho}$ is the one of a mixed system $\hat{\rho}_{\mathrm{mixed}} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ with $p_\alpha \leq 1$ and $\sum_\alpha p_\alpha = 1$, its square reads
$(\hat{\rho}_{\mathrm{mixed}})^2 = (\sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|)(\sum_\beta p_\beta |\psi_\beta\rangle\langle\psi_\beta| = \sum_{\alpha\beta} p_\alpha p_\beta |\psi_\alpha\rangle\langle\psi_\alpha|\psi_\beta\rangle\langle\psi_\beta| = \sum_\alpha p_\alpha^2 |\psi_\alpha\rangle\langle\psi_\alpha|$.
The trace of this operator is $\mathrm{Tr}(\hat{\rho}_{\mathrm{mixed}})^2 = \sum_\alpha p_\alpha^2 < 1$.

A pure quantum state is a state that cannot be written as a probabilistic mixture of other quantum states. There is only one $p_\alpha = 1$ and all the others vanish in (2.47).

Let us express the ensemble average (expectation value) of an observable $\hat{A}$ in a mixed state $\hat{\rho} = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ made out of the pure states

$$|\psi_\alpha\rangle = \sum_n c_\alpha^n |a_n\rangle \qquad \text{with} \qquad c_\alpha^n = \langle a_n|\psi_\alpha\rangle \tag{2.48}$$

where a_n and $|a_n\rangle$ are the eigenvalues and eigenkets of $\hat{A}$ and this is the representation of $|\psi_\alpha\rangle$ in this basis. It reads

$$\begin{aligned}
\langle\hat{A}\rangle_\psi &= \mathrm{Tr}(\hat{\rho}\hat{A}) = \sum_m \langle a_m|\hat{\rho}\hat{A}|a_m\rangle \\
&= \sum_m a_m \langle a_m| \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|a_m\rangle \\
&= \sum_\alpha p_\alpha \sum_m a_m \sum_r c_\alpha^r \langle a_m|a_r\rangle \sum_s (c_\alpha^s)^* \langle a_s|a_m\rangle \\
&= \sum_\alpha p_\alpha \sum_m a_m \sum_r c_\alpha^r \delta_{mr} \sum_s (c_\alpha^s)^* \delta_{sm} \\
&= \sum_\alpha p_\alpha \sum_m a_m |c_\alpha^m|^2
\end{aligned} \tag{2.49}$$

There are two types of averaging here: one is a weighted quantum superposition over the basis kets $|a_n\rangle$ of the pure states, and the other is a statistical (said incoherent) average with the probabilities p_α of those states.

Example

It is important to emphasise the difference between a probabilistic mixture of quantum states and their superposition.

Take a physical system with a two dimensional Hilbert space with basis $|1\rangle$ or $|0\rangle$, and consider that the system can be in any of these two states with equal probability. The density matrix is $\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

On the other hand, a quantum superposition of these two states with equal probability amplitudes results in the pure state $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$, with density operator $|\psi\rangle\langle\psi|$ associated to the density matrix $\rho = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$. Unlike the probabilistic mixture, this superposition can display quantum interference (non-zero non-diagonal elements).

Exercise 2.6 Consider a mixture such that with probability 1/2 one prepares $|0\rangle$ and with probability 1/2 one prepares the state $(|0\rangle + |1\rangle)/\sqrt{2}$. Find the density matrix in the $\{|0\rangle, |1\rangle\}$ basis. Calculate the eigenvalues, check that they are real and positive, that the trace equals one, and whether $|\rho_{nm}|^2 < \rho_{nn}\rho_{mm}$.

Solution

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} = \begin{pmatrix} 3/4 & 1/4 \\ 1/4 & 1/4 \end{pmatrix} \tag{2.50}$$

The eigenvalues and eigenvectors of this matrix are $\lambda_\pm = 1/2 \pm \sqrt{2}/4$ and $|\phi_\pm\rangle = \sqrt{\lambda_\pm}\,|0\rangle \mp \sqrt{1-\lambda_\pm}\,|1\rangle$. The trace of the matrix equals one, $3/4+1/4=1$, and accordingly $\lambda_+ + \lambda_- = 1$. $|\rho_{12}|^2 = (1/4)^2 = 1/16 < \rho_{11}\rho_{22} = (3/4)(1/4) = 3/16$.

When the density operator is just the projector on a pure state, the information content of the density operator is equivalent to that of the state vector (except for the overall phase, which is not of physical significance). Otherwise, it represents an *incoherent superposition of states* and, through the definition, one assigns a probability or weight to each of them. The density operator represents uncertainty 'beyond the minimum required by quantum mechanics'. Like in classical statistical physics, the density operator can be interpreted as representing an ensemble of identical systems in possibly different states.

Exercise 2.7 Prove that in a generic mixed state, $|\rho_{\alpha\beta}|^2 < \rho_{\alpha\alpha}\rho_{\beta\beta}$.

Proof. This result is a consequence of the Cauchy-Schwarz inequality, which holds for any density matrix, since they are all positive semi-definite.
The Cauchy-Schwarz inequality states that for any two complex vectors $|\psi\rangle$ and $|\phi\rangle$, $|\langle\psi|\phi\rangle|^2 \leq |\langle\psi|\psi\rangle||\langle\phi|\phi\rangle|$ and follows from $||\psi\rangle - |\phi\rangle|^2 \geq 0$. This inequality is fundamental in linear algebra and essentially says that the inner product squared between two vectors is bounded by the product of the norms (magnitudes) of the two vectors.
Apply this inequality to the columns of the density matrix in the subspace α, β. The result follows.

Symbol	Name or property
$\hat\rho$	**Density (linear) operator**
$\mathrm{Tr}\hat\rho = 1$	Conservation of probability
$\langle\hat A\rangle = \mathrm{Tr}(\hat A\hat\rho)$	Expectation value of $\hat A$ in $\hat\rho$
$\hat\rho_{\text{pure}} = \|\psi\rangle\langle\psi\|$	Projector on a vector = Pure state
$\mathrm{Tr}\hat\rho^2_{\text{pure}} = 1$	consequence of $\langle\psi\|\psi\rangle = 1$
$\hat\rho_{\text{mixed}} = \sum\limits_\alpha p_\alpha \|\psi_\alpha\rangle\langle\psi_\alpha\|$	Mixed state with $\sum\limits_\alpha p_\alpha = 1$
$\mathrm{Tr}\hat\rho^2_{\text{mixed}} = \sum_\alpha p^2_\alpha < 1$	consequence of $0 \leq p_\alpha \leq 1$
$\hat\rho_{\text{microcanical}} = \frac{1}{N}\sum\limits_n \|\psi_n\rangle\langle\psi_n\|$	$\hat H\|\psi_n\rangle = E_n\|\psi_n\rangle$ and $p_n = \frac{1}{N}$
$\hat\rho_{\text{canonical}} = \dfrac{e^{-\beta\hat H}}{\mathrm{Tr}e^{-\beta\hat H}} = \sum\limits_n \dfrac{e^{-\beta E_n}}{\sum\limits_m e^{-\beta E_m}}\|\psi_n\rangle\langle\psi_n\|$	$\hat H\|\psi_n\rangle = E_n\|\psi_n\rangle$ and $p_n = \dfrac{e^{-\beta E_n}}{\sum\limits_m e^{-\beta E_m}}$
$\mathcal{Z} = \mathrm{Tr}e^{-\beta\hat H}$	Partition function
$F = -\beta\ln\mathcal{Z}$	Free-energy

2.1.7 Statistical Physics

The density operator encapsulates the statistical properties of a system [13,14]. We will discuss this in more detail after studying the quantum formalism for many-body systems, but we can already introduce some special expressions for the density operator of systems in thermal equilibrium.

Microcanonical ensemble

In quantum statistical physics, the microcanonical ensemble describes a closed quantum system with fixed energy, volume, and particle number. This ensemble is used to model isolated systems that are not in contact with any external environment or heat reservoir, for example, an isolated atomic gas.

The system is confined to a narrow range of energy values, denoted as E. In practice, this is represented by an energy shell $[E, E + \delta E]$, where δE is very small. The microcanonical ensemble assumes equal probability for all quantum states within this energy range. The density operator for the microcanonical ensemble is:

$$\hat{\rho} = \frac{1}{\Omega} \sum_{n \in \text{shell}} |n\rangle\langle n|,$$

where $|n\rangle$ are the energy eigenstates, $\Omega =$ number of states in the shell is the total *number of accessible microstates*. The *entropy* S in the microcanonical ensemble is given by the Boltzmann formula:

$$S = k_B \ln \Omega,$$

where k_B is the Boltzmann constant and Ω measures the multiplicity of states at energy E. The *microcanonical temperature* T is defined from the entropy as

$$\frac{1}{T} = \frac{\partial S}{\partial E}.$$

For an observable $\hat{O}$, its expectation value is computed as:

$$\langle \hat{O} \rangle = \mathrm{Tr}(\hat{\rho}\hat{O}) = \frac{1}{\Omega} \sum_{n \in \text{shell}} \langle n|\hat{O}|n\rangle.$$

The microcanonical ensemble embodies the principle of "equal a priori probabilities": all accessible microstates are equally likely since there is no external influence to favor one state over another.

The fields of *Quantum Chaos and Ergodicity* explore how complex quantum systems equilibrate and distribute energy among accessible microstates.

Exercise 2.8 Calculate the expected value of $\hat{\sigma}^z$ for a qubit with Hamiltonian $\hat{H} = -(\hbar\omega/2)\hat{\sigma}^z$, with $\hbar\omega$ the energy splitting between the eigenstates of $\hat{\sigma}_z$ (due to an external magnetic field), in microcanonical equilibrium.

Solution. In the microcanonical ensemble, the system is restricted to a specific energy level E, meaning that only states with this specific energy contribute to the ensemble. The eigenvalues of $\hat{H}$ are $E_0 = -\frac{\hbar\omega}{2}$ (corresponding to the eigenstate $|0\rangle$), $E_1 = +\frac{\hbar\omega}{2}$ (corresponding to the eigenstate $|1\rangle$). Thus, the system can be in one of two distinct energy levels. The microcanonical ensemble assumes the system is strictly confined to one of these energy levels. The expectation value of $\hat{\sigma}_z$ takes two possible values:

- If the energy is $E = -\frac{\hbar\omega}{2}$, the system is in the state $|0\rangle$, the eigenstate of $\hat{\sigma}_z$ with eigenvalue $+1$ and
$$\langle\hat{\sigma}_z\rangle = \langle 0|\hat{\sigma}_z|0\rangle = 1.$$
- If the energy is $E = +\frac{\hbar\omega}{2}$, the system is in the state $|1\rangle$, the eigenstate of $\hat{\sigma}_z$ with eigenvalue -1 and the expectation value of $\hat{\sigma}_z$ is
$$\langle\hat{\sigma}_z\rangle = \langle 1|\hat{\sigma}_z|1\rangle = -1.$$

Canonical ensemble

For a system in thermal equilibrium at temperature T, the density operator ρ is given by the Boltzmann distribution (also called the canonical ensemble):

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{\mathcal{Z}},$$

where H is the Hamiltonian of the system (the total energy operator), $\beta = \frac{1}{k_B T}$, with k_B being the Boltzmann constant and T the temperature, $\mathcal{Z}$ is the *partition function*, defined as:

$$\mathcal{Z} = \mathrm{Tr}(e^{-\beta\hat{H}}) = \sum_n \langle n|e^{-\beta\hat{H}}|n\rangle = \sum_n e^{-\beta E_n},$$

where E_n are the eigenvalues of the Hamiltonian H and $\{|n\rangle\}$ is its associated eigenbasis. The interpretation of this form is similar to the one of classical statistical physics:

- The partition function plays a central role in thermodynamics, as it helps calculate thermodynamic quantities like free energy, entropy, and specific heat. It sums over all possible states of the system, weighted by their Boltzmann factor $e^{-\beta E_n}$.
- The density operator $\hat{\rho}$ describes the state of the system. In the canonical ensemble, the density matrix ρ can be viewed as a weighted sum over the eigenstates of the Hamiltonian, with the weights determined by the Boltzmann factor. Essentially, $\hat{\rho}$ encodes the probability distribution of states in canonical thermal equilibrium.

The density operator gives the probability of the system being in a particular state. For the canonical ensemble, the probability of the system being in the state corresponding to energy E_n is given by the Boltzmann distribution

$$P(E_n) = \frac{e^{-\beta E_n}}{\mathcal{Z}}.$$

Thus, the density operator $\hat{\rho}$ in the eigenbasis of the Hamiltonian can be written as

$$\hat{\rho} = \sum_n P(E_n)|n\rangle\langle n| = \frac{1}{\mathcal{Z}} \sum_n e^{-\beta E_n} |n\rangle\langle n|.$$

Here, $\{|n\rangle\}$ are the eigenstates of the Hamiltonian, and the density matrix with elements ρ_{mn} is diagonal in this basis with entries $e^{-\beta E_n}/\mathcal{Z}$.

The partition function $\mathcal{Z}$ is used to compute the *free energy* F of the system:

$$F = -k_B T \ln \mathcal{Z}.$$

The *internal energy* U is given by

$$U = \langle \hat{H} \rangle = \mathrm{Tr}(\hat{\rho}\hat{H}) = -\frac{\partial}{\partial \beta} \ln \mathcal{Z}.$$

The *entropy* S can be derived from:

$$S = -k_B \mathrm{Tr}(\hat{\rho} \ln \hat{\rho}).$$

The density operator $\hat{\rho}$ and partition function $\mathcal{Z}$ are directly related through the statistical mechanics framework, providing a complete description of the system's thermodynamic behavior.

Exercise 2.9 Calculate the expected value of $\hat{\sigma}^z$ for a qubit with Hamiltonian $\hat{H} = -(\hbar\omega/2)\hat{\sigma}^z$, with $\hbar\omega$ the energy splitting between the eigenstates of $\hat{\sigma}_z$ (due to an external magnetic field), in canonical equilibrium at inverse temperature $\beta = 1/(k_B T)$.

Proof. The matrix representation of the $\hat{\sigma}^z$ is $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. In the canonical ensemble, the density operator is given by

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}(e^{-\beta \hat{H}})},$$

where $\mathrm{Tr}(e^{-\beta \hat{H}})$ is the partition function, which ensures the normalization of $\hat{\rho}$. The eigenvalues of $\hat{H}$ are $-\hbar\omega/2$ and $\hbar\omega/2$, corresponding to the eigenstates $|0\rangle$ and $|1\rangle$, respectively. Thus

$$\mathrm{Tr}(e^{-\beta \hat{H}}) = e^{\beta \frac{\hbar\omega}{2}} + e^{-\beta \frac{\hbar\omega}{2}} = 2\cosh\left(\frac{\beta\hbar\omega}{2}\right).$$

The expectation value of $\hat{\sigma}_z$ is

$$\langle \hat{\sigma}_z \rangle = \mathrm{Tr}(\hat{\rho}\hat{\sigma}_z) = \frac{\mathrm{Tr}(e^{-\beta \hat{H}}\hat{\sigma}_z)}{\mathrm{Tr}(e^{-\beta \hat{H}})}.$$

The matrix σ_z is diagonal in the eigenbasis of $\hat{H}$, with eigenvalues $+1$ and -1. Thus, the trace simplifies

$$\mathrm{Tr}(e^{-\beta \hat{H}}\hat{\sigma}_z) = e^{-\beta \frac{\hbar\omega}{2}}(1) + e^{\beta \frac{\hbar\omega}{2}}(-1) = e^{-\beta \frac{\hbar\omega}{2}} - e^{\beta \frac{\hbar\omega}{2}} = -2\sinh\left(\frac{\beta\hbar\omega}{2}\right).$$

Putting together the two expressions for numerator and denominator

$$\langle\hat{\sigma}_z\rangle = -\tanh\left(\frac{\beta\hbar\omega}{2}\right).$$

At high temperatures ($\beta \to 0$), $\langle\hat{\sigma}_z\rangle \to 0$, as the system becomes equally likely to be in either state. At low temperatures ($\beta \to \infty$), $\langle\hat{\sigma}_z\rangle \to -1$, as the system predominantly occupies the lower-energy state. In the classical limit $\hbar \to 0$, $\lim_{\hbar\to 0}\langle\hat{\sigma}^z\rangle = 0$, which is obvious since $\hat{H} = 0$ in this case.

2.2 Many-body systems

2.2.1 Hilbert space, pure states and linear superposition

The Hilbert space of a system made of two subsystems A and B is

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \tag{2.51}$$

An example with many subsystems is a system of spins sitting on a lattice, with the spins labelled by an integer $i = 1, \dots, N$, and $x = ia$ the position of each lattice site. Then,

$$\mathcal{H} = \bigotimes_{i=1}^{N} \mathcal{H}_i \tag{2.52}$$

A pure state of a system made of N elements, each with K possible states, is

$$|\psi\rangle = \sum_{k_1=1}^{K} \cdots \sum_{k_N=1}^{K} c_{k_1\dots k_N} |\psi_1^{k_1}\rangle \otimes \cdots \otimes |\psi_N^{k_N}\rangle \tag{2.53}$$

with $\sum_{k_1=1}^{K} \cdots \sum_{k_N=1}^{K} |c_{k_1\dots k_N}|^2 = 1$. If we measure all N elements by projecting each onto the $\{|\psi_k\rangle\}$ basis, the probability of obtaining the outcome $|\psi_1^{k_1}\rangle \otimes \cdots \otimes |\psi_N^{k_N}\rangle$ is $|c_{k_1\dots k_N}|^2$. The so-called *computational basis* is also often written as

$$|\psi_{k_1} \dots \psi_{k_N}\rangle = |\psi_1^{k_1}\rangle \otimes \cdots \otimes |\psi_N^{k_N}\rangle \tag{2.54}$$

The pure state is a superposition of all K^N basis states of the system, weighted by complex coefficients that represent the amplitudes. The normalization condition ensures the total probability is 1. This structure applies universally for any N and K.

Example

Take as an example a system made of two qubits or two-state systems.

Classically, each of the two qubits has two possible configurations, 0 and 1, and the system made of the two qubits can be in any of the four possible states $00, 10, 01, 11$.

Quantum mechanically, the basis of the Hilbert space of each of them is

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{2.55}$$

A generic state of the combined set of two bits, is

$$|\psi\rangle = c_{00}|0\rangle \otimes |0\rangle + c_{01}|0\rangle \otimes |1\rangle + c_{10}|1\rangle \otimes |0\rangle + c_{11}|1\rangle \otimes |1\rangle \tag{2.56}$$

and its vector representation is

$$\begin{bmatrix} c_{00} \\ c_{01} \\ c_{10} \\ c_{00} \end{bmatrix} \tag{2.57}$$

The measurement of the full system, obtained by sandwiching the projector $|\psi_{k_1}\rangle\langle\psi_{k_1}| \otimes |\psi_{k_2}\rangle\langle\psi_{k_2}|$ between $\langle\psi|$ and $|\psi\rangle$, can give four different outcomes, labeled by $k_1k_2 = 00, 01, 10, 11$, each with probability $|c_{k_1k_2}|^2$. The system will then be projected on the state $|\psi_{k_1}\rangle \otimes |\psi_{k_2}\rangle$. What is the probability that the first qubit equals $|0\rangle$ after such a measurement? It is $|c_{00}|^2 + |c_{01}|^2$ (the second qubit has not been measured and it can still be in both states).

Imagine now that one measures just the first qubit applying $\hat{\sigma}^z$ to it. The probability of measuring its eigenvalue 1 in this way is also $|c_{00}|^2 + |c_{01}|^2$. The resulting state is

$$|\psi\rangle = \frac{c_{00}|0\rangle \otimes |0\rangle + c_{01}|0\rangle \otimes |1\rangle}{(|c_{00}|^2 + |c_{01}|^2)^{1/2}} \tag{2.58}$$

The probability that a subsequent measurement performed on the second qubit, by now applying $\hat{\sigma}^z$ to it, with the full system already set in this state $|\psi\rangle$, yields -1 is

$$P(\text{1st meas on 1st qubit yields 1, 2nd meas on 2nd qubit yields -1}) = \frac{|c_{01}|^2}{(|c_{00}|^2 + |c_{01}|^2)^{1/2}} \tag{2.59}$$

2.2.2 Reduced density operator

The *reduced density operator* on subsystem A of a total system $A \otimes B$ is

$$\hat{\rho}_A^{\text{red}} \equiv \text{Tr}_B\, \hat{\rho}_{AB} \ . \tag{2.60}$$

Separable states

If the state describing a system made of two sub-systems A and B is separable

$$|\psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \tag{2.61}$$

the density matrix is

$$\begin{aligned} \hat{\rho}_{AB} &= |\psi_{AB}\rangle\langle\psi_{AB}| = |\psi_A\rangle \otimes |\psi_B\rangle\langle\psi_A| \otimes \langle\psi_B| \\ &= |\psi_A\rangle\langle\psi_A| \otimes |\psi_B\rangle\langle\psi_B| = \hat{\rho}_A \otimes \hat{\rho}_B \end{aligned} \tag{2.62}$$

The reduced density matrix of A in this separable state is then

$$\begin{aligned}\hat{\rho}_A^{\text{red}} &= \text{Tr}_B|\psi_{AB}\rangle\langle\psi_{AB}| = \text{Tr}_B\Big(|\psi_A\rangle\otimes|\psi_B\rangle\langle\psi_A|\otimes\langle\psi_B|\Big) = \text{Tr}_B\Big(\hat{\rho}_A\otimes\hat{\rho}_B\Big)\\ &= \hat{\rho}_A\text{Tr}\hat{\rho}_B = |\psi_A\rangle\langle\psi_A| \qquad (2.63)\end{aligned}$$

and it is the one of a pure state. Otherwise, for a non-separable state, it is not the one of a pure state.

Mixed states reduced from pure states

Mixed states arise from pure states of multiple quantum systems, if we consider only one of the systems by itself. Consider a pure non-separable state of two quantum systems A and B. In general, we can write such a state as a superposition

$$|\psi_{AB}\rangle = \sum_{nm} c_{nm}\,|a_n\rangle\otimes|b_m\rangle \qquad (2.64)$$

where $\{|a_n\rangle\}$ and $\{|b_m\rangle\}$ are basis of the Hilbert spaces of A and B. The coefficients c_{nm} are complex numbers and the normalization implies $\sum_{nm}|c_{nm}|^2 = 1$. The density operator of the full system is

$$\begin{aligned}\hat{\rho}_{AB} &= |\psi_{AB}\rangle\langle\psi_{AB}| = \sum_{nmn'm'}\underbrace{c_{nm}c^*_{n'm'}}_{c_{nmn'm'}}\Big(|a_n\rangle\otimes|b_m\rangle\Big)\Big(\langle a_{n'}|\otimes\langle b_{m'}|\Big)\\ &= \sum_{nmn'm'} c_{nm}c^*_{n'm'}\,|a_n\rangle\langle a_{n'}|\otimes|b_m\rangle\langle b_{m'}| \qquad (2.65)\end{aligned}$$

The reduced density operator, by definition, is the trace of $\hat{\rho}_{AB}$ over the states of B:

$$\begin{aligned}\hat{\rho}_A^{\text{red}} &= \sum_{m''}\langle b_{m''}|\hat{\rho}_{AB}|b_{m''}\rangle = \sum_{m''}\langle b_{m''}|\sum_{nmn'm'} c_{nm}c^*_{n'm'}\,|a_n\rangle\langle a_{n'}|\otimes|b_m\rangle\langle b_{m'}|b_{m''}\rangle\\ &= \sum_{m''}\sum_{nmn'm'} c_{nm}c^*_{n'm'}\,|a_n\rangle\langle a_{n'}|\otimes\langle b_{m''}|b_m\rangle\,\delta_{m'm''}\\ &= \sum_{nmn'm'} c_{nm}c^*_{n'm'}\,|a_n\rangle\langle a_{n'}|\,\delta_{m'm}\\ &= \sum_{nmn'} c_{nm}c^*_{n'm}\,|a_n\rangle\langle a_{n'}|\\ &= \sum_{nn'}\bar{c}_{nn'}\,|a_n\rangle\langle a_{n'}| \qquad \text{with} \qquad \bar{c}_{nn'} \equiv \sum_m c_{nm}c^*_{n'm} \qquad (2.66)\end{aligned}$$

The initial state was a pure one but after the trace over B the resulting one is not (note that the sum includes non-diagonal terms $n \neq n'$).

We recover the particular case of a separable state only if $c_{nm} = c_n c_m$,

$$\begin{aligned}\hat{\rho}_A^{\text{red}-\text{sep}} &= \sum_{mnn'} c_n c_m c^*_{n'} c^*_m\,|a_n\rangle\langle a_{n'}| = \sum_m |c_m|^2\sum_{nn'} c_n c^*_{n'}\,|a_n\rangle\langle a_{n'}|\\ &= \sum_{nn'} c_n c^*_{n'}|a_n\rangle\langle a_{n'}| = \sum_n c_n|a_n\rangle\sum_{n'} c^*_{n'}\langle a_{n'}| = |\psi_A\rangle\langle\psi_A| \qquad (2.67)\end{aligned}$$

Example

Take the pure state $|\psi\rangle_{AB} = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |1\rangle_B + |1\rangle_A \otimes |0\rangle_B)$ of a composite system AB. The density operator is

$$\begin{aligned} 2\,\hat{\rho}_{AB} = 2\,|\psi\rangle_{AB}\;{}_{AB}\langle\psi| \;&=\; |0\rangle_A\,{}_A\langle 0| \otimes |1\rangle_B\,{}_B\langle 1| + |0\rangle_A\,{}_A\langle 1| \otimes |1\rangle_B\,{}_B\langle 0| \\ &\quad + |1\rangle_A\,{}_A\langle 0| \otimes |0\rangle_B\,{}_B\langle 1| + |1\rangle_A\,{}_A\langle 1| \otimes |0\rangle_B\,{}_B\langle 0| \end{aligned} \tag{2.68}$$

Take now the trace over the B system and calculate the reduced density operator $\hat{\rho}_A^{\rm red}$. Only the first and last terms survive after sandwiching with ${}_B\langle 1|\ldots|1\rangle_B$ and ${}_B\langle 0|\ldots|0\rangle_B$, respectively. One has

$$2\,\hat{\rho}_A^{\rm red} = 2\,\mathop{\rm Tr}_A \hat{\rho}_{AB} = |0\rangle_A\,{}_A\langle 0| + |1\rangle_A\,{}_A\langle 1| \tag{2.69}$$

and this is a mixed state with $\mathrm{Tr}(\hat{\rho}_A^{\rm red})^2 < 1$:

$$4(\hat{\rho}_A^{\rm red})^2 = (|0\rangle_A\,{}_A\langle 0| + |1\rangle_A\,{}_A\langle 1|)\,(|0\rangle_A\,{}_A\langle 0| + |1\rangle_A\,{}_A\langle 1|) = (|0\rangle_A\,{}_A\langle 0| + |1\rangle_A\,{}_A\langle 1|) \tag{2.70}$$

from where

$$\mathrm{Tr}(\hat{\rho}_A^{\rm red})^2 = \frac{1}{2} \tag{2.71}$$

Purification of mixed states

A mixed state can be purified i.e. treated as a pure state of a larger system.

Take the example of a qubit. To purify a mixed state of it, we need to represent the mixed state as part of a larger Hilbert space in such a way that the mixed state is recovered as the reduced density matrix of the pure state.

Consider the mixed state of a qubit given by:

$$\rho = \begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix},$$

where $p \in [0,1]$. This is a statistical mixture of the states $|0\rangle$ and $|1\rangle$ with probabilities p and $1-p$, respectively.

A purification of ρ is a pure state $|\Psi\rangle$ in a larger Hilbert space (e.g., $\mathcal{H}_A \otimes \mathcal{H}_B$) such that the reduced density matrix of $|\Psi\rangle\langle\Psi|$ on subsystem A is ρ. We define:

$$|\Psi\rangle = \sqrt{p}\,|0\rangle_A \otimes |0\rangle_B + \sqrt{1-p}\,|1\rangle_A \otimes |1\rangle_B,$$

where $|0\rangle_A$ and $|1\rangle_A$ are the basis states of the original qubit (system A), and $|0\rangle_B$ and $|1\rangle_B$ are the basis states of an auxiliary qubit (system B) introduced for purification.

To check that this state purifies ρ, calculate the reduced density matrix of $|\Psi\rangle$ on subsystem A by tracing out B:

$$\rho_A = \mathrm{Tr}_B|\Psi\rangle\langle\Psi|$$

Explicitly:

$$\begin{aligned} |\Psi\rangle\langle\Psi| \;&=\; \left(\sqrt{p}\,|0\rangle_A \otimes |0\rangle_B + \sqrt{1-p}\,|1\rangle_A \otimes |1\rangle_B\right) \\ &\quad \times \left(\sqrt{p}\,\langle 0|_A \otimes \langle 0|_B + \sqrt{1-p}\,\langle 1|_A \otimes \langle 1|_B\right). \end{aligned} \tag{2.72}$$

Tracing out B:

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

This is exactly the original mixed state ρ.

The purification introduces an auxiliary system B *entangled* with A in such a way that the apparent mixedness of ρ on A arises from the entanglement with B. We will introduce and discuss the concept of entanglement below.

Expected values in the reduced system

Calculate now the expected value of an observable $\hat{O}_A$ on sub-system A:

$$\begin{aligned}\langle \hat{O}_A \rangle &= \operatorname*{Tr}_{AB} \hat{O}_A\, \hat{\rho}_{AB} = \sum_{nm} \left(\langle a_n| \otimes \langle b_m| \right) \hat{O}_A\, \hat{\rho}_{AB} \left(|a_n\rangle \otimes |b_m\rangle \right) \\ &= \sum_n \langle a_n| \hat{O}_A \sum_m \langle b_m|\hat{\rho}_{AB}|b_m\rangle\; |a_n\rangle = \sum_n \langle a_n| \hat{O}_A\, \hat{\rho}_A^{\text{red}}\; |a_n\rangle \\ &= \operatorname*{Tr}_{A} \left(\hat{O}_A\, \hat{\rho}_A^{\text{red}} \right) \end{aligned} \tag{2.73}$$

where we used the definition of the reduced density matrix. We have performed a partial trace, an integration over B.

Exercise 2.10 Let us see this calculation at work with an example. Take a system made of two qu-bits and suppose it is in the state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Make a measurement on the qubit A.

> To perform a measurement on qubit A using the reduced density matrix representation, we first compute the reduced density matrix for qubit A by tracing out qubit B. Then, we apply the measurement operators to this reduced density matrix.
> The corresponding density matrix for the full system is
>
> $$\rho = |\Psi\rangle\langle\Psi| = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$
>
> As the only non-zero elements are $\langle 00|\hat{\rho}|00\rangle = \langle 00|\hat{\rho}|11\rangle = \langle 11|\hat{\rho}|00\rangle = \langle 11|\hat{\rho}|11\rangle$, that is, the elements 00, 03, 30 and 33 in the 4×4 matrix above with elements ρ_{nm} and $n = 0,\ldots,3$ and $m = 0,\ldots,3$. The basis elements are ordered $n = 0 \mapsto |00\rangle, n = 1 \mapsto |10\rangle, n = 2 \mapsto |01\rangle, n = 3 \mapsto |11\rangle$.
> These matrix elements can also be labelled $\rho_{ab,a'b'}$:
>
> $$\rho = \begin{pmatrix} \rho_{00,00} & \rho_{00,01} & \rho_{00,10} & \rho_{00,11} \\ \rho_{01,00} & \rho_{01,01} & \rho_{01,10} & \rho_{01,11} \\ & & & \\ \rho_{10,00} & \rho_{10,01} & \rho_{10,10} & \rho_{10,11} \\ \rho_{11,00} & \rho_{11,01} & \rho_{11,10} & \rho_{11,11} \end{pmatrix}$$

In this representation, $a = 0$ and 1 label the first and second line block, respectively. Then, $b = 0, 1$ label the two lines within the block. Concerning the columns, $a' = 0, 1$ determine the first, second block columns, while $b' = 0, 1$ the columns within the blocks.
The reduced density matrix ρ_A is obtained by tracing out the qubit B from ρ:

$$\hat{\rho}_A^{\text{red}} = \text{Tr}_B \hat{\rho} = \langle a0|\hat{\rho}|a'0\rangle + \langle a1|\hat{\rho}|a'1\rangle = \rho_{a0,a'0} + \rho_{a1,a'1}$$

with a and a' the states of A not fixed. This yields a 2×2 matrix, with elements $\rho_{aa'}$

$$\rho_A^{\text{red}} = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = \begin{pmatrix} \rho_{00,00} + \rho_{01,01} & \rho_{00,10} + \rho_{01,11} \\ \rho_{10,00} + \rho_{11,01} & \rho_{10,10} + \rho_{11,11} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1+0 & 0+0 \\ 0+0 & 0+1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Thus, $\rho_A^{\text{red}} = \frac{1}{2}\,\mathbb{I}$, representing a maximally mixed state.
We perform a measurement in the computational basis $\{|0\rangle, |1\rangle\}$ on qubit A. The measurement operators are

$$\hat{P}_0 = |0\rangle\langle 0| \implies \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \hat{P}_1 = |1\rangle\langle 1| \implies \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

The post-measurement state for outcome 0 is:

$$\rho_A^{(0)} = \frac{P_0 \rho_A^{\text{red}} P_0}{\text{Tr}(P_0 \rho_A^{\text{red}})}.$$

Calculate the numerator

$$P_0 \rho_A^{\text{red}} P_0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

and the denominator

$$\text{Tr}(P_0 \rho_A^{\text{red}}) = \frac{1}{2}.$$

Thus:

$$\rho_A^{(0)} = \frac{\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}}{\frac{1}{2}} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

Probability of outcome 0:

$$p_0 = \text{Tr}(P_0 \rho_A) = \frac{1}{2}.$$

Similarly, for P_1:

$$P_1 \rho_A P_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Trace:

$$\text{Tr}(P_1 \rho_A) = \frac{1}{2}.$$

Thus:

$$\rho_A^{(1)} = \frac{\frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}}{\frac{1}{2}} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

and the probability of outcome 1 is

$$p_1 = \mathrm{Tr}(P_1 \rho_A) = \frac{1}{2}.$$

The probabilities for outcomes 0 and 1 are both 1/2. The post-measurement states for qubit A are $|0\rangle\langle 0|$ and $|1\rangle\langle 1|$, depending on the measurement outcome.

2.2.3 Entanglement

Two particles (or systems) form a bound system and are entangled if their quantum states are dependent on each other, regardless of the distance between them. Schrödinger coined the term entanglement (*Verschränkung*) in 1935 [19].

Entangled systems can be perfectly correlated. For example, a subatomic particle decays into an entangled pair of other particles. The decay events obey the various conservation laws, and as a result, the measurement outcomes of one daughter particle must be highly correlated with the measurement outcomes of the other daughter particle. A concrete such case is the one of a pair of entangled particles generated such that their total spin is zero. If one particle is found to have clockwise spin on a first axis, then the spin of the other particle, measured on the same axis, should be anticlockwise.

Historical remarks

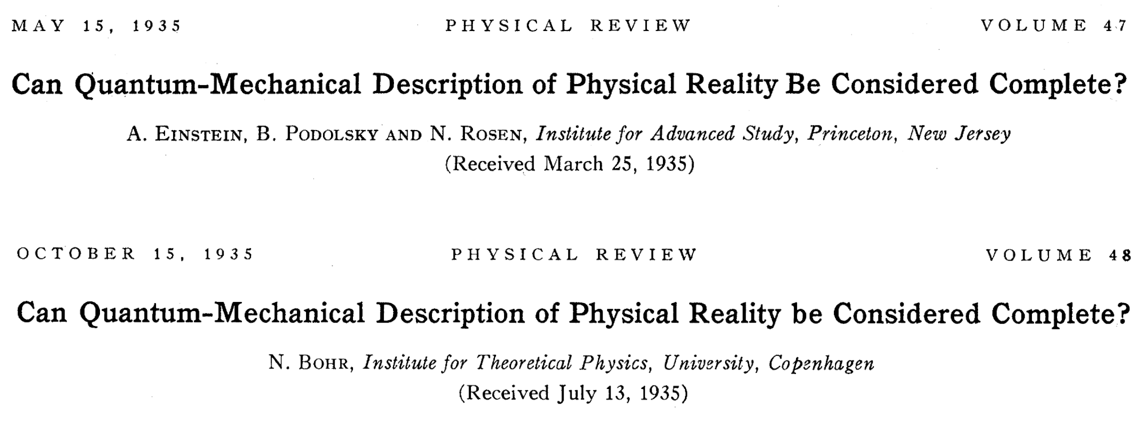
Einstein did not believe that quantum mechanics, which makes probabilistic predictions, could be an ultimate and complete theory. He thought that it had to be completed with hidden variables so far unknown that would yield a more precise description and render the description deterministic. His claims along these lines, when applied to single particle problems, were refuted by Bohr, especially during the 1927 Solvay conference.

Next he focused on the consequence of the laws of quantum mechanics for a two particle system, like the one we described with words in the previous paragraphs, and that we will explain technically in the rest of this subsection. Einstein, Podolsky and Rosen then published a paper, in which they exposed the celebrated EPR paradox [17]. This EPR paper was commented even by the New York Times.

The EPR claim was contradicted by Bohr [18] (in a paper that curiously has the same title as the EPR one, see Fig. 2.2) and Schrödinger [19]. Bohm found a simpler way of stating the EPR paradox which is the one that we will study [20, 21]. For many decades the discussion could not be given a sharp answer.

In 1964 John S. Bell proposed a measurable way of distinguishing between the predictions of quantum mechanics and the one of the hidden variable theory of EPR [22], an experiment that could rule out the existence of a local reality. Clauser was the first to perform the test, which was later improved and perfected by Aspect and Zeilinger. Finally, in the 80s a series of experiments conducted by Aspect and collaborators showed that the hidden variable theory was incorrect [23–26]. These experiments showed that there can be correlation without communication. Entangled systems should be thought of as being a single object. Details on how this works can be found in `https://scienceexchange.caltech.edu/topics/quantum-science-explained/entanglement` and will be discuss below, after introducing the Bell states. In Fig. 2.3 we display a cartoon that illustrates the problem.

It is important to recognize that the peculiarity of quantum entanglement, its perfect correlations independent of distance, motivated Feynman to propose to use it and launched the field of quantum computation [27].



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Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?

A. Einstein, B. Podolsky and N. Rosen, *Institute for Advanced Study, Princeton, New Jersey*
(Received March 25, 1935)

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Can Quantum-Mechanical Description of Physical Reality be Considered Complete?

N. Bohr, *Institute for Theoretical Physics, University, Copenhagen*
(Received July 13, 1935)

Figure 2.2: The EPR and Bohr papers.

Definition

Consider the bases $|\psi_a\rangle_A$ of $\mathcal{H}_A$ and $|\phi_b\rangle_B$ of $\mathcal{H}_B$. (In this section we use a notation in which the subsystem label is written outside the $\langle$ or $\rangle$ symbols in the bras and kets.) A generic pure state of the full system is

$$|\psi\rangle_{AB} = \sum_{ab} c_{ab} |\psi_a\rangle_A \otimes |\phi_b\rangle_B \tag{2.74}$$

A state $|\psi\rangle_{AB}$ is *entangled* if it cannot be written as a *separable* or *product* state

$$|\psi\rangle_{AB} = \Big(\sum_a c_a |\psi_a\rangle_A\Big) \otimes \Big(\sum_b c'_b |\phi_b\rangle_B\Big) = |\psi\rangle_A \otimes |\phi\rangle_B \ , \tag{2.75}$$

that is $c_{ab} \neq c_a c'_b$. An entangled system can thus be defined to be one whose quantum state cannot be factored as a product of states of its constituents.

A measurement made on either of the sub-systems collapses the state of the entire entangled system - and does so instantaneously, before any information about the measurement result could have been communicated to the other subsystem. Indeed, the independent of the distance at which the two subsystems are, made Einstein-Podolsky-Rosen doubt about the correctness of quantum mechanics, since they thought that this conclusion could imply propagation of information faster than the speed of light, and "spooky action at a distance". They proposed a hidden variable theory to solve the potential inconsistency and maintain the idea of local reality. In a hidden variable theory, measurement is actually fundamentally deterministic, but appears to be probabilistic because some degrees of freedom are not precisely known.

Similarly, the density operator of two independent (non-entangled) systems reads

$$\hat{\rho} = \hat{\rho}_A \otimes \hat{\rho}_B \tag{2.76}$$

The density operator of a mixed entangled state is a probabilistic mixture of entangled pure states:

$$\hat{\rho} = \sum_{\alpha} p_\alpha |\psi_\alpha\rangle_{AB}\ {}_{AB}\langle\psi_\alpha| \tag{2.77}$$

with $|\psi_\alpha\rangle_{AB}$ are entangled states and $0 \leq p_\alpha \leq 1$ and $\sum_\alpha p_\alpha = 1$.

For a pure entangled state, the reduced density matrices $\hat{\rho}_A^{\text{red}}$ and $\hat{\rho}_B^{\text{red}}$ are the ones of mixed states, indicating entanglement.

A density operator for a composite system is separable if and only if it can be written in the form

$$\hat{\rho} = \sum_{\alpha} p_\alpha\ \rho_\alpha^A \otimes \rho_\alpha^B \tag{2.78}$$

Unfortunately, given an arbitrary mixed density operator, it is difficult to tell if it corresponds to an entangled state (this turns out to be an NP-hard problem).

Two entangled systems do not have local states that can be treated independently.

Symbol	Name or property
(S_A, S_B)	Composite system made of two parts
$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$	Hilbert space of composite system
$\{\lvert\psi_n^A\rangle \otimes \lvert\psi_m^B\rangle\}$	Orthonormal basis of $\mathcal{H}$
$\lvert\psi\rangle = \sum_{nm} c_{nm} \lvert\psi_n^A\rangle \otimes \lvert\psi_m^B\rangle$ $\neq \lvert\psi^A\rangle \otimes \lvert\psi^B\rangle$	State in $\mathcal{H}$
$\hat{\rho}_{\text{pure}} = \lvert\psi\rangle\langle\psi\rvert \neq \hat{\rho}_A \otimes \hat{\rho}_B$	Pure state of composite system
$\hat{Q}_A \otimes \mathbb{I}_B$	Operator in A
$\mathbb{I}_B \otimes \hat{Q}_B$	Operator in B

The result of a measurement of a single qubit in a Bell state is indeterminate, but upon measuring the first qubit in the z-basis, the result of measuring the second qubit is guaranteed to yield the same value (for the Φ Bell states) or the opposite value (for the Ψ Bell states). This implies that the measurement outcomes are correlated.

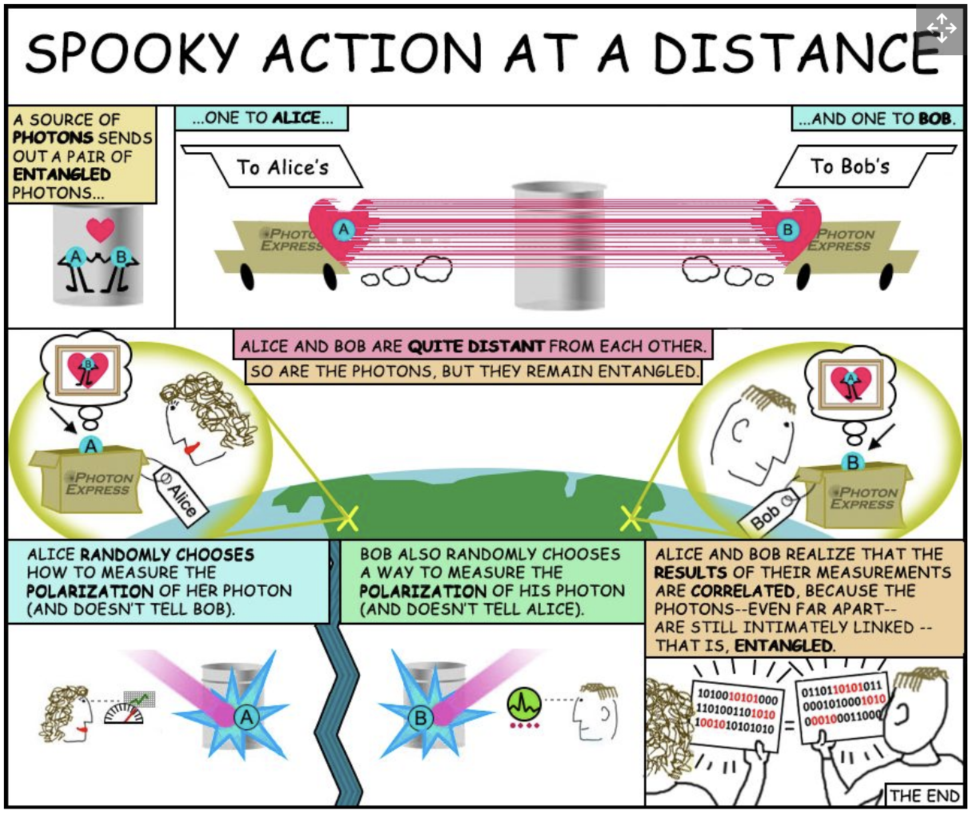

Figure 2.3: Image credit NASA/JPL-Caltech

The Bell states are pure state, but the reduced density operator of the first qubit is a mixed state. The mixed state implies that not all the information on this first qubit is known.

Entanglement is broken when the entangled particles decohere through interaction with the environment; for example, when a measurement is made.

The Bell states

The Bell's states or EPR pairs are entangled quantum states of two qubits. Use the basis $\{|0\rangle, |1\rangle\}$ of eigenvectors with eigenvalues 1 and -1 of the $\hat{\sigma}^z$ operator for each of the two qubits. The four Bell states of a system composed of two qubits are

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle\otimes|0\rangle + |1\rangle\otimes|1\rangle\right) \tag{2.79}$$

$$|\Phi^-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle\otimes|0\rangle - |1\rangle\otimes|1\rangle\right) \tag{2.80}$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle\otimes|1\rangle + |1\rangle\otimes|0\rangle\right) \tag{2.81}$$

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle\otimes|1\rangle - |1\rangle\otimes|0\rangle\right) \tag{2.82}$$

They are normalized basis vectors, $\langle\Phi|\Phi\rangle = 1$ for all of them.

Exercise 2.10 Prove that the Bell states are normalized.

> Take, for example, $|\Phi^+\rangle$ and calculate its inner product with itself. It reads $\langle\Phi^+|\Phi^+\rangle = \frac{1}{2}\left(\langle 0|0\rangle\langle 0|0\rangle + \cancel{\langle 0|1\rangle\langle 0|1\rangle} + \cancel{\langle 1|0\rangle\langle 0|1\rangle} + \langle 1|1\rangle\langle 1|1\rangle\right) = 1$. Similarly, one proves the normalization of the other three Bell states.

Exercise 2.11 Prove that the Bell states are entangled.

> To prove that they are entangled one has to show that they cannot be written as $|\psi_A\rangle\otimes|\psi_B\rangle$. Let us work with $|\Phi^+\rangle$ and assume that it can be written in this separable way:
>
> $$\begin{aligned} |\Phi^+\rangle &= \frac{1}{\sqrt{2}}\Big(|0\rangle\otimes|0\rangle + |1\rangle\otimes|1\rangle\Big) = \Big(a\,|0\rangle_A + b\,|1\rangle_A\Big)\otimes\Big(c\,|0\rangle_B + d\,|1\rangle_B\Big) \\ &= ac\,|0\rangle_A\otimes|0\rangle_B + bc\,|1\rangle_A\otimes|0\rangle_B + bc\,|1\rangle_A\otimes|0\rangle_B + bd\,|1\rangle_B\otimes|1\rangle_B \end{aligned} \tag{2.83}$$
>
> From here we need to set $ad = bc = 0$, $ac \neq 0$ and $bd \neq 0$. There is no solution to these conditions.

Exercise 2.12 Prove that the Bell states cannot be factorized as in Eq. (2.75) and that therefore they are entangled.

> Take, for example, $|\Phi^+\rangle$ and try to equate it to the factorized form:
>
> $$\frac{1}{\sqrt{2}}\Big(|0\rangle\otimes|0\rangle + |1\rangle\otimes|1\rangle\Big) = c_0c_0'|0\rangle\otimes|0\rangle + c_0c_1'|0\rangle\otimes|1\rangle + c_1c_0|1\rangle\otimes|0\rangle + c_1c_1'|1\rangle\otimes|1\rangle\ . \tag{2.84}$$
>
> The conditions are
>
> $$\sqrt{2}c_0c_0' = 1 \qquad \sqrt{2}c_0c_1' = 0 \qquad \sqrt{2}c_1c_0' = 0 \qquad \sqrt{2}c_1c_1' = 1\ . \tag{2.85}$$
>
> The first and last imply that $c_0 \neq 0$, $c_0' \neq 0$, $c_1 \neq 0$ and $c_1' \neq 0$. Therefore, all coefficients must be different from cero and the intermediate conditions cannot be satisfied. The proofs for the other three Bell states follow the same lines of reasoning.

Exercise 2.13 Show that the Bell states are pure states satisfying $(|\Phi^\pm\rangle\langle\Phi^\pm|)^2 = |\Phi^\pm\rangle\langle\Phi^\pm|$.

Bell states are either symmetric or antisymmetric with respect to the exchange of the two subsystems. The exchange of the two subsystems corresponds to swapping the positions of the first and second qubits in each Bell state. Mathematically, this can be viewed as applying the swap operator, which interchanges the states of the two qubits. The $|\Phi^+\rangle$ and $|\Psi^+\rangle$ states are symmetric. $|\Phi^-\rangle$ is also symmetric with respect to the exchange of the two qubits while $|\Psi^+\rangle$ is antisymmetric.

Exercise 2.14 Prove that $|\Phi^-\rangle$ is equal to $1/\sqrt{2}\,(|+-\rangle + |-+\rangle)$ and use this identity to prove its symmetry with respect to the exchange of the two qubits.

In $|\Phi^\pm\rangle$ the two particles always have the same spin (both up or both down) while in $|\Psi^\pm\rangle$ the two particles always have opposite spins (one up and one down). This is important for the use of Bell states to disprove the EPR arguments.

Exercise 2.15 Prove that in $|\Phi^\pm\rangle$ the two particles should have parallel spins in the z direction, while in $|\Psi^\pm\rangle$ they must have antiparallel spin in the z direction.

A way to prove this statement is to calculate the probabilities of the varios events. Take $|\Phi^\pm\rangle$, we have

$$P_{00} = |\Big(\langle 0| \otimes \langle 0|\Big)|\Phi^\pm\rangle|^2 = P_{11} = |\Big(\langle 1| \otimes \langle 1|\Big)|\Phi^\pm\rangle|^2 = \frac{1}{2} \tag{2.86}$$

while

$$P_{01} = |\Big(\langle 0| \otimes \langle 1|\Big)|\Phi^\pm\rangle|^2 = P_{10} = |\Big(\langle 1| \otimes \langle 0|\Big)|\Phi^\pm\rangle|^2 = 0 \tag{2.87}$$

Instead, the states $\Phi^\pm\rangle$ have opposite spins:

$$P_{00} = |\Big(\langle 0| \otimes \langle 0|\Big)|\Psi^\pm\rangle|^2 = P_{11} = |\Big(\langle 1| \otimes \langle 1|\Big)|\Psi^\pm\rangle|^2 = 0 \tag{2.88}$$

while

$$P_{01} = |\Big(\langle 0| \otimes \langle 1|\Big)|\Psi^\pm\rangle|^2 = P_{10} = |\Big(\langle 1| \otimes \langle 0|\Big)|\Psi^\pm\rangle|^2 = \frac{1}{2} \tag{2.89}$$

Exercise 2.16 Prove that the four Bell states are eigenstates of the operators $\hat{\sigma}^z \otimes \hat{\sigma}^a$ with $a = x, y, z$.

Take $|\Phi^+\rangle$ and apply $\hat{\sigma}^z \otimes \hat{\sigma}^z$:

$$\begin{aligned}\hat{\sigma}^z \otimes \hat{\sigma}^z |\Phi^+\rangle &= \hat{\sigma}^z \otimes \hat{\sigma}^z \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\right) = \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |0\rangle + (-1)|1\rangle \otimes (-1)|1\rangle\right) \\ &= \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\right) = |\Phi^+\rangle \end{aligned} \tag{2.90}$$

Take now $|\Phi^-\rangle$ and also apply $\hat{\sigma}^z \otimes \hat{\sigma}^z$:

$$\begin{aligned}\hat{\sigma}^z \otimes \hat{\sigma}^z |\Phi^-\rangle &= \hat{\sigma}^z \otimes \hat{\sigma}^z \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |0\rangle - |1\rangle \otimes |1\rangle\right) = \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |0\rangle - (-1)|1\rangle \otimes (-1)|1\rangle\right) \\ &= \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |0\rangle - |1\rangle \otimes |1\rangle\right) = |\Phi^-\rangle \end{aligned} \tag{2.91}$$

Consider now $|\Psi^\pm\rangle$ and $\hat{\sigma}^z \otimes \hat{\sigma}^z$:

$$\begin{aligned}\hat{\sigma}^z \otimes \hat{\sigma}^z |\Psi^\pm\rangle &= \hat{\sigma}^z \otimes \hat{\sigma}^z \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |1\rangle \pm |1\rangle \otimes |0\rangle\right) = \frac{1}{\sqrt{2}}\left((-1)|0\rangle \otimes |1\rangle \pm (-1)|1\rangle \otimes |0\rangle\right) \\ &= -\frac{1}{\sqrt{2}}\left(|0\rangle \otimes |1\rangle \pm (-1)|1\rangle \otimes |0\rangle\right) = -|\Psi^\pm\rangle \end{aligned} \tag{2.92}$$

The other cases can be treated similarly.

Exercise 2.17 Calculate the expected value of $\hat{\sigma}^z \otimes \mathbb{I}$ and $\hat{\sigma}^z \otimes \hat{\sigma}^z$ in the four Bell states.

Let us first consider

$$\begin{aligned}\langle\Phi^\pm|\hat{\sigma}^z \otimes \mathbb{I}|\Phi^\pm\rangle &= \frac{1}{2}\left(\langle 0|\otimes\langle 0| \pm \langle 1|\otimes\langle 1|\right)\hat{\sigma}^z \otimes \mathbb{I}\left(|0\rangle\otimes|0\rangle \pm |1\rangle\otimes|1\rangle\right)\\ &= \frac{1}{2}\left(\langle 0|\otimes\langle 0| \pm \langle 1|\otimes\langle 1|\right)\left(|0\rangle\otimes|0\rangle \pm (-1)|1\rangle\otimes|1\rangle\right)\\ &= \frac{1}{2}(1-1) = 0 \qquad (2.93)\end{aligned}$$

Next,

$$\begin{aligned}\langle\Psi^\pm|\hat{\sigma}^z \otimes \mathbb{I}|\Psi^\pm\rangle &= \frac{1}{2}\left(\langle 0|\otimes\langle 1| \pm \langle 1|\otimes\langle 0|\right)\hat{\sigma}^z \otimes \mathbb{I}\left(|0\rangle\otimes\langle 1| \pm |1\rangle\otimes|0\rangle\right)\\ &= \frac{1}{2}\left(\langle 0|\otimes\langle 1| \pm \langle 1|\otimes\langle 0|\right)\left(|0\rangle\otimes|1\rangle \pm (-1)|1\rangle\otimes|0\rangle\right)\\ &= \frac{1}{2}(1-1) = 0 \qquad (2.94)\end{aligned}$$

Now, let us calculate

$$\begin{aligned}\langle\Phi^\pm|\hat{\sigma}^z \otimes \hat{\sigma}^z|\Phi^\pm\rangle &= \frac{1}{2}\left(\langle 0|\otimes\langle 0| \pm \langle 1|\otimes\langle 1|\right)\hat{\sigma}^z \otimes \hat{\sigma}^z\left(|0\rangle\otimes|0\rangle \pm |1\rangle\otimes|1\rangle\right)\\ &= \frac{1}{2}\left(\langle 0|\otimes\langle 0| \pm \langle 1|\otimes\langle 1|\right)\left(|0\rangle\otimes|0\rangle \pm |1\rangle\otimes|1\rangle\right)\\ &= \frac{1}{2}(1+1) = 1 \qquad (2.95)\end{aligned}$$

Similarly,

$$\begin{aligned}\langle\Psi^\pm|\hat{\sigma}^z \otimes \hat{\sigma}^z|\Psi^\pm\rangle &= \frac{1}{2}\left(\langle 0|\otimes\langle 1| \pm \langle 1|\otimes\langle 0|\right)\hat{\sigma}^z \otimes \hat{\sigma}^z\left(|0\rangle\otimes|1\rangle \pm |1\rangle\otimes|0\rangle\right)\\ &= \frac{1}{2}\left(\langle 0|\otimes\langle 1| \pm \langle 1|\otimes\langle 0|\right)\left((-1)|0\rangle\otimes|1\rangle \pm (-1)|1\rangle\otimes|0\rangle\right)\\ &= (-1)\frac{1}{2}(1+1) = -1 \qquad (2.96)\end{aligned}$$

The other cases are $\langle\Phi^\pm|\hat{\sigma}^x\otimes\hat{\sigma}^x|\Phi^\pm\rangle = \pm 1$, $\langle\Psi^\pm|\hat{\sigma}^x\otimes\hat{\sigma}^x|\Psi^\pm\rangle = \pm 1$, $\langle\Phi^\pm|\hat{\sigma}^y\otimes\hat{\sigma}^y|\Phi^\pm\rangle = \mp 1$, $\langle\Psi^\pm|\hat{\sigma}^y\otimes\hat{\sigma}^y|\Psi^\pm\rangle = \mp 1$. Individually the particles appear to behave like classical mixtures, but collectively they exhibit quantum correlations.

Exercise 2.18 Calculate the density operators $|\Phi^\pm\rangle\langle\Phi^\pm|$ and $|\Psi^\pm\rangle\langle\Psi^\pm|$. The existence of off-diagonal elements in these matrix operators is the quantum signature of an entangled superposition.

The special feature of Bell states is that when one of the two qubits is measured, it takes on a specific value, and the second qubit is forced to also take on instantaneously a specific value, as the state collapses. Because of the entanglement, measurement of one qubit will "collapse" the other qubit to a state whose measurement will yield one of two possible values. Because of this, Bell states are *maximally entangled* or *fully correlated*. This means that when one traces over one subsystem, the reduced density matrix is proportional to the identity.

Exercise 2.19 Calculate the reduced density matrices of the four Bell states and show that they are maximally entangled.

Proof. Take the Bell state $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B)$ as an example. Its density operator is $\hat{\rho} = \hat{\rho}_{AB} = |\Phi^+\rangle\langle\Phi^+|$. The reduced density operator of the first qubit (A) is $\rho^{\text{red}}_{1\text{st}} = \text{Tr}_{2\text{nd}}\hat{\rho} = \text{Tr}_B\hat{\rho}_{AB}$ which reads

$$\begin{aligned} \text{Tr}_B\hat{\rho}_{AB} = {}& {}_B\langle 0|\left[\tfrac{1}{\sqrt{2}}(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B)\tfrac{1}{\sqrt{2}}({}_A\langle 0| \otimes {}_B\langle 0| + {}_A\langle 1| \otimes {}_B\langle 1|)\right]|0\rangle_B \\ & + {}_B\langle 1|\left[\tfrac{1}{\sqrt{2}}(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B)\tfrac{1}{\sqrt{2}}({}_A\langle 0| \otimes {}_B\langle 0| + {}_A\langle 1| \otimes {}_B\langle 1|)\right]|1\rangle_B \\ = {}& \tfrac{1}{2}(|0\rangle_A \otimes {}_B\langle 0|0\rangle_B)({}_A\langle 0| \otimes {}_B\langle 0|0\rangle_B) + \tfrac{1}{2}(|1\rangle_A \otimes {}_B\langle 1|1\rangle_B)({}_A\langle 1| \otimes {}_B\langle 1|1\rangle_B) \\ = {}& \tfrac{1}{2}|0\rangle_{A\,A}\langle 0| + \tfrac{1}{2}|1\rangle_{A\,A}\langle 1| \end{aligned} \tag{2.97}$$

If we now calculate the elements of the operator matrix in the basis $|0\rangle$ and $|1\rangle$:

$$\rho = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix} = \frac{1}{2}\,\mathbb{I} \tag{2.98}$$

which is proportional to the identity indicating maximal entanglement.

Example

Take the first Bell state $|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\right)$. Measure the first qu-bit and say that the result of the measurement is 0. The state Φ^+ is then collapsed on the first term, $|\Phi^+\rangle \mapsto |0\rangle \otimes |0\rangle$ and the second qu-bit is therefore forced to be in the state $|0\rangle$, it has no more freedom to be in the other state. The same argument applies to the other three Bell states.

But for an uncorrelated (unentangled) pair, measuring the spin of second particle tells us nothing about the first one and just leaves it in its original superposition.

Note that in the examples above $|0\rangle$ and $|1\rangle$ are orthogonal. Let us consider a case in which the quantum states of the two particles are each a superposition of different basis states $|\psi_i\rangle$ and $|\phi_i\rangle$, for the first and second particle, respectively, that do not necessarily form orthonormal sets like spin states. For example, consider the general entangled Bell state defined as

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1 \otimes |\phi_1\rangle + |\psi_2\rangle \otimes |\phi_2\rangle\right) \tag{2.99}$$

Measure now an observable $\hat{B}$ on the second particle. If $|\phi_1\rangle$ and $|\phi_2\rangle$ are orthogonal eigenstates of $\hat{B}$, then the measurement will yield $|\phi_1\rangle$ or $|\phi_2\rangle$ and the state of the first particle will be fully determined after the measurement. This is the case discussed above using the spin example.

However, if $|\phi_1\rangle$ and $|\phi_2\rangle$ are not orthogonal, that is they have non-zero overlap, then we will only get partial information on the first particle after a measurement on the second one. Take as an extreme case the one in which $|\phi_1\rangle$ and $|\phi_2\rangle$ are the same state, then

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1 + |\psi_2\rangle\right) \otimes |\phi_1\rangle \tag{2.100}$$

and by measuring on the second particle we do not learn anything about the first one. Thus the more the elements of the superposition of particle 2 overlap, the less distinguishable they are and the less information we get about particle 1 by measuring particle 2.

Entanglement is a basis-independent result of superposition.

2.2.4 The EPR paradox & Bell's inqualities

The EPR paradox

Consider *Bohm's formulation* of the EPR paradox in which the systems A and B are two spin-half particles in two different regions of space, with their spin degrees of freedom initially in a *spin singlet state*.

- Let an atom with zero spin decay in two photons. Conservation of spin (polarisation of the photons) implies that the spins of the two photons have to be opposite.
- Let these photons separate very very very far away.
- Recall that to measure a spin one has to first choose a direction in three dimensional space and then measure the orientation of the spin along it. Say, if one chooses the z direction, then the measurement of the spin can yield up or down along this direction. If one chooses the x direction, the result of the measurement of the spin can be left or right along this direction. Similarly for the y direction.
- Let Alice measure the spin of the first photon along the z direction. The result will be up with probability $1/2$ or down with probability $1/2$. If, instead, she measures the spin in the x direction, she will get right or left also with probability a half. The same for the y component of the spin.
- Imagine that Alice does not measure but it is Bob who measures. Then he will get similar results as Alice's, that is, up or down in z with $p = 1/2$, right or left in x with $p = 1/2$, and similarly for y.
- Now, if Alice and Bob make their measurements simultaneously, forcefully, Bob has to measure the opposite value of the spin of his photon than the one that Alice gets. Thus, if they measure in the z direction, if Alice measures up (with $p = 1/2$), then Bob measures down with $p = 1$! Instead, if Alice measures down (with $p = 1/2$), Bob measures up with $p = 1$.
- Note that the notion of probabilities makes full sense within an experiment, where these measurements are performed a very large number of times.
- Whatever the direction in which they measure, their results are perfectly correlated.
- Consider that the measurements of Alice and Bob and made so close in time so that not even light can travel between one photon and the other during the time lag. Then, the fact that the two measurements necessarily yield the opposite result could be interpreted as transfer of information faster than light, and this would violate a principle of special relativity. See the sketch in Fig. 2.3.
- EPR claimed that this could not be correct. They argued that the states of the two spins must have been imprinted in the photons when they were created, and that they were attached to them in the form of hidden variables. This is contrary to the Copenhagen interpretation of quantum mechanics which claims that the state of the spin "is not determined" before it is measured.

Another way of presenting the paradox, for the same system of two spins, is the following:

- Suppose σ^z is measured for A. The result allows one to predict σ^z for particle b, since $\sigma^z_B = -\hat{\sigma}^z_A$.
- In the same way, the outcome of a measurement of $\hat{\sigma}^x_A$ allows one to predict $\hat{\sigma}^x_B$ since $\sigma^x_B = -\hat{\sigma}^x_A$. Note, however, there is no way to measure $\hat{\sigma}^z_B$ and $\hat{\sigma}^x_B$ simultaneously on the same system, and therefore no situation in this event and the previous one can be applied to the same particle.
- B is isolated from A, therefore it cannot be affected by measurements carried out on A.
- Consequently, one may conclude that B must simultaneously possess values for both σ^x_B and σ^z_B, namely the values revealed by the corresponding measurements on A, either of which could be carried out in any given experimental run.
- But this contradicts the basic principles of quantum theory, since in the two-dimensional spin space one cannot simultaneously assign values of both σ^x_B and σ^z_B.

You can look at the video `https://www.youtube.com/watch?v=6p2jjLB4GNA` where this is explained in an online lecture by J. Preskill (Caltech).

Bell's inequalities

In 1964 J. Bell figured out a way to distinguish between the hidden variables idea put forward by EPR and the consequences of Bohr's interpretation of quantum mechanics. The idea is to take the point of view of the hidden variables proposal, argue in terms of standard probabilities, and find an inequality that, if violated by the experiments, would disprove this approach.

The spins can be measured in three directions, say x, y and z. If Alice could measure along the three directions simultaneously, although quantum mechanically she cannot since $\hat{\sigma}^a_A$ and $\hat{\sigma}^b_A$ do not commute for $a \neq b$, she would obtain the eight combinations reported in Table 1 each with probability 1/8.

Imagine that Alice measures along x and Bob measures along y. This is allowed quantum mechanically since the measurements are performed on different photons and $\hat{\sigma}^a_A$ and $\hat{\sigma}^b_B$ do commute for $a \neq b$. Since we know that the result for Alice should be the opposite from the result for Bob (since the two photons decayed from a spin-less atom), the outcome of Alice for the y measurement, if she were doing it, should be the opposite of the result obtained by Bob. Thus, one can ask, what is the probability that, for Alice, the two measurements (along x and y) would be the same. This can occur because the two Alice's measurements are $+$ (Alice $+$ and Bob $-$) or the two are $-$ (Alice $-$ and Bob $+$). z remains free and both possibilities have to be taken into account. So, reasoning classically, with standard probability arguments, one has

$$P_{\text{same}}(x, y) = P(+,+,+) + P(+,+,-) + P(-,-,+) + P(-,-,-) \; . \tag{2.101}$$

E	x	y	z
E_1	$+$	$+$	$+$
E_2	$+$	$+$	$-$
E_3	$+$	$-$	$+$
E_4	$+$	$-$	$-$
E_5	$-$	$+$	$+$
E_6	$-$	$+$	$-$
E_7	$-$	$-$	$+$
E_8	$-$	$-$	$-$

Table 1: The eight possible outcomes of Alice's measurements labeled events 1 to 8. The outcomes of Bob's simultaneous measurements would be the opposite of these.

One can repeat this procedure for the directions y and z and get

$$P_{\text{same}}(y,z) = P(+,+,+) + P(-,+,+) + P(+,-,-) + P(-,-,-)\ . \tag{2.102}$$

Finally, for x and z

$$P_{\text{same}}(x,z) = P(+,+,+) + P(x,-,+) + P(-,+,-) + P(-,-,-)\ . \tag{2.103}$$

These probabilities concern Alice. Then, the sum of these probabilities yields:

$$P_{\text{same}}(x,y) + P_{\text{same}}(y,z) + P_{\text{same}}(x,z) = 1 + 2P(+,+,+) + 2P(-,-,-) \geq 1 \tag{2.104}$$

because a sum over all eight cases appears and it equals one. This is one of Bell's inequalities. It confirms that if there are three classical objects (coins) with two possibilities (head or tail), and you throw them, at least two of them have to be equal: the left-hand-side is larger than 1 since it is a sure classical event.

Quantum mechanical violation of Bell's inequality

Let us now see how these probabilities take different values and Bell's inequality is violated in quantum mechanics.

We have seen in an exercise above that the states $|\Psi^{\pm}\rangle$ are such that the spins of the two particles should be opposite. We proved it for the z direction but the proof can be extended to any other direction.

We will need to calculate probabilities of spin measurements, that is, sandwiches of functions of the spin, within those states. We note that while $|\Psi^-\rangle$ is the only Bell state annihilated by $\left(\hat{\sigma}^c \otimes \mathbb{I} + \mathbb{I} \otimes \hat{\sigma}^c\right)|\Psi^-\rangle = 0 \ \ c = x, y, z$, for all Bell states

$$\langle\Phi^{\pm}|\left(\hat{\sigma}^c \otimes \mathbb{I} + \mathbb{I} \otimes \hat{\sigma}^c\right)|\Phi^{\pm}\rangle = \langle\Psi^{\pm}|\left(\hat{\sigma}^c \otimes \mathbb{I} + \mathbb{I} \otimes \hat{\sigma}^c\right)|\Psi^{\pm}\rangle = 0 \tag{2.105}$$

Exercise 2.20 Prove that $\langle\Phi^{\pm}|\hat{\sigma}^c \otimes \mathbb{I}|\Phi^{\pm}\rangle = 0$ for all c.

$$\begin{aligned}
2\langle\Phi^{\pm}|\hat{\sigma}^{z}\otimes\mathbb{I}|\Phi^{\pm}\rangle &= (\langle 0|\otimes\langle 0|\pm\langle 1|\otimes\langle 1|)\,\hat{\sigma}_{z}\otimes\mathbb{I}\,(|0\rangle\otimes|0\rangle\pm|1\rangle\otimes|1\rangle) \\
&= (\langle 0|\otimes\langle 0|\pm\langle 1|\otimes\langle 1|)\;(|0\rangle\otimes|0\rangle\pm(-1)|1\rangle\otimes|1\rangle) \\
&= 1-1=0 \qquad (2.106) \\
2\langle\Phi^{\pm}|\hat{\sigma}^{x}\otimes\mathbb{I}|\Phi^{\pm}\rangle &= (\langle 0|\otimes\langle 0|\pm\langle 1|\otimes\langle 1|)\,\hat{\sigma}_{x}\otimes\mathbb{I}\,(|0\rangle\otimes|0\rangle\pm|1\rangle\otimes|1\rangle) \\
&= (\langle 0|\otimes\langle 0|\pm\langle 1|\otimes\langle 1|)\;(|1\rangle\otimes|0\rangle\pm|0\rangle\otimes|1\rangle) \\
&= 0 \qquad (2.107) \\
2\langle\Phi^{\pm}|\hat{\sigma}^{y}\otimes\mathbb{I}|\Phi^{\pm}\rangle &= (\langle 0|\otimes\langle 0|\pm\langle 1|\otimes\langle 1|)\,\hat{\sigma}_{y}\otimes\mathbb{I}\,(|0\rangle\otimes|0\rangle\pm|1\rangle\otimes|1\rangle) \\
&= (\langle 0|\otimes\langle 0|\pm\langle 1|\otimes\langle 1|)\;(i|1\rangle\otimes|0\rangle\pm(-i)|0\rangle\otimes|1\rangle) \\
&= 0 \qquad (2.108)
\end{aligned}$$

Exercise 2.21 Show Eqs. (2.105)

Having proved the result of the previous exercise, this proof is immediate. We can however do it in an slightly different way.

$$\begin{aligned}
(\hat{\sigma}^{z}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{\sigma}^{z})\,|\Phi^{\pm}\rangle &= \tfrac{1}{\sqrt{2}}\,(\hat{\sigma}^{z}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{\sigma}^{z})\,(|0\rangle\otimes|0\rangle\pm|1\rangle\otimes|1\rangle) \\
&= \tfrac{1}{\sqrt{2}}\,(|0\rangle\otimes|0\rangle\mp|1\rangle\otimes|1\rangle+|0\rangle\otimes|0\rangle\mp|1\rangle\otimes|1\rangle)=\sqrt{2}\;|\Phi^{\mp}\rangle \\
(\hat{\sigma}^{z}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{\sigma}^{z})\,|\Psi^{\pm}\rangle &= \tfrac{1}{\sqrt{2}}\,(\hat{\sigma}^{z}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{\sigma}^{z})\,(|0\rangle\otimes|1\rangle\pm|1\rangle\otimes|0\rangle) \\
&= \tfrac{1}{\sqrt{2}}\,(|0\rangle\otimes|1\rangle\mp|1\rangle\otimes|0\rangle-|0\rangle\otimes|1\rangle\pm|1\rangle\otimes|0\rangle)=0 \\
(\hat{\sigma}^{x}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{\sigma}^{x})\,|\Psi^{\pm}\rangle &= \tfrac{1}{\sqrt{2}}\,(\hat{\sigma}^{x}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{\sigma}^{x})\,(|0\rangle\otimes|1\rangle\pm|1\rangle\otimes|0\rangle) \\
&= \tfrac{1}{\sqrt{2}}\,(|1\rangle\otimes|1\rangle\pm|0\rangle\otimes|0\rangle)+(|0\rangle\otimes|0\rangle\pm|1\rangle\otimes|1\rangle) \\
&= \begin{cases}\sqrt{2}\;|\Phi^{+}\rangle \\ 0\end{cases} \\
(\hat{\sigma}^{y}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{\sigma}^{y})\,|\Psi^{\pm}\rangle &= \tfrac{1}{\sqrt{2}}\,(\hat{\sigma}^{y}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{\sigma}^{y})\,(|0\rangle\otimes|1\rangle\pm|1\rangle\otimes|0\rangle) \\
&= \tfrac{\mathrm{i}}{\sqrt{2}}\,(|1\rangle\otimes|1\rangle\mp|0\rangle\otimes|0\rangle)+(-|0\rangle\otimes|0\rangle\pm|1\rangle\otimes|1\rangle) \\
&= \begin{cases}-\sqrt{2}\,\mathrm{i}\;|\Phi^{-}\rangle \\ 0\end{cases} \qquad (2.109)
\end{aligned}$$

where we used $\hat{\sigma}^{x}|0\rangle=|1\rangle$, $\hat{\sigma}^{x}|1\rangle=|0\rangle$, $\hat{\sigma}^{y}|0\rangle=\mathrm{i}|1\rangle$, and $\hat{\sigma}^{y}|1\rangle=-\mathrm{i}|0\rangle$. Then $\langle\Phi^{\pm}|\hat{\sigma}^{c}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{\sigma}^{c}|\Phi^{\pm}\rangle=0=\langle\Psi^{\pm}|\hat{\sigma}^{c}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{\sigma}^{c}|\Psi^{\pm}\rangle$.

Let us focus on the state $|\Psi^{-}\rangle$ which has opposite spins for the two subsystems, and for which we can write the first identity below. For any two directions $\vec{m}$ and $\vec{n}$ one has

$$\begin{aligned}
\langle\Psi^{-}|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|\Psi^{-}\rangle &= -\langle\Psi^{-}|\hat{\vec{\sigma}}\cdot\vec{m}\;\hat{\vec{\sigma}}\cdot\vec{n}\otimes\mathbb{I}|\Psi^{-}\rangle=-\langle\Psi^{-}|\hat{\sigma}^{a}m^{a}\;\hat{\sigma}^{b}n^{b}\otimes\mathbb{I}|\Phi^{-}\rangle \\
&= -m^{a}n^{b}\;\langle\Psi^{-}|(\delta_{ab}\mathbb{I}+\mathrm{i}\epsilon_{abc}\hat{\sigma}_{c})\otimes\mathbb{I}|\Psi^{-}\rangle \\
&= -m^{a}n^{a}\;\langle\Psi^{-}|\Psi^{-}\rangle=-\vec{m}\cdot\vec{n}=-\cos\theta \qquad (2.110)
\end{aligned}$$

where we used $\hat{\sigma}^{a}\hat{\sigma}^{b}=i\sum_{c}\epsilon_{abc}\hat{\sigma}^{c}$ for $a\neq b$ and $(\hat{\sigma}^{a})^{2}=\mathbb{I}$ for each a and the fact that $\langle\Phi^{\pm}|\hat{\sigma}_{c}\otimes\mathbb{I}|\Phi^{\pm}\rangle=0$ for all c. The same applies to $|\Psi^{\pm}\rangle$. Summation over repeated indices is assumed in the equation above. The angle between the unit vectors $\vec{m}$ and $\vec{n}$ was called θ in the last equality. Thus, the measurement outcomes are always perfectly anti-correlated when we measure both spins along the same axis (since $\vec{m}\cdot\vec{n} = 1$ and $\cos\theta = 1$ in this case). We have also obtained a more general result that applies when the two axes are different.

Exercise 2.22 Prove $\hat{\sigma}^a\hat{\sigma}^b = \mathrm{i}\epsilon_{abc}\hat{\sigma}^c$ for $a \neq b$ with ϵ_{abc} the Levi Civita tensor (that is $\epsilon_{abc} = 1$ if abc are all different and (cyclically) ordered (with $x < y < z$), $\epsilon_{abc} = -1$ if abc are all different and not (cyclically) ordered), and $\epsilon_{abc} = 0$ if two indices are equal.

Exercise 2.23 Prove $\langle\Psi^-|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|\Psi^-\rangle = -\langle\Psi^-|\hat{\vec{\sigma}}\cdot\vec{m}\;\hat{\vec{\sigma}}\cdot\vec{n}\otimes\mathbb{I}|\Psi^-\rangle$ for all $\vec{m}$ and $\vec{n}$.

The Bell states we focus on are $|\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle\otimes|1\rangle \pm |1\rangle\otimes|0\rangle)$. The operators applied are $\hat{\vec{\sigma}}\cdot\vec{m} = m_x\hat{\sigma}_x + m_y\hat{\sigma}_y + m_z\hat{\sigma}_z$, where $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ are Pauli matrices, and $\vec{m} = (m_x, m_y, m_z)$ is a unit vector, and similarly for $\hat{\vec{\sigma}}\cdot\vec{n}$. The tensor product $\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}$ means that the first qubit is measured along $\vec{m}$, and the second qubit along $\vec{n}$, while the other tensor product $\hat{\vec{\sigma}}\cdot\vec{m}\;\hat{\vec{\sigma}}\cdot\vec{n}\otimes\mathbb{I}$ involves both operators acting on the same qubit (via multiplication), with the identity $\mathbb{I}$ acting on the second qubit.
For the Bell states $|\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle\otimes|1\rangle \pm |1\rangle\otimes|0\rangle)$, the left-hand-side reads

$$\langle\Psi^\pm|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|\Psi^\pm\rangle$$

Let us do this calculation in detail (the other ones are similar). Using a compact notation for the two quibit states, and expanding, the left-hand-side is

$$\frac{1}{2}\Big(\langle 01|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|01\rangle + \langle 10|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|10\rangle \pm \langle 01|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|10\rangle \pm \langle 10|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|01\rangle\Big)$$

The first term reads

$$\begin{aligned}
&\langle 01|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|01\rangle = \langle 01|(m_x\hat{\sigma}_x + m_y\hat{\sigma}_y + m_z\hat{\sigma}_z)\otimes(n_x\hat{\sigma}_x + n_y\hat{\sigma}_y + n_z\hat{\sigma}_z)|01\rangle\\
&= \Big(\langle 0|\otimes\langle 1|\Big)\Big[\Big(m_x|1\rangle + \mathrm{i}m_y|1\rangle + m_z|0\rangle\Big)\otimes\Big(n_x|0\rangle - \mathrm{i}n_y|0\rangle - n_z|1\rangle\Big)\Big]\\
&= m_z(-n_z) = -m_z n_z.
\end{aligned} \tag{2.111}$$

Similarly, the second term reads

$$\langle 10|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|10\rangle = (-m_z)n_z = -m_z n_z.$$

The cross terms are

$$\begin{aligned}
\langle 01|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|10\rangle &= \langle 01|(m_x\hat{\sigma}_x + m_y\hat{\sigma}_y + m_z\hat{\sigma}_z)\otimes(n_x\hat{\sigma}_x + n_y\hat{\sigma}_y + n_z\hat{\sigma}_z)|10\rangle\\
&= \langle 01|(m_x|0\rangle - \mathrm{i}m_y|0\rangle - m_z|1\rangle)\otimes(n_x|1\rangle + \mathrm{i}n_y|1\rangle + n_z|0\rangle)\\
&= m_x n_x + m_x\mathrm{i}n_y - n_x\mathrm{i}m_y + m_y n_y
\end{aligned} \tag{2.112}$$

since the left-hand-side selects the terms $|01\rangle$. The other cross term is

$$\begin{aligned}
\langle 10|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|01\rangle &= \langle 10|(m_x\hat{\sigma}_x + m_y\hat{\sigma}_y + m_z\hat{\sigma}_z)\otimes(n_x\hat{\sigma}_x + n_y\hat{\sigma}_y + n_z\hat{\sigma}_z)|01\rangle\\
&= \langle 10|(m_x|1\rangle + \mathrm{i}m_y|1\rangle + m_z|0\rangle)\otimes(n_x|0\rangle - \mathrm{i}n_y|0\rangle - n_z|1\rangle)\\
&= m_x n_x - m_x\mathrm{i}n_y + n_x\mathrm{i}m_y + m_y n_y
\end{aligned} \tag{2.113}$$

since the left-hand-side selects the terms $|10\rangle$. Now, putting the four contributions together

$$\begin{aligned}\frac{1}{2}\Big[&-m_z n_z - m_z n_z \pm \Big(m_x n_x + m_x i n_y - n_x i m_y + m_y n_y\Big) \pm \Big(m_x n_x - m_x i n_y + n_x i m_y + m_y n_y\Big)\Big]\\ &= \frac{1}{2}\Big[-2 m_z n_z \pm \Big(m_x n_x + m_y n_y\Big) \pm \Big(m_x n_x + m_y n_y\Big)\Big]\\ &= \Big[-m_z n_z \pm \Big(m_x n_x + m_y n_y\Big)\Big] = \begin{cases} -m_z n_z + m_x n_x + m_y n_y & \text{for } |\Psi^+\rangle \\ -\vec{m}\cdot\vec{n} & \text{for } |\Psi^-\rangle \end{cases}\end{aligned} \tag{2.114}$$

Concerning the right-hand-side, when the operator $\hat{\vec{\sigma}}\cdot\vec{m}\;\hat{\vec{\sigma}}\cdot\vec{n}\otimes\mathbb{I}$ acts on the same qubit, the calculation in the main text yields

$$\langle\Psi^{\pm}|\hat{\vec{\sigma}}\cdot\vec{m}\;\hat{\vec{\sigma}}\cdot\vec{n}\otimes\mathbb{I}|\Psi^{\pm}\rangle = \vec{m}\cdot\vec{n}.$$

Combining the two results:

$$\langle\Psi^{-}|\hat{\vec{\sigma}}\cdot\vec{m}\otimes\hat{\vec{\sigma}}\cdot\vec{n}|\Psi^{-}\rangle = -\langle\Psi^{-}|\hat{\vec{\sigma}}\cdot\vec{m}\;\hat{\vec{\sigma}}\cdot\vec{n}\otimes\mathbb{I}|\Psi^{-}\rangle.$$

The probability that the measurement yields up (down) spin along the $\hat{m}$ direction for Alice and up (down) along the $\hat{n}$ direction for Bob is obtained by sandwiching the projectors

$$\tfrac{1}{2}\Big(\mathbb{I}\pm\,\vec{m}\cdot\hat{\vec{\sigma}}\Big)\otimes\tfrac{1}{2}\Big(\mathbb{I}\pm\vec{n}\cdot\hat{\vec{\sigma}}\Big) \tag{2.115}$$

with the first factor acting on A and the second on B.

Exercise 2.24 Prove that $\frac{1}{2}(\mathbb{I}\pm\hat{\sigma}^z)$ is the projection operator for the eigenstates of $\hat{\sigma}^z$ with eigenvalue ±1.

Proof. The operators $\frac{1}{2}(I\pm\hat{\sigma}^z)$ are

$$\tfrac{1}{2}\Big(\mathbb{I}\pm\hat{\sigma}^z\Big) = \tfrac{1}{2}\Big[(|0\rangle\langle0| + |1\rangle\langle1|) \pm (|0\rangle\langle0| - |1\rangle\langle1|)\Big] = \begin{cases} |0\rangle\langle0| \\ |1\rangle\langle1| \end{cases} = \hat{P}_{\pm} \tag{2.116}$$

which, as expected, are Hermitian, idempotent, and normalized.

We have

$$\begin{aligned}&\langle\Phi^{\pm}|\tfrac{1}{2}\Big(\mathbb{I}\pm\vec{m}\cdot\hat{\vec{\sigma}}_A\Big)\otimes\tfrac{1}{2}\Big(\mathbb{I}\pm\vec{n}\cdot\hat{\vec{\sigma}}_B\Big)|\Phi^{\pm}\rangle\\ &\quad= \frac{1}{4}\left(\langle0|\otimes\langle0|\pm\langle1|\otimes\langle1|\right)\Big[\Big(\mathbb{I}\pm\vec{m}\cdot\hat{\vec{\sigma}}\Big)\otimes\Big(\mathbb{I}\pm\vec{n}\cdot\hat{\vec{\sigma}}\Big)\Big]\left(|0\rangle\otimes|0\rangle\pm|1\rangle\otimes|1\rangle\right)\\ &\quad= \frac{1}{4}\left(1-\cos\theta\right) = P_{\text{same A, B measurement}}\end{aligned} \tag{2.117}$$

We have used

$$\begin{aligned}&\frac{1}{2}\Big(\mathbb{I}\pm\vec{m}\cdot\hat{\vec{\sigma}}\Big)\otimes\frac{1}{2}\Big(\mathbb{I}\pm\vec{n}\cdot\hat{\vec{\sigma}}\Big)\\ &\qquad= \frac{1}{4}\Big(\mathbb{I}\otimes\mathbb{I}\;\pm\;\vec{m}\cdot\hat{\vec{\sigma}}\otimes\mathbb{I}\pm\mathbb{I}\otimes\vec{n}\cdot\hat{\vec{\sigma}}+\vec{m}\cdot\hat{\vec{\sigma}}\otimes\vec{n}\cdot\hat{\vec{\sigma}}\Big)\end{aligned} \tag{2.118}$$

There are therefore four terms, but the "cross" ones vanish as shown in an exercise above. The double identity operator yields one, and the result of the product of the two non-trivial operators has been calculated in Eq. (2.110) and yields the $-\cos\theta$ (we noted $\vec{m}$ and $\vec{n}$ unit vectors to avoid using a hat whch could be confused with an operator). Here "same" means the same orientation (plus, right) for A and B, in their measurements along $\vec{m}$ and $\vec{n}$, respectively. Similarly,

$$\begin{aligned}&\langle\Phi^{\pm}|\tfrac{1}{2}\left(\mathbb{I}\pm\vec{m}\cdot\hat{\vec{\sigma}}_A\right)\otimes\tfrac{1}{2}\left(\mathbb{I}\mp\vec{n}\cdot\hat{\vec{\sigma}}_B\right)|\Phi^{\pm}\rangle\\ &=\frac{1}{4}\left(1+\cos\theta\right)=P_{\text{opposite A, B measurement}}\end{aligned}\tag{2.119}$$

Now, we will choose three axes in the xz plane, with 120° angles between them:

$$\begin{aligned}&\hat{n}_1=(1,0,0)\qquad\hat{n}_2=\left(-\frac{1}{2},0,\frac{\sqrt{3}}{2}\right)\qquad\hat{n}_3=\left(-\frac{1}{2},0,-\frac{\sqrt{3}}{2}\right)\qquad\Rightarrow\\ &\hat{n}_1=(1,0)\qquad\hat{n}_2=\left(-\frac{1}{2},\frac{\sqrt{3}}{2}\right)\qquad\hat{n}_3=\left(-\frac{1}{2},-\frac{\sqrt{3}}{2}\right)\end{aligned}\tag{2.120}$$

One checks that $\cos\theta=\hat{n}_1\cdot\hat{n}_2=-1/2$, $\cos\theta=\hat{n}_1\cdot\hat{n}_3=-1/2$, $\cos\theta=\hat{n}_2\cdot\hat{n}_3=-1/2$. Of course other choices are possible but this is convenient.

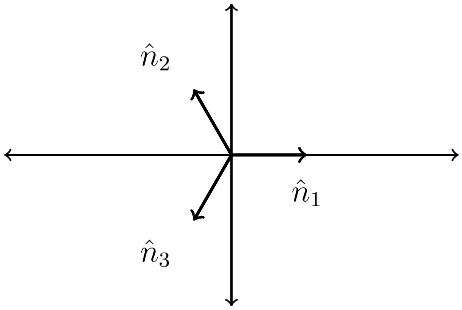

Figure 2.4: Sketch of three vectors on a plane with $120^o=2\pi/3$ angles between them.

We then have that the probability of Alice having the same result on the two axes is equal to the probability of A and B getting different results:

$$P_{\text{A same}}(\hat{n}_1,\hat{n}_2)=P_{\text{opposite A, B measurement}}(\hat{n}_1,\hat{n}_2)=\frac{1}{4}(1+\cos\theta)=\frac{1}{4}\left(1-\frac{1}{2}\right)=\frac{1}{8}\tag{2.121}$$

One can then calculate the various quantum probabilities appearing in Bell's inequality and obtain

$$P_{\text{A same}}(\hat{n}_1,\hat{n}_2)+P_{\text{A same}}(\hat{n}_2,\hat{n}_3)+P_{\text{A same}}(\hat{n}_1,\hat{n}_3)=3\,\frac{1}{8}=\frac{3}{8}<1\tag{2.122}$$

Experimental verification

This violation was measured experimentally by A. Aspect (affiliation at the time of the award: Institut d'Optique Graduate School - Université Paris-Saclay, Paris, France and École Polytechnique, Palaiseau, France), who shared the 2022 Nobel Prize, testing a slightly different version of Bell's inequality and finding that it is violated by the polarization of two entangled photons, see Fig. 2.5.

A. Aspect's Nobel Lecture can be watched here

`https://www.nobelprize.org/prizes/physics/2022/aspect/lecture/`

Non-locality

The conclusion is that the two photons are characterized by a single wave function all along the preparation and evolution. The state created quantum mechanically is *non local*.

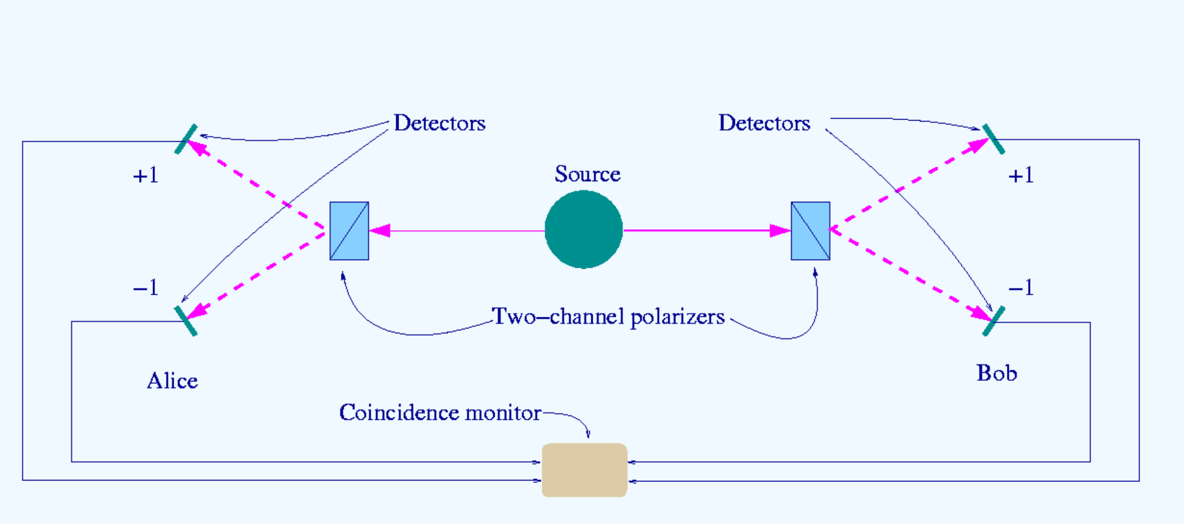

Figure 2.5: Aspect's experimental set-up. Source: Wikipedia.

Construction of a Bell state

The idea is to use the (simple) quantum circuit in Fig. 2.6 to create a Bell state from a simple initial state.

The first qubit is passed through a Hadamard gate and then both qubits are entangled by a CNOT gate. If the input to the circuit is $|\psi\rangle = |0\rangle \otimes |0\rangle$ then the circuit changes the

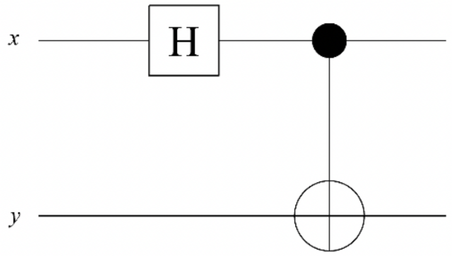

Figure 2.6: The quantum circuit that builds a Bell state.

state to

$$\begin{aligned} \text{CNOT}\, \mathbb{H}_1 |0\rangle \otimes |0\rangle &= \text{CNOT} \left(\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \otimes |0\rangle \right) = \frac{1}{\sqrt{2}} (|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle) \\ &= |\Phi^+\rangle \end{aligned} \tag{2.123}$$

Exercise 2.24 Prove that the operations CNOT $\mathbb{H}_1$ on the inputs $|0\rangle \otimes |1\rangle$, $|1\rangle \otimes |0\rangle$ and $|1\rangle \otimes |1\rangle$ yield $|\Phi^-\rangle$, $|\Psi^+\rangle$, and $|\Psi^-\rangle$, respectively.

2.2.5 Entanglement entropy

In classical physics, the entropy is $k_B \ln$ of the number of microstates which are compatible with the macrostate of the system. It is a measure of uncertainty, or the lack of information needed to identify the microstate of a system.

In quantum mechanics positive entropies may arise even without lack of information, as we show below.

The most common definitions of entropy are the following. The Von Neumann entropy associated to the density matrix $\hat{\rho}$, i.e.

$$S_{\text{vN}} = -\text{Tr}\, \hat{\rho} \ln \hat{\rho}\ . \tag{2.124}$$

The Rényi entropies are defined as

$$S_q = -\frac{1}{1-q} \ln \text{Tr}\, \hat{\rho}^q\ . \tag{2.125}$$

The entanglement entropy is a measure of the degree of quantum entanglement between two subsystems constituting a composite quantum system. The entropy of entanglement is the Von Neumann entropy of the reduced density matrix for any of the subsystems:

$$S_{vN} = -\text{Tr} \hat{\rho}_A^{\text{red}} \ln \hat{\rho}_A^{\text{red}} = -\text{Tr} \hat{\rho}_B^{\text{red}} \ln \hat{\rho}_B^{\text{red}}\ . \tag{2.126}$$

For a separable state, the entanglement entropy vanishes. If it is non-zero, i.e. the subsystem is in a mixed state, it indicates the two subsystems are entangled.

Let us show that for a separable state the entanglement entropy vanishes. A state $\hat{\rho}$ is separable if it can be written as a convex combination of product states:

$$\hat{\rho} = \sum_{\alpha} p_\alpha \, \hat{\rho}_A^\alpha \otimes \hat{\rho}_B^\alpha,$$

where $p_\alpha \geq 0$ and $\sum_\alpha p_\alpha = 1$ are probabilities and $\hat{\rho}_A^{(i)}$ and $\hat{\rho}_B^{(i)}$ are the density matrices for the subsystems A and B, respectively. The reduced density matrix for a separable state:

$$\hat{\rho}_A^{\text{red}} = \mathrm{Tr}_B \, \hat{\rho} = \sum_\alpha p_\alpha \, \mathrm{Tr}_B(\hat{\rho}_B^\alpha) \, \hat{\rho}_A^\alpha = \sum_\alpha p_\alpha \, \hat{\rho}_A^\alpha$$

since $\mathrm{Tr}_B(\hat{\rho}_B^{(i)}) = 1$ (each $\hat{\rho}_B^{(i)}$ is a normalized density matrix). Thus, for a separable state, $\hat{\rho}_A^{\text{red}}$ represents a classical probabilistic mixture of the $\hat{\rho}_A^\alpha$ states. In this case, the entropy S_A reflects the classical probability distribution p_α, rather than quantum entanglement. If the state is truly separable, the reduced density operator $\hat{\rho}_A^{\text{red}}$ corresponds to a pure state (or can be diagonalized into a single pure-state component with certainty). This aligns with the intuition that separable states have no quantum entanglement, as entanglement entropy measures correlations beyond classical ones.

Exercise 2.25

Take two qubits, each of them in the states:

$$|\psi_1\rangle = \frac{3}{5}|0\rangle + \frac{4}{5}|1\rangle \qquad\qquad |\psi_2\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle \tag{2.127}$$

and claim that the joint state of the two qubits is

$$\begin{aligned} |\psi\rangle &= |\psi_1\rangle \otimes |\psi_2\rangle = \left(\frac{3}{5}|0\rangle + \frac{4}{5}|1\rangle\right) \otimes \left(\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle\right) \\ &= \frac{1}{5\sqrt{2}}\Big(3|0\rangle \otimes |0\rangle + 4|1\rangle \otimes |0\rangle - 3|0\rangle \otimes |1\rangle - 4|1\rangle \otimes |1\rangle\Big) \end{aligned} \tag{2.128}$$

Check that this state is correctly normalized. Calculate the entanglement entropy of one spin with respect to the other and prove that it vanishes so that this state is not entangled.

Exercise 2.26

Consider now that the state of the composite system is the *Bell state*

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|00\rangle + |11\rangle\Big) \tag{2.129}$$

Note that Bell states are maximally entangled but not all entangled states are Bell ones. For example,

$$|\psi\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle \qquad \text{with} \quad \theta \in (0, \pi/4) \tag{2.130}$$

are all entangled but are not Bell-states.

Properties

Some properties of von Neumann and Rényi entropies are:

- $S_A^{(n)}$ is insensitive to unitary transformations which act separately within A or the complement of A which we call $\overline{A}$, such as local changes of basis in the quantum many-body system, since these leave the eigenvalues of the reduced density matrix unchanged.
- $0 \leq S_A^{(n)} \leq \ln D$ where $D = \min(D_A, D_{\overline{A}})$.
- $S_A^{(n)}$ is zero if subsystem A is pure and may be described with $\hat{\rho}_A = |\psi\rangle\langle\psi|$ and is maximized if the reduced density matrix for the smaller of the two subsystems is I_D/D where I_D is the $D \times D$ identity matrix (in this case we say that this subsystem is in a maximally-mixed state). In the former case, we will say that the two subsystems are disentangled.
- Writing $\hat{\rho}_A = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ as a probabilistic mixture of orthonormal pure states, with probabilities $p_\alpha = \lambda_\alpha$, the von Neumann entropy $S_A = -\sum_\alpha p_\alpha \ln p_\alpha$ is the classical Shannon entropy of this distribution.

The von Neumann entropy is often preferred to other Rényi entropies as a measure of entanglement since it satisfies additional properties, such as sub-additivity, strong sub-additivity, and concavity which are natural if we wish to give SA an information-theoretic interpretation.

Heuristically, the entanglement entropy between complementary sets quantifies (the logarithm of) the number of terms required to write a pure state as a superposition of product states between A and $\overline{A}$. Formally, $|\psi\rangle$ may be written in the Schmidt form $|\psi\rangle = \sum_\alpha \sqrt{\lambda_\alpha}|\phi_\alpha\rangle\langle\psi_\alpha|$ where $|\phi_\alpha\rangle$ and $|\psi_\alpha\rangle$ are orthonormal sets of states in the two subsystems, and α runs over at most $\min(D_A, D_{\overline{A}})$ values. The distinct Rényi entropies correspond to distinct "counts" of the Schmidt values that discount smaller values of λ_α to a greater or lesser extent.

A key point is that low-entanglement states can be expressed (or approximated) by keeping a number of Schmidt states that is much smaller than D. A generalization of this idea to *Matrix Product States* for chains means that there is a direct relation between the entanglement of a 1D quantum state and the cost of storing it as a Matrix Product State.

A typical quantum state will asymptotically satisfy a *volume law*, in which the entanglement entropy scales with the volume of the selected subsystem. A quantum state satisfies an *area law* if the leading term of the entanglement entropy grows at most proportionally with the boundary between the two partitions (and not with the volume of the selected part).

Area laws are remarkably common for ground states of local gapped quantum many-body systems. These states are therefore non-generic. They emerge in the context of black hole physics, quantum information science, and quantum many-body physics and have been proven rigorously for lattice models in one and higher spatial dimensions. They have important implications, especially on the numerical simulation of lattice models, since they reduce the complexity of quantum many-body systems. The *density matrix renormalization group* and *matrix product states* rely on such area laws.

The holographic principle is the conjecture that the information contained in a volume of space can be represented by a theory which lives in the boundary of that region. It could be related to the area law of the entanglement entropy in microscopic theories.

The emergence of an area law [**?**] then provides support for the intuition that short ranged interactions require that quantum correlations between a distinguished region and its exterior are established via its boundary surface.

That a strict area law emerges is by no means obvious from the decay of two-point correlators.

In contrast to thermal states this entanglement entropy does not originate from a lack of knowledge about the microstate of the system. Even at zero temperature we will encounter a non-zero entropy. This quite intriguing trait of quantum mechanics gives rise to correlations even in situations where the randomness cannot be traced back to a mere lack of knowledge.

In one dimensional systems the entanglement entropy can often be calculated exactly. Whether an area law holds or not, will largely depend on whether the system is at a quantum critical point or not.

The entanglement entropy can also be used to define a basis-independent measure of correlations between subsystems A and B whose union is not necessarily the entire system. This "mutual information" is defined as

$$I_{AB} = S_A + S_B - S_{A\cup B} \tag{2.131}$$

Practical uses

The entanglement entropy is currently being used to

- In systems near criticality, the entanglement entropy often scales logarithmically:

  $$S \sim \frac{c}{3} \ln L$$

  where c is the central charge of the underlying Conformal Field Theory.
- Characterise and distinguish quantum topological phases [73] with no order parameter [74], because it encodes information about both local and non-local quantum correlations in a system and therefore the entanglement entropy that set them apart from conventional phases. In systems with topological order (e.g., fractional quantum Hall states or spin liquids), the entanglement entropy includes a universal, non-local term:

  $$S \sim \alpha L - \gamma$$

  with α a non-universal coefficient related to boundary contributions, L the size of the subsystem boundary (obeys the "area law"), and γ the "topological entanglement entropy", which is a constant and reflects the total quantum dimension of the system's topological excitations. The term γ is directly tied to the underlying topological phase and does not depend on microscopic details. Its value can distinguish between different topological phases.

- Characterise Anderson localised states in electronic systems with local disorder (like random fields) and no interactions [75]. In these systems there is a transition between delocalized and localized phases at a critical disorder strength. The exact value depends on the dimensionality of the system and the nature of the disorder. In one-dimensional systems, even infinitesimal disorder can induce localization, while in higher dimensions, a finite critical disorder strength is required.
  The entanglement entropy of such systems depends on the disorder strength.
  - For weak disorder, the system is in the delocalized phase, where entanglement entropy grows according to the volume law, similar to extended states in non-disordered systems. The entanglement entropy scales with the size of the subsystem.
  - As disorder increases toward the localization transition, the system enters a critical regime. Here, the entanglement entropy growth deviates from the volume law and transitions toward the area law. This intermediate phase often shows logarithmic or sublinear scaling with subsystem size.
  - For strong disorder, the system becomes Anderson localized, and the entanglement entropy adheres to the area law. This means it is proportional to the boundary of the subsystem rather than its volume. The localized nature of the states limits quantum correlations to distances shorter than a characteristic one ξ, reducing entanglement. This behavior reflects the exponential decay of wavefunctions, preventing long-range entanglement. For finite size subsystem with linear size L, there is a crossover. For $L < \xi$ the entanglement entropy scales as in a clean system. Instead, for $L \gg \xi$, disorder dominates and the area law is recovered.

  Summarizing, the entanglement entropy S typically behaves as:
  - $S \sim L^{d-1}$ (area law) in the localized phase.
  - $S \sim L^{d}$ (volume law) in the delocalized phase.
  - $S \sim \ln L$ or sublinear scaling near criticality.

  with L the linear size of the subsystem. Numerical studies of Anderson localization often show a clear crossover from high entanglement in weak disorder to significantly reduced entanglement in the strong disorder regime. Experimental realizations, such as cold atomic gases in disordered potentials, have provided further evidence of these trends.

2.2.6 Modern applications

Quantum computation

A quantum computation acts on an assemble of N qubits, the many-body system. One prepares them in an initial state such as $|1\rangle \otimes \cdots \otimes |1\rangle$. One then applies a unitary transformation $\hat{U}$ to the N qubits. (The transformation $\hat{U}$ is constructed as a product of standard quantum gates, unitary transformations that act on just a few qubits at a time). One next measures all of the qubits by projecting onto the $\{|0\rangle, |1\rangle\}$ basis. The measurement outcome is the output of the computation.

The algorithm performed by the quantum computer is a probabilistic algorithm: one could run exactly the same program twice and obtain different results, because of the randomness of the quantum measurement process. The quantum algorithm actually generates a probability distribution of possible outputs. (This poses no problem since in many cases it is easy to verify whether the solutions are correct.)

A classical computer can accomplish any task that a quantum computer does. The gain can be in the time (in terms of number of operations) and storage needed to achieve the goal. A state of $N = 100$ qubits would need $2^{100} \sim 10^{30}$ complex numbers to characterize it. It is huge.

Quantum circuits

Quantum circuits are collections of local quantum gates, which perform some unitary operators on one qubit (or n qubits arranged in a lattice), interconnected by quantum wires. The evolution occurs on discrete-time. In general, each local operation is not close to the identity and energy is not conserved. These operations are followed by a local quantum measurement element.

Quantum circuits are a fashionable playground for quantum many-body physics. They allow one to explore universal collective phenomena far-from-equilibrium, and they shed light on longstanding questions about thermalization and chaos, and on the underlying universal dynamics of quantum information and entanglement. They also exhibit new dynamical phases in quantum systems that are monitored by an external observer. They allow for experimental progress in building digital quantum simulators.

Randomness in the circuit elements allows a high level of theoretical control, with a key theme being mappings between real-time quantum dynamics and effective classical lattice models or dynamical processes. Many of the universal phenomena that can be identified in this tractable setting apply to much wider classes of more structured many-body dynamics. A recent review is [15] and an example of a very simple quantum circuit is shown in Fig. 2.7.

A minimally-structured unitary quantum circuit which lacks any symmetries or other special properties will rapidly bring the system into a steady-state that is locally completely disordered, in the sense that local observables reproduce an infinite-temperature statistical ensemble. The search for universal phenomena in this setting thus requires going beyond traditional probes of quantum condensed matter involving correlations between specially-chosen local operators. Instead, interesting universal features of the evolving state can be usefully quantified with information-theoretic quantities such as the entanglement entropy and the quantum mutual information, measures of correlations that are non-linear in the reduced density matrix for a subsystem.

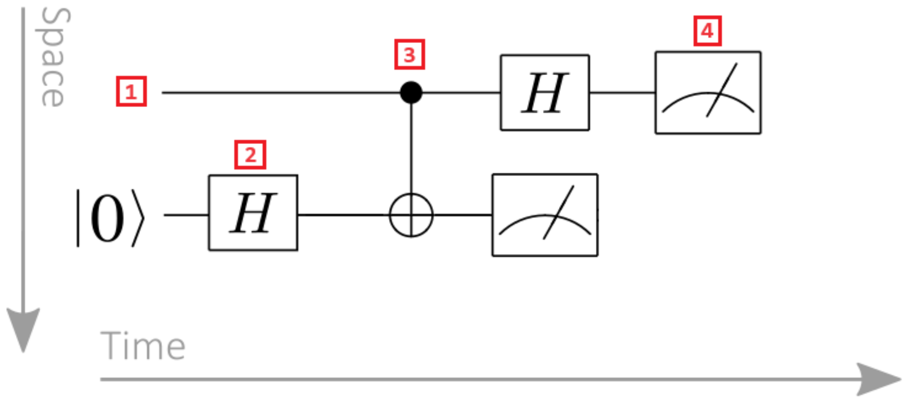

Figure 2.7: An example of a quantum circuit, with the gates drawn according to the convention in the figure where all the gates are listed, Fig. 2.1.

Example
What happens to the quantum state of two qubits when we apply a single qubit gate to one of them? Suppose we apply a Hadamard gate (2.19) to the first qubit in the superposition:

$$|\psi\rangle = \frac{1}{2}|00\rangle - \frac{\mathrm{i}}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|11\rangle \tag{2.132}$$

We have

$$\begin{aligned} \mathbb{H}|\psi\rangle &= \frac{1}{2}\left(\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|10\rangle\right) - \frac{\mathrm{i}}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|11\rangle\right) + \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}|01\rangle - \frac{1}{\sqrt{2}}|11\rangle\right) \\ &= \frac{1}{\sqrt{2}}\left[\frac{1}{2}|00\rangle + \frac{1}{2}|10\rangle + \frac{1-\mathrm{i}}{\sqrt{2}}|01\rangle - \frac{1+\mathrm{i}}{\sqrt{2}}|11\rangle\right] \end{aligned} \tag{2.133}$$

Specific to a two qubit system is the CNOT *gate.* The first bit of a CNOT gate is the “control bit”, the second one is the “target bit”. The control bit never changes, while the target bit flips if and only if the control bit is in state $|1\rangle$.

Though the CNOT gate looks very simple, any unitary transformation on two qubits can be closely approximated by a sequence of CNOT gates and single qubit gates.

Quantum information and technology

Quantum information is not local. Classical bits store information locally, and each classical bit is independent of every other bit. Quantum information is typically stored in the relationships between individual qubits, and a qubit is typically not independent of the others.

For instance, engineers can prepare a pair of qubits in a state such that if we measured one qubit as a 0, the other would have to be a 1, and vice versa. In theory, engineers can build up systems with as many qubits as they want, where each qubit's state depends on many other qubits' states, and all are part of a complex entangled system.

Two sources of difficulties are inherent to quantum information. First, there are more ways for errors to creep into the system. Second, coupling to an environment can corrupt information stored, since entanglement with the surrounding can let the stored information be lost. Moreover, quantum error correction is more challenging than the classical one, since a problem that affects one qubit can end up corrupting the entire system.

The weird property of entanglement is at the basis of quantum technologies. For example, in cryptography, the idea that *safe key distribution* may profit from entanglement is clear. If one produces a series of N entangled pairs atoms and sends each of the members of the pairs to Alice and Bob, at their measurements they will get the same results, that is, the same series of 1 and 0. Before their measurement, the series does not really exist and that is why the transmission is safe [28].

2.3 Time evolution

We here discuss the description of the evolution of a quantum system using the two well-known pictures: the one named Schrödinger, in which operators are time independent, while states depend on time and the one called Heisenberg in which operators depend on time, while states do not. The interaction picture, which is mixed and both states and operators depend on time, is also useful to know.

2.3.1 Schrödinger picture

In the Schrödinger picture of quantum mechanics, the *Schrödinger equation* giving the time evolution of states, is postulated:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi,t\rangle = \hat{H}|\psi,t\rangle,$$

where $\hat{H}$ is the Hamiltonian operator, which encodes the energy of the system.

The *time evolution operator*, $\hat{U}(t,t_0)$, which describes the evolution of the quantum state over time, is defined from

$$|\psi,t\rangle = \hat{U}(t,t_0)|\psi,t_0\rangle.$$

can be derived. The linearity of the Schrödinger equation implies that the time evolution operator $\hat{U}(t,t_0)$ must also be linear.

Reversibility

Quantum mechanics is time-reversible for closed systems, that if the evolution fromt_0 to t is governed by $\hat{U}(t,t_0)$, the reverse evolution from t to t_0 must also be possible. Therefore $\hat{U}(t,t_0)$ must have an inverse

$$\hat{U}^{-1}(t,t_0)\hat{U}(t_0,t) = \hat{U}(t,t_0)\hat{U}^{-1}(t,t_0) = \mathbb{I}$$

Unitarity & conservation of probability

If the system is represented by a state, the conservation of its normalization implies

$$|\langle\psi,t|\psi,t\rangle|^2 = |\langle\psi,t_0|\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)|\psi,t_0\rangle|^2 = |\langle\psi,t_0|\psi,t_0\rangle|^2 \;, \tag{2.134}$$

which is ensured by

$$\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = \hat{U}(t,t_0)\hat{U}^\dagger(t,t_0) = \mathbb{I}$$

Let us represent a state with an expansion on the eigenstates $|a_\alpha\rangle$ of an operator $\hat{A}$. At times t_0 and t:

$$|\psi,t_0\rangle = \sum_\alpha c_\alpha(t_0)|a_\alpha\rangle \qquad\qquad |\psi,t\rangle = \sum_\alpha c_\alpha(t)|a_\alpha\rangle \tag{2.135}$$

Conservation of probability, ensured by the unitary evolution, implies

$$\sum_\alpha |c_\alpha(t_0)|^2 = \sum_\alpha |c_\alpha(t)|^2 \;. \tag{2.136}$$

In the more general case in which the state of the system is represented by a density operator, in order to ensure probability conservation, its trace must equal 1. The evolution of the density operator follows from the one of the states (see below):

$$\hat{\rho}(t) = \hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t,t_0)$$

Therefore

$$\begin{aligned} 1 &= \mathrm{Tr}\,\hat{\rho}(t) = \mathrm{Tr}\,[\hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t,t_0)] \\ &= \mathrm{Tr}\,[\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)\hat{\rho}(t_0)] = \mathrm{Tr}\,[\hat{\rho}(t_0)\hat{U}(t,t_0)\hat{U}^\dagger(t,t_0)] = \mathrm{Tr}\hat{\rho}(t_0) \end{aligned} \tag{2.137}$$

and this implies that the evolution operator must be unitary

$$\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = \hat{U}(t,t_0)\hat{U}^\dagger(t,t_0) = \mathbb{I}$$

Composition

Another requirement is the composition property

$$\hat{U}(t,t_1)\hat{U}(t_1,t_0) = \hat{U}(t,t_0) \qquad t \geq t_1 \geq t_0 \tag{2.138}$$

Continuity

The continuity condition is

$$\lim_{dt\to 0} \hat{U}(t+dt,t) = \mathbb{I} \tag{2.139}$$

Evolution equation

These properties are satisfied by

$$\hat{U}(t+dt,t) = \mathbb{I} - \frac{\mathrm{i}}{\hbar}\hat{H}(t)dt \qquad\qquad \hat{H}(t) = \hat{H}^{\dagger}(t) \tag{2.140}$$

One can now use this expression to derive the equation ruling the time evolution of the evolution operator:

$$\begin{aligned}\hat{U}(t+dt,t_0) &= \underbrace{\hat{U}(t+dt,t)\hat{U}(t,t_0)}_{\text{composition}} = \underbrace{\left(\mathbb{I} - \frac{\mathrm{i}}{\hbar}\hat{H}(t)dt\right)}_{\text{continuity, unitarity \& Schrod}} \hat{U}(t,t_0) \\ &= \hat{U}(t,t_0) - \frac{\mathrm{i}}{\hbar}\hat{H}(t)\hat{U}(t,t_0)dt\end{aligned}$$

that implies

$$\frac{\hat{U}(t+dt,t_0) - \hat{U}(t,t_0)}{dt} = -\frac{\mathrm{i}}{\hbar}\hat{H}(t)\hat{U}(t,t_0) \quad \Rightarrow \quad \mathrm{i}\hbar\frac{d\hat{U}(t,t_0)}{dt} = \hat{H}(t)\hat{U}(t,t_0) \tag{2.141}$$

This is the *Schrödinger equation* for the time-evolution operator.

Explicit expression

The solution to Eq. (2.141) is, in complete generality,

$$\hat{U}(t,t_0) = \mathbb{I} + \sum_{n=1}^{\infty}\left(\frac{-\mathrm{i}}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \; \hat{H}(t_1)\hat{H}(t_2)\ldots\hat{H}(t_n) \tag{2.142}$$

where the $\hat{H}(t)$ could be time dependent and the factors evaluated at different times not commute. In particular cases it simplifies considerably:

$$\hat{U}(t,t_0) = e^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t-t_0)} \qquad \hat{H} \;\; \text{time independent} \tag{2.143}$$

$$\hat{U}(t,t_0) = e^{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} dt'\hat{H}(t')} \qquad \hat{H} \;\; \text{time dependent but } \; [\hat{H}(t_1),\hat{H}(t_2)] = 0 \tag{2.144}$$

In the first case one can also express the evolution operator as

$$e^{-\frac{\mathrm{i}}{\hbar}\hat{H}t} = \sum_{\alpha} e^{-\frac{\mathrm{i}}{\hbar}E_\alpha t}|\psi_\alpha\rangle\langle\psi_\alpha| \qquad\qquad \hat{H}|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle \tag{2.145}$$

and this implies that the evolution of a generic ket reads

$$\begin{aligned}e^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t-t_0)}|\psi,t_0\rangle &= \sum_{\alpha} e^{-\frac{\mathrm{i}}{\hbar}E_\alpha(t-t_0)}|\psi_\alpha\rangle\langle\psi_\alpha|\sum_{\beta}c_\beta(t_0)|\psi_\beta\rangle \\ &= \sum_{\alpha,\beta} e^{-\frac{\mathrm{i}}{\hbar}E_\alpha(t-t_0)}c_\beta(t_0)|\psi_\alpha\rangle\delta_{\alpha,\beta} \\ &= \sum_{\alpha} e^{-\frac{\mathrm{i}}{\hbar}E_\alpha(t-t_0)}c_\alpha(t_0)|\psi_\alpha\rangle \\ &= \sum_{\alpha} c_\alpha(t)|\psi_\alpha\rangle \quad \text{with} \quad c_\alpha(t) = e^{-\frac{\mathrm{i}}{\hbar}E_\alpha(t-t_0)}c_\alpha(t_0)\end{aligned} \tag{2.146}$$

While the modulus of these coefficients do not change in time, their relative phases do.

For time-dependent Hamiltonians which do not commute at different times, the expression of the evolution operator is more complex and typically involves a time-ordered exponential,

$$\hat{U}(t,t_0) = \mathcal{T}\exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\hat{H}(t')\,dt'\right),$$

where $\mathcal{T}$ is the time-ordering operator.

The fact that the evolution operator is unitary one can see now that it follows from the fact that the Hamiltonian is Hermitian. For example, for the special case in which $\hat{H}$ is time independent but commuting at different times, $\hat{U}^\dagger(t,t_0) = e^{\frac{\mathrm{i}}{\hbar}\hat{H}^\dagger(t-t_0)} = e^{\frac{\mathrm{i}}{\hbar}\hat{H}(t-t_0)}$, and then

$$\hat{U}(t,t_0)\hat{U}^\dagger(t,t_0) = \hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = \mathbb{I}\,. \tag{2.147}$$

For the more general case, the proof is similar.

Naturally, we can recover the Schrödinger equation for the states evolution from the equation for the evolution operator. Indeed, multiplying Eq. (2.141) by $|\psi,t_0\rangle$:

$$\mathrm{i}\hbar\,\frac{d\hat{U}(t+dt,t_0)|\psi,t_0\rangle}{dt} = \hat{H}\hat{U}(t,t_0)|\psi,t_0\rangle \quad\Rightarrow\quad \mathrm{i}\hbar\,\frac{d|\psi,t\rangle}{dt} = \hat{H}|\psi,t\rangle \tag{2.148}$$

Exercise 2.27 Take $\hat{H}(t)$ a Hamiltonian which can depend explicitly on time. Prove that the evolution is linear, that is the superposition principle holds: if $|\psi_{1,2},t\rangle$ are two solutions of the Schrödinger equation with initial conditions $|\psi_{1,2},0\rangle$ then one can construct the state $|\psi,t\rangle = c_1|\psi_1,t\rangle + c_2|\psi_2,t\rangle$ which is again solution of the Schrödinger equation with initial condition $|\psi,t\rangle = c_1|\psi_1,0\rangle + c_2|\psi_2,0\rangle$.

Exercise 2.29 Obtain an expression for the time-derivative of the expectation of the Hamiltonian, $d\langle\hat{H}\rangle/dt$. Does it vanish? Under which condition does it vanish?

2.3.2 Heisenberg picture

Here observables, rather than states, vary with time:

$$\hat{A}_H(t,t_0) \equiv \hat{U}^\dagger(t,t_0)\hat{A}_S\hat{U}(t,t_0) \tag{2.149}$$

where $\hat{A}_S = \hat{A}_H(t_0)$ is the Schrödinger picture operator $\hat{A}$. The states, instead, remain unchanged. (This will also apply to the density operator.)

The expectation value is the same in the two pictures

$$\langle\hat{A}\rangle(t) = \langle\psi,t|\hat{A}_S|\psi,t\rangle = \langle\psi,t_0|\hat{U}^\dagger(t,t_0)\hat{A}_S\hat{U}(t,t_0)|\psi,t_0\rangle = \langle\psi,t_0|\hat{A}_H(t,t_0)|\psi,t_0\rangle \tag{2.150}$$

Heisenberg's equation

The fundamental equation of motion in the Heisenberg picture is the following. Assume that $\hat{A}_S$ does not depend explicitly on time. Then,

$$\begin{aligned}\frac{d\hat{A}_H(t,t_0)}{dt} &= \frac{d\hat{U}^\dagger(t,t_0)}{dt}\hat{A}_S\hat{U}(t,t_0) + \hat{U}^\dagger(t,t_0)\hat{A}_S\frac{d\hat{U}(t,t_0)}{dt} \\ &= -\frac{1}{\mathrm{i}\hbar}\hat{U}^\dagger(t,t_0)\hat{H}_S\hat{A}_S\hat{U}(t,t_0) + \hat{U}^\dagger(t,t_0)\hat{A}_S\frac{1}{i\hbar}\hat{H}_S\hat{U}(t,t_0) \\ &= -\frac{1}{\mathrm{i}\hbar}\Big(\hat{U}^\dagger(t,0)\hat{H}_S\hat{U}(t,t_0)\hat{U}^\dagger(t,t_0)\hat{A}_S\hat{U}(t,0) \\ &\qquad -\hat{U}^\dagger(t,t_0)\hat{A}_S\hat{U}(t,t_0)\hat{U}^\dagger(t,0)\hat{H}_S\hat{U}(t,t_0)\Big) \\ &= \frac{1}{\mathrm{i}\hbar}\Big(-\hat{H}_H(t,t_0)\hat{A}_H(t,t_0) + \hat{A}_H(t,t_0)\hat{H}_H(t,t_0)\Big)\ . \end{aligned} \tag{2.151}$$

We note that if $\hat{U}(t,t_0) = e^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t-t_0)}$, then $\hat{H}_H = \hat{H}_S = \hat{H}$, and the equation becomes

$$\frac{d\hat{A}_H(t,t_0)}{dt} = \frac{1}{\mathrm{i}\hbar}\left[\hat{A}_H(t,t_0),\hat{H}\right] \tag{2.152}$$

2.3.3 Interaction picture

The interaction or *Dirac picture* is an intermediate representation between the Schrödinger picture and the Heisenberg picture in which both states and operators carry part of the time dependence of observables. Take a total time-independent Hamiltonian made of the sum of two terms

$$\hat{H}_T = \hat{H}_0 + \hat{H}_{\text{int}} \tag{2.153}$$

Then

$$|\psi_{\mathrm{I}},t\rangle = e^{-\frac{\mathrm{i}}{\hbar}\hat{H}_{\text{int}}t}|\psi_S,t\rangle \qquad\qquad \hat{O}_{\mathrm{I}}(t) = e^{\frac{\mathrm{i}}{\hbar}\hat{H}_0 t}\,\hat{O}_S\,e^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0 t} \tag{2.154}$$

where $|\psi_S,t\rangle$ and $\hat{O}_S$ are a state and an operator in the Schrödinger picture. We set $t_0 = 0$ for simplicity here. Typically $\hat{H}_0$ is a simple (e.g. quadratic) Hamiltonian and $\hat{H}_{\text{int}}$ carries the non-trivial interactions.

The advantage of the interaction picture is that it separates the dynamics due to the "free" Hamiltonian H_0 (which is solved exactly) from the dynamics due to the interaction Hamiltonian $H_{\mathrm{I}}(t)$ (which is treated perturbatively).

2.3.4 The density operator

The time evolution of a generic density operator $\hat{\rho}(t,t_0) = \sum_\alpha p_\alpha|\psi_\alpha,t\rangle\langle\psi_\alpha,t|$ of a system with $\hat{H} = \hat{H}^\dagger$ is

$$\mathrm{i}\hbar\frac{d\hat{\rho}}{dt} = [\hat{H},\hat{\rho}] \equiv \hat{\mathcal{L}}\hat{\rho} \tag{2.155}$$

in the Schrödinger picture. This is called the *Liouville-von Neumann* or *master equation*. $\hat{\mathcal{L}}$ is the *Liouvillian superoperator* called this way since it describes a linear transformation on an operator: it operates on both sides of $\hat{\rho}$. The proof is straightforward, it only uses the Schrödinger equation for each of the states $|\psi_\alpha\rangle$, $\mathrm{i}\hbar\frac{d|\psi_\alpha,t\rangle}{dt} = \hat{H}|\psi_\alpha,t\rangle$.

In the Schrödinger picture that we used above, although $\hat{\rho}$ is an operator, it evolves in time because it represents the state of the system, and not an observable. Instead, if we worked in the Heisenberg picture it would be time-independent.

Exercise 2.30 Prove that the density operator transforms to the interaction picture as any other operator, Eq. (2.154), $\hat{\rho}_{\mathrm{I}}(t) = \hat{U}_0^\dagger(t,0)\hat{\rho}_S\hat{U}_0(t,t_0)$ with the evolution operator involving $\hat{H}_0$.

Exercise 2.31 Prove that the evolution of the density operator in the interaction picture is given by

$$\frac{d\hat{\rho}_{\mathrm{I}}(t)}{dt} = -\frac{\mathrm{i}}{\hbar}\left[\hat{H}^{\mathrm{I}}_{\mathrm{int}}(t),\hat{\rho}_{\mathrm{I}}(t)\right] . \tag{2.156}$$

Exercise 2.32 Prove that the Hamiltonian dynamics does not change the purity of a system. This result illustrates that the mixing rate of a state does not change due to the quantum evolution.

In the Schrödinger picture,

$$\begin{aligned}\frac{d\,\mathrm{Tr}\hat{\rho}^2(t)}{dt} &= \mathrm{Tr}\,\frac{d\hat{\rho}^2(t)}{dt} = \mathrm{Tr}\,2\,\hat{\rho}(t)\,\frac{d\hat{\rho}(t)}{dt} = 2\,\mathrm{Tr}\,\hat{\rho}(t)\left(\frac{-\mathrm{i}}{\hbar}\left[\hat{H}(t),\hat{\rho}(t)\right]\right)\\ &= -\frac{2\mathrm{i}}{\hbar}\,\mathrm{Tr}\,\hat{\rho}(t)\left(\hat{H}(t)\hat{\rho}(t)-\hat{\rho}(t)\hat{H}(t)\right) = 0\end{aligned} \tag{2.157}$$

using the cyclic property of the trace.

Exercise 2.33 Show that the entropy remains constant for unitary evolution with $\hat{H}(t)$. In particular, show that for a pure state the entropy vanishes and remains zero under unitary evolution. The result of the previous exercise and this one suggest that for closed systems the quantum information is never really lost.

Exercise 2.34 Consider a two-level system with Hamiltonian $\hat{H} = e_0|0\rangle\langle 0| + \hbar\Omega(|0\rangle\langle 1| + |1\rangle\langle 0|) + e_1|1\rangle\langle 1|$, where Ω is the frequency of driving that coherently switches between both states. Calculate the populations ρ_{00} and ρ_{11} as a function of time. Show that system is driven between the states, and the populations present Rabi oscillations.

2.3.5 Gibbs-Boltzmann

The density operator of a pure state representing a closed system vanishes and remains zero henceforth under unitary evolution.

Consider a small subsystem of a large, interacting quantum system, in a pure state. The subsystem can exhibit an apparent loss of information due to the spreading of entanglement between the subsystem and the rest. The reduced density operator can display

$$\lim_{t\to\infty}\lim_{N_B\to\infty}\hat{\rho}_A(t) = \hat{\rho} \qquad \text{stationary} \tag{2.158}$$

In this stationary limit, $\hat{\rho}$ must be independent of time and $\hat{\rho}$ must commute with $\hat{H}$, because of the Liouville equation. This is true iff we can simultaneously diagonalize $\hat{\rho}$ and $\hat{H}$. Hence, the eigenstates of $\hat{\rho}$ can be assumed to be energy eigenstates.

Any function of $\hat{H}$ commutes with $\hat{H}$. Furthermore, if the system has continuous symmetries then there exist other operators that also commute with $\hat{H}$. For example, if the system is invariant under translations then the momentum operator will commute with $\hat{H}$. If it is invariant under rotations then the angular momentum operator will commute with $\hat{H}$. So, in equilibrium, the density operator can be a function of these various operators. In practice, we are usually interested in systems for which boundary conditions break translational and rotational symmetry e.g. a gas in a cubic box. In such a situation, one can argue that any operator which commutes with $\hat{H}$ must be a function of $\hat{H}$ only. So, in equilibrium, the density operator must be a function of the Hamiltonian operator $\hat{H}$.

Arguing in this way one justifies the equilibrium density operator in the canonical ensemble

$$\lim_{t\to\infty}\lim_{N_B\to\infty}\hat{\rho}_A(t)=\frac{e^{-\beta\hat{H}_A}}{\mathcal{Z}}\qquad \text{Gibbs}-\text{Boltzmann} \tag{2.159}$$

(with the addition in the exponential of other terms like $\mu\hat{N}$, etc if there are other finite number of constants to consider).

2.3.6 No cloning theorem

The no-cloning theorem states that it is impossible to create an independent and identical copy of an arbitrary unknown quantum state. It turns out to be a consequence of unitary evolution [63, 64]. A dual of this theorem is called the *no deleting theorem*. They both have deep consequences in the field of *quantum computation*. The no-cloning theorem (as generally understood) concerns only pure states whereas the generalised statement regarding mixed states is known as the *no-broadcasting* theorem.

Let us prove this statement. Take a system A which can be in two possible states, say $|0\rangle$ and $|1\rangle$ and ask whether one can copy its state on another two-state system B, that, without loss of generality we initialise in $|0\rangle$. Note that the two systems share the Hilbert space and $\mathcal{H}_A\otimes\mathcal{H}_B=\mathcal{H}\otimes\mathcal{H}$.

We can manipulate the composite system with two permissible quantum operations:

- Perform an observation, which irreversibly collapses the system into some eigenstate of an observable, corrupting the information contained in the system.
- Evolve with a judicious choice of evolution operator constructed with the Hamiltonian of the combined system.

The first option is not what we want. Let us see how would the second one work.

First, consider that the system to be copied is in an eigenstate of $\hat{\sigma}^z$, that is $|0\rangle_A$ or $|1\rangle_A$, that we combine with another qubit in the state $|0\rangle_B$. We evolve with a $\hat{U}$ the full system, and we assume that there is a $\hat{U}$ such that

$$\hat{U}(|0\rangle_A \otimes |0\rangle_B) = |0\rangle_A \otimes |0\rangle_B \qquad \hat{U}(|1\rangle_A \otimes |0\rangle_B) = |1\rangle_A \otimes |1\rangle_B \tag{2.160}$$

that is, the state of B becomes identical to the one of A, and the state of A does not change. We simplify the notation and we do not write the t_0 and t for the initial and final times.

Imagine now that the particle A is in a superposition state

$$|\psi\rangle_A = \frac{1}{\sqrt{2}}\left(|1\rangle_A + |0\rangle_A\right) \tag{2.161}$$

and ask whether the same $\hat{U}$ operator above clones the state of A. Acting with $\hat{U}$

$$\hat{U}\left[\frac{1}{\sqrt{2}}\left(|1\rangle_A + |0\rangle_A\right) \otimes |0\rangle_B\right] = \frac{1}{\sqrt{2}}\left(|1\rangle_A \otimes |1\rangle_B + |0\rangle_A \otimes |0\rangle_B\right) \tag{2.162}$$

which is the *entangled Schrödinger-cat state*, one if the Bell states, while the expected cloning would have been

$$\begin{aligned} &\frac{1}{\sqrt{2}}\left(|1\rangle_A + |0\rangle_A\right) \otimes \frac{1}{\sqrt{2}}\left(|1\rangle_B + |0\rangle_B\right) \\ &\qquad \frac{1}{2}\left(|1\rangle_A \otimes |1\rangle_B + |1\rangle_A \otimes |0\rangle_B + |0\rangle_A \otimes |1\rangle_B + |0\rangle_A \otimes |0\rangle_B\right) \end{aligned} \tag{2.163}$$

$\hat{U}$ acts non-locally, and thus induces entanglement between the two systems. Note that there is no problem with the cloning of the basis states, the problem is in also cloning more general states. In conclusion, there is no unitary operator to clone all states.

Another proof of the theorem can be found in the web site
`https://en.wikipedia.org/wiki/No-cloning_theorem`

2.3.7 Development of entaglement

Imagine that one starts with $\hat{\rho}(0) = \hat{\rho}_A(0) \otimes \hat{\rho}_B(0)$ at $t = 0$, with $\hat{\rho}_A(0)$ and $\hat{\rho}_A(0)$ the ones of two pure states. The subsystems A and B are initially uncorrelated (not entangled).

As systems A and B become entangled with each other they will individually become mixed states in the sense that we can no longer define either of them by a state vector. However, the overall combined system described by $\hat{\rho}$ will remain in a pure state.

Example

Let us consider a simple system of two qubits interacting via a time-dependent Hamiltonian. This example demonstrates how the entanglement between two initially separable qubits develops over time. We start with two qubits in an unentangled, separable state:

$$|\psi, 0\rangle = |0\rangle \otimes |1\rangle = |01\rangle$$

where $|0\rangle$ and $|1\rangle$ are the standard computational basis states. Assume the qubits interact through an exchange interaction, described by the Hamiltonian:

$$\hat{H} = \frac{\hbar\omega}{2}\left(\hat{\sigma}_x^{(A)}\hat{\sigma}_x^{(B)} + \hat{\sigma}_y^{(A)}\hat{\sigma}_y^{(B)}\right),$$

where $\hat{\sigma}_x^{(A,B)}$ and $\hat{\sigma}_y^{(A,B)}$ are the Pauli operators for qubits A and B and ω is the interaction strength (frequency). This Hamiltonian generates entanglement between the two qubits over time. The time evolution of the system is governed by the Schrödinger equation:

$$|\psi, t\rangle = e^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}|\psi, 0\rangle.$$

To compute the evolution, note that the Hamiltonian acts in the basis of two qubits: $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$. The interaction effectively couples these states. Applying the Hamiltonian, the time-evolved state becomes

$$|\psi, t\rangle = \cos(\omega t)|01\rangle - \mathrm{i}\sin(\omega t)|10\rangle.$$

and it is a superposition of $|01\rangle$ and $|10\rangle$. The degree of entanglement between the two qubits can be quantified using the concurrence or the von Neumann entropy of the reduced density matrix. Tracing out one qubit gives the reduced density matrix for the other qubit:

$$\hat{\rho}_A(t) = \mathrm{Tr}_B\left(|\psi(t)\rangle\langle\psi(t)|\right).$$

After tracing over the second qubit:

$$\rho_A(t) = \begin{pmatrix} \sin^2(\omega t) & 0 \\ 0 & \cos^2(\omega t) \end{pmatrix}.$$

This reduced density matrix correctly satisfies $\rho_{00} + \rho_{11} = 1$, and it is mixed for $t \neq n\pi/(2\omega)$ with $n \in \mathbb{Z}$, indicating entanglement, since taking $\rho_A^2(t)$ and its trace

$$\mathrm{Tr}\rho_A^2(t) = \mathrm{Tr}\begin{pmatrix} \sin^4(\omega t) & 0 \\ 0 & \cos^4(\omega t) \end{pmatrix} = \sin^4(\omega t) + \cos^4(\omega t) < 1 \qquad \text{if } \; t \neq n\pi/(2\omega) \tag{2.164}$$

The entanglement oscillates periodically due to the coherent interaction described by the Hamiltonian. At $t = \pi/(4\omega)$, the state becomes $|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle - \mathrm{i}|10\rangle\right)$, a maximally entangled (Bell) state while at $t = \pi/(2\omega)$ the state returns to a separable form.

2.3.8 Quantum quenches

Quantum quenches is the name given to the protocol such that a parameter in the Hamiltonian, say $\lambda(t)$, is changed from an initial value λ_0 at times, say $t < 0$, to another value λ_1 at a later time t_1 following some functional form, $\lambda(t)$ such that $\lambda(0) = \lambda_0$ and $\lambda(t_1) = \lambda_1$. For example,

$$\lambda(t) = \lambda_0\theta(-t) + \lambda_1\theta(t) \qquad \text{instantaneous quench}\,. \tag{2.165}$$

Two common choices for the system at time $t = 0$ are (i) the ground state of the Hamiltonian $\hat{H}(\lambda_0)$ at time $t = 0$

$$|\psi, 0\rangle = |\psi, \lambda_0\rangle_{\mathrm{GS}} \tag{2.166}$$

or (ii) canonical equilibrium with the Hamiltonian $\hat{H}(\lambda_0)$:

$$\hat{\rho}(0) = \frac{e^{-\beta \hat{H}(\lambda_0)}}{\mathcal{Z}_0} \ , \tag{2.167}$$

with $\mathcal{Z}_0$ the partition function of the unperturbed system. The system is then evolved in isolation with the Hamiltonian $\hat{H}(\lambda(t))$ at times $t > 0$,

$$|\psi, t\rangle = e^{-\frac{\mathrm{i}}{\hbar}\int_0^t dt' \hat{H}(\lambda(t'))} |\psi, \lambda_0\rangle_{\mathrm{GS}} \tag{2.168}$$

If $\lambda(t) = \lambda_0$ there is no quench, the initial state is an eigenstate of the Hamiltonian and the dynamics is trivial. The interesting cases are the ones that deviate from this case, for which $|\psi, \lambda_0\rangle_{\mathrm{GS}}$ is not an eigenstate of $\hat{H}(\lambda(t))$ and the dynamics is non-trivial.

A typical choice of $\hat{H}(\lambda(t))$ is

$$\hat{H}(\lambda(t)) = \hat{H}_0 + \lambda(t)\hat{Q}(t) \qquad\qquad \lambda(t) = \overline{\lambda}(t)\theta(t) \ . \tag{2.169}$$

The time-dependent parameter $\overline{\lambda}(t)$ couples to an observable $\hat{Q}$ of the system.

Example

Let us examine a quantum quench in a single qubit. Before the quench ($t < 0$), the Hamiltonian is

$$\hat{H}_i = -\frac{\hbar\omega}{2}\hat{\sigma}^z,$$

where $\hat{\sigma}^z$ is the Pauli z-operator and $\omega > 0$ is a constant frequency. The qubit is initially in the ground state of $\hat{H}_i$:

$$|\psi, 0\rangle = |0\rangle,$$

where $|0\rangle$ is the eigenstate of $\hat{\sigma}^z$ with eigenvalue $+1$. At $t = 0$, the Hamiltonian is suddenly quenched to

$$\hat{H}_f = -\frac{\hbar\omega}{2}\hat{\sigma}^x,$$

where $\hat{\sigma}^x$ is the Pauli x-operator. This represents an abrupt change in the direction of the external field. The time evolution is governed by the Schrödinger equation:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi, t\rangle = \hat{H}_f|\psi, t\rangle.$$

The eigenstates of $\hat{H}_f$ are the eigenstates of $\hat{\sigma}^x$, given by

$$|\pm\rangle_x = \frac{1}{\sqrt{2}}\big(|0\rangle \pm |1\rangle\big),$$

with eigenvalues $\mp\frac{\hbar\omega}{2}$, respectively. The initial state $|0\rangle$ can be written as a superposition of the eigenstates of $\hat{H}_f$:

$$|0\rangle = \frac{1}{\sqrt{2}}\big(|+\rangle_x + |-\rangle_x\big).$$

After the quench ($t \geq 0$), the time-evolved state is

$$|\psi, t\rangle = \frac{1}{\sqrt{2}}\left(e^{\mathrm{i}\frac{\omega t}{2}}|+\rangle_x + e^{-\mathrm{i}\frac{\omega t}{2}}|-\rangle_x\right).$$

Substituting back the eigenstates $|\pm\rangle_x$ into the computational basis

$$|\psi, t\rangle = \frac{1}{\sqrt{2}}\left[e^{\mathrm{i}\frac{\omega t}{2}}\frac{|0\rangle + |1\rangle}{\sqrt{2}} + e^{-\mathrm{i}\frac{\omega t}{2}}\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] = \cos\left(\frac{\omega t}{2}\right)|0\rangle - \mathrm{i}\sin\left(\frac{\omega t}{2}\right)|1\rangle.$$

The Probability of Measuring $|0\rangle$ and $|1\rangle$ are

$$P_0(t) = |\langle 0|\psi(t)\rangle|^2 = \cos^2\left(\frac{\omega t}{2}\right) \qquad P_1(t) = |\langle 1|\psi(t)\rangle|^2 = \sin^2\left(\frac{\omega t}{2}\right)$$

At $t = 0$, $P_0 = 1$, and the qubit is in state $|0\rangle$, as expected. Over time, the qubit oscillates between states $|0\rangle$ and $|1\rangle$ due to the sudden change in the Hamiltonian. The frequency of oscillation is $\omega/2$.

This example demonstrates a fully solvable case of a quantum quench applied to a single qubit, highlighting the interplay between the initial and final Hamiltonians.

2.3.9 Quantum chaos

Since the discovery of *deterministic classical chaos*, it is known that reserving the velocities of a system after a time t, and letting it evolve 'backwards' in time towards $2t$, will not recover the same initial state. Typical systems of many particles possess exponential sensitivity on the variation of initial condition. Arbitrarily small but non-vanishing perturbations of the initial condition, or of the equations of motion (e.g. introducing a small external force field like gravity), drive the returning orbit away and the trajectory will not return back to the initial phase space point. The *classical Lyapunov exponent*, λ, quantifies the rate of exponential divergence of nearby trajectories in phase space. It is a key feature of chaotic systems, reflecting the sensitivity to initial conditions.

This, however, is not the case in quantum mechanics. First of all, the notion of a trajectory in phase space does not strictly exist in quantum mechanics due to the uncertainty principle. Moreover, due to the linearity and unitarity of the quantum dynamics, the latter is always stable against small variations of the initial state. Yet, small variation in the Hamiltonian can produce non-trivial effects.

Quantum chaos is characterized by properties such as:

- The first characterizations of chaos emerged from the analysis of the quantization of classical chaotic systems such as billiards. It was observed that the statistical distribution of energy levels differs being the Wigner-Dyson statistics of random matrices for chaotic systems, and Poisson for integrable ones. This is the Bohigas-Giannoni-Schmidt conjecture [61] which was found to apply to all known problems so far.
- The behavior of quantum observables, such as the fidelity, the Loschmidt echo or the out-of-time-ordered correlators (OTOCs), which are used to study quantum analogs of classical chaos.

We give the definitions and properties of these diagnostics below. Before doing it, let us discuss some points.

The relationship between the Lyapunov exponent of a quantum chaotic system and that of its classical counterpart is complex and depends on the context in which the Lyapunov exponent is being considered.

In the semiclassical limit ($\hbar \to 0$), the quantum system is expected to reflect the behavior of its classical counterpart. Here, certain quantum quantities, like the decay rate of the Loschmidt echo or the growth rate of OTOCs, can be linked to the classical Lyapunov exponent. For example:

$$F(t) \propto e^{-2\lambda t},$$

for the Lodschmidt echo where λ is the classical Lyapunov exponent.

In the fully quantum regime (away from the semiclassical limit), the classical concept of Lyapunov exponents becomes less meaningful. Quantum coherence, interference, and the finite size of the Hilbert space alter the behavior. For instance, exponential divergence is replaced by saturation or other forms of growth due to quantum effects.

The quantum Lyapunov exponent λ_{Q} approaches, in the semiclassical limit, $\lambda_{\mathrm{Q}} \approx \lambda$, the classical Lyapunov exponent, but in strongly quantum regimes, λ_{Q} can differ significantly. Maldacena, Shenker, and Stanford derived a universal bound for quantum Lyapunov exponents in systems satisfying certain conditions (e.g., holographic systems): $\lambda_{\mathrm{Q}} \leq 2\pi k_B T/\hbar$, where T is the temperature. This bound suggests that in certain cases, λ_{Q} is constrained in ways unrelated to the classical Lyapunov exponent.

Instead, *classical integrable systems*, when quantized, exhibit a more stable behaviour under perturbations due to the regularity of their dynamics. The decay of the Loschmidt echo or growth of the OTOC should be qualitatively slower. For small perturbations, power-law behaviour are expected

$$F(t) \propto t^{-\alpha},$$

where α depends on the perturbation strength and system specifics. The absence of exponential divergence in the classical phase space is reflected in this slower decay. For long times, saturation of the OTOC similarly to chaotic systems but at a higher value due to the reduced sensitivity of the integrable dynamics to perturbations is expected. In some cases, integrable systems may exhibit quasiperiodic revivals of fidelity due to the coherent evolution of the quantum states.

The absence of exponential decay/growth in the Loschmidt echo/OTOCs indicates that integrable systems do not *"scramble" information* efficiently, preserving local structures and correlations over time. This behavior contrasts with chaotic systems, where information spreads rapidly and irreversibly.

Let us now present the definitions of the fidelity, Lodschmidt echo and OTOCs.

Fidelity

The fidelity is a measure of the *closeness* or *overlap* of two quantum states whether they are pure or mixed. For two generic states with density operators $\hat{\rho}$ and $\hat{\varrho}$, respectively, the fidelity is defined as

$$F(\hat{\rho}, \hat{\varrho}) = \left(\mathrm{Tr} \sqrt{\sqrt{\hat{\rho}}\hat{\varrho}\sqrt{\hat{\rho}}} \right)^2 \ . \tag{2.170}$$

If one of the states is pure, say $\hat{\rho} = |\psi\rangle\langle\psi|$, and the other one is not, the fidelity simplifies,

$$F(|\psi\rangle, \hat{\varrho}) = \langle\psi|\hat{\varrho}|\psi\rangle.$$

For two pure states it boils down to the overlap between the two states

$$F(\ \psi\rangle, |\phi\rangle) = |\langle\psi|\phi\rangle|^2 \ . \tag{2.171}$$

Some properties of the fidelity are the following.

- It is constant under unitary transformation,

  $$F(\hat{U}\hat{\rho}\hat{U}^\dagger, \hat{U}\hat{\varrho}\hat{U}^\dagger) = F(\hat{\rho}, \hat{\varrho}),$$

  where $\hat{U}$ is a unitary operator. This property holds because unitary transformations preserve the eigenvalues of the density matrices and the structure of the overlap between quantum states. This invariance is a static property and is not directly related to time evolution. It simply states that fidelity does not change if both states are transformed in the same way.
- It is symmetric in its arguments, i.e. $F(\hat{\rho}, \hat{\varrho}) = F(\hat{\varrho}, \hat{\rho})$. The proof relies on the following properties:
  - The cyclic property of the trace $\mathrm{Tr}(\hat{A}\hat{B}\hat{C}) = \mathrm{Tr}(\hat{C}\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{C}\hat{A})$, for any set of operators $\hat{A}, \hat{B}, \hat{C}$ (as long as the products are well-defined).
  - The square root of a positive semi-definite Hermitian operator $\hat{A}$ (denoted $\sqrt{\hat{A}}$) and multiplied by another Hermitian operator as below satisfies: $(\sqrt{\hat{A}}\hat{B}\sqrt{\hat{A}})^\dagger = \sqrt{\hat{A}}^\dagger \hat{B}^\dagger \sqrt{\hat{A}}^\dagger = \sqrt{\hat{A}}\hat{B}\sqrt{\hat{A}}$ Thus, $\sqrt{\hat{\rho}}\hat{\varrho}\sqrt{\hat{\rho}}$ and $\sqrt{\hat{\varrho}}\hat{\rho}\sqrt{\hat{\varrho}}$ are Hermitian.
  - Equivalent Inner Products. Consider the expression $\sqrt{\hat{\rho}}\hat{\varrho}\sqrt{\hat{\rho}}$. Since $\hat{\rho}$ and $\hat{\varrho}$ are density operators (positive semi-definite and Hermitian), there exists a mathematical equivalence such that:

    $$\sqrt{\sqrt{\hat{\rho}}\hat{\varrho}\sqrt{\hat{\rho}}} \quad \text{and} \quad \sqrt{\sqrt{\hat{\varrho}}\hat{\rho}\sqrt{\hat{\varrho}}}$$

    have the same spectrum of eigenvalues. This equivalence arises because the square roots of $\hat{\rho}$ and $\hat{\varrho}$ commute under the trace and spectral decomposition ensures symmetry between the two arguments.

  Finally, since the fidelity depends only on the trace of the square root, we find that the fidelity is symmetric with respect to its arguments. $F(\hat{\rho}, \hat{\varrho}) = F(\hat{\varrho}, \hat{\rho})$.
- $F(\hat{\rho}, \hat{\varrho})$ lies in $[0, 1]$ by the Cauchy-Schwarz inequality. $F = 1$ indicates that the states are identical, and $F = 0$ means they are orthogonal (completely distinguishable).

- The fidelity does not increase under any quantum operation $\mathcal{E}$:

  $$F(\mathcal{E}(\hat{\rho}_1), \mathcal{E}(\hat{\rho}_2)) \leq F(\hat{\rho}_1, \hat{\rho}_2).$$

  This property is called monotonicity under Completely positive trace-preserving maps.
- It is related to the trace distance $D(\hat{\rho}_1, \hat{\rho}_2) = \frac{1}{2}\|\hat{\rho}_1 - \hat{\rho}_2\|_1$ by

  $$1 - \sqrt{F(\hat{\rho}_1, \hat{\rho}_2)} \leq D(\hat{\rho}_1, \hat{\rho}_2) \leq \sqrt{1 - F(\hat{\rho}_1, \hat{\rho}_2)}.$$

  The definition of $||\hat{A}||_1$ is $||\hat{A}||_1 = \mathrm{Tr}\sqrt{\hat{A}^\dagger \hat{A}}$.
- For product states $\hat{\rho}_1 = \hat{\rho}_A \otimes \hat{\rho}_B$ and $\hat{\rho}_2 = \hat{\varrho}_A \otimes \hat{\varrho}_B$:

  $$F(\hat{\rho}_1, \hat{\rho}_2) = F(\hat{\rho}_A, \hat{\varrho}_A)\, F(\hat{\rho}_B, \hat{\varrho}_B).$$

The fidelity measures how well a prepared quantum state matches the desired target state. It can evaluate the quality of a quantum process, such as quantum gates in quantum computing, it helps quantifying the impact of noise or decoherence on a quantum system, it plays a role in determining the minimum time required to evolve between two quantum states. It can reveal critical points in quantum phase transitions by measuring the change in ground-state overlap.

The fidelity between two states, be them pure or mixed, *evolves over time* due to the quantum evolution of the states. The fidelity remains constant in some special cases: for evolution with identical Hamiltonians, or when the evolution is done with different Hamiltonians $\hat{H}$ and $\hat{H} + \delta\hat{H}$, and $\delta\hat{H}$ commutes with $\hat{H}$. Then, the dynamics do not mix states in a way that reduces the fidelity, and $F(t)$ can remain constant.

The fidelity decay provides insight into the stability of quantum dynamics against perturbations. The key quantity is $F(\psi, \psi_\delta; t) = |\langle\psi, t|\psi_\delta, t\rangle|^2$ where $|\psi_\delta, t\rangle$ is the state evolved with the Hamiltonian used to evolve $|\psi\rangle$ but perturbed in some way that has strength δ.

Example

If the system is a single qubit, $\hat{\rho}$ and $\hat{\varrho}$ have 2×2 matrix representations. The fidelity is then

$$F(\hat{\rho}, \hat{\varrho}) = \mathrm{Tr}(\rho\varrho) + 2\sqrt{\det(\rho)\det(\varrho)} \tag{2.172}$$

This formula takes advantage of the small dimensionality of the Hilbert space, allowing for explicit computation. The proof goes as follows. Any qubit density matrix ρ can be written in the Bloch representation:

$$\rho = \frac{1}{2}\left(I + \vec{r} \cdot \vec{\sigma}\right),$$

where $\vec{r}$ is the Bloch vector ($|\vec{r}| \leq 1$), I is the 2×2 identity matrix, and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. For any density matrix ρ: $\mathrm{Tr}\rho = 1$, and for the qubit $\det\rho = \frac{1}{4}(1 - |\vec{r}|^2)$. Using the Bloch representation, the fidelity simplifies to:

$$F(\rho, \varrho) = \frac{1}{2}\left(1 + \vec{r}_\rho \cdot \vec{r}_\varrho + \sqrt{(1 - |\vec{r}_\rho|^2)(1 - |\vec{r}_\varrho|^2)}\right),$$

where $\vec{r}_\rho$ and $\vec{r}_\varrho$ are the Bloch vectors of ρ and ϱ, respectively. This compact form is particularly useful when working with two-level systems, as it directly relates the fidelity to the geometric properties of the Bloch vectors.

Exercise 2.34 Calculate the fidelity between two pure states $|\psi_1\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}|1\rangle$ and $|\psi_2\rangle = \cos\frac{\phi}{2}|0\rangle + \sin\frac{\phi}{2}|1\rangle$.

Solution. $F(|\psi_1\rangle, |\psi_2\rangle) = |\langle\psi_1|\psi_2\rangle|^2 = \left(\cos\frac{\theta}{2}\cos\frac{\phi}{2} + \sin\frac{\theta}{2}\sin\frac{\phi}{2}\right)^2$. Using the trigonometric identity $\cos a\cos b + \sin a\sin b = \cos(a-b)$, the fidelity is

$$F(|\psi_1\rangle, |\psi_2\rangle) = \cos^2\left(\frac{\theta-\phi}{2}\right).$$

Exercise 2.35 Calculate the fidelity between the pure state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, and the mixed state $\hat{\rho} = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1|$.

The fidelity is $F(|\psi\rangle, \hat{\rho}) = \langle\psi|\hat{\rho}|\psi\rangle = p|\langle 0|\psi\rangle|^2 + (1-p)|\langle 1|\psi\rangle|^2$. For $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, we have $|\langle 0|\psi\rangle|^2 = |\alpha|^2$ and $|\langle 1|\psi\rangle|^2 = |\beta|^2$. Thus,

$$F(|\psi\rangle, \hat{\rho}) = p|\alpha|^2 + (1-p)|\beta|^2.$$

If $|\psi\rangle = |0\rangle$ $(\alpha = 1, \beta = 0)$, then $F = p$, showing fidelity depends directly on the mixed state's weighting of $|0\rangle$.

Exercise 2.36 Let us calculate the fidelity between two mixed states

$$\hat{\rho}_1 = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1|, \qquad \hat{\rho}_2 = q|0\rangle\langle 0| + (1-q)|1\rangle\langle 1|.$$

Diagonal matrices simplify the computation. For $\hat{\rho}_1$ and $\hat{\rho}_2$, the fidelity simplifies to

$$F(\hat{\rho}_1, \hat{\rho}_2) = \left(\sqrt{pq} + \sqrt{(1-p)(1-q)}\right)^2.$$

Exercise 2.37 Fidelity after a quantum gate. Suppose a qubit starts in the state

$$|\psi\rangle = |0\rangle,$$

and undergoes a Hadamard gate

$$\hat{H}|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

Calculate the fidelity between the final and initial state.

The fidelity between the initial state $|0\rangle$ and the final state $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ is:

$$F(|0\rangle, |+\rangle) = |\langle 0|+\rangle|^2 = \frac{1}{\sqrt{2}}(\langle 0|0\rangle + \langle 0|1\rangle)|^2 = \frac{1}{2}$$

Exercise 2.38 Fidelity after decoherence. Suppose a qubit starts in a pure state

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

and undergoes dephasing, resulting in the mixed state

$$\hat{\rho} = |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1|.$$

Calculate the fidelity between the final and the initial state.

The fidelity between the initial state $|\psi\rangle$ and the dephased state $\hat{\rho}$ is

$$F(|\psi\rangle, \hat{\rho}) = \langle\psi|\hat{\rho}|\psi\rangle = |\alpha|^4 + |\beta|^4,$$

since the cross-terms decay under dephasing. This reflects the loss of coherence.

Loschmidt echo

Let us focus on cases in which the Hamiltonian does not depend on time explicitly.

The Loschmidt echo is a measure of the revival occurring when an imperfect time-reversal procedure is applied to a complex quantum system. It allows to quantify the sensitivity of quantum evolution to perturbations. An initial quantum state $|\psi, 0\rangle$ evolves during a time t under a Hamiltonian $\hat{H}_1$ reaching the state $|\psi, t\rangle$. Aiming to recover the initial state $|\psi, 0\rangle$ a new Hamiltonian $-\hat{H}_2$ is applied between t and $2t$. Perfect recovery of $|\psi, 0\rangle$ would be achieved by choosing $\hat{H}_2 = \hat{H}_1$. This is not possible in realistic setups, and there always appears a difference between $\hat{H}_2$ and $\hat{H}_1$, leading to a non-perfect recovery of the initial state. The forward evolution between t and $2t$ under the Hamiltonian $-\hat{H}_2$ is equivalent to a backward evolution from t to 0 under $\hat{H}_2$, which embodies the notion of time-reversal. The Loschmidt echo studies are focused on the cases where the dynamics induced by the Hamiltonians $\hat{H}_1$ and $\hat{H}_2$ are non-trivial, or sufficiently complex (like that of a classically chaotic one-particle system or a many-body system which is quantized).

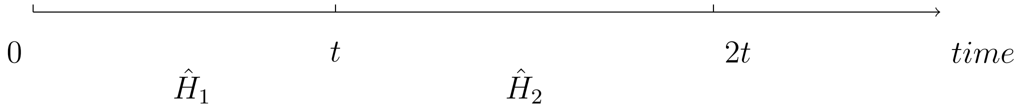

Figure 2.8: Sketch of the Loschmidt echo procedure.

The Loschmidt echo is defined as

$$M(t) = |\langle\psi, t|\psi, 0\rangle|^2 = |\langle\psi, 0|e^{\frac{\mathrm{i}}{\hbar}\hat{H}_2 t - \frac{\mathrm{i}}{\hbar}\hat{H}_1 t}|\psi, 0\rangle|^2 \tag{2.173}$$

It is the (square of the absolute value of) the overlap between the initial state and the one recovered after the forward and backward evolution with the Hamiltonians $\hat{H}_1$ and $\hat{H}_2$, respectively. It is a particular case of fidelity.

The Loschmidt echo is used to quantify quantum chaos but also the effects of decoherence induced by a coupling to an environment.

Out of time order correlations

The Out of Time Order Correlators (OTOC) were first introduced in the analysis of superconductors [65] and were recently considered as a measure of the magnitude of quantum chaos [66]. They measure the sensitivity of a quantum system to small perturbations and is a key quantity in studying quantum chaos and scrambling.

The generic definition is

$$C(t) = \langle [\hat{W}(t), \hat{V}(0)]^\dagger [\hat{W}(t), \hat{V}(0)] \rangle = \mathrm{Tr}\left([\hat{W}(t), \hat{V}(0)]^\dagger [\hat{W}(t), \hat{V}(0)] \hat{\rho} \right) \tag{2.174}$$

where $\hat{W}(t)$ and $\hat{V}(0)$ are two operators in the Heisenberg representation and $\hat{\rho}$ is the density operator. They depend on time and temperature and can be used in systems with or without classical analogue.

The definition above holds for an arbitrary pair of operators and density operator. However, one typically restricts to Hermitian operators and works with

$$C(t) = -\langle [\hat{W}(t), \hat{V}(0)]^2 \rangle \tag{2.175}$$

Moreover, one uses a thermal density operator $\hat{\rho} = \mathcal{Z}^{-1} e^{-\beta \hat{H}}$ and then $C(t)$ depends on time and tempeature.

Sometimes regularizations, that change slightly the definition above and are supposed to not modify the long-time limit (though this is not obvious and sometimes not even true) are used

$$C_{\mathrm{reg}}(t) = \mathrm{Tr}\left(\hat{\rho}^{1/2} [\hat{W}(t), \hat{V}(0)]^\dagger \hat{\rho}^{1/2} [\hat{W}(t), \hat{V}(0)] \right) \tag{2.176}$$

$$C_{\mathrm{reg}}(t) = \mathrm{Tr}\left([\hat{\rho}^{1/4} \hat{W}(t), \hat{\rho}^{1/4} \hat{V}(0)]^\dagger \hat{\rho}^{1/2} [\hat{W}(t), \hat{V}(0)] \right) \tag{2.177}$$

The relation to chaos can be justified from the semiclassical limit. Consider position and momentum operators, $\hat{x}(t)$ and $\hat{p}(t)$, in a quantum system. Their OTOC is $C(t) = -\langle [\hat{x}(t), \hat{p}(0)]^2 \rangle$. In the semiclassical limit one can replace the commutator by the Poisson bracket

$$[\hat{x}(t), \hat{p}(0)] \mapsto \mathrm{i}\hbar \{x(t), p(0)\} = \mathrm{i}\hbar \frac{\delta x(t)}{\delta x(0)} \ , \tag{2.178}$$

which measures the sensitivity of $x(t)$ to changes in the initial condition. For a classically chaotic system with a Lyapunov exponent λ, one has $\delta x(t)/\delta x(0) \sim e^{\lambda t}$. The reason to include the square in the definition is that, assuming that one can replace the commutator by the Poisson bracket in the semiclassical limit, the growth would be $e^{\lambda t}$ but with no definite sign. The thermal average would then yield a vanishing result as positive and negative contributions would cancel. Thus, the analogy states that the OTOC should grow as $\hbar^2 e^{2\lambda t}$ and the Lyapunov exponent λ of the quantum system could be read from it.

The growth of the OTOC is associated with the spread of quantum information. This is shown by choosing $\hat{W}$ and $\hat{V}$ to be operators that act locally in space-like separated regions (so that $[\hat{W}, \hat{V}] = 0$). A visual example is the one of a chain with nearest-neighbour interactions, $\hat{W}$ located at the middle of the chain, and $\hat{V}$ ℓ sites away to the left. The Baker-Campbell-Hausdorff formula for the expansion of $\hat{W}(t)$ yields the nested commutator expression

$$\hat{W}(t) = \sum_{k=0}^{\infty} \frac{(it)^k}{k!} \underbrace{[\hat{H}, \dots [\hat{H}}_{k}, \hat{W}] \dots] \tag{2.179}$$

The operator $\hat{W}$ spreads over the chain as time elapses. with an increasing number of sites around the initial one being involved. There is a symmetric propagation cone. Eventually the site of the operator $\hat{V}$ is reached by the propagation. The OTOC is expected to depend on $x - vt$ with velocity v limited by the Lieb-Robinson bound [71] for the speed of correlations spreading in non-relativistic quantum systems.

The OTOC of quantum systems does not grow unbounded but saturates at the Ehrenfest time t_E. The Ehrenfest time is defined by the time scale beyond which the wave function spreads over the whole system. It is roughly characterized as a boundary between a particle-like behavior and a wave-like behavior of the wave function.

Maldacena, et al. conjectured in 2016 the existence of an upper bound to the growth-rate of the OTOC, essentially given by the temperature of the system [67]. This bound can be viewed as a consequence of the fluctuation-dissipation theorem [68]. Systems saturating the bound, as black holes do, are called *fast scramblers*. In the Sachdev-Ye-Kitaev model [69,70] (which is a kind of spin-glass model) for strongly correlated fermions the bound is also saturated [70].

In summary,

- Integrable systems: The OTOC remains near its initial value or oscillates, indicating little scrambling.
- Chaotic Systems: The OTOC decays exponentially at early times, indicating rapid scrambling of quantum information. The decay rate is related to the system's Lyapunov exponent in the classical analog, a hallmark of chaos.
- Thermal Systems: The OTOC can saturate at long times, reflecting thermal equilibrium and loss of detailed quantum information.

Example

Consider a single qubit, $\hat{W} = \hat{\sigma}^x$ and $\hat{V} = \hat{\sigma}^z$, with the qubit governed by the Hamiltonian

$$\hat{H} = \frac{\hbar\omega}{2}\hat{\sigma}_z.$$

Using the Heisenberg equation of motion

$$\frac{d\hat{W}(t)}{dt} = \frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{W}(t)],$$

we find that the Pauli operators evolve under $\hat{H}$ as:

$$\hat{\sigma}^x(t) = e^{\mathrm{i}\hat{H}t/\hbar}\hat{\sigma}^x e^{-\mathrm{i}\hat{H}t/\hbar}.$$

For $\hat{H} = \frac{\hbar\omega}{2}\hat{\sigma}_z$, the commutator $[\hat{H}, \hat{\sigma}_x]$ gives:

$$[\hat{H}, \hat{\sigma}_x] = -i\hbar\omega\hat{\sigma}_y.$$

Iterating the Heisenberg equation, we find

$$\hat{\sigma}^x(t) = \hat{\sigma}^x\cos(\omega t) - \hat{\sigma}^y\sin(\omega t).$$

We now compute OTOC(t) for $\hat{W} = \hat{\sigma}^x$ and $\hat{V} = \hat{\sigma}^z$. Substituting the time-evolved $\hat{W}(t) = \hat{\sigma}^x(t)$:

$$\text{OTOC}(t) = \langle \hat{\sigma}^x(t)\hat{\sigma}^z\hat{\sigma}^x(t)\hat{\sigma}^z \rangle.$$

Substitute $\hat{\sigma}^x(t) = \hat{\sigma}^x\cos(\omega t) - \hat{\sigma}^y\sin(\omega t)$:

$$\hat{\sigma}_x(t)\hat{\sigma}^z = (\hat{\sigma}^x\cos(\omega t) - \hat{\sigma}^y\sin(\omega t))\,\hat{\sigma}^z.$$

Using the Pauli matrix commutation relations:

$$\hat{\sigma}^x\hat{\sigma}_z = -\hat{\sigma}_z\hat{\sigma}^x, \quad \hat{\sigma}^y\hat{\sigma}^z = -\hat{\sigma}^z\hat{\sigma}^y$$

we find

$$\hat{\sigma}^x(t)\hat{\sigma}^z = -\hat{\sigma}^z\hat{\sigma}^x\cos(\omega t) + \hat{\sigma}^z\hat{\sigma}^y\sin(\omega t).$$

Squaring this:

$$\hat{\sigma}^x(t)\hat{\sigma}^z\hat{\sigma}^x(t)\hat{\sigma}^z = \cos^2(\omega t) + \sin^2(\omega t) = 1.$$

For this specific case, the OTOC is:

$$\text{OTOC}(t) = 1.$$

This indicates no scrambling of quantum information, as expected for a single qubit governed by a simple integrable Hamiltonian. In more complex systems (e.g., multi-qubit systems with chaotic interactions), the OTOC typically decays over time, indicating scrambling.

Example

A simple solvable example where the OTOC decays over time involves two interacting qubits with a coupling term that can generate entanglement and quantum scrambling.
Consider a system of two qubits with the Hamiltonian:

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{\sigma}_z^{(A)} + \hat{\sigma}_z^{(B)}) + J\hat{\sigma}_z^{(A)}\hat{\sigma}_z^{(B)},$$

with the same notation as in the previous example, and J the interaction strength (Ising-type coupling). This Hamiltonian is diagonal in the computational basis, making it solvable while still capable of exhibiting non-trivial OTOC decay. Choose the operators: $\hat{W} = \hat{\sigma}_x^{(A)}$ (acting on qubit A) and $\hat{V} = \hat{\sigma}_z^{(B)}$ (acting on qubit B). The OTOC is

$$\text{OTOC}(t) = \langle \hat{\sigma}_x^{(A)}(t)\hat{\sigma}_z^{(B)}\hat{\sigma}_x^{(A)}(t)\hat{\sigma}_z^{(B)} \rangle,$$

where $\hat{\sigma}_x^{(A)}(t) = \hat{\sigma}_x^{(A)}(t) = e^{\mathrm{i}\hat{H}t/\hbar}\hat{\sigma}_x^{(A)}e^{-\mathrm{i}\hat{H}t/\hbar}$ is the time-evolved $\hat{\sigma}_x^{(A)}$ in the Heisenberg picture. Using the commutator $[\hat{H}, \hat{\sigma}_x^{(A)}]$, we find

$$\hat{\sigma}_x^{(A)}(t) = \hat{\sigma}_x^{(A)}\cos(2Jt) + \hat{\sigma}_y^{(A)}\hat{\sigma}_z^{(B)}\sin(2Jt).$$

This shows that $\hat{\sigma}_x^{(A)}(t)$ depends explicitly on the coupling J and introduces correlations with $\hat{\sigma}_z^{(B)}$, a necessary ingredient for OTOC decay. Substituting $\hat{\sigma}_x^{(A)}(t)$ in the product of first two factors within the OTOC:

$$\hat{\sigma}_x^{(A)}(t)\hat{\sigma}_z^{(B)} = \left(\hat{\sigma}_x^{(A)}\cos(2Jt) + \hat{\sigma}_y^{(A)}\hat{\sigma}_z^{(B)}\sin(2Jt)\right)\hat{\sigma}_z^{(B)}$$

and using the Pauli matrix commutation rules,

$$\hat{\sigma}_z^{(B)}\hat{\sigma}_z^{(B)} = \mathbb{I}, \quad \hat{\sigma}_y^{(A)}\hat{\sigma}_z^{(B)} = -\hat{\sigma}_z^{(B)}\hat{\sigma}_y^{(A)},$$

we find

$$\hat{\sigma}_x^{(A)}(t)\hat{\sigma}_z^{(B)} = \hat{\sigma}_x^{(A)}\cos(2Jt) - \hat{\sigma}_y^{(A)}\sin(2Jt).$$

Squaring this expression to compute the full OTOC:

$$\hat{\sigma}_x^{(A)}(t)\hat{\sigma}_z^{(B)}\hat{\sigma}_x^{(A)}(t)\hat{\sigma}_z^{(B)} = \cos^2(2Jt) + \sin^2(2Jt) - [\text{cross terms decay under expectation values}].$$

For initial product states like $|00\rangle$, the cross terms vanish, and the OTOC simplifies to:

$$\text{OTOC}(t) = \cos^2(2Jt).$$

This demonstrates oscillatory decay of the OTOC, reflecting how the interaction strength J generates scrambling of information between the two qubits. While not exponential (as in chaotic systems), the decay shows sensitivity to the coupling and time evolution, making it a simple example of entanglement and scrambling dynamics.

3 Correlation functions

In this Section we introduce some generic points: the no-cloning theorem, correlation and linear response functions and we discuss several of their properties.

Linear response functions are especially important since they are measured experimentally. For example, the electrical conductivity is the response to a weak applied field, the thermal conductivity the response to a thermal gradient, etc.

Some correlation functions have analytic properties that do not depend on the microscopic model considered. It is very important to keep them in mind to check whether approximation schemes satisfy these exact properties and, when formulating phenomenological models, be sure that they are consistent. Approximate calculations do not always satisfy all known exact relations, and one then has to choose violating the less harmful ones.

A detailed discussion of linear response theory and the symmetry properties of correlations and Green functions can be found in [29].

Under equilibrium conditions linear response function are related to some correlation functions. These relations are called fluctuation-dissipation theorems, and they also have to be preserved in any treatment of model systems in equilibrium.

3.1 Expectation values and correlation functions

We focus on systems with time-independent Hamiltonians. Go to the Heisenberg picture in which the operators depend on time while states do not. A generic operator $\hat{A}$ in the Schödinger picture transforms into the Heisenberg one

$$\hat{A}(t) = e^{\mathrm{i}\hat{H}t/\hbar}\hat{A}e^{-\mathrm{i}\hat{H}t/\hbar} = \hat{U}^\dagger(t)\hat{A}\hat{U}(t) \; . \tag{3.180}$$

The expected value of $\hat{A}$ is

$$\langle \hat{A}(t)\rangle = \mathrm{Tr}[\hat{A}(t)\hat{\rho}_0] \tag{3.181}$$

where $\hat{\rho}_0$ is the (already normalised) initial density operator. In Boltzmann equilibrium at inverse temperature β,

$$\hat{\rho}_0 = \frac{e^{-\beta\hat{H}}}{\mathrm{Tr}e^{-\beta\hat{H}}} \; . \tag{3.182}$$

In these cases, the evolution operators $e^{\pm i\hat{H}t/\hbar}$ in $\hat{A}(t)$ commute with $\hat{\rho}_0$ and using the cyclic property of the trace they cancel each other. Then,

$$\langle \hat{A}(t)\rangle = \mathrm{Tr}[\hat{A}\hat{\rho}_0] \; . \tag{3.183}$$

A bit more generally, *one-time observables* are *time-independent* in any system with $\hat{\rho}_0(\hat{H})$.

The term *Green function* refers specifically to correlators of field operators or creation and annihilation operators. In this respect, *correlation functions* are more general as they correlate any kind of observables. Still, the two terms are sometimes used interchangeably. The *zero-temperature time-ordered self-correlation function* of an operator $\hat{A}$ is defined as

$$C_{AA}(t,t') \equiv \langle 0|\mathcal{T}[\hat{A}(t)\hat{A}(t')]|0\rangle \tag{3.184}$$

where $\hat{A}(t)$ and $\hat{A}(t')$ are time-dependent and $|0\rangle$ is the ground state of $\hat{H}$ which does not depend on time. $\mathcal{T}$ is the time-ordering operator

$$\mathcal{T}[\hat{A}(t)\hat{A}(t')] = \hat{A}(t)\hat{A}(t')\theta(t-t') + \hat{A}(t')\hat{A}(t)\theta(t'-t) \tag{3.185}$$

($\theta(y) = 1$ for $y > 0$, $\theta(y) = 0$ for $y < 0$, and there is some freedom in the choice of $\theta(0)$ which we take to be $\theta(0) = 1/2$.)

The *finite-temperature time-ordered self-correlation function* of the operator $\hat{A}$ is defined as

$$C_{AA}(t,t') = \frac{\text{Tr}\ \{\mathcal{T}[\hat{A}(t)\hat{A}(t')]e^{-\beta\hat{H}}\}}{\text{Tr}\ e^{-\beta\hat{H}}} = \frac{\sum_n \langle n|\mathcal{T}[\hat{A}(t)\hat{A}(t')]e^{-\beta E_n}|n\rangle}{\sum_n e^{-\beta E_n}}\ , \tag{3.186}$$

where $|n\rangle$ is a complete set of eigenstates of $\hat{H}$ and each matrix element is weighted with the corresponding Boltzmann factor.

Note that one could define time-ordered correlation functions in out of equilibrium systems by using a $\hat{\rho}_0$ which is not the Boltzmann one.

These definitions can be straightforwardly extended to cases with two (or more) different operators $\hat{A}$ and $\hat{B}$.

The (equilibrium) two-time correlation is *stationary,* that is, depends only on $t-t'$, as can be checked from its very definition. Take the generic case of two different operators $\hat{A}$ and $\hat{B}$, and choose $t > t'$. Then, replacing the Heisenberg operators by their expressions in terms of time-independent ones:

$$\begin{aligned} C_{AB}(t,t') &= \frac{\text{Tr}[e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}e^{i\hat{H}t'/\hbar}\hat{B}e^{-i\hat{H}t'/\hbar}e^{-\beta\hat{H}}]}{\text{Tr}e^{-\beta\hat{H}}} \\ &= \frac{\text{Tr}[e^{i\hat{H}(t-t')/\hbar}\hat{A}e^{-i\hat{H}(t-t')/\hbar}\hat{B}e^{-\beta\hat{H}}]}{\text{Tr}e^{-\beta\hat{H}}} \\ &= C_{AB}(t-t',0) \ = \ \overline{C}_{AB}(t-t')\ . \end{aligned} \tag{3.187}$$

(The overline is just to indicate that the functional form is different from the starting one, which was a function of two variables. This distinction is often ignored.) The cyclic property of the trace, and the commutation of the evolution operator with the Boltzmann factor (same $\hat{H}$ involved) allowed one to rewrite all evolution operators as functions of $t-t'$. A similar procedure can be used in the case $t' > t$. One usually uses the same notation (C_{AB}) for the function of two times in the left-hand-side and the one of only one time-difference in the right-hand-side though these are two different functions. The stationarity property is also called *time translation invariance* since

$$C_{AB}(t,t') = C_{AB}(t+\delta t, t'+\delta t) \qquad \text{for any} \quad \delta t \tag{3.188}$$

if C_{AB} depends only on the time difference.

We note that the very much studied *quantum quenches* - both theoretically and experimentally - consist in preparing an initial state with one Hamiltonian, $\hat{H}_1$, and evolving it with another Hamiltonian, $\hat{H}_2$. in these cases, the correlation functions need not be stationary.

The term Green function, is usually reserved to the correlation of fields, or creation and annihilation operators. e.g. $\hat{c}(t)$ and $\hat{c}^\dagger(t')$, with the latter creating an excitation at t' and the former destroying it at t. At zero temperature the two-point Green function or *propagator* is

$$G(t,t') = i\langle 0|\mathcal{T}c(t)c^\dagger(t')|0\rangle \tag{3.189}$$

and the finite temperature generalisation is obvious. A good summary of the properties of Green functions is here
`https://en.wikipedia.org/wiki/Green%27s_function_(many-body_theory)`

3.2 Linear response and the Kubo formula

We start by giving the definition of the *instantaneous linear response* of an Hermitian observable $\hat{A}$ to a perturbation linearly coupled to another Hermitian observable $\hat{B}$, in such a way that $\hat{H} \mapsto \hat{H} - h\hat{B}$ between the instants t' and $t'+\epsilon$ with ϵ infinitesimal. We then calculate it by treating the strength of the change, h, as a perturbation, taking the full interacting Hamiltonian of the system $\hat{H}$ as the unperturbed Hamiltonian.

First, we write $\langle \hat{A}(t)\rangle_B$ with the evolution generated by $\hat{H}$ from time 0 to t', $\hat{H}-h\hat{B}$ from t' to $t'+\epsilon$, and $\hat{H}$ from $t'+\epsilon$ to t. Note that we are assuming $t \geq t'$. The full evolution operator is then

$$\begin{aligned} \hat{U}_h(t,0) &= e^{-i\hat{H}(t-t'-\epsilon)/\hbar} e^{-i(\hat{H}-h\hat{B})\epsilon/\hbar} e^{-i\hat{H}t'/\hbar} \,, \\ \hat{U}_h^\dagger(t,0) &= e^{i\hat{H}t'/\hbar} e^{i(\hat{H}-h\hat{B})\epsilon/\hbar} e^{i\hat{H}(t-t'-\epsilon)/\hbar} \,. \end{aligned} \tag{3.190}$$

Note that we used $\hat{B}^\dagger = \hat{B}$. We do not worry about the possible non-commutativity of $\hat{H}$ and $\hat{B}$ since both $h \to 0$ and $\epsilon \to 0$ let us factorise the exponentials. Moreover, we can Taylor expand the exponential of $\hat{B}$ in the middle factor and get

$$\begin{aligned} \hat{U}_h(t,0) &\sim e^{-i\hat{H}(t-t'-\epsilon)/\hbar} e^{-i\hat{H}\epsilon/\hbar}[1 + i(h\epsilon/\hbar)\hat{B} + \mathcal{O}((\epsilon h)^2)] e^{-i\hat{H}t'/\hbar} \\ &\sim e^{-i\hat{H}(t-t')/\hbar}[1 + i(h\epsilon/\hbar)\hat{B} + \mathcal{O}((\epsilon h)^2)] e^{-i\hat{H}t'/\hbar} \end{aligned} \tag{3.191}$$

and similarly for $\hat{U}_h^\dagger$. Then,

$$\begin{aligned} \left.\frac{\delta}{\delta\epsilon h}\hat{U}_h(t,0)\right|_{h=0} &= e^{-i\hat{H}(t-t')/\hbar}\frac{\mathrm{i}}{\hbar}\hat{B}e^{-i\hat{H}t'/\hbar} \,, \\ \left.\frac{\delta}{\delta\epsilon h}\hat{U}_h^\dagger(t,0)\right|_{h=0} &= -e^{i\hat{H}t'/\hbar}\frac{\mathrm{i}}{\hbar}\hat{B}e^{i\hat{H}(t-t')/\hbar} \,, \end{aligned} \tag{3.192}$$

where we already dropped higher order contributions in h which vanish for $h \to 0$. The *instantaneous linear response function* is defined as

$$R_{AB}(t,t') \equiv \left.\frac{\delta \langle \hat{A}(t)\rangle_B}{\delta \epsilon h}\right|_{h=0} = \left.\frac{\delta}{\delta \epsilon h} \mathrm{Tr}[\hat{U}_h^\dagger(t,0)\hat{A}\hat{U}_h(t,0)\hat{\rho}_0]\right|_{h=0} , \tag{3.193}$$

and the information about the coupling to $\hat{B}$ is in the $\hat{U}_h$ and $\hat{U}_h^\dagger$. The first contribution comes from the variation of the $\hat{U}_h^\dagger$:

$$\begin{aligned} \mathrm{Tr}\left[\frac{\delta}{\delta\epsilon h}\left(\hat{U}_h^\dagger(t,0)\right)\hat{A}\hat{U}_0(t,0)\hat{\rho}_0\right]\Bigg|_{h=0} &= -\frac{\mathrm{i}}{\hbar}\mathrm{Tr}\left[e^{i\hat{H}t'/\hbar}\hat{B}e^{i\hat{H}(t-t')/\hbar}\hat{A}\hat{U}_0(t,0)\hat{\rho}_0\right] \\ = -\frac{\mathrm{i}}{\hbar}\mathrm{Tr}\left[e^{i\hat{H}t'/\hbar}\hat{B}e^{i\hat{H}(t-t')/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}\hat{\rho}_0\right] &= -\frac{\mathrm{i}}{\hbar}\langle\hat{B}(t')\hat{A}(t)\rangle \end{aligned} \tag{3.194}$$

and the second one from the variation of $\hat{U}_h$

$$\begin{aligned} \mathrm{Tr}\left[\hat{U}_0^\dagger(t,0)\hat{A}\frac{\delta}{\delta\epsilon h}\left(\hat{U}_h(t,0)\right)\hat{\rho}_0\right]\Bigg|_{h=0} &= \frac{\mathrm{i}}{\hbar}\mathrm{Tr}\left[\hat{U}_0^\dagger(t,0)\hat{A}e^{-i\hat{H}(t-t')/\hbar}\hat{B}e^{-i\hat{H}t'/\hbar}\hat{\rho}_0\right] \\ = \frac{\mathrm{i}}{\hbar}\mathrm{Tr}\left[e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}(t-t')/\hbar}\hat{B}e^{-i\hat{H}t'/\hbar}\hat{\rho}_0\right] &= \frac{\mathrm{i}}{\hbar}\langle\hat{A}(t)\hat{B}(t')\rangle . \end{aligned} \tag{3.195}$$

In the end we have

$$R_{AB}(t,t') = \frac{\mathrm{i}}{\hbar}\langle[\hat{A}(t),\hat{B}(t')]\rangle\theta(t-t') \tag{3.196}$$

where we introduced the θ function that ensures *causality*, since the system cannot respond to a perturbation which has not been applied yet. The square brackets denote the commutator of $\hat{A}$ and $\hat{B}$ and we stress the fact that the right-hand-side is calculated without the external perturbation. In cases in which the observables $\hat{A}$ and $\hat{B}$ are simply replaced by say creation and annihilation operators, the right-hand-side is related to the *retarded Green function*.

We note that this is a model independent *Kubo formula*. Nowhere in this derivation we used a particular form of $\hat{\rho}_0$. This relation is actually valid beyond any equilibrium hypothesis. The proof above can be applied to field theories, in which the perturbation can be localised in space.

Linear response theory implies that the influence of two subsequent kicks of time-length ϵ is equal to the one of a single kick of time-length 2ϵ, that is, the effect of the perturbations is *additive*. In this way, one derives the time-delayed *susceptibility*

$$\chi_{AB}(t,t') = \int_{t'}^{t} dt''\ R_{AB}(t,t'') \tag{3.197}$$

as the result of a perturbation applied during a finite (and not infinitesimal) time-interval going from t' to t.

Another way of writing the linear response relation is

$$\langle \hat{A}(t)\rangle_B = \int_{-\infty}^{\infty} dt''\, R_{AB}(t,t'')h(t'') \tag{3.198}$$

which is just the integral version of the instantaneous (3.193). If we focus on stationary situations, the right-hand-side is a time convolution. In Fourier

$$\tilde{R}_{AB}(\omega) = \int dt\, e^{i\omega t} R_{AB}(t)\ , \qquad\qquad R_{AB}(t) = \int \frac{d\omega}{2\pi}\, e^{-i\omega t}\tilde{R}_{AB}(\omega)\ , \tag{3.199}$$

the relation above then reads

$$\langle \tilde{A}(\omega)\rangle_B = \tilde{R}_{AB}(\omega)\tilde{h}(\omega) \tag{3.200}$$

and is *local in ω*: the response is at the same frequency as the external field. This feature does not survive if higher order terms in the perturbation are kept to calculate non-linear responses.

Under equilibrium conditions, $\hat{\rho}_0 \propto e^{-\beta\hat{H}}$, one finds that the linear response is stationary, as any other correlation function.

3.3 Linear response and Onsager relations

The response function is expressed in terms of a commutator of Hermitian operators times a theta function that imposes causality. Let us focus on the first factor and define

$$\hbar R''_{AB}(t,t') \equiv \langle [\hat{A}(t), \hat{B}(t')]\rangle\ . \tag{3.201}$$

The response$''$ of the operator $\hat{B}$ to an external perturbation that couples to $\hat{A}$ is simply related to the response$''$ of $\hat{A}$ to a perturbation that couples to $\hat{B}$; in other words, the operators have reversed roles:

$$\left.\begin{array}{l} \hbar R''_{AB}(t,t') = \langle [\hat{A}(t), \hat{B}(t')]\rangle \\ \hbar R''_{BA}(t',t) = \langle [\hat{B}(t'), \hat{A}(t)]\rangle \end{array}\right\} \quad \Longrightarrow \quad R''_{AB}(t,t') = -R''_{BA}(t',t)\ . \tag{3.202}$$

These are *Onsager's reciprocity relations*.

3.4 Causality and the Kramers-Kronig relations

The causality of the real-time linear response is ensured by the analyticity of $\mathrm{Im}\tilde{R}_{AB}(\omega)$ in the upper half complex plane. This is proved as follows. Write

$$R_{AB}(t,t') = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')}\tilde{R}_{AB}(\omega) \tag{3.203}$$

where we assumed that the linear response is stationary.[1] Focus on $t - t' < 0$, extend $\omega \to z \in \mathbb{C}$ and close the contour in the upper half plane. The exponential $e^{-i\omega(t-t')} \propto e^{-iiz_I(t-t')} = e^{z_I(t-t')}$ falls off exponentially and, if we take $\tilde{R}_{AB}(z)$ to be analytic in this half plane, the resulting integral vanishes. This argument shows that analyticity is a sufficient condition to get $R_{AB}(t,t') \propto \theta(t-t')$. One can also argue for necessity (we will not show it here).

Assuming now that $\tilde{R}_{AB}(\omega)$ is analytic in the upper half plane, and hence $R_{AB}(t,t')$ is causal, one can derive the Kramers-Kronig relations which relate real and imaginary parts of the response functions and read

$$\begin{aligned} \mathrm{Re}\tilde{R}_{AB}(\omega) &= -P\int \frac{d\omega'}{\pi}\,\frac{\mathrm{Im}R_{AB}(\omega')}{\omega-\omega'}\ , \\ \mathrm{Im}\tilde{R}_{AB}(\omega) &= \ \ P\int \frac{d\omega'}{\pi}\,\frac{\mathrm{Re}R_{AB}(\omega')}{\omega-\omega'}\ . \end{aligned} \tag{3.204}$$

The proof goes as follows. First,

$$\begin{aligned} \int \frac{d\omega'}{\pi}\frac{1}{\omega'-\omega-i\eta}\,\tilde{R}_{AB}(\omega') &= 2i\oint \frac{dz}{2\pi i}\frac{1}{z-\omega-i\eta}\,\tilde{R}_{AB}(z) \\ &= 2i\tilde{R}_{AB}(\omega+i\eta) \end{aligned} \tag{3.205}$$

where we assumed that $\tilde{R}_{AB}(z)$ falls to zero sufficiently fast at infinity.

Next, the identity

$$\begin{aligned} \lim_{\eta\to 0}\frac{1}{\omega \mp i\eta} = \lim_{\eta\to 0}\frac{\omega \pm i\eta}{\omega^2+\eta^2} &= \lim_{\eta\to 0}\left[\frac{\omega}{\omega^2+\eta^2} \pm \frac{i\eta}{\omega^2+\eta^2}\right] \\ &= P\frac{1}{\omega} \pm i\pi\delta(\omega) \end{aligned} \tag{3.206}$$

P is the *principal part*. (Take this as a definition of the principal part.)

Now, applying (3.206) to (3.205) in the limit $\eta \to 0$, and taking the real part of the result of the lhs:

$$\begin{aligned} \mathrm{lhs} &= \mathrm{Re}\lim_{\eta\to 0}\int \frac{d\omega'}{\pi}\frac{1}{\omega'-\omega-i\eta}\,\tilde{R}_{AB}(\omega') \\ &= -P\int \frac{d\omega'}{\pi}\frac{1}{\omega-\omega'}\,\mathrm{Re}\tilde{R}_{AB}(\omega') + \mathrm{Im}\tilde{R}_{AB}(\omega) \end{aligned} \tag{3.207}$$

and of the rhs

$$\mathrm{rhs} = 2\mathrm{Im}\lim_{\eta\to 0}\tilde{R}_{AB}(\omega+i\eta) = 2\mathrm{Im}\tilde{R}_{AB}(\omega)\ . \tag{3.208}$$

---

[1] In non-stationary cases one can rewrite the two time dependence as a dependence on t' and $t - t'$ and Fourier transform with respect to the time difference. The results below also apply in these cases at fixed t'.

Thus, the equality between the two yields the first Kramers-Kronig relation in (3.204). The imaginary part of the same operation yields

$$\begin{aligned}
\text{lhs} &= \text{Im}\lim_{\eta\to 0}\int\frac{d\omega'}{\pi}\frac{1}{\omega'-\omega-i\eta}\,\tilde{R}_{AB}(\omega') \\
&= -P\int\frac{d\omega'}{\pi}\frac{1}{\omega-\omega'}\,\text{Im}\tilde{R}_{AB}(\omega')+\text{Re}\tilde{R}_{AB}(\omega) \qquad (3.209)
\end{aligned}$$

and of the rhs

$$\text{rhs} = 2\text{Re}\lim_{\eta\to 0}\tilde{R}_{AB}(\omega+i\eta) = 2\text{Re}\tilde{R}_{AB}(\omega) \qquad (3.210)$$

and hence the second Kramers-Kronig relation in (3.204).

For the *spectral representation* of the linear response see [29].

3.5 The KMS relations

The cyclic properties of the trace and a Boltzmann density operator yield the so-called KMS (Kadanoff-Martin-Schwinger) relations. Take a canonical equilibrium correlation between two operators measured at different times,

$$C_{AB}(t,t') = \langle\hat{A}(t)\hat{B}(t')\rangle = \frac{\text{Tr}[e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}e^{i\hat{H}t'/\hbar}\hat{B}e^{-i\hat{H}t'/\hbar}e^{-\beta\hat{H}}]}{\text{Tr}e^{-\beta\hat{H}}}\ . \qquad (3.211)$$

Inserting identities and moving the factors around one can show

$$\langle\hat{A}(t)\hat{B}(t')\rangle = \langle\hat{B}(t')\hat{A}(t+i\beta\hbar)\rangle = \langle\hat{B}(-t-i\beta\hbar)\hat{A}(-t')\rangle \qquad (3.212)$$

which can also be written as

$$C_{AB}(t,t') = C_{BA}(t',t+i\beta\hbar) = C_{BA}(-t-i\beta\hbar,-t')\ . \qquad (3.213)$$

As way of example, let us prove the first of these expressions.

$$\begin{aligned}
C_{AB}(t,t') &= \frac{\text{Tr}[e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}e^{i\hat{H}t'/\hbar}\hat{B}e^{-i\hat{H}t'/\hbar}e^{-\beta\hat{H}}]}{\text{Tr}e^{-\beta\hat{H}}} \\
&= \frac{\text{Tr}[e^{i\hat{H}t/\hbar}e^{-\beta\hat{H}}e^{\beta\hat{H}}\hat{A}e^{\beta\hat{H}}e^{-\beta\hat{H}}e^{-i\hat{H}t/\hbar}e^{i\hat{H}t'/\hbar}\hat{B}e^{-i\hat{H}t'/\hbar}e^{-\beta\hat{H}}]}{\text{Tr}e^{-\beta\hat{H}}} \\
&= \frac{\text{Tr}[e^{i\hat{H}(t+i\beta\hbar)/\hbar}\cancel{e^{\beta\hat{H}}}\hat{A}e^{-i\hat{H}(t+i\beta\hbar)/\hbar}e^{-\beta\hat{H}}e^{i\hat{H}t'/\hbar}\hat{B}e^{-i\hat{H}t'/\hbar}\cancel{e^{-\beta\hat{H}}}]}{\text{Tr}e^{-\beta\hat{H}}} \\
&= \frac{\text{Tr}[e^{i\hat{H}t'/\hbar}\hat{B}e^{-i\hat{H}t'/\hbar}e^{i\hat{H}(t+i\beta\hbar)/\hbar}\hat{A}e^{-i\hat{H}(t+i\beta\hbar)/\hbar}e^{-\beta\hat{H}}]}{\text{Tr}e^{-\beta\hat{H}}} \\
&= \langle\hat{B}(t')\hat{A}(t+i\beta\hbar)\rangle\ . \qquad (3.214)
\end{aligned}$$

The other relations follow from similar steps.

Having assumed equilibrium conditions the correlation functions are stationary, and depend only on the difference between the two times involved, e.g. $C_{AB}(t,t') = C_{AB}(t-t')$. They can then be Fourier transformed,

$$C_{AB}(t-t') = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \tilde{C}_{AB}(\omega) \tag{3.215}$$

as well as the full KMS relations (3.213), which in Fourier space read

$$\tilde{C}_{AB}(\omega) = e^{\beta\hbar\omega} \tilde{C}_{BA}(-\omega) \; . \tag{3.216}$$

3.6 The fluctuation-dissipation theorem

Let us define *symmetrized and anti-symmetrized* correlation functions

$$\begin{aligned} C_{[A,B]}(t,t') &= \frac{1}{2}\langle [\hat{A}(t), \hat{B}(t')] \rangle \; , \\ C_{\{A,B\}}(t,t') &= \frac{1}{2}\langle \{\hat{A}(t), \hat{B}(t')\} \rangle \; , \end{aligned} \tag{3.217}$$

which we assume are also *time-translational invariant*. Fourier transforming

$$\begin{aligned} 2\tilde{C}_{[A,B]}(\omega) &= [1 - e^{-\beta\hbar\omega}] \tilde{C}_{AB}(\omega) \; , \\ 2\tilde{C}_{\{A,B\}}(\omega) &= [1 + e^{-\beta\hbar\omega}] \tilde{C}_{AB}(\omega) \; . \end{aligned} \tag{3.218}$$

Taking the ratio between these two,

$$\tilde{C}_{[A,B]}(\omega) = \tanh\left(\frac{\beta\hbar\omega}{2}\right) \tilde{C}_{\{A,B\}}(\omega) \; . \tag{3.219}$$

We go back to the Kubo relation to replace the commutator by the linear response. However, one has to be careful, because these two, though proportional to each other in the time domain, have in front the theta function which ensures causality. Therefore, the Fourier transform has to be taken with care. One can replace in the right-hand-side of Eq. (3.196) the Fourier representation of the commutator, taken to be stationary since in equilibrium,

$$\begin{aligned} R_{AB}(t,t') &= \frac{\mathrm{i}}{\hbar} \theta(t-t') \int \frac{d\omega}{2\pi} \, e^{-i\omega(t-t')} \, 2\tilde{C}_{[A,B]}(\omega) \\ &= \frac{\mathrm{i}}{\hbar} \theta(t-t') \int \frac{d\omega}{2\pi} \, e^{-i\omega(t-t')} \tanh\left(\frac{\beta\hbar\omega}{2}\right) \, 2\tilde{C}_{\{A,B\}}(\omega) \; . \end{aligned} \tag{3.220}$$

This is the *quantum fluctuation-dissipation theorem* in a mixed time-frequency domain. Applying now

$$\int_0^\infty dt \, e^{i\omega t} = \lim_{\epsilon \to 0^+} \frac{\mathrm{i}}{\omega + i\epsilon} = \pi\delta(\omega) + i\frac{P}{\omega} \tag{3.221}$$

with P the principal part, we deduce

$$\tilde{R}_{AB}(\omega) = -\frac{1}{\hbar} \lim_{\epsilon \to 0^+} \int \frac{d\omega'}{\pi} \frac{1}{\omega - \omega' + i\epsilon} \tanh\left(\frac{\beta\hbar\omega'}{2}\right) 2C_{\{A,B\}}(\omega') \tag{3.222}$$

from which we derive the imaginary and real parts

$$\begin{aligned} \mathrm{Im}\tilde{R}_{AB}(\omega) &= \frac{1}{\hbar} \tanh\left(\frac{\beta\hbar\omega}{2}\right) \tilde{C}_{\{A,B\}}(\omega) , \\ \mathrm{Re}\tilde{R}_{AB}(\omega) &= -\frac{1}{\hbar} P \int \frac{d\omega'}{\pi} \frac{1}{\omega - \omega'} \tanh\left(\frac{\beta\hbar\omega'}{2}\right) \tilde{C}_{\{A,B\}}(\omega') . \end{aligned} \tag{3.223}$$

This is the statement of the *fluctuation-dissipation theorem*, linking a linear response to its associated correlation function, in this case written in Fourier space. This relation is valid under equilibrium conditions only.

One can now take the limit $\beta\hbar \to 0$ to recover the classical limit. Let us focus on Eq. (3.220)

$$\begin{aligned} R_{AB}(t-t') \;&\to\; \frac{\mathrm{i}}{\hbar}\theta(t-t') \int \frac{d\omega}{\pi} e^{-i\omega(t-t')} \frac{\beta\hbar\omega}{2} \tilde{C}_{AB}(\omega) \\ &= \; -\beta \frac{dC_{AB}(t-t')}{d(t-t')} \theta(t-t') . \end{aligned} \tag{3.224}$$

Another way of writing the fluctuation dissipation theorem, in the complex time domain, is

$$C_{\{A,B\}}(t_c) + C_{[A,B]}(t_c) = C_{\{A,B\}}(t_c^*) - C_{[A,B]}(t_c^*) \tag{3.225}$$

where $t_c = t + i\beta\hbar/2$.

The fluctuation dissipation theorem is a model independent relation between two-time correlation and linar response, written in the form of the expectation of the commutator of two operators, which extend to the quantum realm the fluctuation dissipation relations of classical statistical physics. It does not depend on the particular Hamiltonian of the system but it does on the equilibrium assumption.

4 Open systems

Closed systems are just an idealisation of real systems, as in Nature nothing can be isolated (apart from the full Universe itself!). The interaction of the system of interest with the environment cannot be avoided. The goal is to infer the equations of motions of a reduced system, that is a selected part of the full isolated system, from the equations of motion of the total system. For practical purposes, the reduced equations of motion should be easier to solve than the full dynamics of the system. Several approximations are usually made in the derivation of the reduced dynamics.

In this section we first revisit a few aspects of equilibrium classical statistical physics that are not commonly discussed and that become important for our purposes. We also present a derivation of the classical Langevin equation for the evolution of a system in contact with an equilibrium environment. Properties of Langevin processes are also discussed in the text but will not be presented in detail in the lectures since they are taught in the Stochastic Processes lectures.

Next we move on to discuss the description of quantum open systems. In this context we first discuss the dynamics of a system connected to several baths modelled by a Markovian interaction (a strong assumption), the Lindblad master equation acting on the density operator of the system of interest (also called Gorini-Kossakowski-Sudarshan-Lindblad equation). This equation is used in quantum optics, condensed matter, atomic physics, quantum information, and quantum biology. Then we introduce more general formalisms that go beyond the Markovian assumption.

4.1 Coherence and decoherence

The first paper on decoherence written by Zeh dates from 1970 [30] and there is a nice review by the same author published as Seminaire Poincaré proceedings in 2005 [31].

Quantum *coherence* describes the ability of a quantum mechanical system to stably maintain its quantum mechanical states. This allows accurate measurement and control of the quantum mechanical properties of the system. As long as there exists a definite phase relation between between components in a superposition, the system is said to be coherent.

However, interactions with the environment always cause incoherence. Such interactions lead to phase shifts and uncertainty in the quantum mechanical states, causing the coherence to fade and the system to become decoherent. Quantum coherence can only be maintained for limited times in many quantum mechanical systems.

If a quantum system were perfectly isolated, it would maintain coherence indefinitely, but it would be impossible to manipulate or investigate it. If it is not perfectly isolated, for example during a measurement, coherence is shared with the environment and the one of the system appears to be lost with time; a process called quantum decoherence or environmental decoherence. As a result of this process, quantum behavior is apparently lost, just as energy appears to be lost by friction in classical mechanics.

Example

Consider a single qubit in the superposition state $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$. The density matrix is

$$\begin{bmatrix} |c_0|^2 & c_0c_1^* \\ c_0^*c_1 & |c_1|^2 \end{bmatrix} \tag{4.1}$$

The diagonal elements represent the probabilities of the qubit being in $|0\rangle$, $|1\rangle$, respectively. The off-diagonal elements encode the coherence. These terms capture the relative phase and amplitude of the superposition.

Decoherence can be viewed as the loss of quantum information from a system into the environment (often modelled as a heat bath), since every system is loosely coupled with the energetic state of its surroundings. Therefore, the system's dynamics are always non-unitary (although the combined system plus environment evolves in a unitary fashion). Thus the dynamics of the system are irreversible. As with any coupling, entanglements are generated between the system and the environment. These have the effect of sharing quantum information with – or transferring it to – the surroundings.

Take a system described by a pure state $|\psi\rangle = \sum_n c_n|\psi_i\rangle$, where $\{|\psi_n\rangle\}$ is a basis of the Hilbert space. Its density operator is

$$\hat{\rho} = |\psi\rangle\langle\psi| = \sum_{nm} c_n c_m^* |\psi_n\rangle\langle\psi_m| = \underbrace{\sum_n |c_n|^2 |\psi_n\rangle\langle\psi_n|}_{\text{diagonal}} + \underbrace{\sum_{i\neq j} c_n c_m^* |\psi_i\rangle\langle\psi_m|}_{\text{off diagonal}} \tag{4.2}$$

The first term (corresponding to just the diagonal terms in the density matrix) looks like a mixed state, whereas the second term is the interference and gives the off-diagonal elements. The second term tends to disappear during decoherence, turning a pure state (quantum) with off-diagonal elements present to a mixed state (classical) with diagonal elements only.

Preserving quantum coherence is critical for applications in quantum technology, including quantum computing, quantum communications, and precision measurements. Researchers are working on strategies to minimize decoherence, such as improved quantum sensor isolation, error correction techniques, and quantum error tolerance protocols. Understanding and controlling quantum coherence are therefore key challenges in quantum physics and for the development of powerful quantum-based technologies.

Under decoherence quantum systems convert to systems which can be explained by classical mechanics. However, the way in which this transition occurs is complex and not fully understood. The theory of decoherence treats how quantum superposition states disappear at the macroscopic scale.

To experiment with the forms of quantum decoherence, scientists use "Schrödinger's kittens". These are a collection of about ten photons that can be observed transitioning from a quantum form with multiple states to a form with a single state, which is thought to result from decoherence. Such kittens are created in several ways, for example, with a box inside which mirrors force photons to bounce billions of times. Serge Haroche, received the Nobel Prize in Physics in 2012 for realizing such experiments. It is possible to observe a photon in superposed states lose this characteristic more or less quickly; with 10 photons introduced into the box, decoherence is almost instantaneous.

The *decoherence time* depends on the size of the system, the size of the bath and the coupling between the two. For example, nuclear spin relaxation can be from one-tenth of a second to a year, whereas the decoherence time is more like 10^{-3} s in the case of electron spin. It is approximately 10^{-6} s for a quantum dot, and around 10^{-9} s for an electron in certain solid state implementations. The biggest quantum computing challenge, arguably, is qubit decoherence. Qubits are extremely sensitive to their environment, and even small disturbances can cause them to lose their quantum properties. Therefore, to overcome the problem of quantum decoherence, it is necessary to be capable of performing *error correction*. This means analyzing the system to determine which disturbances have occurred and then reversing them.

When the decoherence theory was proposed, there was no need to observe quantum properties on a macroscopic scale, and this theory was not given much value. The need to build a quantum computer and maintain quantum coherence for a certain period of time to perform quantum calculations drove interest in investigating the factors that cause decoherence on quantum systems and how to reduce it.

Quantum decoherence explains why we tend to see definite states rather than superpositions at the macroscopic level. Interactions quickly destroy coherence between superimposed states. The process can be seen as a *transfer of information* about the state of the system to the environment. This information becomes inaccessible and coherence is lost. The rate of non-uniformity depends on the strength of the interaction between the system and the environment. Stronger coupling to the medium leads to faster misalignment.

4.2 Generic features

Consider a system of interest coupled to an environment with which it can exchange energy. The total energy of the full system is conserved but the contributions from the system, bath and interaction are not.

Classical and quantum environments are usually modelled as large ensembles of non-interacting variables (e.g., oscillators [35], spins [36]) with chosen distributions of coupling constants and energies.

4.3 The classical reduced partition function

We analyze the statistical *static* properties of a *classical canonical system* in equilibrium at inverse temperature β and itself formed by two sub-parts, one that will be treated as an environment (not necessarily of infinite size) and another one that will be the (sub-)system

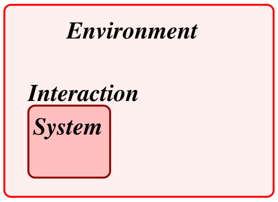

Figure 4.1: Sketch of the system and bath coupling.

of interest. We study the *partition function* or Gibbs functional, Z_T:

$$Z_T[\eta] = \sum_{\substack{\text{conf env}\\ \text{conf syst}}} \exp(-\beta H_T - \beta\eta x) \tag{4.3}$$

where the sum represents an integration over the phase space of the full system, i.e. the system's and the environmental ones. η is a source. We take

$$H_T = H_{\text{syst}} + H_{\text{env}} + H_{\text{int}} + H_{\text{counter}} = H_{\text{syst}} + \tilde{H}_{\text{env}} \ . \tag{4.4}$$

For simplicity we use a single particle moving in $d = 1$: H_{syst} is the Hamiltonian of the isolated particle,

$$H_{\text{syst}} = \frac{p^2}{2M} + V(x) \ , \tag{4.5}$$

with p and x its momentum and position. H_{env} is the Hamiltonian of a 'thermal bath' that, for simplicity, we take to be an ensemble of N independent harmonic oscillators [34, 35] with masses m_a and frequencies ω_a, $a = 1, \dots, N$

$$H_{\text{env}} = \sum_{a=1}^{N} \frac{\pi_a^2}{2m_a} + \frac{m_a\omega_a^2}{2} q_a^2 \tag{4.6}$$

with π_a and q_a their momenta and positions. This is indeed a very usual choice since it may represent phonons. (These oscillators could be the normal modes of a generic Hamiltonian expanded to quadratic order around its absolute minimum, written in terms of other pairs of conjugate variables; the bath could be, for instance, a chain of harmonic oscillators with nearest-neighbor couplings.) H_{int} is the coupling between system and environment. We will restrict the following discussion to a linear interaction in the oscillator coordinates, q_a, and in the particle coordinate,

$$H_{\text{int}} = x \sum_{a=1}^{N} c_a q_a \ , \tag{4.7}$$

with c_a the coupling constants. The counter-term H_{counter} is added to avoid the generation of a negative harmonic potential on the particle due to the coupling to the oscillators (that may render the dynamics unstable). We choose it to be

$$H_{\rm counter} = \frac{1}{2} \sum_{a=1}^{N} \frac{c_a^2}{m_a \omega_a^2} x^2 \; . \tag{4.8}$$

The generalization to more complex systems and/or to more complicated baths and higher dimensions is straightforward. The calculations can also be easily generalized to an interaction of the oscillator coordinate with a more complicated dependence on the system's coordinate, $\mathcal{V}(x)$, that may be dictated by the symmetries of the system at the expense of modifying the counter-term. Non-linear functions of the oscillator coordinates cannot be used since they render the problem unsolvable analytically.

Having chosen a quadratic bath and a linear coupling, the integration over the oscillators' coordinates and momenta can be easily performed. This yields the *reduced* Gibbs functional

$$Z_{\rm red}[\eta] \propto \sum_{\text{conf syst}} \exp \left[-\beta \left(H_{\rm syst} + H_{\rm count} + \eta x - \frac{1}{2} \sum_{a=1}^{N} \frac{c_a^2}{m_a \omega_a^2} \, x^2 \right) \right] \; . \tag{4.9}$$

The 'counter-term' $H_{\rm count}$ is chosen to cancel the last term in the exponential and it avoids the renormalization of the coefficient of the quadratic term in the potential due to the coupling to the environment that could have even destabilized the potential by taking negative values. An alternative way of curing this problem would be to take a vanishingly small coupling to the bath in such a way that the last term must vanish by itself (say, all $c_a \to 0$). However, this might be problematic when dealing with the stochastic dynamics since a very weak coupling to the bath implies also a very slow relaxation. It is then conventional to include the counter-term to cancel the mass renormalization. One then finds

$$\boxed{Z_{\rm red}[\eta] \propto \sum_{\text{conf syst}} \exp \left[-\beta \left(H_{\rm syst} + \eta x \right) \right] = Z_{\rm syst}[\eta] \; .} \tag{4.10}$$

For a non-linear coupling $H_{\rm int} = \sum_{a=1}^{N} c_a q_a \mathcal{V}(x)$ the counter-term is $H_{\rm count} = \frac{1}{2} \sum_{a=1}^{N} \frac{c_a^2}{m_a \omega_a^2} [\mathcal{V}(x)]^2$.

The interaction with the reservoir does not modify the statistical properties of the particle since $Z_{\rm red} \propto Z_{\rm syst}$, independently of the choices of c_a, m_a, ω_a and N.

If one is interested in the *dynamics* of a coupled problem, the characteristics of the sub-system that will be considered to be the bath have an influence on the reduced dynamic equations found for the system, that are of generic Langevin kind, as explained in Sect. 4.5.2.

Quantum mechanically the reduced partition function depends explicitly on the properties of the bath. The interaction with quantum harmonic oscillators introduces non-local interactions (along the Matsubara time direction) and there is no physical way to introduce a counter-term to correct for this feature. We will see these feature arise in the Sec. **??**.

The *dynamics of quantum systems* has all these difficulties.

4.4 Classical dissipative processes (1h)

Examples of experimental and theoretical interest in condensed matter and biophysics in which quantum fluctuation can be totally neglected are manifold. In this context one usually concentrates on systems in contact with an environment: one selects some relevant degrees of freedom and treats the rest as a bath. It is a canonical view. Among these instances are colloidal suspensions which are particles suspended in a liquid, typically salted water, a 'soft condensed matter' example; spins in ferromagnets coupled to lattice phonons, a 'hard condensed matter' case; and proteins in the cell a 'biophysics' instance. These problems are modelled as stochastic processes with Langevin equations [45, 46, 48–51, 54], the Kramers-Fokker-Planck formalism or master equations depending on the continuous or discrete character of the relevant variables and analytic convenience.

The Langevin equation was originally proposed to model the motion of a colloidal particle in a liquid but it was soon realised that generalisations of it can be used in a much wider context to describe, e.g. the motion of ions in water of the reorientation of dipolar molecules, or some collective variable of a macroscopic system. It is a stochastic differential equation that describes phenomenologically a large variety of problems. It models the time evolution of a set of slow variables coupled to a much larger set of fast variables that are usually (but not necessarily) assumed to be in thermal equilibrium at a given temperature. We first introduce it in the context of Brownian motion in Sect. 4.4.1 and we derive it in more generality in Sect. 4.4.2. A detailed description of Langevin processes can be consulted in [50].

4.4.1 Langevin's Langevin equation

The Langevin equation[2] for a particle moving in one dimension in contact with a *white-noise* bath reads

$$\boxed{m\dot{v} + \gamma_0 v = F + \xi \; , \qquad\qquad v = \dot{x} \; ,} \tag{4.11}$$

with x and v the particle's position and velocity.

The fluctuating force ξ is supposed to come from occasional impacts of the Brownian particle with molecules of the surrounding medium. The force during an impact is supposed to vary with extreme rapidity over the time of any observation. Then the effects of the fluctuating force can be summarised by giving its first and second moments, as time averages over an infinitesimal time interval. ξ is then a Gaussian white noise with zero mean $\langle \xi(t) \rangle$ and correlation $\langle \xi(t)\xi(t') \rangle = 2\gamma_0 k_B T \delta(t-t')$. The delta function in time indicates that there is no correlation between impacts in any distinct time intervals around t and t'. $\gamma_0 v$ is a friction force that opposes the motion of the particle. The force

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[2] P. Langevin, *Sur la théorie du mouvement brownien*, Comptes-Rendus de l'Académie des Sciences **146**, 530-532 (1908).

F designates all external deterministic forces and depends, in the most common cases, on the position of the particle x only. In cases in which the force derives from a potential, $F = -dV/dx$. The generalization to higher dimensions is straightforward. Note that γ_0 is the parameter that controls the strength of the coupling to the bath (it appears in the friction term as well as in the noise term). In the case $\gamma_0 = 0$ one recovers Newton equation of motion. The relation between the friction term and thermal correlation is non-trivial. Langevin fixed it by requiring $\langle v^2(t)\rangle \to \langle v^2\rangle_{eq}$. We will give a different argument for it in the next section.

4.4.2 Derivation of the Langevin equation

Let us take a system in contact with an environment. The interacting system+environment ensemble is 'closed' while the system is 'open'. The nature of the environment, *e.g.* whether it can be modeled by a classical or a quantum formalism, depends on the problem under study. We focus here on the classical problem defined by H_T. A derivation of a generalized Langevin equation with memory is very simple starting from Newton dynamics of the full system [5, 34, 51].

The generalization to more complex systems and/or to more complicated baths and higher dimensions is straightforward. The calculations can also be easily generalized to an interaction of the oscillator coordinate with a more complicated dependence on the system's coordinate, $\mathcal{V}(x)$, that may be dictated by the symmetries of the system, see **Ex. 2.1**.

Hamilton's equations for the particle are

$$\dot{x}(t) = \frac{p(t)}{m} \; , \qquad \dot{p}(t) = -V'[x(t)] - \sum_{a=1}^{N} c_a q_a(t) - \sum_{a=1}^{N} \frac{c_a^2}{m_a\omega_a^2} x(t) \tag{4.12}$$

(the counter-term yields the last term) while the dynamic equations for each member of the environment read

$$\dot{q}_a(t) = \frac{\pi_a(t)}{m_a} \; , \qquad \dot{\pi}_a(t) = -m_a\omega_a^2 q_a(t) - c_a x(t) \; , \tag{4.13}$$

showing that they are all stable harmonic oscillators *forced by the chosen particle*. These equations are readily solved by

$$q_a(t) = q_a(0)\cos(\omega_a t) + \frac{\pi_a(0)}{m_a\omega_a}\sin(\omega_a t) - \frac{c_a}{m_a\omega_a}\int_0^t dt' \sin[\omega_a(t-t')]x(t') \tag{4.14}$$

with $q_a(0)$ and $\pi_a(0)$ the initial coordinate and position at time $t = 0$ when the particle is set in contact with the bath. It is convenient to integrate by parts the last term. The replacement of the resulting expression in the last term in the rhs of eq. (4.12) yields

$$\boxed{\dot{p}(t) = -V'[x(t)] + \xi(t) - \int_0^t dt' \; \Gamma(t-t')\dot{x}(t') \; ,} \tag{4.15}$$

with the *symmetric and stationary kernel* Γ given by

$$\boxed{\Gamma(t-t') = \sum_{a=1}^{N} \frac{c_a^2}{m_a\omega_a^2} \cos[\omega_a(t-t')] \ ,} \tag{4.16}$$

$\Gamma(t-t') = \Gamma(t'-t)$, and the *time-dependent force* ξ given by

$$\boxed{\xi(t) = -\sum_{a=1}^{N} c_a \left[\frac{\pi_a(0)}{m_a\omega_a} \sin(\omega_a t) + \left(q_a(0) + \frac{c_a x(0)}{m_a\omega_a^2} \right) \cos(\omega_a t) \right] \ .} \tag{4.17}$$

This is the equation of motion of the *reduced* system. It is still *deterministic*.

$\xi(t)$ is a sum of oscillating functions of time. The third term on the rhs of eq. (4.15) represents a rather complicated *friction force*. Its value at time t depends explicitly on the history of the particle at times $0 \leq t' \leq t$ and makes the equation *non-Markovian*. One can rewrite it as an integral running up to a total time $\mathcal{T} > \max(t,t')$ introducing the *retarded friction*:

$$\boxed{\gamma(t-t') = \Gamma(t-t')\theta(t-t') \ .} \tag{4.18}$$

Until this point the dynamics of the system remain deterministic and are completely determined by its initial conditions as well as those of the reservoir variables. Two important points can be make here. On the one hand, one can check, by simple numerical generation, that the function ξ at, say, fixed t resembles more and more a random variable as the number of oscillators increases (for incommensurate frequencies ω_a). The initial conditions for the oscillators are the seeds of the random number generator. This is similar to what happens with random number generators in the sense that these are, ultimately, periodic functions with a finite recurrence time that, however, can be made sufficiently long for computational purposes. Therefore, ξ is a *pseudo random number*. On the other hand, one can directly introduce the *statistical element* into play when one realizes that it is impossible to know the initial configuration of the large number of oscillators with great precision and one proposes that the initial coordinates and momenta of the oscillators have a canonical distribution at an *inverse temperature* β. (Note that one needs to assume that the oscillators interacted in the past to establish ergodicity and reach this pdf, though they do not do any longer.) Then, one chooses $\{\pi_a(0), q_a(0)\}$ to be initially distributed according to a canonical phase space distribution:

$$\boxed{P(\{\pi_a(0), q_a(0)\}, x(0)) = 1/\tilde{\mathcal{Z}}_{\text{env}}[x(0)] \ e^{-\beta \tilde{H}_{\text{env}}[\{\pi_a(0), q_a(0)\}, x(0)]}} \tag{4.19}$$

with $\tilde{H}_{\text{env}} = H_{\text{env}} + H_{\text{int}} + H_{\text{count}}$, that can be rewritten as

$$\tilde{H}_{\text{env}} = \sum_{a=1}^{N} \left[\frac{m_a\omega_a^2}{2} \left(q_a(0) + \frac{c_a}{m_a\omega_a^2} x(0) \right)^2 + \frac{\pi_a^2(0)}{2m_a} \right] \ . \tag{4.20}$$

Again, the presence of $H_{\rm count}$ here is for convenience. The randomness in the initial conditions gives rise to a random force acting on the reduced system. Indeed, ξ is now a *Gaussian random variable*, that is to say a noise, with

$$\langle \xi(t) \rangle = 0 \, , \qquad \langle \xi(t)\xi(t') \rangle = k_B T \, \Gamma(t-t') \, . \tag{4.21}$$

One can easily check that higher-order correlations vanish for an odd number of ξ factors and factorize as products of two time correlations for an even number of ξ factors. In consequence ξ has Gaussian statistics. Defining the inverse of Γ over the interval $[0,t]$, $\int_0^t dt'' \; \Gamma(t-t'')\Gamma^{-1}(t''-t') = \delta(t-t')$, one has the Gaussian pdf:

$$P[\xi] = \mathcal{Z}^{-1} e^{-\frac{1}{2k_BT} \int_0^t dt \int_0^t dt' \; \xi(t)\Gamma^{-1}(t-t')\xi(t')} \, . \tag{4.22}$$

$\mathcal{Z}$ is the normalization. A random force with non-vanishing correlations on a finite support is usually called a *coloured noise*. Equation (4.15) is now a genuine Langevin equation. A *multiplicative retarded noise* arises from a model in which one couples the coordinates of the oscillators to a generic function of the coordinates of the system, see **Ex. 2.1**.

The use of an *equilibrium measure* for the oscillators implies the relation between the friction kernel and the noise-noise correlation, which are proportional, with a constant of proportionality of value $k_B T$. This is a generalized form of the *fluctuation-dissipation relation*, and it applies to the environment.

About the bath

One last comment is in order here. A closed ensemble of harmonic oscillators is an integrable system that does not equilibrate in strict sense. Still, we are using it as a model for a thermal bath. One can argue that the oscillators were in interaction in the past, before being connected to the system, and that this allowed them to reach the Boltzmann probability distribution that is used for their initial states in this calculation. Or else, one can follow the calculations by Mazur & Montroll and see that in the limit of a large number of degrees of freedom the *Poincaré recurrence time* for the system of non-interacting harmonic oscillators becomes so large that it lies beyond any relevant time for the relaxation of the system that is coupled to the oscillator bath[3].

About the counterterm.

Had we not added the counter term the equation would read

$$\dot{p}(t) = -V'[x(t)] + \sum_{a=1}^{N} \frac{c_a^2}{m_a \omega_a^2} x(t) + \xi(t) - \int_0^t dt' \; \Gamma(t-t')\dot{x}(t') \, , \tag{4.23}$$

that is like eq. (4.15) for $V \mapsto V - \frac{1}{2}\sum_{a=1}^N \frac{c_a^2}{m_a\omega_a^2} x^2$, as we found with the analysis of the partition sum. Note that, as we will take $c_a = \tilde{c}_a/\sqrt{N}$, with $\tilde{c}_a$ of $O(1)$, the constant

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[3] P. Mazur and E. Montroll, *Poincaré cycles, ergodicity, and irreversibility in assemblies of coupled harmonic oscillators*, J. Math. Phys. **1**, 70 (1960).

resulting from the sum over a is $O(1)$. For the distribution of the initial values we can still use $\widetilde{H}_{\rm env}$ or we can choose a Maxwell-Boltzmann distribution with $H_{\rm env} + H_{\rm int}$ alone. The result will be the same, as the supplementary term goes into the normalisation constant for $P_{\rm env}(0)$.

The bath kernel Γ*.*

Different choices of the environment are possible by selecting different ensembles of harmonic oscillators [4]. The simplest one, that leads to an approximate Markovian equation, is to consider that the oscillators are coupled to the particle via coupling constants $c_a = \tilde{c}_a/\sqrt{N}$ with $\tilde{c}_a$ of order one. One defines

$$\boxed{S(\omega) \equiv \tfrac{1}{N} \sum_{a=1}^{N} \tfrac{\tilde{c}_a^2}{m_a \omega_a} \; \delta(\omega - \omega_a)} \tag{4.24}$$

a function of ω, of order one with respect to N, and rewrites the kernel Γ as

$$\boxed{\Gamma(t - t') = \int_0^\infty d\omega \, \frac{S(\omega)}{\omega} \, \cos[\omega(t - t')] \; .} \tag{4.25}$$

The spectral density $S(\omega)$ is a weighted sum over the frequencies of the oscillators in the bath. For all finite N it is then just a discrete sum of delta functions. In the limit $N \to \infty$ it can become, instead, a regular function of ω. Assuming this limit is taken, several proposals for the resulting function $S(\omega)$ are made. A common choice is

$$\boxed{\frac{S(\omega)}{\omega} = \frac{2\gamma_0}{\pi} \left(\frac{|\omega|}{\tilde{\omega}} \right)^{\alpha - 1} \; f_c\left(\frac{|\omega|}{\Lambda} \right) \; .} \tag{4.26}$$

The function $f_c(x)$ is a high-frequency cut-off of typical width Λ and is usually chosen to be an exponential. The frequency $\tilde{\omega} \ll \Lambda$ is a reference frequency that allows one to have a coupling strength γ_0 with the dimensions of viscosity. If $\alpha = 1$, the friction is said to be *Ohmic*, $S(\omega)/\omega$ is constant when $|\omega| \ll \Lambda$ as for a white noise. This name is motivated by the electric circuit analog exposed in Sec. **??**. When $\alpha > 1$ ($\alpha < 1$) the bath is *superOhmic* (*subOhmic*). The exponent α is taken to be > 0 to avoid divergencies at low frequency. For the exponential cut-off the integral over ω can be computed for $\alpha = 1$ and $\alpha \neq 1$. In the former Ohmic case one finds

$$\Gamma(t) = \frac{2\gamma_0}{\pi} \, \frac{\Lambda}{[1 + (\Lambda t)^2]} \; . \tag{4.27}$$

In the $\Lambda \to \infty$ limit one approaches the Stratonovich limit and $\Gamma(t)$ becomes a delta-function, $\Gamma(t) \to 2\gamma_0 \delta(t)$ such that $\int_0^t dt' \; \Gamma(t - t') = 2\gamma_0 \arctan(\Lambda t) \to \gamma_0$ for $\Lambda \to \infty$. In

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[4] See, G. W. Ford, M. Kac, and P. Mazur, *Statistical mechanics of assemblies of coupled oscillators*, J. Math. Phys. **6**, 504 (1965), for a detailed analysis.

the latter non-Ohmic case the integral over ω yields

$$\Gamma(t) = \frac{2\gamma_0}{\pi} \tilde{\omega}^{-\alpha+1} \, \Gamma_{\rm E}(\alpha) \, \Lambda^\alpha \, \frac{\cos[\alpha \arctan(\Lambda t)]}{[1+(\Lambda t)^2]^{\alpha/2}} \tag{4.28}$$

with $\Gamma_{\rm E}(\alpha)$ the Euler Gamma-function. At long times, for any $\alpha > 0$ and $\alpha \neq 1$, one has

$$\lim_{\Lambda t \to \infty} \Gamma(t) \quad = \quad \frac{2\gamma_0}{\pi} \tilde{\omega} \, \cos(\alpha\pi/2) \Gamma_{\rm E}(\alpha) \, (\tilde{\omega} t)^{-\alpha} \, , \tag{4.29}$$

a *power law decay*.

4.5 Quantum dissipative processes

4.5.1 The Ramsey interferometer

The Ramsey interferometer is a fundamental tool in quantum mechanics to measure quantum coherence and is often used in experiments involving atomic or qubit systems. When coupled to an environment, it serves as a prime example of how decoherence emerges

Take a single qubit and consider its evolution in isolation or coupled to another qubit which acts as the bath. We will see how the latter may drastically modify the evolution of the former, a very simple quantum system [33].

The unitary evolution of the isolated system is

$$\begin{aligned} |0\rangle \xrightarrow{\hat{U}_0} \frac{1}{\sqrt{2}}\Big(|0\rangle + |1\rangle\Big) \xrightarrow{\hat{U}_\phi} \frac{1}{\sqrt{2}}\Big(|0\rangle + e^{i\phi}|1\rangle\Big) \xrightarrow{\hat{U}_0} \frac{1}{2}\Big[\Big(|0\rangle + |1\rangle\Big) + e^{i\phi}\Big(-|0\rangle + |1\rangle\Big)\Big] \\ = e^{i\phi/2}\left(-i \sin\frac{\phi}{2}|1\rangle + \cos\frac{\phi}{2}|0\rangle\right) \end{aligned} \tag{4.30}$$

with

$$\hat{U}_0 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \qquad\qquad \hat{U}_\phi = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix} \tag{4.31}$$

This sequence of unitary operations, $\hat{U}|\psi\rangle$, realizes a Ramsey interferometer. $\hat{U}_0$ corresponds to a $\pi/2$ pulse and $\hat{U}_\phi$ to free evolution. The probability to obtain the spin-up (spin-down) outcome is a sine (cosine) function of ϕ: Ramsey fringes are obtained when measuring spin-up (spin-down).

Let us add now a coupling to the environment in between the first $\pi/2$ pulse ($\hat{U}_0$) and the free evolution ($\hat{U}_\phi$) period. We suppose that the spin and the environment, which is initially in $|0\rangle_E$, evolve unitarily such that $|1\rangle \otimes |0\rangle_E \to |1\rangle \otimes |e_1\rangle_E$ and $|0\rangle \otimes |0\rangle_E \to |0\rangle \otimes |e_0\rangle_E$ (the "system" does not change and the environment changes to two states for the moment not fixed). The full sequence becomes

$$\begin{aligned}|0\rangle \otimes |0\rangle_E &\xrightarrow{\hat{U}_0} \frac{1}{\sqrt{2}}\Big(|0\rangle \otimes |e_0\rangle_E + |1\rangle \otimes |e_1\rangle_E\Big) \xrightarrow{\hat{U}_\phi} \frac{1}{\sqrt{2}}\Big(|0\rangle \otimes |e_0\rangle_E + e^{i\phi}|1\rangle \otimes |e_1\rangle_E\Big)\\ &\xrightarrow{\hat{U}_0} \frac{1}{2}\left[(|0\rangle + |1\rangle) \otimes |e_0\rangle_E + e^{i\phi}\left(-|0\rangle + |1\rangle\right) \otimes |e_1\rangle_E\right]\\ &= \frac{1}{\sqrt{2}}\left[|\uparrow_x\rangle \otimes |e_0\rangle_E - e^{i\phi}|\downarrow_x\rangle \otimes |e_1\rangle_E\right]\end{aligned}$$

(In the last two steps only the system was modified.)

The final measurement can be decomposed as a projective measurement of the environment followed by a projective measurement of the spin. There are two extreme cases depending on the angle between the two environment states $|e_0\rangle_E$ and $|e_1\rangle_E$. If the states are identical, then the environment state can be factored out and the projective measurement of the environment does not modify the state of the spin: Ramsey oscillations with full contrast are still observed.

Instead, if the environment states are orthogonal and therefore perfectly distinguishable, the first measurement ($|e_0\rangle_E$) prepares the spin in

$$|\uparrow_x\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle),$$

an eigenvector with eigenvalue 1 of $\hat{\sigma}^x$. If, instead, the environment is projected on $|e_1\rangle_E$, then

$$|\downarrow_x\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

the eigenvector with eigenvalue -1 of $\hat{\sigma}^x$. Both outcomes happen with probability $1/2$. The final measurement then leads to spin up and down outcomes with probability $1/2$, independently of the value of ϕ, and the Ramsey oscillations are washed out. This exemplifies some important features of an open quantum system:

- Once the environment is measured, the state of the system is, in general, in a mixture of states. It cannot be represented as a ket of the Hilbert space but by a density matrix.
- The evolution of a quantum system in the presence of an environment is, in general, not unitary and is called a *quantum map*. Here, we have obtained a map where the coherence is completely lost: the initial pure state $|0\rangle$ is mapped onto a fully mixed state. This happens because the qubit and the environment have become maximally entangled. This loss of coherence of the qubit is irreversible. There is no quantum operation acting on the qubit alone that can restore the coherence and the fringe contrast.

4.5.2 The Lindblad master equation

The Lindblad master equation is a *Markovian linear master equation* which describes the evolution of the density operator of an open quantum system. It should be noted that there is no unique way of implementing a Markov approximation. Instead, there exists a continuous family of distinct approximations that result in a Markovian dynamics, all with error bounds of the same order in a control parameter.

The resulting dynamics is no longer unitary, but for some approximation is still trace-preserving and completely positive for any initial condition (not for others in the literature). It results in dissipation of energy into the surroundings, causing decay and randomization of phase.

The Lindblad equation takes the diagonal form

$$\frac{d\hat{\rho}_S^{\rm red}}{dt} = -\frac{\rm i}{\hbar}[\hat{H}, \hat{\rho}_S^{\rm red}] + \sum_{i=1}^{N^2-1} \gamma_i \left(\hat{L}_i \hat{\rho}_S^{\rm red} \hat{L}_i^\dagger - \frac{1}{2} \left\{ \hat{L}_i^\dagger \hat{L}_i, \hat{\rho}_S^{\rm red} \right\} \right) \tag{4.32}$$

Here, $\hat{H}$ is a Hamiltonian describing the unitary aspects of the dynamics. It is not necessarily equal to the bare system's Hamiltonian since it may also incorporate effective unitary dynamics arising from the system-environment interaction,

$$\hat{H} = \hat{H}_S + \hat{\Lambda}(\{\gamma_i\}) \tag{4.33}$$

The extra term $\hat{\Lambda}(\{\gamma_i\})$ is Hermitian. It has the same origin as the potential renormalization that we saw arising in the derivation of the Langevin equation, after the integration of the harmonic oscillators. The $N^2 - 1$ operators $\{\hat{L}_i\}$ (in a Hilbert space of N dimensions) are a set of jump operators, which describe how the environment acts on the system and induce dissipation. (There need be no limitation on the number of terms in the sum, but this can always be reduced to a sum of $N^2 - 1$ terms.) They must either be determined from microscopic models of the system-environment coupling or be phenomenologically proposed. The damping rates $\gamma_i \geq 0$ are real and non-negative. If all $\gamma_i = 0$ the von Neumann equation $\dot{\hat{\rho}}_S = -(i/\hbar)[\hat{H}_S, \hat{\rho}_S]$ describing unitary dynamics with the systems's Hamiltonian $\hat{H}_S$ is recovered. Otherwise, tracing over the environment introduces non-unitary effects on the system's dynamics.

Sometimes the more general GKSL (for Gorini-Kossakowski-Sudarshan-Lindblad) equation is used

$$\frac{d\hat{\rho}_S^{\rm red}}{dt} = -\frac{\rm i}{\hbar}[\hat{H}, \hat{\rho}_S^{\rm red}] + \sum_{n,m} h_{nm} \left(\hat{A}_n \hat{\rho}_S^{\rm red} \hat{A}_m^\dagger - \frac{1}{2} \left\{ \hat{A}_m^\dagger \hat{A}_n, \hat{\rho}_S^{\rm red} \right\} \right) \tag{4.34}$$

where $\{\hat{A}_m\}$ are arbitrary operators and $\{h_{mn}\}$ are the elements of a positive semidefinite matrix. The latter is a strict requirement to have trace-preserving and positive dynamics. The number of $\{\hat{A}_m\}$ operators is arbitrary (but can be reduced as above), and they do not have to satisfy any special properties. This equation can be reduced to Eq. (4.32) after a diagonalization of the matrix h with elements h_{nm} and a change of variables.

Exercise 4.1 Establish the conditions under which Eq. (4.34) can be taken to the form in Eq. (4.32).

Properties

The Lindblad equation (or Lindblad master equation) conserves the positivity of the density operator $\hat\rho_S^{\text{red}}$, ensuring it remains a valid quantum state during its evolution. Important properties of the Lindblad equation are:

(a) The equation should conserve the Hermiticity of the density operator. This imposes constraints on the coefficients γ_i or h_{nm} in the more generic equation.
(b) Trace preservation: The total probability is conserved ($\text{Tr}\hat\rho_S^{\text{red}} = 1$).
(c) Positivity preservation: $\hat\rho_S^{\text{red}}$ remains a positive semidefinite operator, meaning that for all vectors $|\psi\rangle$, $\langle\psi|\hat\rho_S^{\text{red}}|\psi\rangle \geq 0$. The dissipative terms in the equation ($\hat L_k \hat\rho_S^{\text{red}} \hat L_k^\dagger - \frac{1}{2}\{\hat L_k^\dagger \hat L_k, \hat\rho_S^{\text{red}}\}$) are constructed in a way that ensures positivity. The positivity of the density operator is a key requirement for it to represent a quantum state, and the Lindblad equation is explicitly designed to meet this requirement.

The operators $\{\hat L_i\}$ are in general arbitrary. Their explicit form depends on the concrete bath and interaction with the system that one wants to model.

Mathematical proofs of the Lindblad equation only use the properties listed above as conditions and leave the form of the operators $\hat L_i$ totally free.

Other proofs are start from a specific form of bath-system coupling and bath model and derive it through a number of approximations. This is a "physical" in the sense that the assumptions made, and hence the range of validity of the Lindblad equation, are clearer.

These two proofs are described in detail in [2]. We present the second derivation here, since it is indeed very close in spirit to the derivation of the classical Langevin equation that we have already discussed. First we present some examples.

Exercise 4.2 Prove the properties listed above.

(a) Hermiticity. Take the Hermitian transform of the Lindblad equation:

$$\frac{d\hat\rho^\dagger}{dt} = +\frac{\mathrm{i}}{\hbar}(\hat\rho^\dagger \hat H^\dagger - \hat H^\dagger \hat\rho^\dagger) + \sum_{i=1}^{N^2-1} \gamma_i^* \left[\hat L_i \hat\rho^\dagger \hat L_i^\dagger - \frac{1}{2}\left(\hat\rho^\dagger \hat L_i^\dagger \hat L_i + \hat L_i^\dagger \hat L_i \hat\rho^\dagger\right)\right]$$

where we did not write the upper-script $^{\text{red}}$ and lower-script $_S$ in $\hat\rho^\dagger$ to make the notation lighter. Since the Hamiltonian $\hat H$ is Hermitian, for $\gamma_i^* = \gamma_i$, the right-hand side is transformed in the same operator as in the original equation acting now on $\hat\rho^\dagger$. So $\hat\rho$ and $\hat\rho^\dagger$ satisfy the same equation and we can consider them equal at all times if they are initially.
(b) Trace. We know that the trace of the first term in the right-hand-side vanishes. What about the trace of the second one? It vanishes for any $\{\hat L_i, \hat L_i^\dagger\}$ as a consequence of the cyclic property of the trace.
(c) Positivity. It can be seen that no negative eigenvalues can be generate in time, just from the structure of each term in the right-hand-side.

Example. Unitary jump

Take a system characterized by a state $|\psi, t\rangle$ at time t and suppose that in the infinitesimal interval dt it has probability λdt of changing to $e^{-\mathrm{i}\hat{G}}|\psi,t\rangle$ and probability $1-\lambda dt$ of being unchanged. $\hat{G}$ is a Hermitian operator and $e^{-\mathrm{i}\hat{G}} \neq \hat{\mathbb{I}}$.

The density operator at time $t+dt$ is

$$\hat{\rho}(t+dt) = (1-\lambda dt)\hat{\rho}(t) + \lambda dt\, e^{-\mathrm{i}\hat{G}}\hat{\rho}(t)e^{\mathrm{i}\hat{G}},$$

so its evolution equation is

$$\frac{d}{dt}\hat{\rho}(t) = -\lambda[\hat{\rho}(t) - e^{-\mathrm{i}\hat{G}}\hat{\rho}(t)e^{\mathrm{i}\hat{G}}].$$

This is of the Lindblad form, with one Lindblad operator $\hat{L} \equiv \sqrt{2\lambda}e^{-\mathrm{i}\hat{G}}$ and $\gamma = 1/2$. Here and in the next examples we denote the density operator of the system simply $\hat{\rho}$ (and not $\hat{\rho}_S^{\mathrm{red}}$ as in the main text).

For the density matrix components, if the operator $\hat{G}$ is diagonal with elements g_1 and g_2, the last term reads

$$\begin{bmatrix} e^{-\mathrm{i}g_1} & 0 \\ 0 & e^{-\mathrm{i}g_2} \end{bmatrix} \begin{bmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{bmatrix} \begin{bmatrix} e^{\mathrm{i}g_1} & 0 \\ 0 & e^{\mathrm{i}g_2} \end{bmatrix} = \begin{bmatrix} e^{-\mathrm{i}g_1} & 0 \\ 0 & e^{-\mathrm{i}g_2} \end{bmatrix} \begin{bmatrix} \rho_{11}e^{\mathrm{i}g_1} & \rho_{12}e^{\mathrm{i}g_2} \\ \rho_{21}e^{\mathrm{i}g_1} & \rho_{22}e^{\mathrm{i}g_2} \end{bmatrix}$$
$$= \begin{bmatrix} \rho_{11} & \rho_{12}e^{\mathrm{i}(g_2-g_1)} \\ \rho_{21}e^{\mathrm{i}(g_1-g_2)} & \rho_{22} \end{bmatrix} \tag{4.35}$$

Plugging this result in the master equation

$$\frac{d\rho_{ii}}{dt} = 0 \qquad \frac{d}{dt}\rho_{12}(t) = -\lambda\rho_{12}(t)\left[1 - e^{\mathrm{i}(g_2-g_1)}\right].$$

The diagonal elements remain constant but the off-diagonal elements decay at the fixed rate $\lambda[1-\cos(g_2-g_1)]$ and their phases change.

Example. State exchange

Suppose that in time dt, with probability λdt, a state vector $|\psi,t\rangle$ in a two dimensional Hilbert space becomes $\hat{\sigma}^y|\psi,t\rangle$ while it remains unchanged with probability $1-\lambda dt$. Here, $\hat{\sigma}^y$ is the second Pauli operator, with matrix representation

$$\begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix} \tag{4.36}$$

In an infinitesimal interval

$$\hat{\rho}(t+dt) = (1-\lambda dt)\,\hat{\rho}(t) + \lambda dt\,\hat{\sigma}^y\,\hat{\rho}(t)\,\hat{\sigma}^y$$

which in the continuous time limit yields the differential equation which governs the evolution of the density operator

$$\frac{d}{dt}\hat{\rho}(t) = -\lambda\left[\hat{\rho}(t) - \hat{\sigma}^y\,\hat{\rho}(t)\,\hat{\sigma}^y\right]$$

This equation is of the Lindblad form,

$$\frac{d\hat{\rho}}{dt} = -\frac{\mathrm{i}}{\hbar}[\hat{H},\hat{\rho}] + \sum_{i=1}^{N^2-1}\gamma_i\left(\hat{L}_i\hat{\rho}\hat{L}_i^\dagger - \frac{1}{2}\left\{\hat{L}_i^\dagger\hat{L}_i,\hat{\rho}\right\}\right) \tag{4.37}$$

with one Hermitian Lindblad operator $\hat{L} \equiv \sqrt{2\lambda}\hat{\sigma}^y$. Indeed,

- $\hat{H} = 0$,
- $\hat{L}\hat{\rho}\hat{L}^\dagger = 2\lambda\hat{\sigma}^y\hat{\rho}\hat{\sigma}^y$,
- $\{\hat{L}^\dagger\hat{L},\hat{\rho}\} = 2\lambda[(\hat{\sigma}^y)^2\hat{\rho} + \hat{\rho}(\hat{\sigma}^y)^2] = 2\lambda[\mathbb{I}\hat{\rho} + \hat{\rho}\mathbb{I}] = 4\lambda\hat{\rho}$

and with $\gamma = -1/2$ we obtain the expression above.

The density matrix elements therefore satisfy

$$\frac{d}{dt}\rho_{11}(t) = -\frac{d}{dt}\rho_{22}(t) = -\lambda[\rho_{11}(t) - \rho_{22}(t)]\ ,$$
$$\frac{d}{dt}\rho_{12}(t) = -\frac{d}{dt}\rho_{21}(t) = -\lambda[\rho_{12}(t) - \rho_{21}(t)]\ ,$$

obtained just by performing explicitly the matrix products in the last term. The diagonal density matrix elements change in this example, decaying to 1/2. The off-diagonal matrix elements keep their real parts while the imaginary parts decay to 0.

Example. OTOCs

Achieving exponential decay of the OTOC typically requires introducing decoherence, dissipation, or chaotic dynamics. A simple solvable model that incorporates decoherence, leading to exponential decay of the OTOC is the following.

Consider a single qubit subject to a pure dephasing channel. The qubit evolves under a Hamiltonian combined with a dephasing term:

$$\hat{H} = \frac{\hbar\omega}{2}\hat{\sigma}_z,$$

with dephasing described by the Lindblad operator $\hat{L} = \sqrt{\gamma}\hat{\sigma}_z$, where ω is the frequency of the qubit and γ is the dephasing rate and sets the timescale for decoherence. The system evolves according to the Lindblad master equation

$$\frac{d\hat{\rho}(t)}{dt} = -\frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{\rho}(t)] + \gamma\left(\hat{\sigma}_z\hat{\rho}(t)\hat{\sigma}_z - \hat{\rho}(t)\right).$$

This dephasing channel causes the off-diagonal elements of the density matrix to decay exponentially at a rate 2γ. We choose the operators $\hat{W} = \hat{\sigma}_x$ and $\hat{V} = \hat{\sigma}_z$. The OTOC is

$$\mathrm{OTOC}(t) = \langle\hat{\sigma}_x(t)\hat{\sigma}_z\hat{\sigma}_x(t)\hat{\sigma}_z\rangle,$$

where $\hat{\sigma}_x(t)$ is the time-evolved $\hat{\sigma}_x$ in the presence of dephasing. The dynamics of $\hat{\sigma}_x$ under the Lindblad equation can be solved directly. Using the commutator $[\hat{H}, \hat{\sigma}_x] = i\hbar\omega\hat{\sigma}_y$ and the effect of the dephasing term, we find

$$\hat{\sigma}_x(t) = \hat{\sigma}_x e^{-\gamma t}\cos(\omega t) - \hat{\sigma}_y e^{-\gamma t}\sin(\omega t).$$

This result shows that the dephasing channel causes the decay of both $\hat{\sigma}_x$ and $\hat{\sigma}_y$ with a rate γ. Substitute $\hat{\sigma}_x(t)$ into the OTOC:

$$\mathrm{OTOC}(t) = \langle\hat{\sigma}_x(t)\hat{\sigma}_z\hat{\sigma}_x(t)\hat{\sigma}_z\rangle.$$

Using $\hat{\sigma}_z\hat{\sigma}_x = -\hat{\sigma}_x\hat{\sigma}_z$ and expanding

$$\hat{\sigma}_x(t)\hat{\sigma}_z = \big(\hat{\sigma}_x e^{-\gamma t}\cos(\omega t) - \hat{\sigma}_y e^{-\gamma t}\sin(\omega t)\big)\hat{\sigma}_z.$$

Squaring this

$$\hat{\sigma}_x(t)\hat{\sigma}_z\hat{\sigma}_x(t)\hat{\sigma}_z = e^{-2\gamma t}\big(\cos^2(\omega t) + \sin^2(\omega t)\big).$$

Since $\cos^2(\omega t) + \sin^2(\omega t) = 1$, the OTOC decays exponentially with a rate 2γ

$$\mathrm{OTOC}(t) = e^{-2\gamma t}.$$

This example demonstrates that dephasing (or other forms of noise) can lead to exponential decay of the OTOC. In this case, the decay reflects the loss of coherence due to the environment, rather than chaotic dynamics. It provides a clear and simple case for teaching OTOC behavior in the presence of dissipation.

The system-environment model

The Hamiltonian has three terms, one concerns the system, another one the environment, and finally an interaction term:

$$\hat{H}_T = \hat{H}_S \otimes \mathbb{I}_E + \mathbb{I}_S \otimes \hat{H}_E + \alpha \hat{H}_I \ , \tag{4.38}$$

with $\hat{H}_S$ acting on $\mathcal{H}_S$, $\hat{H}_E$ acting on $\mathcal{H}_E$, and $\hat{H}_I$ acting on $\mathcal{H}_T$. We assume, for simplicity, that none of them is explicitly time dependent. The coefficient α is a measure of the strength of the system-environment coupling. Without loss of generality, the interaction term can be decomposed as

$$\hat{H}_I = \sum_i \gamma_i \hat{S}_i \otimes \hat{E}_i = \sum_i \gamma_i \hat{S}_i^\dagger \otimes \hat{E}_i^\dagger \ , \tag{4.39}$$

with $\hat{S}_i$ and $\hat{E}_i$ Hermitian operators acting on $\mathcal{H}_S$ and $\mathcal{H}_E$, respectively, and γ_i real coefficients. Of course, one can absorb the parameter α in the individual γ_i, but we keep it in explicit form since it is easier to follow in this way the order of the effect of the bath-system interaction. Each term above is referred to as a (quantum) *noise channel*. From now on we will not write the identity operators explicitly when they can be inferred from the context.

Derivation

We derive the Lindblad equation for a system coupled to its environment or a measurement apparatus. One first derives the Born-Markov master equation and then traces out the degrees of freedom of the "surroundings". The Lindbladian emerges naturally as a consequence of the Markov approximation.

It is important to note that a decay of the environmental correlations, an assumption that we will repeatedly use in the derivation, can only be strictly valid for an environment which is infinitely large and involves a continuum of frequencies. In the typical situation, like the one we discussed when we derived the Langevin equation, the reservoir is provided by a collection of harmonic oscillator modes with frequencies ω_n and the $\hat{E}_i$ are given by linear combinations of the modes $\hat{q}_n$.

In the weak-coupling limit derivation that we discuss below, one typically assumes:

(a) The correlations of the system with the environment develop slowly.
(b) The excitations of the environment caused by the system decay very quickly.
(c) The terms which are fast-oscillating when compared to the system's timescale of interest can be neglected.

The names *Born, Markov*, and *rotating wave* are associated to these approximations as indicated below.

Take a total isolated system T and its Hilbert space $\mathcal{H}_T$. The evolution of its density operator is given by the von Neumann equation:

$$\frac{d\hat{\rho}_T(t)}{dt} = -\frac{\mathrm{i}}{\hbar}\left[\hat{H}_T, \hat{\rho}_T(t)\right] \, . \tag{4.40}$$

Consider now that the total system is made of our system of interest S with its Hilbert space $\mathcal{H}_S$, and the environment E with its Hilbert space $\mathcal{H}_E$. As we are interested in the dynamics of the system, without the environment, we will trace over the environment degrees of freedom to obtain the reduced density matrix of the system $\hat{\rho}_S^{\mathrm{red}} = \mathrm{Tr}_E \hat{\rho}_T$ and search for the equation that rules its time evolution.

The goal is to write an equation for $\hat{\rho}_S^{\mathrm{red}}$. There exists several approximation schemes for obtaining it [2,54–59]. While useful in their respective regimes of applicability, each of these methods has its limitations which can be due to physical limitations on the regime of applicability, or because of practical issues associated with the numerical implementation.

It is useful to work in the interaction picture, in which any operator $\hat{O}$ evolves with time with the system and environment Hamiltonian.

$$\hat{O}_{\mathrm{I}}(t) = e^{\frac{\mathrm{i}}{\hbar}(\hat{H}_S+\hat{H}_E)t}\ \hat{O}\ e^{-\frac{\mathrm{i}}{\hbar}(\hat{H}_S+\hat{H}_E)t} \tag{4.41}$$

Here we signal with a subindex $_{\mathrm{I}}$ the interaction picture. Some simple calculations lead to the evolution equation of the total density matrix in the interaction picture

$$\frac{d\hat{\rho}_T(t)}{dt} = -\frac{\mathrm{i}}{\hbar}\alpha\left[\hat{H}_I(t), \hat{\rho}_T(t)\right] \tag{4.42}$$

with

$$\hat{H}_I(t) = e^{\frac{\mathrm{i}}{\hbar}(\hat{H}_S+\hat{H}_E)t}\ \hat{H}_I\ e^{-\frac{\mathrm{i}}{\hbar}(\hat{H}_S+\hat{H}_E)t} \tag{4.43}$$

$$\underbrace{\hat{\rho}_T(t)}_{\text{Interaction}} = e^{\frac{\mathrm{i}}{\hbar}(\hat{H}_S+\hat{H}_E)t}\ \underbrace{\hat{\rho}_T(t)}_{\text{Schrodinger}}\ e^{-\frac{\mathrm{i}}{\hbar}(\hat{H}_S+\hat{H}_E)t} \tag{4.44}$$

We do not attach a subindex $_I$ to $\hat{\rho}_T(t)$ to lighten the notation.

Exercise 4.3 Derive the von Neumann equation in the interaction picture.

The interaction picture density operator $\hat{\rho}_{\mathrm{I}}(t)$ is defined as

$$\hat{\rho}_{\mathrm{I}}(t) = \hat{U}_0^{\dagger}(t)\hat{\rho}(t)\hat{U}_0(t),$$

where $\hat{\rho}$ is the Schrödinger picture density operator (we do not write a sub-index $_S$ to lighten the notation), $\hat{U}_0(t)$ is the unitary evolution operator for the "free" Hamiltonian

$$\hat{U}_0(t) = e^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0 t}$$

and $\hat{H}_0 = \hat{H}_S + \hat{H}_E$. We start with the Schrödinger picture equation for the total density operator,

$$\frac{d\hat{\rho}(t)}{dt} = -\frac{\mathrm{i}}{\hbar}[\hat{H}_T, \hat{\rho}(t)] \, ,$$

where we substitute the total Hamiltonian $\hat{H}_T = \hat{H}_0 + \alpha \hat{H}_I(t)$, and we obtain

$$\frac{d\hat{\rho}(t)}{dt} = -\frac{\mathrm{i}}{\hbar}[\hat{H}_0, \hat{\rho}(t)] - \frac{\mathrm{i}}{\hbar}\alpha[\hat{H}_I(t), \hat{\rho}(t)] \ . \tag{4.45}$$

We now transform to the interaction picture using $\hat{\rho}_{\mathrm{I}}(t) = \hat{U}_0^\dagger(t)\hat{\rho}(t)\hat{U}_0(t)$. The time derivative of $\hat{\rho}_{\mathrm{I}}(t)$ is:

$$\frac{d\hat{\rho}_{\mathrm{I}}(t)}{dt} = \frac{d}{dt}\left(\hat{U}_0^\dagger(t)\hat{\rho}(t)\hat{U}_0(t)\right).$$

that using the product rule becomes

$$\frac{d\hat{\rho}_{\mathrm{I}}(t)}{dt} = \frac{d\hat{U}_0^\dagger(t)}{dt}\hat{\rho}(t)\hat{U}_0(t) + \hat{U}_0^\dagger(t)\frac{d\hat{\rho}(t)}{dt}\hat{U}_0(t) + U_0^\dagger(t)\rho_S(t)\frac{dU_0(t)}{dt}.$$

Using now $d\hat{U}_0(t)/dt = -\frac{\mathrm{i}}{\hbar}\hat{H}_0\hat{U}_0(t)$ and $d\hat{U}_0^\dagger(t)/dt = \frac{\mathrm{i}}{\hbar}\hat{U}_0^\dagger(t)\hat{H}_0$:

$$\frac{d\hat{\rho}_{\mathrm{I}}(t)}{dt} = \frac{\mathrm{i}}{\hbar}\hat{U}_0^\dagger(t)\hat{H}_0\hat{\rho}(t)\hat{U}_0(t) + \hat{U}_0^\dagger(t)\frac{d\hat{\rho}(t)}{dt}\hat{U}_0(t) - \frac{\mathrm{i}}{\hbar}\hat{U}_0^\dagger(t)\hat{\rho}(t)\hat{H}_0\hat{U}_0(t).$$

In the first and third terms in the right-hand-side we see the commutator $[\hat{H}_0, \hat{\rho}(t)]$ appear between $\hat{U}_0^\dagger$ (left) and $\hat{U}_0$ (right). In the term in the middle there is $\frac{d\hat{\rho}(t)}{dt}$ which we can substitute using (4.45). The terms involving the commutator cancel and we are left with

$$\frac{d\hat{\rho}_{\mathrm{I}}(t)}{dt} = -\frac{\mathrm{i}}{\hbar}\alpha\hat{U}_0^\dagger(t)[\hat{H}_I(t), \hat{\rho}(t)]\hat{U}_0(t)$$

The operator $\hat{H}_I$ and $\hat{\rho}$ in the right hand side are still in the Schrödinger picture. But opening the commutator and inserting identities $\hat{U}_0\hat{U}_0^\dagger$ one transforms them both into the interaction picture. Then,

$$\frac{d\hat{\rho}_{\mathrm{I}}(t)}{dt} = -\frac{\mathrm{i}}{\hbar}\alpha[\hat{H}_I(t), \hat{\rho}_{\mathrm{I}}(t)]$$

where $\hat{H}_I(t)$ is also in the interaction picture here (but we do not write the $_{\mathrm{I}}$ to make the notation less heavy. This equation shows that the dynamics in the interaction picture are driven solely by the interaction Hamiltonian $\hat{H}_I(t)$ in the interaction picture.

This equation can be formally time-integrated to yield

$$\hat{\rho}_T(t) = \hat{\rho}_T(0) - \frac{\mathrm{i}}{\hbar}\alpha\int_0^t ds\left[\hat{H}_I(s), \hat{\rho}_T(s)\right]. \tag{4.46}$$

In principle one could trace over the environment here and obtain an exact expression for $\hat{\rho}_S^{\mathrm{red}}(t)$ but this is in general unfeasible. It is also inconvenient (though unavoidable at the exact level) that the resulting $\hat{\rho}_S^{\mathrm{red}}(t)$ will depend on the integration of the density matrix over all previous times.

Equation (4.46) is the starting point of an iterative approach. Let us introduce it in the right-hand-side of Eq. (4.42),

$$\frac{d\hat{\rho}_T(t)}{dt} = -\frac{\mathrm{i}}{\hbar}\alpha\left[\hat{H}_I(t), \hat{\rho}_T(0)\right] - \frac{\alpha^2}{\hbar^2}\int_0^t ds\left[\hat{H}_I(t), \left[\hat{H}_I(s), \hat{\rho}_T(s)\right]\right] \ . \tag{4.47}$$

By applying this method once more we obtain

$$\frac{d\hat{\rho}_T(t)}{dt} = -\frac{\mathrm{i}}{\hbar}\alpha\left[\hat{H}_I(t),\hat{\rho}_T(0)\right] - \frac{\alpha^2}{\hbar^2}\int_0^t ds\left[\hat{H}_I(t),\left[\hat{H}_I(s),\hat{\rho}_T(0)\right]\right] + O(\alpha^3/\hbar^3). \tag{4.48}$$

After this substitution, the integration of the previous states of the system, $\hat{\rho}_T(s)$ appears only in the terms that are $O(\alpha^3/\hbar^3)$ or higher.

Let us go back to the integro-differential equation (4.47), which is exact, and trace over the environment degrees of freedom:

$$\begin{aligned}\frac{d\hat{\rho}_S^{\mathrm{red}}(t)}{dt} &\equiv \mathrm{Tr}_E\left[\frac{d\hat{\rho}_T(t)}{dt}\right]\\ &= -\frac{\mathrm{i}}{\hbar}\alpha\mathrm{Tr}_E\left[\hat{H}_I(t),\hat{\rho}_T(0)\right] - \frac{\alpha^2}{\hbar^2}\int_0^t ds\ \mathrm{Tr}_E\left[\hat{H}_I(t),\left[\hat{H}_I(s),\hat{\rho}_T(s)\right]\right]\end{aligned} \tag{4.49}$$

This is not a closed time-evolution equation for $\hat{\rho}_S^{\mathrm{red}}(t)$, because the full density matrix $\hat{\rho}_T(s)$ still appears in the right-hand-side. To proceed, we need to make some assumptions.

Assume now that at $t=0$ the system and the environment are in a separable state of the form

$$\hat{\rho}_T(0) = \hat{\rho}_S(0)\otimes\hat{\rho}_E(0)\ . \tag{4.50}$$

This may be the case if the system and the environment have not interacted before $t=0$ or if the correlations between them are very short-lived. Moreover, at the initial time $\hat{\rho}_S(0) = \hat{\rho}_S^{\mathrm{red}}(0)$.

By using the assumption (4.50) and the factorized $\hat{H}_I$ in (4.39), we can now focus on the environment only. The first element of the r.h.s of Eq. (4.49) reads

$$\mathrm{Tr}_E\left[\hat{H}_I(t),\hat{\rho}_T(0)\right] = \sum_i\left\{\hat{S}_i(t)\hat{\rho}_S(0)\mathrm{Tr}_E\left[\hat{E}_i(t)\hat{\rho}_E(0)\right] - \hat{\rho}_S(0)\hat{S}_i(t)\mathrm{Tr}_E\left[\hat{\rho}_E(0)\hat{E}_i(t)\right]\right\}\ .$$

We can now use that $\langle\hat{E}_i\rangle = \mathrm{Tr}[\hat{E}_i\hat{\rho}_E(0)] = 0$ for all i. This looks like a strong assumption, but it is not. If the total Hamiltonian does not fulfil it, we can always rewrite it as $\hat{H}_T = \left(\hat{H}_S + \alpha\sum_i\langle\hat{E}_i\rangle\hat{S}_i\right) + \hat{H}_E + \alpha\hat{H}'_i$, with $\hat{H}'_i = \sum_i S_i\otimes(\hat{E}_i - \langle\hat{E}_i\rangle)$. It is clear that now $\langle\hat{E}'_i\rangle = 0$, with $\hat{E}'_i = \hat{E}_i - \langle\hat{E}_i\rangle$, and the system Hamiltonian is changed just by the addition of an energy shift that does no affect the system's dynamics. Using the cyclic property of the trace, it is easy to prove that this term vanishes.

The equation of motion (4.49) reduces to

$$\frac{d\hat{\rho}_S^{\mathrm{red}}(t)}{dt} = -\frac{\alpha^2}{\hbar^2}\int_0^t ds\ \mathrm{Tr}_E\left[\hat{H}_I(t),\left[\hat{H}_I(s),\hat{\rho}_T(s)\right]\right]. \tag{4.51}$$

In order to unravel the system from the environment in the r.h.s. we need a further assumption. As we are working in the weak coupling regime, $\alpha\ll 1$, we may assume that the timescales of correlation of the environment with the system (τ_{SE}) and relaxation of the environment (τ_E) are much shorter than the typical system's timescale (τ_S). This *Born approximation* rests on the largeness of the bath and the relative weakness of the coupling, and states that the environment state is always decoupled from the system's state,

$$\hat{\rho}_T(t) = \hat{\rho}_S^{\text{red}}(t) \otimes \hat{\rho}_E(0) \tag{4.52}$$

and remains unaltered. The systems' state does not and this is why we write here $\hat{\rho}_S^{\text{red}}(t)$ instead of $\hat{\rho}_S(t)$ which would be the evolved density operator in the absence of coupling to the environment. Equation (4.51) then transforms to

$$\frac{d\hat{\rho}_S^{\text{red}}(t)}{dt} = -\frac{\alpha^2}{\hbar^2}\int_0^t ds\, \text{Tr}_E\left[\hat{H}_I(t), \left[\hat{H}_I(s), \hat{\rho}_S^{\text{red}}(s) \otimes \hat{\rho}_E(0)\right]\right] \tag{4.53}$$

This is a closed linear integro-differential for $\hat{\rho}_S^{\text{red}}$ which is still very hard to solve. This equation is still non-Markovian, as it displays an integration over time running from the initial $s = 0$ to the measuring $s = t$ in the r.h.s.

A further approximation, now going in the direction of *Markovianity*, is that one makes the time derivative of the system's density matrix depend only on its current state, and not on its past. This assumption is valid under fast bath dynamics, wherein correlations within the bath are lost extremely quickly, and amounts to replacing

$$\hat{\rho}_S^{\text{red}}(s) \to \hat{\rho}_S^{\text{red}}(t)$$

under the integral

$$\frac{d\hat{\rho}_S^{\text{red}}(t)}{dt} = -\frac{\alpha^2}{\hbar}\int_0^t ds\, \text{Tr}_E\left[\hat{H}_I(t), \left[\hat{H}_I(s), \hat{\rho}_S^{\text{red}}(t) \otimes \hat{\rho}_E(0)\right]\right] . \tag{4.54}$$

Another way of justifying this replacement is to invoke the weak coupling limit, recognizing that that the time-derivative of $\hat{\rho}_S^{\text{red}}$ is already $O(\alpha^2/\hbar^2)$, hence $\hat{\rho}_S^{\text{red}}(s)$ cannot change much in the interval, and replace it by $\hat{\rho}_S^{\text{red}}(t)$. This is sometimes called the *Redfield* or *Born-Markov master equation*. It is now local in time, concerning $\hat{\rho}_S^{\text{red}}(t)$. One should notice, however, that it no longer guarantees the conservation of positivity of the density matrix due to the approximations we have made, and it may therefore yield un-physical solutions, with negative or diverging probabilities. This problem is corrected after making an explicit choice for $\hat{H}_I$ and working out its consequences.

We now change the integration variable from s to $t-s$, with no change of the integration bounds,

$$\frac{d\hat{\rho}_S^{\text{red}}(t)}{dt} = -\frac{\alpha^2}{\hbar^2}\int_0^t ds\ \text{Tr}_E\left[\hat{H}_I(t), \left[\hat{H}_I(t-s), \hat{\rho}_S^{\text{red}}(t) \otimes \hat{\rho}_E(0)\right]\right] . \tag{4.55}$$

We can now understand that the time s indicates how far we go backwards in time to account for memory effects, which can be the characteristic timescale over which correlations in the bath decay, τ_E. Claiming that the bath correlation will decay sufficiently fast we can extend the upper limit of the integral to infinity. We will not do it for now.

The issue now is to perform the trace over the environmental states. We will do it in two ways.

"White bath" approximation

We open the commutators.

$$\begin{aligned}
-\frac{\hbar^2}{\alpha^2}\frac{d\hat{\rho}_S^{\rm red}(t)}{dt} &= \int_0^t ds\ {\rm Tr}_E\left[\hat{H}_I(t),\left[\hat{H}_I(s),\hat{\rho}_S^{\rm red}(t)\otimes\hat{\rho}_E(0)\right]\right]\\
&= \int_0^t ds\,{\rm Tr}_E\Big\{\hat{H}_I(t)\left[\hat{H}_I(s),\hat{\rho}_S^{\rm red}(t)\otimes\hat{\rho}_E(0)\right]-\left[\hat{H}_I(s),\hat{\rho}_S^{\rm red}(t)\otimes\hat{\rho}_E(0)\right]\hat{H}_I(t)\Big\}\\
&= \int_0^t ds\,{\rm Tr}_E\Big\{\hat{H}_I(t)\hat{H}_I(s)\ \hat{\rho}_S^{\rm red}(t)\otimes\hat{\rho}_E(0)-\hat{H}_I(t)\ \hat{\rho}_S^{\rm red}(t)\otimes\hat{\rho}_E(0)\ \hat{H}_I(s)\\
&\qquad -\hat{H}_I(s)\ \hat{\rho}_S^{\rm red}(t)\otimes\hat{\rho}_E(0)\ \hat{H}_I(t)+\hat{\rho}_S^{\rm red}(t)\otimes\hat{\rho}_E(0)\ \hat{H}_I(s)\hat{H}_I(t)\Big\}
\end{aligned}$$

and we replace the explicit form of $\hat{H}_I$, using one form in one factor and the other (daggered) form in the other factor. For example,

$$\begin{aligned}
\hat{H}_I(t)\hat{H}_I(s) &= \sum_i\gamma_i\hat{S}_i^\dagger(t)\otimes\hat{E}_i^\dagger(t)\sum_j\gamma_j\hat{S}_j(s)\otimes\hat{E}_j(s)\\
&= \sum_{ij}\gamma_i\gamma_j\hat{S}_i^\dagger(t)\hat{S}_j(s)\otimes\hat{E}_i^\dagger(t)\hat{E}_j(s)
\end{aligned}$$

One finds

$$\begin{aligned}
-\frac{\hbar^2}{\alpha^2}\frac{d\hat{\rho}_S^{\rm red}(t)}{dt} = \sum_{i,j}\gamma_i\gamma_j\int_0^t ds\ \Big\{&\hat{S}_i^\dagger(t)\hat{S}_j(s)\hat{\rho}_S^{\rm red}(t)\ {\rm Tr}_E\hat{E}_i^\dagger(t)\hat{E}_j(s)\hat{\rho}_E(0)\\
&-\hat{S}_i(t)\hat{\rho}_S^{\rm red}(t)\hat{S}_j^\dagger(s)\ {\rm Tr}_E\hat{E}_i(t)\hat{\rho}_E(0)\hat{E}_j^\dagger(s)\\
&-\hat{S}_j(s)\hat{\rho}_S^{\rm red}(t)\hat{S}_i^\dagger(t)\ {\rm Tr}_E\hat{E}_j(s)\hat{\rho}_E(0)\hat{E}_i^\dagger(t)\\
&+\hat{\rho}_S^{\rm red}(t)\hat{S}_j^\dagger(s)\hat{S}_i(t)\ {\rm Tr}_E\hat{\rho}_E(0)\hat{E}_j^\dagger(s)\hat{E}_i(t)\Big\} \qquad (4.56)
\end{aligned}$$

Since we assumed from the start that $\hat{S}_i$ and $\hat{E}_i$ are Hermitian it may seem superfluous to carry the daggers. We do it to find a more general expression for the Lindblad equation. We now use the cyclic property of traces and propose

$$\begin{aligned}
{\rm Tr}_E\hat{E}_j(s)\hat{\rho}_E(0)\hat{E}_i^\dagger(t) = {\rm Tr}_E\hat{\rho}_E(0)\hat{E}_i^\dagger(t)\hat{E}_j(s) = {\rm Tr}_E\hat{E}_i^\dagger(t)\hat{E}_j(s)\hat{\rho}_E(0) \equiv \Gamma_{ij}(t,s)\\
{\rm Tr}_E\hat{E}_i(t)\hat{\rho}_E(0)\hat{E}_j^\dagger(s) = {\rm Tr}_E\hat{\rho}_E(0)\hat{E}_j^\dagger(s)\hat{E}_i(t) = {\rm Tr}_E\hat{E}_j^\dagger(s)\hat{E}_i(t)\hat{\rho}_E(0) \equiv \Gamma_{ji}(s,t)
\end{aligned}$$

These correlations are not equal. Indeed,

$$\Gamma_{ji}(s,t) = {\rm Tr}_E\hat{E}_j^\dagger(s)\hat{E}_i(t)\hat{\rho}_E(0) = {\rm Tr}_E\hat{E}_j(s)\hat{E}_i^\dagger(t)\hat{\rho}_E(0) = {\rm Tr}_E\hat{E}_i^\dagger(t)\hat{\rho}_E(0)\hat{E}_j(s) \neq \Gamma_{ij}(t,s)$$

Instead,

$$
\begin{aligned}
\Big(\Gamma_{ji}(s,t)\Big)^{\dagger} &= \mathrm{Tr}_E \hat{\rho}_E(0)\Big(\hat{E}_j^{\dagger}(s)\hat{E}_i(t)\Big)^{\dagger} = \mathrm{Tr}_E \hat{\rho}_E(0)\hat{E}_i^{\dagger}(t)\hat{E}_j(s) \\
&= \mathrm{Tr}_E \hat{E}_i^{\dagger}(t)\hat{E}_j(s)\hat{\rho}_E(0) = \Gamma_{ij}(t,s)
\end{aligned}
$$

Assuming *stationarity* for the bath, a rather reasonable assumption in many relevant cases, the correlations $\Gamma_{ij}(t,s)$ and $\Gamma_{ji}(s,t)$ depend on time-differences only:

$$
\Gamma_{ij}(t,s) = \Gamma_{ij}(t-s) \qquad\qquad \Gamma_{ji}(s,t) = \Gamma_{ji}(s-t)
$$

One can also suppose that they depend on the absolute value of the time difference, $\Gamma_{ji}(|t-s|)$. Changing $i \leftrightarrow j$ in the second group of terms,

$$
\begin{aligned}
-\frac{\hbar^2}{\alpha^2}\frac{d\hat{\rho}_S^{\mathrm{red}}(t)}{dt} &= \sum_{i,j}\gamma_i\gamma_j \int_0^t ds\, \Big\{ \Big[\hat{S}_i^{\dagger}(t)\hat{S}_j(s)\hat{\rho}_S^{\mathrm{red}}(t) - \hat{S}_j(s)\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_i^{\dagger}(t)\Big]\,\Gamma_{ij}(t-s) \\
&\qquad + \Big[-\hat{S}_i(t)\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_j^{\dagger}(s) + \hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_j^{\dagger}(s)\hat{S}_i(t)\Big]\,\Gamma_{ji}(s-t)\ \Big\} \\
&= \sum_{i,j}\gamma_i\gamma_j \int_0^t ds\, \Gamma_{ij}(|t-s|)\, \Big\{ \Big[\hat{S}_i^{\dagger}(t)\hat{S}_j(s)\hat{\rho}_S^{\mathrm{red}}(t) - \hat{S}_j(s)\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_i^{\dagger}(t)\Big] \\
&\qquad + \Big[-\hat{S}_j(t)\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_i^{\dagger}(s) + \hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_i^{\dagger}(s)\hat{S}_j(t)\Big]\ \Big\} \qquad (4.57)
\end{aligned}
$$

At this stage one can redefine the bath correlations $\gamma_i\gamma_j\Gamma_{ij} \mapsto \Gamma_{ij}$. In some cases, a further assumption is made

$$
\Gamma_{ij}(t,s) = h_{ij}\ \delta(t-s) \qquad\qquad \Gamma_{ji}(s,t) = h_{ji}\ \delta(t-s) \qquad (4.58)
$$

that is, that correlations within the bath die out so quickly compared to the system's evolution that one ignores them completely. The h_{ij} factors are general numerical factors which result from performing the trace over the bath. This is another consequence of the weak system-bath interaction and the Markov approximation. The first and third terms combine together and the second and fourth as well. The master equation simplifies to

$$
\begin{aligned}
-\frac{\hbar^2}{\alpha^2}\frac{d\hat{\rho}_S^{\mathrm{red}}(t)}{dt} &= \sum_{i,j}\frac{h_{ij}}{2}\Big[\hat{S}_i^{\dagger}(t)\hat{S}_j(t)\hat{\rho}_S^{\mathrm{red}}(t) - \hat{S}_j(t)\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_i^{\dagger}(t) \\
&\qquad + \hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_i^{\dagger}(t)\hat{S}_j(t) - \hat{S}_j(t)\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_i^{\dagger}(t)\Big] \\
&= \sum_{i,j} h_{ij}\Big[-\hat{S}_j(t)\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_i^{\dagger}(t) + \frac{1}{2}\{\hat{S}_i^{\dagger}(t)\hat{S}_j(t), \hat{\rho}_S^{\mathrm{red}}(t)\}\Big] \qquad (4.59)
\end{aligned}
$$

The factor 1/2 in the first line comes from the fact that the integral goes until t the same time at which the delta function is evaluated.

After diagonalization of the matrix h_{ij} with an orthogonal transformation, we define new coefficients $\Gamma_i\delta_{ij} = \Gamma_{ij} = \sum_{kl} d_{ik}h_{kl}d^*_{lj}$,

$$\Gamma_i\delta_{ij} = \sum_{kl} d_{ik}h_{kl}d^*_{lj} \qquad \hat{L}_i(t) = \sum_k d_{ik}\hat{S}_k(t) \tag{4.60}$$

Moving back to the Schrödinger picture,

$$\underbrace{\hat{\rho}_S^{\mathrm{red}}(t)}_{\text{Schrodinger}} = \hat{U}(t)\ \underbrace{\hat{\rho}_S^{\mathrm{red}}(t)}_{\text{Interaction}}\ \hat{U}^\dagger(t) \tag{4.61}$$

with $\hat{U}(t) = e^{\frac{\mathrm{i}}{\hbar}\hat{H}_S t}$, the Lindblad equation takes its usual form:

$$\frac{d\hat{\rho}_S^{\mathrm{red}}}{dt} = -\frac{\mathrm{i}}{\hbar}[\hat{H}_S, \hat{\rho}_S^{\mathrm{red}}] + \frac{\alpha^2}{\hbar^2}\sum_i \Gamma_i \left[\hat{L}_i\hat{\rho}_S^{\mathrm{red}}\hat{L}_i^\dagger - \frac{1}{2}\{\hat{L}_i^\dagger\hat{L}_j, \hat{\rho}_S^{\mathrm{red}}\}\right] \tag{4.62}$$

$\hat{H}_S$ is here the Hamiltonian of the system alone. Often a factor $\alpha/\hbar$ is absorbed in a definition of the operators $\hat{L}_i$.

The delta functions in (4.58) for the environmental operator correlations is quite a brutal approximation. Better ones are often used. We discuss them below.

Rotating wave approximation

One can be a bit more careful with the treatment of the bath correlation function and not just assume they are delta-correlated in time.

Let us now look at the operators $\hat{S}$ acting on the system. Let us denote by $|\epsilon\rangle$ the eigenstates of $\hat{H}_S$ and expand any of the $\hat{S}$ in the Schrödinger picture as

$$\hat{S} = \sum_{\epsilon,\epsilon'} S_{\epsilon\epsilon'}|\epsilon\rangle\langle\epsilon'|\ .$$

In the interaction frame, these operators are touched only by the exponential in $\hat{H}_E$ and we obtain

$$\hat{S}_{\mathrm{I}}(t) = \sum_{\epsilon\epsilon'} S_{\epsilon\epsilon'}\,|\epsilon\rangle\langle\epsilon'|\,e^{-\mathrm{i}(\epsilon-\epsilon')t/\hbar} = \sum_\omega \hat{S}(\omega)\,e^{-\mathrm{i}\omega t}$$

where the sum over ω is over all the possible transition frequencies $(\epsilon-\epsilon')/\hbar$ that appear in the spectrum of $\hat{H}_S$ and $\hat{S}(\omega) = S_{\epsilon\epsilon'}\,|\epsilon\rangle\langle\epsilon'|$ with ω thus defined. The operators $\hat{S}(\omega)$ are in general non-Hermitian, they satisfy $\hat{S}^\dagger(\omega) = \hat{S}(-\omega)$.

Putting these two ingredients together, the interaction Hamiltonian in the interaction picture can be rewritten as

$$\hat{H}_I(t) = \sum_i \gamma_i \sum_\omega e^{-\mathrm{i}\omega t}\hat{S}_i(\omega)\otimes\hat{E}_i(t) = \sum_i \gamma_i \sum_\omega e^{\mathrm{i}\omega t}\hat{S}_i^\dagger(\omega)\otimes\hat{E}_i^\dagger(t) \tag{4.63}$$

with

$$\hat{E}_i(t) = e^{\mathrm{i}\hat{H}_E t/\hbar}\hat{E}_i e^{-\mathrm{i}\hat{H}_E t/\hbar} \tag{4.64}$$

the operators acting on the environment in its own interaction picture. Replacing in the master equation in the form (4.55) with the upper limit of integration extended to ∞, and absorbing the parameters $\gamma_i\gamma_j$ in the definition og Γ_{ij},

$$\begin{aligned} -\frac{\hbar^2}{\alpha^2}\frac{d\hat{\rho}_S^{\mathrm{red}}(t)}{dt} &= \sum_{ij}\sum_{\omega\omega'}\Gamma_{ij}(\omega)e^{\mathrm{i}(\omega-\omega')t}\Big(\hat{S}_i^\dagger(\omega)\hat{S}_j(\omega')\hat{\rho}_S^{\mathrm{red}}(t)-\hat{S}_i(\omega)\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_j^\dagger(\omega') \\ &\qquad +\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_i^\dagger(\omega)\hat{S}_j(\omega')-\hat{S}_i(\omega')\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_j^\dagger(\omega)\Big) \end{aligned} \tag{4.65}$$

The correlations $\Gamma_{ij}(\omega)$ are defined as

$$\Gamma_{ij}^t(\omega)\equiv\gamma_i\gamma_j\int_0^\infty ds\, e^{-\mathrm{i}\omega s}\,\mathrm{Tr}_E\left[\hat{E}_i^\dagger(t)\hat{E}_j(s)\,\hat{\rho}_E(0)\right]$$

and similarly for the others. We note that the integration over s has been extended here to ∞. These are, in general, time-dependent functions. However, one assumes that they are not and drops the superindex t. In the typical situation in which the reservoir is a collection of harmonic oscillator modes, if the frequency spectrum ω_n of the reservoir modes is discrete (as in the classical case) these correlation functions are quasi-periodic functions of t. A rapid decay of the reservoir correlations therefore requires a continuum of frequencies.

The *secular approximation* consists in neglecting all the terms that rapidly oscillate in the sum over ω and ω', that is the omission of all terms with $\omega\neq\omega'$. One keeps only the contributions from $\omega=\omega'$, which leads to

$$-\frac{\hbar^2}{\alpha^2}\frac{d\rho_S^{\mathrm{red}}(t)}{dt}=\sum_{ij}\sum_{\omega}\Gamma_{ij}(\omega)\left(\hat{S}_j(\omega)\hat{\rho}_S^{\mathrm{red}}\hat{S}_i^\dagger(\omega)-\frac{1}{2}\{\hat{S}_i(\omega)^\dagger\hat{S}_j(\omega),\hat{\rho}_S^{\mathrm{red}}(t)\}\right).$$

We now split the real and imaginary parts of the bath correlations as

$$\Gamma_{ij}(\omega)=\frac{1}{2}\gamma_{ij}(\omega)+\mathrm{i}\pi_{ij}(\omega) \tag{4.66}$$

with

$$\pi_{ij}(\omega) = -\frac{\mathrm{i}}{2}(\Gamma_{ij}(\omega)-\Gamma^*(\omega)) \tag{4.67}$$

$$\gamma_{ij}(\omega) = \Gamma_{ij}(\omega)+\Gamma_{ij}^*(\omega) \tag{4.68}$$

The real and imaginary parts $\gamma_{ij}(\omega)$ and $\pi_{ij}(\omega)$ of the complex function Γ_{ij} verify the Kramers-Kronig relations.

Inserting the expression (4.66) of Γ_{ij} in the last equation, we arrive at a master equation in the Lindblad form

$$\begin{aligned} \frac{d\hat{\rho}_S^{\mathrm{red}}(t)}{dt} &= -\frac{\mathrm{i}}{\hbar}\sum_{\omega}\sum_{ij}\ \pi_{ij}(\omega)\,[\hat{S}_i^\dagger(\omega)\hat{S}_j(\omega),\rho_S^{\mathrm{red}}(t)] \\ &\quad+\sum_{\omega}\sum_{ij}\gamma_{ij}(\omega)\left(\hat{S}_j(\omega)\hat{\rho}_S^{\mathrm{red}}(t)\hat{S}_i^\dagger(\omega)-\frac{1}{2}\{\hat{S}_i^\dagger(\omega)\hat{S}_j(\omega),\hat{\rho}_S^{\mathrm{red}}(t)\}\right). \end{aligned} \tag{4.69}$$

where we have absorbed a factor $\alpha/\hbar$ in each $\hat{S}_i$. This master equation is still expressed in the interaction picture, it can be transformed back to the Schrödinger picture by adding the system Hamiltonian H_S to the coherent part of the dynamics in the first line.

The coupling to the bath has two effects:

- The Hamiltonian of the system is shifted by a quantity $\sum_\omega \pi_{ij}(\omega)\hat{S}_i^\dagger(\omega)\hat{S}_j(\omega)$. This term is often called the *Lamb shift* term by analogy to the shift of the atomic levels that arises from the coupling of the atom to its electromagnetic environment. Note the similarity with what happened when we derived the classical Langevin equation and we found a renormlization of the quadratic potential due to the coupling to the bath. It represents the small corrections to the energy levels of the system that arise due to the coupling to the bath.
- *Jump operators* appear, which induce transitions between the eigenstates of $\hat{H}_S$. In the secular approximation, the energy exchanged between the system and the bath during a jump is perfectly defined. The rate associated with the jump where a quantum of energy $\hbar\omega$ is exchanged between the system and the bath is given by the functions $\gamma_{ij}(\omega)$.

4.5.3 Interaction with the radiation field

In the case of an atom interacting with the quantized radiation field, the Hamiltonian for the latter is given by a sum of harmonic oscillators,

$$\hat{H}_E = \sum_{\vec{k}\lambda} \omega_{\vec{k}}\, \hat{a}^\dagger_{\vec{k}\lambda}\hat{a}_{\vec{k}\lambda}, \tag{59}$$

where λ is the polarization index [?]. If the wavelength of the radiation field is much larger than the spatial extent of the atomic wavefunction, the dominant interaction term is given by the electric dipole term,

$$\hat{H}_I = -\vec{d}\cdot\vec{\mathcal{E}} = -\vec{d}\cdot i\sqrt{\frac{\hbar\omega_k}{V}}\vec{\epsilon}_\lambda(\hat{a}^\dagger_{\vec{k}\lambda} - \hat{a}_{\vec{k}\lambda})$$

where $\vec{d}$ is the dipole operator of the atom and $\vec{E}$ is the quantized electric field.

If the reference state of the bath, $\hat{\rho}_E$, is the vacuum without any photons, the reservoir correlations are

$$\langle a_{\vec{k}\lambda}a_{\vec{k}'\lambda'}\rangle = \langle a^\dagger_{\vec{k}\lambda}a^\dagger_{\vec{k}'\lambda'}\rangle = \langle a^\dagger_{\vec{k}\lambda}a_{\vec{k}'\lambda'}\rangle = 0 \qquad \langle a_{\vec{k}\lambda}a^\dagger_{\vec{k}'\lambda'}\rangle = \delta_{\vec{k}\vec{k}'}\delta_{\lambda\lambda'}$$

$$\sum_\lambda e^i_{k\lambda}e^j_{k\lambda} = \delta_{ij} - \frac{k_ik_j}{k^2}\,. \tag{4.70}$$

The spectral correlation tensor becomes

$$\Gamma_{ij}(\omega) = \sum_{\vec{k}} \frac{\hbar\omega_k}{V}\left(\delta_{ij} - \frac{k_ik_j}{k^2}\right)\cdot\int ds\; e^{-i(\omega_k-\omega)s}$$

Going to the continuum limit, we can use:

$$\sum_{\vec{k}} \to \frac{V}{(2\pi)^3}\int d^3k = \frac{V}{(2\pi)^3 c^3}\int d\omega_k \omega_k^2 \int d\Omega \tag{4.71}$$

$$\int d\Omega \left(\delta_{ij} - \frac{k_i k_j}{k^2}\right) = \frac{8\pi}{3}\delta_{ij} \tag{4.72}$$

The spectral correlation tensor is in diagonal form. For the s-integration,

$$\int_0^\infty ds\, e^{-i(\omega_k-\omega)s} = \pi\delta(\omega_k - \omega) + \mathrm{PV}\frac{1}{\omega_k - \omega},$$

where PV denotes the Cauchy principal value. We can thus split the spectral correlation tensor into its real and imaginary parts to obtain the decay rate and the Lamb shift, respectively. The Lamb shift is divergent as we have neglected relativistic effects that become relevant for large values of ω_k. Since this only gives a slight renormalization of the energy levels of the atom, we neglect it in the following (this is similar to what was done at the classical level when adding a counter-term in the derivation of the Langevin equation).

We focus on the transition between two atomic levels differing by the frequency ω. The Lindblad equation reads

$$\frac{d}{dt}\hat{\rho}_S = \gamma\left(\hat{\sigma}_-\hat{\rho}_S\hat{\sigma}_+ - \frac{1}{2}\{\hat{\sigma}_+\hat{\sigma}_-, \hat{\rho}_S\}\right) ,$$

where we have used the spontaneous emission rate

$$\gamma = \frac{4\omega^3 d^2}{3\hbar c^3} ,$$

and the spin flip operators:

$$\hat{\sigma}_\pm = \frac{1}{2}(\hat{\sigma}_x \pm i\hat{\sigma}^y) .$$

The master equation can be solved by expanding it into Pauli matrices. The vector $\langle\vec{\sigma}\rangle$ is known as the Bloch vector, and the equations of motion for its components decouple

$$\frac{d}{dt}\langle\hat{\sigma}_x\rangle = -\frac{\gamma}{2}\langle\hat{\sigma}_x\rangle , \qquad \frac{d}{dt}\langle\hat{\sigma}^y\rangle = -\frac{\gamma}{2}\langle\hat{\sigma}^y\rangle , \qquad \frac{d}{dt}\langle\hat{\sigma}_z\rangle = -\gamma(\langle\hat{\sigma}_z\rangle + 1) .$$

From this, we see that the off-diagonal elements of the density matrix decay exponentially with the rate $\gamma/2$, a phenomenon called decoherence. The z-component of the Bloch vector decays exponentially with the rate γ to a steady state of $\langle\hat{\sigma}_z\rangle = -1$, i.e., the atom ends up in the state with lower energy.

5 Generating functionals

Concise presentations of the path integral formalism can be found in the lecture notes by B. Simons [76] and D. J. Amit's book [77]. The method was suggested by Dirac in the 30s and then developed by Feynman in the 40s.

The path integral method provides a way to write the matrix element of the evolution operator, or *amplitude* to find the particle at x at time t knowing that it was at x' at time t',

$$\langle x, t|x', t'\rangle = \langle x|\hat{U}(t, t')|x'\rangle = U(x, t; x', t') \ , \tag{5.73}$$

as an *integral over classical paths*. (Extensions to spins, fields or other kinds of variables also exist.) Before presenting its construction we take a few paragraphs to explain how functional integration methods were introduced in the context of stochastic processes

5.1 The Wiener construction for Langevin equations

We open a parenthesis and comment on a classical analogy of what Feynman did quantum mechanically. It concerns the description of stochastic processes developed by Wiener in the 20s. Consider a time-dependent random process as described, for example, by the over-damped Langevin equation

$$\frac{dx(t)}{dt} = \xi(t) \ . \tag{5.74}$$

The right-hand-side is a random function, and its statistical properties have to be specified. A usual choice is Gaussian, as a zero mean white noise, that is, $\langle\xi(t'')\rangle = 0$ and $\langle\xi(t'')x(t''')\rangle = 2k_BT\delta(t'' - t''')$ for all t'' and t'''. The angular brackets represent here the average over the Gaussian probability distribution of the noise. This noise has *no memory* or, in other terms, the process is *Markovian*. We will come back to what this means below. The friction coefficient has been absorbed in a time redefinition and T is the temperature of the bath. The particle has fixed initial condition $x(t') = x'$ and it evolves according to (5.74). Observables are noise averages of the particle's position and can be readily calculated from the solution of the above equation, $x(t) = x(t') + \int_{t'}^{t} dt''\, \xi(t'')$. For example, $\langle x(t)\rangle = x'$ and $\langle(x(t) - x(t'))^2\rangle = 2D(t - t')$ with diffusion coefficient $D = k_BT$.

Time is now discretized in infinitesimal steps of length $\delta t = (t - t')/N$ with $t_k = t' + k\,\delta t$ and $k = 0, \ldots, N$; then $t_0 = t'$ and $t_N = t$. The evaluation of the position at the discrete time will be denoted $x_k = x(t_k)$. Equation (5.74) then reads

$$\delta x_k \equiv x_{k+1} - x_k = \delta t\ \xi_k \ . \tag{5.75}$$

(We adopt here what is called Ito's discretization scheme in which the noise is evaluated in the pre-point.) The Gaussian white noise has joint probability distribution

$$P(\xi) \equiv P(\{\xi_k\}) = \prod_k \frac{1}{(2\pi\ 2k_BT/\delta t)^{1/2}}\ e^{-\frac{1}{2}\frac{\delta t}{2k_BT}\xi_k^2} \ . \tag{5.76}$$

This ensures that

$$\langle \xi_k \rangle = 0 \; , \qquad\qquad \langle \xi_k \xi_{k'} \rangle = 2k_B T \, \frac{1}{\delta t} \, \delta_{kk'} \tag{5.77}$$

giving the scalings $\xi_k = \mathcal{O}(\delta t^{-1/2})$ and $x_{k+1} - x_k = \mathcal{O}(\delta t^{1/2})$ typical of over-damped (no second time derivative) white noise processes. The weird normalization of the Kronecker delta in the second relation ensures that it approaches the Dirac delta in the continuous time limit. The noise average of a generic function O of the variable x is then,

$$\langle O \rangle = \int \mathcal{D}\xi \; O(x^{(\xi)}) \, P(\xi) \tag{5.78}$$

where $O(x^{(\xi)})$ indicates that x has to be expressed as a solution of the Langevin equation, in terms of the noise, the measure $\mathcal{D}\xi$ is just $\prod_k d\xi_k$ and all integrals over the noise run from $-\infty$ to ∞.

Thanks to the Markov property of the process, the probability to find the particle at a position $x = x_N$ at time $t = t_N$ knowing that it departed from $x' = x_0$ at time $t' = t_0$ is

$$\begin{aligned} & p(x,t|x',t') \\ & \quad = \int_{-\infty}^{\infty} dx_{N-1} \cdots \int_{-\infty}^{\infty} dx_1 \; p(x_N = x, t_N = t | x_{N-1}, t_{N-1}) \dots p(x_1, t_1 | x' = x_0, t_0 = t') \; . \end{aligned} \tag{5.79}$$

The evolution over an infinitesimal time step is ruled by Eq. (5.75). Take the first time-step $x_1 = x_0 + \delta t \, \xi_0$. x_0 is fixed to x', and x_1 is just a linear function of ξ_0. One has

$$\begin{aligned} p(x_1, t_1 | x_0, t_0) &= \int d\xi_0 \; \delta(x_1 - (x_0 + \delta t \, \xi_0)) \, \frac{1}{(2\pi \; 2k_B T/\delta t)^{1/2}} \; e^{-\frac{1}{2} \frac{\delta t}{2k_B T} \, \xi_0^2} \\ &= \frac{1}{(2\pi \; 2k_B T/\delta t)^{1/2}} \int d\xi_0 \; \delta(x_1 - x_0 - \delta t \, \xi_0)) \; e^{-\frac{1}{2} \frac{\delta t}{2k_B T} \, \xi_0^2} \\ &= \frac{1}{(2\pi \; 2k_B T/\delta t)^{1/2}} \, \frac{1}{\delta t} \int d\overline{\xi}_0 \; \delta(\overline{\xi}_0 - (x_1 - x_0)) \; e^{-\frac{1}{2} \frac{\delta t}{2k_B T} \left(\frac{\overline{\xi}_0}{\delta t} \right)^2} \\ &= \frac{1}{(2\pi \; 2k_B T \delta t)^{1/2}} \; e^{-\frac{1}{2} \frac{\delta t}{2k_B T} \left(\frac{x_1 - x_0}{\delta t} \right)^2} \; . \end{aligned} \tag{5.80}$$

Replacing now in (5.79)

$$\begin{aligned} p(x,t|x',t') &= \frac{1}{(2\pi \; 2k_B T \; \delta t)^{(N-1)/2}} \int_{-\infty}^{\infty} dx_{N-1} \cdots \int_{-\infty}^{\infty} dx_1 \; e^{-\frac{1}{2} \frac{1}{2k_B T} \; \delta t \, \sum_k \left(\frac{x_{k+1} - x_k}{\delta t} \right)^2} \\ &= \int \mathcal{D}x \; e^{-\frac{1}{2} \frac{1}{2k_B T} \int_{t'}^{t} dt'' \left(\frac{dx(t'')}{dt''} \right)^2} \; . \end{aligned} \tag{5.81}$$

The compact notation $\int \mathcal{D}x$ represents

$$\int \mathcal{D}x \; \dots \; = \; \frac{1}{(2\pi \; 2k_B T \; \delta t)^{(N-1)/2}} \int_{-\infty}^{\infty} dx_{N-1} \cdots \int_{-\infty}^{\infty} dx_1 \; \dots \tag{5.82}$$

We have expressed the transition probability as a sum over all paths (in the x variable) linking the initial value $x_0 = x'$ to the final one $x_N = x$.

For the generalization of this construction to stochastic Langevin equations with deterministic forces and also multiplicative noise, see [79, 80].

5.2 The Feynman construction for quantum systems

Take an *orthonormal complete basis* of eigenstates, $|x\rangle$, of the position operator, $\hat{x}$, that is $\hat{x}|x\rangle = x|x\rangle$, with $\langle x'|x\rangle = \delta(x - x')$.

Going back to the quantum problem, the (forward) propagator is

$$\langle x|\hat{U}(t,t')|x'\rangle = U(x,t;x',t') \qquad \hat{U}(t,t') = e^{-\mathrm{i}\hat{H}(t-t')/\hbar} \; . \tag{5.83}$$

The idea is to write it as a sum over all paths leading from, in the Lagrangian representation, $x' = x(t')$ to $x = x(t)$ with $t > t'$ weighted with the exponential of the action (times $\mathrm{i}/\hbar$). The formalism is well-suited to compute any type of time-ordered correlation since the evolution is done towards the future.

The idea is to discretise the real time interval $[t', t]$, with the definitions

$$t_k = t' + k\,\delta t \qquad k = 0, \dots, N \quad \text{and} \quad \delta t = (t - t')/N \tag{5.84}$$

in such a way that $t' = t_0$ and $t = t_N$. Eventually one takes $\delta t \to 0$ and $N \to \infty$ with $t - t'$ fixed.

We first factorize the evolution operator

$$e^{-\mathrm{i}\hat{H}(t-t')/\hbar} = e^{-\mathrm{i}\hat{H}\delta t/\hbar} \; \dots \; e^{-\mathrm{i}\hat{H}\delta t/\hbar} \tag{5.85}$$

in N factors such that $N\delta t = t - t'$. The Hamiltonian $\hat{H}$ commutes with itself so this is a licit expansion. Then we introduce resolutions of the identity in position space

$$\mathbb{I} = \int dx_k \; |x_k\rangle\langle x_k| \tag{5.86}$$

and we derive

$$\begin{aligned} e^{-\mathrm{i}\hat{H}(t-t')/\hbar} \quad &= \int dx_{N-1}|x_{N-1}\rangle\langle x_{N-1}|e^{-\mathrm{i}\hat{H}\delta t/\hbar} \int dx_{N-2}|x_{N-2}\rangle\langle x_{N-2}|e^{-\mathrm{i}\hat{H}\delta t/\hbar} \; \dots \\ & \dots \int dx_1|x_1\rangle\langle x_1|e^{-\mathrm{i}\hat{H}\delta t/\hbar} \end{aligned} \tag{5.87}$$

Sandwiched between $\langle x|$ and $|x'\rangle$, this expression can also be written as

$$\begin{aligned} \langle x,t|x',t'\rangle = \int dx_{N-1} \; \dots \int dx_2 \int dx_1 \; U(x,t;x_{N-1},t_{N-1}) \\ U(x_{N-1},t_{N-1};x_{N-2},t_{N-2}) \dots U(x_2,t_2;x_1,t_1) U(x_1,t_1;x',t') \; . \end{aligned} \tag{5.88}$$

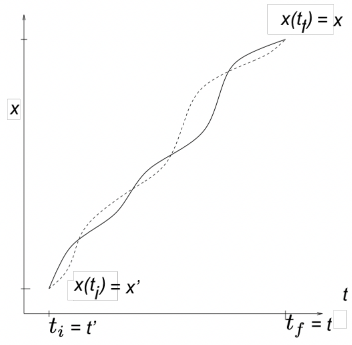

Figure 5.2: Two paths out of many contributing to the path integral that represents the bracket of the evolution operator between an initial and a final state at times t_i and t_f respectively.

Each factor in the product is

$$\langle x_k|\hat{U}(t_k,t_{k-1})|x_{k-1}\rangle = U(x_k,t_k;x_{k-1},t_{k-1}) \ . \tag{5.89}$$

Inserting now identities in momentum space $\mathbb{I} = \int \frac{dp_k}{2\pi\hbar}\,|p_k\rangle\langle p_k|$

$$\begin{aligned} U(x_k,t_k;x_{k-1},t_{k-1}) &= \langle x_k|e^{-\mathrm{i}\hat{H}\delta t/\hbar}|x_{k-1}\rangle = \int \frac{dp_k}{2\pi\hbar}\,\langle x_k|p_k\rangle\,\langle p_k|e^{-\mathrm{i}\hat{H}\delta t/\hbar}|x_{k-1}\rangle \\ &= \int \frac{dp_k}{2\pi\hbar}\,\exp\left[\frac{\mathrm{i}}{\hbar}\left(p_k\dot{x}_k - H(p_k,x_k)\right)\delta t\right] \end{aligned} \tag{5.90}$$

where we have dropped any $\mathcal{O}(\delta t^2)$ contribution. The matrix element is calcutaed in detail in App. B. Inserting this expression in the product of evolution functions and using a continuous time notation

$$U(x,t;x',t') = \int \mathcal{D}p \int_{x(t')=x'}^{x(t)=x} \mathcal{D}x\ \exp\left\{\frac{i}{\hbar}\int_{t'}^{t} dt''\,[p(t'')\dot{x}(t'') - H(p(t''),x(t''))]\right\} \tag{5.91}$$

If the kinetic energy is quadratic in p, the two p-dependent terms in the exponential can be combined to form a Gaussian weight:

$$p\dot{x} - \frac{p^2}{2m} = -\frac{1}{2m}(p-m\dot{x})^2 + \frac{m}{2}\dot{x}^2 \ . \tag{5.92}$$

After translation $p - m\dot{x} \mapsto p$, the momentum can be integrated out and yields a simple factor $m/(2\pi\mathrm{i}\hbar\delta t)^{N/2}$ which can be absorbed in the measure $\mathcal{D}x$ (similarly to what we have done in the stochastic case). Then,

$$U(x,t;x',t') = \int_{x(t')=x'}^{x(t)=x} \mathcal{D}x\ \exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t'}^{t} dt''\left[\frac{m}{2}\dot{x}^2(t'') - V(x(t''))\right]\right\} \ . \tag{5.93}$$

In the exponential we recognise the *classical action*,

$$S = \int_{t'}^{t} dt'' \; L(\dot{x}, x) \; , \tag{5.94}$$

with $L(\dot{x}, x)$ the *Lagrangian*.

5.2.1 Wick's rotation

Make now an analytic continuation from real to *imaginary time*

$$t \mapsto -\mathrm{i}\tau \tag{5.95}$$

This is also called a *Wick rotation*. The expression above becomes

$$U(x, -\mathrm{i}\tau; x', -\mathrm{i}\tau') = \int_{x(-\mathrm{i}\tau')=x'}^{x(-\mathrm{i}\tau)=x} \mathcal{D}x \; \exp\left\{ \frac{\mathrm{i}}{\hbar} \int_{-\mathrm{i}\tau'}^{-\mathrm{i}\tau} d(-\mathrm{i}\tau'') \left[\frac{m}{2} \left(\frac{dx(-\mathrm{i}\tau'')}{d(-\mathrm{i}\tau'')} \right)^2 - V(x(-\mathrm{i}\tau'')) \right] \right\}$$

Renaming $x(-\mathrm{i}\tau) \mapsto x(-\tau)$ and $U(x, -\mathrm{i}\tau; x', -\mathrm{i}\tau') \mapsto U(x, -\tau; x', -\tau')$, and noticing that

$$\int_{-\mathrm{i}\tau'}^{-\mathrm{i}\tau} d(-\mathrm{i}\tau'') \; f(-\tau'') = \mathrm{i} \int_{\tau'}^{\tau} d\tau'' \; f(\tau'') \tag{5.96}$$

$$\frac{dx(-\mathrm{i}\tau'')}{d(-\mathrm{i}\tau'')} = \frac{1}{(-\mathrm{i})} \frac{dx(-\mathrm{i}\tau'')}{d\tau''} \mapsto \mathrm{i} \; \frac{dx(\tau'')}{d\tau''} = \mathrm{i} \; \dot{x}(\tau'') \tag{5.97}$$

one derives

$$U(x, \tau; x', \tau') = \int_{x(\tau')=x'}^{x(\tau)=x} \mathcal{D}x \; \exp\left\{ -\frac{1}{\hbar} \int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2} \left(\dot{x}(\tau'') \right)^2 + V(x(\tau'')) \right] \right\}$$

and the expression in the exponential is just the classical energy integrated over time (times $-1/\hbar$). This form is also called the *Euclidean action*

$$S_E = \int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2} \left(\dot{x}(\tau'') \right)^2 + V(x(\tau'')) \right] \tag{5.98}$$

(in contrast with a Minkowskian one in which temporal and spatial contributions come with different signs). Tracing over the “initial=final” states

$$\int dx \; \int_{x(\tau')=x}^{x(\tau)=x} \mathcal{D}x \; \exp\left\{ -\frac{1}{\hbar} \int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2} \left(\dot{x}(\tau'') \right)^2 + V(x(\tau'')) \right] \right\} \; . \tag{5.99}$$

That is, we must use boundary conditions such that the initial and final states are the same state, and we need to sum over all such states. This is the reason why we integrate over dx after setting $x(\tau') = x(\tau) = x$. We are getting closer to finding a representation of the partition sum. But what about the times τ and τ'?

- The choice of the “initial” time τ' is arbitrary. We can simply set it to zero, $\tau' = 0$.

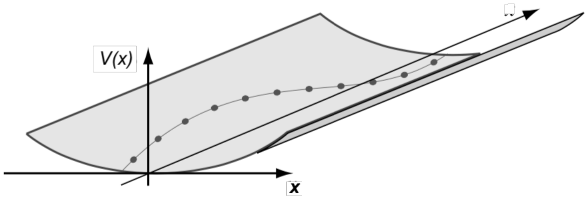

Figure 3.2 A string held under tension and confined to a potential well V.

Figure 5.3: Figure copied from [78], representing the elastic string (think of a polymer made of individual beads labelled by τ). The translation is such that the coordinate along the string is τ. The displacement of each "bead" is $x(\tau)$.

- What about the "final" time τ? We started by representing elements of the evolution operator $e^{-\mathrm{i}\hat{H}t/\hbar}$. If we want to obtain the partition function $e^{-\beta\hat{H}}$ we need the imaginary time $\tau = \mathrm{i}t$ to be related to the inverse temperature β as $\tau = \beta\hbar$.

The *partition function* is therefore

$$\mathcal{Z} = \int dx \int_{x(\tau')=x}^{x(\tau)=x} \mathcal{D}x \, \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau'' \left[\frac{m}{2}\left(\dot{x}(\tau'')\right)^2 + V(x(\tau''))\right]\right\} . \tag{5.100}$$

This problem is equivalent to the classical mechanics of an *elastic string* with $x(\tau)$ the transverse displacement with respect to the internal coordinate along the string represented by τ. The length of the string is $\tau - \tau'$ and its ends are forced to be at $x(\tau') = x$ and $x(\tau) = x$, but otherwise the string can fluctuate. Its elastic energy is

$$E_{\text{elast}} = m\int_{\tau'}^{\tau} d\tau'' \left\{\left[1 + \left(\frac{dx(\tau'')}{d\tau''}\right)^2\right]^{1/2} - 1\right\} \approx \frac{m}{2}\int_{\tau'}^{\tau} d\tau'' \left(\frac{dx(\tau'')}{d\tau''}\right)^2 , \tag{5.101}$$

and it is added to the external potential V to get the full potential energy. Thus, the analytic continuation to imaginary time has transformed the quantum mechanical problem of a single particle moving in a one dimensional space into the statistical physics one of a one dimensional object with transverse displacements. The generalisation to higher dimensions is straightforward. This is another way of deriving the

d-dimensional quantum mechanics – $d+1$ dimensional statistical physics correspondence with the association $t \mapsto -\mathrm{i}\tau$ and $\beta \leftrightarrow 1/\hbar$

One can always interpret the imaginary time generating functional of the quantum problem in d dimensions as the equilibrium Gibbs-Boltzmann partition function of the classical model at finite inverse temperature in $d+1$ dimensions. The classical model, though, is *anisotropic*, since the direction associated to the imaginary time has different interactions from the truly spatial ones.

Mathematically, the imaginary time path integral is a better behaved object than its real time counterpart, since it is a sum of positive quantities, the statistical weights.

In practice, the sum over trajectories which are periodic in imaginary time, can only be done exactly for simple systems. In general, one has to resort to some form of perturbation theory or other approximation scheme.

The Euclidean action is usually non-negative, which implies that if the action corresponding to some $x(\tau)$ is large, its contribution is very small. This fact dramatically improves the convergence of the path integral. The classical path is the one with the maximal contribution since it yields the minimal value to the action.

Example. The ground state

Take a quantum system with Hamiltonian $\hat{H}$ in canonical equilibrium at inverse temperature β (to keep the notation we were using so far). The elements of the (un-normalized) density matrix are

$$\langle x|e^{-\beta\hat{H}}|x'\rangle \ . \tag{5.102}$$

Inserting a complete set of energy eigenstates $|n\rangle$,

$$\begin{aligned}\langle x|e^{-\beta\hat{H}}|x'\rangle &= \sum_{n=0}^{\infty}\langle x|e^{-\beta\hat{H}}|n\rangle\langle n|x'\rangle = \sum_{n=0}^{\infty}e^{-\beta E_n}\langle x|n\rangle\langle n|x'\rangle \\ &= \sum_{n=0}^{\infty}e^{-\beta E_n}\psi_n^*(x)\psi_n(x')\end{aligned} \tag{5.103}$$

with E_n the energy of the nth state and $\psi_n(x)$ its wave function. Taking the limit $\beta\to\infty$ the sum is dominated by the ground state contribution. One can then use

$$\lim_{\beta\to\infty}\mathcal{Z} = \int dx\ \lim_{\beta\to\infty}\langle x|e^{-\beta\hat{H}}|x\rangle = e^{-\beta E_0}\int dx\ |\psi_0(x)|^2 = e^{-\beta E_0} \tag{5.104}$$

which implies

$$E_0 = -\lim_{\beta\to\infty}\frac{1}{\beta}\ln\mathrm{Tr}\, e^{-\beta\hat{H}} \ . \tag{5.105}$$

We can now use the path integral expression for the trace of the density operator or partition function, Eq. (5.100), and therefore get the ground state energy in this way.

5.3 Semi-classical calculation

In the correspondence limit, $\hbar\to 0$, the only history (or possibly histories) that contribute significantly to the path integral must be those that leave the action S stationary. Otherwise, the rapidly oscillating contributions would add up to zero. Thus, in the classical limit there is only one history $x_{\mathrm{cl}}(t)$ linking $x_{\mathrm{cl}}(t') = x'$ and $x_{\mathrm{cl}}(t) = x$ which contributes and it is the one that makes $\delta S = 0$, the *least action principle*. The classical trajectory satisfies the *Euler-Lagrange equation*

$$\left.\frac{\delta S}{\delta x(t'')}\right|_{x_{\rm cl}(t'')} = \frac{\partial L}{\partial x(t'')} - \frac{d}{dt''}\frac{\partial L}{\partial \dot{x}(t'')} = 0 \tag{5.106}$$

with the condition

$$\left.\frac{\delta^2 S}{\delta x(t'')\delta x(t''')}\right|_{x_{\rm cl}(t)} \quad \text{positive definite} . \tag{5.107}$$

Since the classical action satisfies $\delta S/\delta x = 0$ by construction, the action of an arbitrary trajectory satisfies

$$\begin{aligned} S[x(t)] &= S[x_{\rm cl}(t) + \delta x(t)] \\ &= S[x_{\rm cl}(t)] + \int dt'' \left.\frac{\delta S}{\delta x(t'')}\right|_{x_{\rm cl}} \delta x(t'') + \frac{1}{2}\int dt'' \int dt''' \left.\frac{\delta^2 S}{\delta x(t'')\delta x(t''')}\right|_{x_{\rm cl}} \delta x(t'')\delta x(t''') + \ldots \\ &\simeq S[x_{\rm cl}(t)] + \frac{1}{2}\int dt'' \int dt''' \left.\frac{\delta^2 S}{\delta x(t'')\delta x(t''')}\right|_{x_{\rm cl}} \delta x(t'')\delta x(t''') . \end{aligned} \tag{5.108}$$

In the last line we cut the expansion at the second order. The Gaussian integral characterises the *quantum quadratic fluctuations* and it can be calculated interpreting the Hessian as a *differential operator* acting in the space of functions $y(t)$ with boundary conditions $\delta x(0) = \delta x(\tau) = 0$, since the boundary conditions are imposed on the classical solution. The quadratic term can then be integrated over and the final calculation is put in the form of the evaluation of a functional determinant:

$$\left[\det \left.\frac{\delta^2 S}{\delta x(t'')\delta x(t''')}\right|_{x_{\rm cl}}\right]^{-1/2} \tag{5.109}$$

We will not carry out this calculation here since it goes beyond the scope of these lectures.

5.4 The harmonic oscillator

We now derive the quantum partition function of the harmonic oscillator using the path integral formalism.

Take the quantum harmonic oscillator

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 \tag{5.110}$$

with Lagrangian

$$L(\dot{x}, x) = K(\dot{x}) - V(x) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 . \tag{5.111}$$

The classical equation of motion is

$$\ddot{x}_{\rm cl} + \omega^2 x_{\rm cl} = 0 . \tag{5.112}$$

A generic trajectory is $x(t) = x_{\rm cl}(t) + \delta x(t)$. We impose the boundary conditions on the classical trajectory $x_{\rm cl}(t') = x'$ and $x_{\rm cl}(t) = x$. Therefore $\delta x(t') = \delta x(t) = 0$.

For the harmonic oscillator, terms of higher than quadratic order vanish and

$$S[x(t)] = S[x_{\rm cl}(t)] + S[\delta x(t)] \tag{5.113}$$

with the second term being identical to the original action, but evaluated on the perturbation of the classical trajectory. Then,

$$U(x,t;x',0) = e^{\frac{\rm i}{\hbar}S[x_{\rm cl}]} \int_{\delta x(t')=0}^{\delta x(t)=0} \mathcal{D}\delta x \; \exp\left\{\frac{\rm i}{\hbar}\int_{t'}^{t} dt'' \left[\frac{m}{2}\left(\frac{d\delta x(t'')}{dt''}\right)^2 - \frac{m\omega^2}{2}(\delta x(t''))^2\right]\right\} .$$

The calculation of the remaining functional integral can be found in the Feynman-Hibbs book, for example, or other traditional references on path integrals. The real time propagator reads

$$U(x,t|x',t') = \sqrt{\frac{m\omega}{2\pi {\rm i}\hbar\sin(\omega t)}} \; \exp\left\{\frac{{\rm i}m\omega}{2\hbar\sin(\omega t)}\left[(x^2+x'^2)\cos(\omega t) - 2xx'\right]\right\} \tag{5.114}$$

where we already set $t'=0$. We now set $x'=x$, $t'=0$ and $t=-{\rm i}\tau$, and we use $\sin(-{\rm i}z) = \frac{1}{2{\rm i}}(e^{-{\rm ii}z} - e^{{\rm ii}z}) = -\frac{\rm i}{2}(e^z - e^{-z}) = -{\rm i}\sinh z$ and $\cos(-{\rm i}z) = \frac{1}{2}(e^{-{\rm ii}z} + e^{{\rm ii}z}) = \frac{1}{2}(e^z + e^{-z}) = \cosh z$ to obtain

$$U(x,-{\rm i}\tau|x,0) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\tau)}} \; \exp\left\{-\frac{m\omega}{\hbar\sinh(\omega\tau)}\left[\cosh(\omega\tau)-1\right]x^2\right\} . \tag{5.115}$$

Finally, at $\tau = \beta\hbar$,

$$U(x,-{\rm i}\beta\hbar|x,0) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\beta\hbar)}} \; \exp\left\{-\frac{m\omega}{\hbar\sinh(\omega\beta\hbar)}\left[\cosh(\omega\beta\hbar)-1\right]x^2\right\} . \tag{5.116}$$

The integral over x needed to calculate the partition sum $\mathcal{Z}_q$ is just a Gaussian integral

$$\begin{aligned}
\mathcal{Z}_q &= \int dx\; U(x,-{\rm i}\beta\hbar|x,0) \\
&= \frac{1}{\sqrt{2[\cosh(\beta\hbar\omega)-1]}} \\
&= \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}} \\
&= \sum_{n=0} e^{-\beta(n+1/2)\hbar\omega}
\end{aligned} \tag{5.117}$$

and we recover the well-known result.

5.5 Tunneling and instantons

Consider a quantum particle in a double well potential $V(x)$ as the one sketched in Fig. 5.4. A particular formula with this form is the familiar $\lambda\phi^4$,

$$V(x) = \frac{r^2}{4u} + \frac{r}{2}x^2 + \frac{u}{4}x^4 \;, \tag{5.118}$$

with $r < 0$. The minima and the maximum are at

$$x_{\rm min} = \pm(-r/u)^{1/2} \equiv \pm x_0 \qquad\qquad x_{\rm max} = 0 \;. \tag{5.119}$$

For convenience, we added the constant $r^2/(4u)$ so that $V(\pm x_0) = 0$. Consequently, $V(x_{\rm max}) = r^2/(4u)$. We note that r^2/u controls the height of the barrier and $(-r/u)^{1/2}$ the distance between the two minima, that is, the thickness of the barrier. If one compares the two, one sees that the larger r the "steeper" the barrier.

Some quantum mechanics

Classically, if the total energy of the particle is lower than the height of the barrier, the particle's motion is oscillatory within the well where it is placed initially. The minimal energy configuration is doubly degenerate, and static at the bottom of each well, with vanishing kinetic and potential energies.

Quantum mechanically, if there were no coupling across the barrier, the Hamiltonian would have two independent, oscillator-like sets of low-lying eigenstates sitting in the two local minima, see the parabola approximating the left well and the equidistant levels in the sketch in Fig. 5.4, with energies $E_n = (n + 1/2)\hbar\omega$, as in (5.117). Allowing for a weak inter-barrier coupling, the oscillator ground states (like all higher states) split into a *doublet* of a symmetric and an antisymmetric eigenstate, $|S\rangle$ and $|A\rangle$ with energies E_S and E_A, respectively. In this case, there is a small tunnelling probability and the particle can be found with non-vanishing probability in the well where it was not initially. The transition amplitudes between the left and the right well, and the one to remain in the right well, from time 0 to an imaginary time $-\mathrm{i}\tau$ are

$$\begin{aligned} U(x_0, -\mathrm{i}\tau, \pm x_0, 0) &= \langle x_0| e^{-\hat{H}\tau/\hbar} | \pm x_0\rangle \\ &\sim \langle x_0| \left(|S\rangle e^{-E_S\tau/\hbar} \langle S| + |A\rangle e^{-E_A\tau/\hbar}\langle A| \right) | \pm x_0\rangle \end{aligned} \tag{5.120}$$

Setting

$$E_{A/S} = \frac{\omega\hbar}{2} \pm \frac{\Delta}{2} \;, \tag{5.121}$$

with Δ the energy splitting between the symmetric and anti-symmetric states, and using the symmetry properties $|\langle x_0|S\rangle|^2 = |\langle -x_0|S\rangle|^2 = C/2$ and $\langle x_0|A\rangle\langle A| - x_0\rangle = -|\langle x_0|A\rangle|2 = -C/2$,

$$\begin{aligned} U(x_0, -\mathrm{i}\tau, \pm x_0, 0) &\sim \frac{C}{2}\left(e^{-(\hbar\omega-\Delta)\tau/(2\hbar)} \pm e^{-(\hbar\omega+\Delta)\tau/(2\hbar)} \right) \\ &= C e^{-\omega\tau/2} \left\{ \begin{array}{l} \cosh(\Delta\tau/\hbar) \\ \sinh(\Delta\tau/\hbar) \end{array} \right. \end{aligned} \tag{5.122}$$

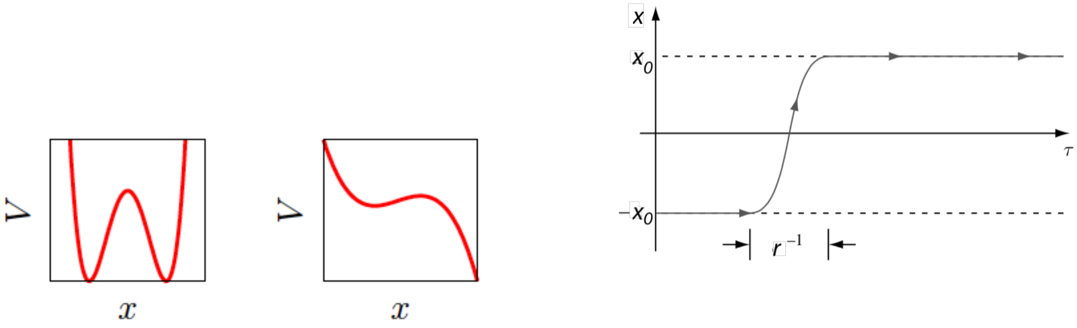

Figure 5.4: Figures copied from [78]. The left panel represents the double well potential $V(x)$ and its reversed $-V(x)$. The minima/maxima have $V = 0$. The right panel plots a typical instanton, with width $|r|^{-1}$ taking the particle from the left well (top of the left hill) to the right one (top of the right hill).

The splitting between the ground and first excited states Δ determines the *tunnelling rate*.

The path integral calculation

In the path integral calculation, we go to imaginary time in part because the evaluation of the path integral by saddle point is better controled.

The transition amplitude between a point x' at (imaginary) time τ' and another point x at (imaginary) time τ is given by

$$U(x, \tau; x', \tau') = \int_{x(\tau')=x'}^{x(\tau)=x} \mathcal{D}x \, \exp \left\{ -\frac{1}{\hbar} \int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2} \left(\dot{x}(\tau'') \right)^2 + V(x(\tau'')) \right] \right\} \tag{5.123}$$

and one has to sum over all possible paths in imaginary time. In the literature one does not write the $(-\mathrm{i})$ in front of the time τ so we will henceforth not do it and follow the usual notation, as already done above. For "thick" enough barriers, the leading contributions can be obtained by a *semi-classical* $\hbar \to 0$ *approximation*, which corresponds to a quadratic expansion around the trajectories with *minimal action*:

$$\left. \frac{\delta S[x(\tau'')]}{\delta x(\tau)} \right|_{x_{\rm cl}(\tau)} = 0 \qquad \text{and} \qquad \left. \frac{\delta^2 S[x(\tau'')]}{\delta x(\tau) \delta x(\tau')} \right|_{x_{\rm cl}(\tau)} \quad \text{positive definite} \, . \tag{5.124}$$

Note that here there is no ambiguity about the need to look for a minimum of the action. Writing $x(\tau) = x_{\rm cl}(\tau) + y(\tau)$, the result is

$$\begin{aligned} U \;&\approx\; \underbrace{e^{-\frac{1}{\hbar} S[x_{\rm cl}(\tau)]}}\, \underbrace{\int \mathcal{D}y \, \exp \left\{ -\frac{1}{2\hbar} \int_{\tau'}^{\tau} d\tau'' \int_{\tau'}^{\tau} d\tau''' \, y(\tau'') \left. \frac{\delta^2 S[x(\tau)]}{\delta x(\tau'') \delta x(\tau''')} \right|_{x_{\rm cl}} y(\tau''') \right\}} \\ &= \quad U_{\rm cl} \qquad\qquad \times \qquad\qquad U_{\rm q} \end{aligned} \tag{5.125}$$

and it is written as the product of a classical contribution $U_{\rm cl}$ and a quantum one $U_{\rm q}$. The Gaussian integral yields the one over the square root of the *determinant* of the Hessian operator:

$$U_{\rm q} \propto \left[\det \left. \frac{\delta^2 S[x(\tau)]}{\delta x(\tau'')\delta x(\tau''')} \right|_{x_{\rm cl}} \right]^{-1/2} . \tag{5.126}$$

The first equation in (5.124) imposes the extreme condition on the trajectory and yields

$$-m \frac{d^2 x_{\rm cl}(\tau'')}{d\tau''^2} + V'(x_{\rm cl}(\tau'')) = 0 \qquad\qquad \tau'' \in [\tau', \tau] . \tag{5.127}$$

with the boundary conditions $x_{\rm cl}(\tau') = x'$ and $x_{\rm cl}(\tau) = x$.

Equation (5.127) is identical to:

- The equation for a *domain wall* in the Ginzburg-Landau field theoretical approach to the one dimensional Ising model (with τ representing the spatial direction). We see, once again, a connection between a quantum problem in $d = 0$ spatial dimensions in this case with a classical one in $d = 0{+}1$ dimension. The domain wall corresponds to a trajectory describing the tunnelling of the particle from one to the other potential well.

- The saddle-point equation (5.127) describes the classical trajectory of a particle moving in the *inverted potential* $-V(x)$, see Fig. 5.4. At the initial instant the particle is, say, at the top of the left hill. At the final time τ it should arrive at, and stay there ever after, the top of the right hill. This classical trajectory should let the particle roll down the hill to the right and climb up the second hill with just enough kinetic energy to reach the top and stay there.

Note that this equation represents energy conservation in a system with potential energy $-V$:

$$E = \frac{m}{2} \left(\frac{dx_{\rm cl}(\tau'')}{d\tau''} \right)^2 - V(x_{\rm cl}(\tau'')) = \text{const} \qquad\qquad \tau'' \in [\tau', \tau] . \tag{5.128}$$

The procedure to obtain this condition is the following. Multiply the saddle-point equation $d^2 x_{\rm cl}(\tau'')/d\tau''^2 = V'(x_{\rm cl}(\tau''))$ by $dx_{\rm cl}(\tau'')/d\tau''$. Then, $(1/2)\, d(dx_{\rm cl}(\tau'')/d\tau'')^2/d\tau'' = dV(x_{\rm cl}(\tau''))/d\tau''$. Integrate now over τ'' to find Eq. (5.128). Now, we set the additive integration constant to zero since $\dot x_{\rm cl} = V(x_{\rm cl}) = 0$ at the extremes of integration, where $x_{\rm cl} = -x_0$ and $x_{\rm cl} = x_0$, for the problem we want to study. Thus

$$\frac{m}{2} \left(\frac{dx_{\rm cl}(\tau'')}{d\tau''} \right)^2 = V(x_{\rm cl}(\tau'')) . \tag{5.129}$$

This is equivalent to stating that we are interested in classical trajectories with $E = 0$ in the mechanical problem with inverted potential. Note that Eq. (5.129) is a *first order differential equation* while the Euler-Lagrange, or Newton equations, are second order ones.

Another way to obtain Eq. (5.129) - and in general first order differential equations - for topological configurations in field theories, is the so-called *Bogomol'nyi trick* [?]. The idea is to re-write the action as (possibly a sum of) square(s) plus a constant and then minimize it by requiring that what is squared vanishes. In this problem, this method amounts to rewriting the imaginary time action as

$$\begin{aligned} S &= \int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2} \left(\dot{x} \mp \sqrt{\frac{2V(x)}{m}} \right)^2 \pm m\dot{x}\sqrt{\frac{2V(x)}{m}} \right] \\ &= \int_{\tau'}^{\tau} d\tau'' \, \frac{m}{2} \left(\dot{x} \mp \sqrt{\frac{2V(x)}{m}} \right)^2 \pm \sqrt{m} \int_{-x_0}^{x_0} dx \, \sqrt{2V(x)} \, . \end{aligned} \tag{5.130}$$

The last term yields a constant which depends on the potential energy form but not on the trajectory. The first one is set to zero by the condition (5.129) when the upper sign is selected which corresponds to the boundary conditions chosen.

A trivial solution to Eq. (5.129) would be the constant $x_{\rm cl}(\tau) = \pm x_0$, but it does not respect the boundary conditions $x_{\rm cl}(\tau') = -x_0$ and $x_{\rm cl}(\tau) = x_0$.

Another solution is one in which $x_{\rm cl}(\tau)$ smoothly connects $x_{\rm cl}(\tau') = -x_0$ and $x_{\rm cl}(\tau) = x_0$ with $dx_{\rm cl}(\tau)/d\tau = 0$ at τ' and τ. This so-called *instanton* is a *topological* trajectory, in the sense that it interpolates between two inequivalent ground states $-x_0$ and x_0 and it cannot be smoothly deformed to the trivial constant situations x_0 or $-x_0$.

From Eq. (5.129) the non-trivial trajectories are explicitly given by

$$\int_{x'}^{x} \frac{dx_{\rm cl}}{[2V(x_{\rm cl})/m]^{1/2}} = \tau - \tau' \, . \tag{5.131}$$

They have action

$$S_{\rm cl} = S[x_{\rm cl}] = \int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2} \left(\frac{dx_{\rm cl}(\tau'')}{d\tau''} \right)^2 + V(x_{\rm cl}(\tau'')) \right] \tag{5.132}$$

with $x_{\rm cl}$ solving the classical equation of motion. We have already shown that the first and second terms are identical, thanks to Eq. (5.129). We then uncover that the classical instanton action is

$$\begin{aligned} S_{\rm cl} &= m \int d\tau'' \left(\frac{dx_{\rm cl}(\tau'')}{d\tau''} \right) \left(\frac{dx_{\rm cl}(\tau'')}{d\tau''} \right) = m \int d\tau'' \left(\frac{dx_{\rm cl}(\tau'')}{d\tau''} \right) \left(\frac{2V(x_{\rm cl}(\tau''))}{m} \right)^{1/2} \\ &= m^{1/2} \int_{-x_0}^{x_0} dx_{\rm cl} \, [2V(x_{\rm cl})]^{1/2} = m^{1/2} \int_{-x_0}^{x_0} du \, [2V(u)]^{1/2} \, , \end{aligned} \tag{5.133}$$

which is the same as the last term in Eq. (5.130) and is fully determined by the form of the potential. Surprisingly enough, it does not depend on the particular form of the trajectory $x_{\rm cl}$, and it is *finite*.

For a generic double well potential $V(x)$ one cannot find an explicit solution $x_{\rm cl}$. Still, one can derive some generic features of it. Taylor expanding $V(x)$ close to its minima, $V(x) \sim (1/2)V''(\pm x_0)(x-x_0)^2 \equiv m\omega^2(x-x_0)^2/2$, with ω the oscillator frequency of the (symmetric) minima. When the particle is close to any of these minima the equation of motion becomes $dx_{\rm cl}/d\tau \sim -\omega(x_{\rm cl}-x_0)$ and the solution is $x_{\rm cl}(\tau) \sim x_0 - e^{-\omega\tau}$. Thus, the *duration* of the instanton is determined by $\omega^2 = V''(\pm x_0)/m$. The instanton is therefore confined to a narrow interval of time, $\tau_W \sim 1/\omega = [m/V''(\pm x_0)]^{1/2}$. (We have already seen some similar when studying the domain wall width in the Landau theory.)

For a quartic potential, Eq. (5.131) is solved exactly by

$$x_{\rm cl}(\tau) = \pm x_0 \tanh[(\tau-\tau_0)/\tau_W] \qquad\qquad \tau_W \propto (m/r)^{1/2} \; , \tag{5.134}$$

with $x_0 > 0$, taking sign opposed values at the two limits $\tau \to \pm\infty$. One such solution, with positive sign is shown in the right panel in Fig. 5.4. τ_W is the *width* of the *instanton* which decreases with the *thickness* of the barrier, and is proportional to $|r|^{-1/2}$. We note that $V''(\pm x_0) = 2r + 3ux_0^2 = 2r + 3u(-r/u) = -r$, in agreement with the argument for the generic potential, $\tau_W \sim 1/[V''(\pm x_0)]^{1/2}$. The instanton can occur at any imaginary time τ_0. Such parameters are called *zero modes*, as they do not change the zero energy character of the trajectory.

The density in the classical action for a quartic potential can be evaluated explicitly. It is

$$\left(\frac{dx_{\rm cl}(\tau'')}{d\tau''}\right)^2 = \frac{x_0^2}{\tau_W^2}\,{\rm sech}^4[(\tau''-\tau_0)/\tau_W] \; . \tag{5.135}$$

It is located around the center of the instanton and rapidly vanishes away from it. The total action, in the limit $\tau' \to -\infty$ and $\tau \to \infty$, reads

$$S_{\rm cl} = \frac{x_0^2}{\tau_W^2}\int_{-\infty}^{\infty} d\tau''\,{\rm sech}^4[(\tau''-\tau_0)/\tau_W] = \frac{x_0^2}{\tau_W}\int_{-\infty}^{\infty} du''\,{\rm sech}^4 u'' = \frac{4x_0^2}{3\tau_W} \; . \tag{5.136}$$

Note that a naïve perturbation theory around one of the two minima of the double well potential would never show the non-perturbative tunneling effect.

If one has to impose periodic boundary conditions, one has to combine this configuration with the *anti-instanton* in which the particle transits back from x_0 to $-x_0$. This, of course, can occur an even number of times in the considered time interval. Having noticed the possibility of getting (approximate) solutions of the saddle-point equations, one can build a gas of instantons and sum all possible combinations of them to evaluate the full instantonic contribution to the partition sum. The detailed evaluation will be carried out in TD6, see also [**?**, 78].

The Arrhenius law

Going back to classical stochastic dynamics as described by, for example, a Langevin process, a similar question can be asked: what is the probability of a particle, initialized in a well of a double well potential, to jump over the barrier and move to the other well? If temperature is non-zero, the thermal noise will kick the particle and increase its energy until an eventual sufficiently strong one takes it to the other well. The time needed to do is the so-called Arrhenius time which scales exponentially with the height of the barrier, $t_A \sim t_0 e^{B/T}$. This time-scale can be estimated with an analysis of the path-integral for the stochastic process similar to the one described above for the quantum one [43].

5.6 The reduced system

Imagine that you take a system of interest, say a quantum particle, in contact with an ensemble of independent quantum harmonic oscillators, which could represent phonons. One can be interested in, for example, calculating the partition function in sequential way, in the sense of first integrating the degrees of freedom of the "bath", that is to say, the phonons, and only later the ones of the particle [35].

We follow the same route as in the derivation of the classical Langevin equation by coupling the system to an ensemble of quantum harmonic oscillators,

$$[\hat{\pi}_a, \hat{q}_b] = -i\hbar\delta_{ab} \ . \tag{5.137}$$

The equilibrium density matrix reads

$$\rho_T(x, q_a; x', q'_a) = \frac{1}{Z_T} \langle x, q_a | \, e^{-\beta \hat{H}_T} \, | x', q'_a \rangle \ , \tag{5.138}$$

with the partition function given by $Z_T = \text{Tr} e^{-\beta \hat{H}_T}$ and the trace taken over all the states of the full system. (Note that here and it what follows q_a represents the ensemble of oscillators.) The density matrix can be represented by a functional integral in imaginary time,

$$\rho_T(x, q_a; x', q'_a) = \frac{1}{Z_T} \int_{x(0)=x'}^{x(\hbar\beta)=x} \mathcal{D}x \int_{q_a(0)=q'_a}^{q_a(\hbar\beta)=q_a} \mathcal{D}q_a \; e^{-\frac{1}{\hbar} S_T} \ . \tag{5.139}$$

The Euclidean action S_T has contributions from the system, the reservoir, the interaction and the counter-term: $S_T = S_S + S_E + S_I + S_C$. The environment action is

$$S_E = \sum_{a=1}^{N} \int_0^{\beta\hbar} d\tau \, \left\{ \frac{m_a}{2} [\dot{q}_a(\tau)]^2 + \frac{m_a \omega_a^2}{2} [q_a(\tau)]^2 \right\} \ , \tag{5.140}$$

that is to say, we choose an ensemble of independent oscillators. For simplicity we take a linear coupling with the couplings constants $c_a = O(1)$,

$$S_E = \int_0^{\beta\hbar} d\tau \; x(\tau) \, \frac{1}{N^{1/2}} \sum_{a=1}^{N} c_a q_a(\tau) \tag{5.141}$$

but others, are also possible. The path integral over the oscillators' coordinates and positions is quadratic. The calculation of expectation values involves a trace over states of the full system. For operators that depend only on the particle, as $A(\hat{x})$, the trace over the oscillators can be done explicitly. Hence, if one constructs the *reduced equilibrium density operator* $\hat{\rho}_S^{\rm red} = {\rm Tr}_E\ \hat{\rho}_T$ that acts on the system's Hilbert space, the expectation value of the observables of the system is given by

$$\langle A(\hat{x})\rangle = \frac{{\rm Tr}_S\ A(\hat{x})\hat{\rho}_S^{\rm red}}{{\rm Tr}\hat{\rho}_T}\ . \tag{5.142}$$

In the path-integral formalism this amounts to performing the functional integral over periodic functions $q_a(\tau)$. From the point of view of the oscillators the system's coordinate is an external τ-dependent force. Using a Fourier representation,

$$q_a(\tau) = \sum_{n=-\infty}^{\infty} q_a^{(n)}\ e^{i\nu_n\tau} \tag{5.143}$$

with

$$\nu_n = \frac{2\pi n}{\beta\hbar} \tag{5.144}$$

the *Matsubara frequencies*, the integration over the $q_a(\tau)$ can be readily done. A long series of steps, very carefully explained in [81] allow one to obtain the reduced density matrix:

$$\begin{aligned} \rho_S^{\rm red}(x,x') &= \langle x|{\rm Tr}_E\ \hat{\rho}_T\ |x\rangle \\ &= \frac{1}{Z_S^{\rm red}} \int_{x(0)=x'}^{x(\hbar\beta)=x} \mathcal{D}x\ \ e^{-\frac{1}{\hbar}S_S-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int_0^\tau d\tau'\ x(\tau)K(\tau-\tau')x(\tau')} \end{aligned} \tag{5.145}$$

where $Z_S^{\rm red}$ is the partition function of the reduced system, $Z_S^{\rm red} = Z_T/Z_E$ and Z_E the partition function of the isolated ensemble of oscillators. The interaction with the reservoir generated a renormalization of the parameter in the quadratic in x^2 term of S_S – cancelled by the counter-term – but also a retarded interaction in the effective action controlled by the kernel

$$K(\tau) = \frac{2}{\pi\hbar\beta}\sum_{n=-\infty}^{\infty}\int_0^\infty d\omega\ \frac{S(\omega)}{\omega}\ \frac{\nu_n^2}{\nu_n^2+\omega^2}\ e^{i\nu_n\tau}\ , \tag{5.146}$$

with $S(\omega)$ the *spectral density* of the bath,

$$S(\omega) \equiv \frac{1}{N}\sum_{a=1}^{N}\frac{c_a^2}{m_a\omega_a}\ \delta(\omega-\omega_a) \tag{5.147}$$

Just as in the derivation of the classical Langevin equation, different choices of the environment are possible by selecting different ensembles of harmonic oscillators. A common choice is

$$\frac{S(\omega)}{\omega} = 2\gamma_0\left(\frac{|\omega|}{\tilde{\omega}}\right)^{\alpha-1}\ f_c\left(\frac{|\omega|}{\Lambda}\right)\ . \tag{5.148}$$

The function $f_c(x)$ is a high-frequency cut-off of typical width Λ and is usually chosen to be an exponential. The frequency $\tilde{\omega} \ll \Lambda$ is a reference frequency that allows one to have a coupling strength γ_0 with the dimensions of viscosity. If $\alpha = 1$, the friction is said to be *Ohmic*, $S(\omega)/\omega$ is constant when $|\omega| \ll \Lambda$ as for a white noise. When $\alpha > 1$ ($\alpha < 1$) the bath is *superOhmic* (*subOhmic*). The exponent α is taken to vary in the interval $(0, 2)$ to avoid divergencies.

The last retarded interaction in (5.145) remains. The imaginary time dependence of K varies according to $S(\omega)$. Power laws in S lead to power-law decays in K and thus to a long-range interaction in the imaginary-time direction.

The effect of the quantum bath is more cumbersome than in the classical case and it can lead to rather spectacular effects. A well-known example is the *localization transition*, as function of the coupling strength to an Ohmic bath in the behaviour of a quantum particle in a double well potential [82–84]. This means that quantum tunneling from the well in which the particle is initially located to the other one is completely suppressed by sufficiently strong couplings to the bath. In the context of interacting macroscopic systems, *e.g.* ferromagnets or spin-glasses, the locus of the transition between the ordered and the disordered phase depends strongly on the coupling to the bath and on the type of bath considered [85, 86].

5.7 Closed time path

We shall see that the distinction between the effect of a reservoir on the statistical properties of a classical and quantum system is absent from a fully dynamic treatment. In both classical and quantum problems, the coupling to an environment leads to a *retarded* interaction. In classical problems one generally argues that the retarded interaction can be simply replaced by a local one due to the very short correlation times involved in cases of interest, *i.e* one uses white baths, but in the quantum problems one cannot do the same.

5.7.1 Schwinger-Keldysh path integral

The Schwinger-Keldysh formalism [3, 87] allows one to analyse the real-time dynamics of a quantum system. The starting point is the time dependent density operator

$$\hat{\rho}(t) = T\ e^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}\ \hat{\rho}(0)\ \overline{T}\ e^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\ . \tag{5.149}$$

We have set the initial time to be $t_o = 0$. Introducing identities, an element of the time-dependent density matrix reads

$$\begin{aligned} &\rho(x'', x'; t) = \\ &\int_{-\infty}^{\infty} dX dX'\ \langle x''|\ T\ e^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}\ |X\rangle\ \langle X|\ \hat{\rho}(0)\ |X'\rangle \\ &\qquad \times \langle X'|\ \overline{T}\ e^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\ |x'\rangle\ . \end{aligned} \tag{5.150}$$

The first and third factors are the coordinate representation of the evolution operators $e^{-i\hat{H}t/\hbar}$ and $e^{i\hat{H}t/\hbar}$, respectively, and they can be represented as functional integrals:

$$\langle x''|\, T\, e^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}\,|X\rangle = \int_X^{x''} \mathcal{D}x^+ \; e^{\frac{\mathrm{i}}{\hbar}S^+} \tag{5.151}$$

$$\langle X'|\,\overline{T} e^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\,|x'\rangle = \int_{x'}^{X'} \mathcal{D}x^- \; e^{-\frac{\mathrm{i}}{\hbar}S^-} \; . \tag{5.152}$$

Interestingly enough, the evolution operator in eq. (5.213) gives rise to a path integral going backwards in time, from $x^-(t) = x'$ to $x^-(0) = X'$. The full time-integration can then be interpreted as being closed, going forwards from $t_0 = 0$ to t and then backwards from t to $t_0 = 0$. This motivates the name *closed time-path formalism*. A doubling of degrees of freedom (x^+, x^-) appeared and it is intimately linked to the introduction of Lagrange multipliers in the functional representation of the Langevin dynamics in the classical limit. The action of the system has two terms, one evaluated in x^+ and the other in x^-.

$$S_S^{\pm}[\eta^+] = \pm \int_0^t dt' \; \left[\frac{m}{2}\left(\dot{x}^{\pm}(t')\right)^2 - V(x^{\pm}(t')) + \eta^{\pm}(t')x^{\pm}(t') \right] \tag{5.153}$$

where we have introduced two time-dependent sources $\eta^{\pm}(t)$, that appear in the exponential with the sign indeicated.

5.7.2 Green functions

We define the *position and fermionic* Green functions

$$G^B_{ab}(t,t') \equiv -i\langle T_C \; x_a(t) x_b(t')\rangle \tag{5.154}$$

$$G^F_{ab}(t,t') \equiv -i\langle T_C \; \psi_a(t) \psi^\dagger_b(t')\rangle \tag{5.155}$$

where $a, b = \pm$ and T_C is time ordering on the close contour.

The definitions (5.154) and (5.155) and the fact that the insertion evaluated at the later time can be put on the upper (+) or lower (−) branch indistinctively *** GIVE EXAMPLE WITH DRAWING *** yield the following relations between different Green functions

$$G_{++}(t,t') = G_{-+}(t,t')\theta(t-t') + G_{+-}(t,t')\theta(t'-t) \; , \tag{5.156}$$

$$G_{--}(t,t') = G_{+-}(t,t')\theta(t-t') + G_{-+}(t,t')\theta(t'-t) \; , \tag{5.157}$$

that hold for the bosonic and fermionic cases as well. We thus erase the superscripts B, F that become superflous. Adding the last two identities one finds

$$G_{++} + G_{--} - G_{+-} - G_{-+} = 0 \qquad \text{for all } t \text{ and } t' \; . \tag{5.158}$$

In both cases one defines *MSRDJ-like fields*. For bosons these are

$$\sqrt{2}\; x(t) = x_+(t) + x_-(t) \; , \qquad \sqrt{2}\hbar\; \hat{x}(t) = x_+(t) - x_-(t) \; , \tag{5.159}$$

while for fermions they are

$$
\begin{array}{ll}
\sqrt{2}\;\psi(t) \equiv \psi^{+}(t) + \psi^{-}(t) & \qquad \sqrt{2}\hbar\;\hat{\psi}(t) \equiv \psi^{+}(t) - \psi^{-}(t) \\
\sqrt{2}\;\psi^{\dagger}(t) \equiv \psi^{+\dagger}(t) + \psi^{-\dagger}(t) & \qquad \sqrt{2}\hbar\;\hat{\psi}^{\dagger}(t) \equiv \psi^{+\dagger}(t) - \psi^{-\dagger}(t)\;.
\end{array}
$$

One then constructs the Green functions

$$
\begin{aligned}
G^B_{xx}(t,t') &\equiv -i\langle T_C\; x(t)x(t')\rangle = \frac{1}{2}\left(G^B_{++} + G^B_{--} + G^B_{-+} + G^B_{+-}\right) \\
&\equiv -2i\; G^B_K(t,t') \\
G^B_{x\hat{x}}(t,t') &\equiv -i\langle T_C\; x(t)\hat{x}(t')\rangle = \frac{1}{2\hbar}\left(G^B_{++} - G^B_{--} + G^B_{-+} - G^B_{+-}\right) \\
&\equiv -G^B_R(t,t') \\
G^B_{\hat{x}x}(t,t') &\equiv -i\langle T_C\; \hat{x}(t)x(t')\rangle = \frac{1}{2\hbar}\left(G^B_{++} - G^B_{--} - G^B_{-+} + G^B_{+-}\right) \\
&\equiv -\;G^B_A(t,t') \\
G^B_{\hat{x}\hat{x}}(t,t') &\equiv -i\langle T_C\; \hat{x}(t)\hat{x}(t')\rangle = \frac{1}{2\hbar^2}\left(G^B_{++} + G^B_{--} - G^B_{-+} - G^B_{+-}\right) \\
&\equiv -\;G^B_4(t,t') = 0\;, \qquad (5.160)
\end{aligned}
$$

and the fermionic ones

$$
\begin{aligned}
G^F_{\psi\psi}(t,t') &\equiv -i\langle T_C\; \psi(t)\psi^{\dagger}(t')\rangle = \frac{1}{2}\left(G^F_{++} + G^F_{--} + G^F_{-+} + G^F_{+-}\right) \\
&\equiv -2iG^F_K(t,t')\;, \\
G^F_{\psi\hat{\psi}}(t,t') &\equiv -i\langle T_C\; \psi(t)\hat{\psi}^{\dagger}(t')\rangle = \frac{1}{2\hbar}\left(G^F_{++} - G^F_{--} + G^F_{-+} - G^F_{+-}\right) \\
&\equiv -G^F_R(t,t')\;, \\
G_{\hat{\psi}\psi}(t,t') &\equiv -i\langle T_C\; \hat{\psi}(t)\psi^{\dagger}(t')\rangle = \frac{1}{2\hbar}\left(G^F_{++} - G^F_{--} - G^F_{-+} + G^F_{+-}\right) \\
&\equiv -G^F_A(t,t')\;, \\
G^F_{\hat{\psi}\hat{\psi}}(t,t') &\equiv -i\langle T_C\; \hat{\psi}(t)\hat{\psi}^{\dagger}(t')\rangle = \frac{1}{2\hbar^2}\left(G^F_{++} + G^F_{--} - G^F_{-+} - G^F_{+-}\right) \\
&\equiv -G^F_4(t,t') = 0\;, \qquad (5.161)
\end{aligned}
$$

From the definition of G^B_K it is obvious that

$$
G^B_K(t,t') = G^B_K(t',t) \quad \in\; \mathrm{Re}\;. \qquad (5.162)
$$

Using eq. (5.158) the 'rotated' Green functions are rewritten as

$$
G_K = \frac{\mathrm{i}}{2}(G_{++} + G_{--}) = \frac{\mathrm{i}}{2}(G_{+-} + G_{-+})\;, \qquad (5.163)
$$

$$
G_R = -\frac{1}{\hbar}(G_{++} - G_{+-}) = \frac{1}{\hbar}(G_{--} - G_{-+})\;, \qquad (5.164)
$$

$$
G_A = -\frac{1}{\hbar}(G_{++} - G_{-+}) = \frac{1}{\hbar}(G_{--} - G_{+-})\;. \qquad (5.165)
$$

Using eqs. (5.156)-(5.157) one also finds

$$G_R(t,t') = -\frac{1}{\hbar}[G_{+-}(t,t') - G_{-+}(t,t')]\ \theta(t-t')\ , \tag{5.166}$$
$$G_A(t,t') = \frac{1}{\hbar}[G_{+-}(t,t') - G_{-+}(t,t')]\ \theta(t'-t)\ . \tag{5.167}$$

which show explicitly the *retarded* and *advanced* character of G_R and G_A, respectively. Moreover,

$$G^B_R(t,t') = G^B_A(t't) \quad \in \text{ Re}\ , \tag{5.168}$$
$$G^F_R(t,t') = [G^F_A(t',t)]^*\ , \tag{5.169}$$
$$G^F_K(t,t') = [G^F_K(t',t)]^*\ . . \tag{5.170}$$

Inverting the above relations one has

$$\begin{array}{ll} iG_{++} = G_K - i\hbar(G_R+G_A)/2\ , & iG_{+-} = G_K + i\hbar(G_R-G_A)/2\ , \\ iG_{-+} = G_K - i\hbar(G_R-G_A)/2\ , & iG_{--} = G_K + i\hbar(G_R+G_A)/2\ . \end{array} \tag{5.171}$$

Going back to an operational formalism

$$G^B_R(t,t') \;\equiv\; \frac{2i}{\hbar}\theta(t-t')\ \langle[\hat{x}(t),\hat{x}(t')]\rangle\ , \tag{5.172}$$
$$G^B_K(t,t') \;\equiv\; \langle\{\hat{x}(t),\hat{x}(t')\}\rangle\ , \tag{5.173}$$

for bosons (see App. **??**), where one recognizes the *Kubo formulæ* in the first two lines, and

$$G^F_R(t,t') \;\equiv\; \frac{2i}{\hbar}\theta(t-t')\ \langle\{\hat{\psi}(t),\hat{\psi}^\dagger(t')\}\rangle\ , \tag{5.174}$$
$$G^F_K(t,t') \;\equiv\; \langle[\hat{\psi}(t),\hat{\psi}^\dagger(t')]\rangle\ , \tag{5.175}$$

for fermions.

5.7.3 Generic correlations

A generic two time correlation that depends only on the system is given by

$$\langle\hat{A}(t)\hat{B}(t')\rangle = \frac{1}{Z^{\text{red}}_S}(0)\ \text{Tr}\hat{A}(t)\hat{B}(t')\hat{\rho}^{\text{red}}_S(0)\ . \tag{5.176}$$

Clearly $\langle\hat{A}(t)\hat{B}(t')\rangle \neq \langle\hat{B}(t')\hat{A}(t)\rangle$ and one can define symmetrized and anti-symmetrized correlations:

$$C_{\{A,B\}}(t,t') \;=\; \langle\hat{A}(t)\hat{B}(t') + \hat{B}(t')\hat{A}(t)\rangle/2\ , \tag{5.177}$$
$$C_{[A,B]}(t,t') \;=\; \langle\hat{A}(t)\hat{B}(t') - \hat{B}(t')\hat{A}(t)\rangle/2\ , \tag{5.178}$$

respectively.

Within the Keldysh path-integral representation these correlations can be written as

$$\begin{aligned} C_{\{A,B\}}(t,t') &= \langle A[x^+](t)\{B[x^+](t') + B[x^-](t')\}\rangle/2 \; , \\ C_{[A,B]}(t,t') &= \langle A[x^+](t)\{B[x^+](t') - B[x^-](t')\}\rangle/2 \; , \end{aligned} \tag{5.179}$$

5.7.4 Linear response and Kubo relation

The linear response is defined as the variation of the averaged observable A at time t due to a change in the Hamiltonian operated at time t' in such a way that $\hat{H} \to \hat{H} - f_B \hat{B}$. In linear-response theory, it can be expressed in terms of the averaged commutator:

$$R_{AB}(t,t') \equiv \left. \frac{\delta \langle \hat{A}(t) \rangle}{\delta f_B(t')} \right|_{f_B=0} = \frac{2i}{\hbar} \theta(t-t') \langle [\hat{A}(t), \hat{B}(t')] \rangle \; . \tag{5.180}$$

In the case $\hat{A} = \hat{x}$ and $\hat{B} = \hat{x}$ this implies $R_{xx}(t,t') = G_R^B(t,t')$. The path-integral representation is in terms of the Keldysh fields x^+, x^-:

$$R_{AB}(t,t') = i \langle A[x^+](t) \; \big\{ B[x^+](t') - B[x^-](t') \big\} \rangle / \hbar \; . \tag{5.181}$$

5.7.5 Quantum FDT

Proofs and descriptions of the quantum FDT can be found in several textbooks [**?**,5]. We first present a standard derivation that applies to bosonic and fermionic Green functions in the canonical and grand-canonical ensembles. We next show it for generic correlations and linear responses in the bosonic case. In so doing we recall its expression in the time-domain and in a mixed time-Fourier notation that gave us insight as to how to extend it to the case of glassy non-equilibrium dynamics [88].

Canonical ensemble

Let us consider the canonical ensemble and let us write

$$iG_{+-}(t,t') = \langle T_C \; \phi^+(t) \phi^-(t') \rangle \tag{5.182}$$

where $\phi^+ = x^+$ and $\phi^- = x^-$ (bosons) or $\phi^+ = \psi^+$ and $\phi^- = \psi^{-\dagger}$ (fermions). This is equal to

$$iG_{+-}(t,t') = (-1)^\zeta \; \langle \phi^-(t') \phi^+(t) \rangle \tag{5.183}$$

with $\zeta = 1$ for fermions and $\zeta = 0$ for bosons. Using the *analytic properties* of Green functions, we have

$$iG_{+-}(t + i\beta\hbar, t') = (-1)^\zeta \; \langle \phi^-(t') \phi^+(t + i\beta\hbar) \rangle \; . \tag{5.184}$$

In the canonical ensemble, $\langle \cdots \rangle \propto \text{Tr} \cdots \rho_0 \propto \text{Tr} \cdots e^{-\beta H}$ and after expanding $\phi^+(t + i\beta\hbar) = \rho_0 \phi^+(t) \rho_0^{-1}$ (in the Heisenberg representation) we get

$$iG_{+-}(t + i\beta\hbar, t') = (-1)^\zeta \; \frac{\text{Tr}\,[\phi^-(t')\rho_0\phi^+(t)]}{\text{Tr}\rho_0} \; . \tag{5.185}$$

Using the *cyclic property* of the trace

$$iG_{+-}(t + i\beta\hbar, t') = (-1)^\zeta \langle \phi^+(t)\phi^-(t')\rangle \tag{5.186}$$

and we recognize

$$G_{+-}(t + i\beta\hbar, t') = (-1)^\zeta \; G_{-+}(t, t') \tag{5.187}$$

If the systen has reached equilibrium, *time translational invariance* implies

$$G_{+-}(t - t' + i\beta\hbar) = (-1)^\zeta \; G_{-+}(t - t') \; . \tag{5.188}$$

After Fourier transforming with respect to $t - t'$ we get the *KMS relation*

$$G_{+-}(\omega) e^{\beta\hbar\omega} = (-1)^\zeta \; G_{-+}(\omega) \; . \tag{5.189}$$

Using eqs. (5.171), we have on the one hand

$$\hbar[G_R(\omega) - G_A(\omega)] = G_{+-}(\omega) - G_{-+}(\omega) \; . \tag{5.190}$$

Inserting the KMS relation (5.189) we get

$$\hbar[G_R(\omega) - G_A(\omega)] = G_{+-}(\omega)[1 - (-1)^\zeta e^{\beta\hbar\omega}] \tag{5.191}$$

On the other hand,

$$G_K(\omega) \;\; = \;\; \frac{\text{i}}{2}[G_{+-}(\omega) + G_{-+}(\omega)] = \frac{\text{i}}{2} G_{+-}(\omega)[1 + (-1)^\zeta e^{\beta\hbar\omega}] \; . \tag{5.192}$$

Combining this relation with eq. (5.189) we obtain the quantum FDTs

$$\boxed{G_K(\omega) = \frac{i\hbar}{2} \; [G_R(\omega) - G_A(\omega)] \left[\frac{1 + (-1)^\zeta e^{\beta\hbar\omega}}{1 - (-1)^\zeta e^{\beta\hbar\omega}} \right]} \tag{5.193}$$

Using $G_R(\omega) - G_A(\omega) = R(\omega) - R^*(\omega) = 2i\text{Im}G_R(\omega)$ for bosons and fermions:

$$G_K^F(\omega) = -\frac{i\hbar}{2} \; [G_R^F(\omega) - G_A^F(\omega)] \;\; \tanh \frac{\beta\hbar\omega}{2} \tag{5.194}$$

$$\boxed{G_K^F(\omega) = \hbar \; \text{Im}G_R^F(\omega) \;\; \tanh \tfrac{\beta\hbar\omega}{2} \; ,} \tag{5.195}$$

$$G^B_K(\omega) = -\frac{i\hbar}{2}\left[G^B_R(\omega) - G^B_A(\omega)\right] \mathrm{cotanh}\frac{\beta\hbar\omega}{2} \tag{5.196}$$

$$\boxed{G^B_K(\omega) = \hbar\ \mathrm{Im}G^B_R(\omega)\ \mathrm{cotanh}\tfrac{\beta\hbar\omega}{2}\ .} \tag{5.197}$$

In the case of bosons the FDT can be easily extended to

$$C_{\{A,B\}}(\omega) = \hbar\ \mathrm{Im}R^B_{AB}(\omega)\ \mathrm{cotanh}\frac{\beta\hbar\omega}{2}\ . \tag{5.198}$$

Grand canonical ensemble

In the grand-canonical ensemble, the proof remains essentially the same. The initial density operator reads $\hat\rho_0 \propto e^{-\beta\hat H+\beta\mu\hat N}$, where $\hat N$ is the number operator which commutes with $\hat H$ (the number of particules is conserved in non-relativistic quantum mechanics). For concreteness, let us focus on fermions The three first steps in the proof presented above imply

$$G^F_{+-}(t+i\beta\hbar,t') = -\mathrm{Tr}\left[\hat\psi^{-\dagger}(t')e^{-\beta\hat H}\hat\psi^{+}(t)e^{\beta\mu\hat N}\right]/\mathrm{tr}\hat\rho_0 \tag{5.199}$$

Since $\hat H$ and $\hat N$ commute and since for any operator $f(\hat N)$, one has the property that $\hat\psi f(\hat N) = f(\hat N+1)\hat\psi$, we have

$$\hat\psi^{+}(t)e^{\beta\mu\hat N} = e^{\beta\mu(\hat N+1)}\hat\psi^{+}(t) \tag{5.200}$$

and so

$$G^F_{+-}(t+i\beta\hbar,t') = -e^{\beta\mu}\ \mathrm{Tr}\left[\psi^{-\dagger}(t')\rho_0\psi^{+}(t)\right]/\mathrm{Tr}\rho_0\ . \tag{5.201}$$

At this point, we can follow the same steps as in the proof for the canonical ensemble, namely use the cyclic property of the trace, time-translational invariance and a Fourier transform, to obtain the fermionic KMS relation in the grand-canonical ensemble

$$G^F_{+-}(\omega)e^{\beta\hbar\omega} = -e^{\beta\mu}G^F_{-+}(\omega)\ . \tag{5.202}$$

and the grand-canonical fermionic quantum FDT relation

$$G^F_K(\omega) = -\frac{i\hbar}{2}[G^F_R(\omega) - G^F_A(\omega)]\tanh\left(\beta\frac{\hbar\omega-\mu}{2}\right) \tag{5.203}$$

or, equivalently

$$\boxed{G^F_K(\omega) = \hbar\ \mathrm{Im}R(\omega)\ \ \tanh\left(\beta\tfrac{\hbar\omega-\mu}{2}\right)} \tag{5.204}$$

FDT for generic observables in the time-domain

If at time t' the system is characterized by a density functional $\rho(t')$, the two-time correlation functions are given by eq. (5.176), (5.177) and (5.178). In linear response theory $R_{AB}(t,t')$ and the correlation $C_{[A,B]}(t,t')$ are related by the Kubo formula (5.180). If the system has reached equilibrium with a heat-bath at temperature T at time t', the density functional $\rho_S(t')$ is just the Boltzmann factor $\exp(-\beta H_S)/Z_S$. It is then immediate to show that, in equilibrium, time-translation invariance, $C_{AB}(t,t') = C_{AB}(t-t')$, and the KMS properties

$$C_{AB}(t,t') \;=\; C_{BA}(t', t+i\beta\hbar) = C_{BA}(-t-i\beta\hbar, -t') \tag{5.205}$$

hold. Using now these identities and assuming, for definiteness, that $t > 0$ it is easy to verify the following equation

$$C_{\{A,B\}}(\mathcal{T}) + \frac{i\hbar}{2} R_{AB}(\mathcal{T}) = C_{\{A,B\}}(\mathcal{T}^*) - \frac{i\hbar}{2} R_{AB}(\mathcal{T}^*) \;, \tag{5.206}$$

where $\mathcal{T} = t + i\beta\hbar/2$. This is a way to express FDT through an analytic continuation to complex times.

In terms of the Fourier transform defined in App. **??** the KMS relations read $C_{AB}(\omega) = \exp(-\beta\hbar\omega)C_{BA}(-\omega)$ and lead to $2C_{[A,B]}(\omega) = \left(1 - e^{\beta\hbar\omega}\right) C_{AB}(\omega)$, $2C_{\{A,B\}}(\omega) = \left(1 + e^{\beta\hbar\omega}\right) C_{AB}(\omega)$ and $C_{[A,B]}(\omega) = -\tanh(\beta\hbar\omega/2)\, C_{\{A,B\}}(\omega)$. Back in the Kubo relation this implies

$$\boxed{R_{AB}(t-t') = -\tfrac{\mathrm{i}}{\hbar}\, \theta(t-t') \int_{-\infty}^{\infty} \tfrac{d\omega}{\pi}\; e^{i\omega(t-t')}\; \tanh(\beta\hbar\omega/2)\, C_{\{A,B\}}(\omega)\;.} \tag{5.207}$$

(recall $C_{\{A,B\}}(\omega) = C_{\{A,B\}}(-\omega)$.) Using $\int_0^\infty dt\, \exp(-i\omega t) = \lim_{\epsilon\to 0^+} \frac{\mathrm{i}}{-\omega+i\epsilon} = \pi\delta(\omega) - i\frac{P}{\omega}$ one has

$$R_{AB}(\omega) = -\frac{1}{\hbar} \lim_{\epsilon\to 0^+} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{1}{\omega - \omega' + i\epsilon} \tanh\frac{\beta\hbar\omega'}{2}\, C_{\{A,B\}}(\omega') \tag{5.208}$$

from which we obtain the real and imaginary relations

$$\begin{aligned} \mathrm{Im} R_{AB}(\omega) &= \frac{1}{\hbar} \tanh\frac{\beta\hbar\omega}{2}\, C_{\{A,B\}}(\omega') \;, \\ \mathrm{Re} R_{AB}(\omega) &= -\frac{1}{\hbar} P \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{1}{\omega - \omega'} \tanh\left(\frac{\beta\hbar\omega'}{2}\right) C_{\{A,B\}}(\omega') \;. \end{aligned} \tag{5.209}$$

If $\beta\hbar\omega/2 \ll 1$, $\tanh(\beta\hbar\omega/2) \sim \beta\hbar\omega/2$ and eq. (5.207) becomes the classical FDT:

$$R_{AB}(t-t') = -\frac{1}{k_B T} \frac{dC_{AB}(t-t')}{dt}\, \theta(t-t') \;. \tag{5.210}$$

5.7.6 The influence functional

As in the derivation of the Langevin equation we model the environment as an ensemble of many non-interaction variables that couple to the relevant system's degrees of freedom in some convenient linear way. The choice of the environment variables depends on the type of bath one intends to consider. Phonons are typically modeled by independent quantum harmonic oscillators that can be dealt with exactly. We then consider a system $(\hat{x}, \hat{p})$ coupled to an environment made of independent harmonic oscillators $(\hat{q}_a, \hat{\pi}_a)$. An element of the total density function reads

$$\begin{aligned} &\rho(x'', q''_a; x', {q'}_a; t) = \\ &\int_{-\infty}^{\infty} dX dX' dQ_a dQ'_a \, \langle x'', q''_a | \, T \; e^{-\frac{\mathrm{i}}{\hbar}\hat{H}_{tot}t} \, |X, Q_a\rangle \, \langle X, Q_a | \, \hat{\rho}_{tot}(0) \, |X', Q'_a\rangle \\ &\qquad \times \langle X', Q'_a | \, \overline{T} \; e^{\frac{\mathrm{i}}{\hbar}\hat{H}_{tot}t} \, |x', q'_a\rangle \; . \end{aligned} \tag{5.211}$$

The first and third factors are the coordinate representation of the evolution operators $e^{-i\hat{H}_{tot}t/\hbar}$ and $e^{i\hat{H}_{tot}t/\hbar}$, respectively, and they can be represented as functional integrals:

$$\langle x'', q''_a | \, T \; e^{-\frac{\mathrm{i}}{\hbar}\hat{H}_{tot}t} \, |X, Q_a\rangle = \int_X^{x''} \mathcal{D}x^+ \int_{Q_a}^{q''_a} \mathcal{D}q_a^+ \; e^{\frac{\mathrm{i}}{\hbar}S^+_{tot}} \tag{5.212}$$

$$\langle X', Q'_a | \, \overline{T} e^{\frac{\mathrm{i}}{\hbar}\hat{H}_{tot}t} \, |x', q'_a\rangle = \int_{x'}^{X'} \mathcal{D}x^- \int_{q'_a}^{Q'_a} \mathcal{D}q_a^- \; e^{-\frac{\mathrm{i}}{\hbar}S^-_{tot}} \; . \tag{5.213}$$

The action S_{tot} has the usual four contributions, from the system, the reservoir, the interaction and the counterterm.

As usual we are interested in the dynamics of the system under the effect of the reservoir. Hence, we compute the reduced density matrix

$$\rho_S^{\mathrm{red}}(x'', x'; t) = \int_{-\infty}^{\infty} dq_a \, \langle x'', q_a | \, \hat{\rho}_{tot}(t) \, |x', q_a\rangle \; . \tag{5.214}$$

5.7.7 Initial conditions

Factorization

The initial density operator $\hat{\rho}_{tot}(0)$ has the information about the initial state of the whole system. If one assumes that the system and the bath are set in contact at the initial time, the operator *factorizes*

$$\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_E(0) \; . \tag{5.215}$$

(Other initial preparations, where the factorization does not hold, can also be considered and may be more realistic in certain cases [81] and see below.) If the environment is initially in equilibrium at an inverse temperature β,

$$\hat{\rho}_E(0) = Z_E^{-1} \; e^{-\beta\hat{H}_E} \; , \tag{5.216}$$

the dependence on the bath variables is quadratic; they can be traced away to yield the reduced density matrix:

$$\begin{aligned}\rho_S^{\rm red}(x'',x';t) &= \int_{-\infty}^{\infty} dX \int_{-\infty}^{\infty} dX' \int_{x^+(0)=X}^{x^+(t)=x''} \mathcal{D}x^+ \int_{x^-(0)=X'}^{x^-(t)=x'} \mathcal{D}x^- \\ &\qquad \times e^{\frac{\rm i}{\hbar}S_{eff}} \, \langle X| \, \hat\rho_S(0) \, |X'\rangle \end{aligned} \tag{5.217}$$

with the effective action $S_{\rm eff} = S_S^+ - S_S^- + S_{\rm B}$. The last term has been generated by the interaction with the environment and it reads [81]

$$\begin{aligned}\frac{\rm i}{\hbar} S_{\rm B} = -i \int_0^{\mathcal{T}} dt' \int_0^{\mathcal{T}} dt'' \, \frac{[x^+(t') - x^-(t')]}{\hbar} \, 4\eta(t'-t'') \, \frac{[x^+(t'') + x^-(t'')]}{2} \\ - \int_0^{\mathcal{T}} dt' \int_0^{\mathcal{T}} dt'' \, \frac{[x^+(t') - x^-(t')]}{\hbar} \, \hbar\nu(t'-t'') \, \frac{[x^+(t'') - x^-(t'')]}{\hbar} \; . \end{aligned} \tag{5.218}$$

The noise and dissipative kernels ν and η are given by

$$\nu(t) = \int_0^\infty d\omega \; S(\omega) \, \coth\left(\frac{1}{2}\beta\hbar\omega\right) \, \cos(\omega t) \; , \tag{5.219}$$

$$\eta(t) = \theta(t) \frac{d\Gamma(t)}{dt} = -\theta(t) \int_0^\infty d\omega \; S(\omega) \, \sin(\omega t) \; . \tag{5.220}$$

One can easily check that $\nu(t) = \nu(-t)$ and $\eta(t)$ is causal; moreover they verify the bosonic FDT, as they should since the bath was assumed to be in equilibrium. η is like a response and ν is a correlation One can also write the bath-generated action in the form

$$S_{\rm B} \equiv - \sum_{a,b=\pm} \frac{1}{2} \int \int dt dt' \; x^a(t) \Sigma_{ab}(t,t') x^b(t') \, , \tag{5.221}$$

with

$$\Sigma_{++} = 2\eta - i\nu \quad \Sigma_{+-} = 2\eta + i\nu \; , \tag{5.222}$$

$$\Sigma_{-+} = -2\eta + i\nu \quad \Sigma_{--} = -2\eta - i\nu \tag{5.223}$$

and $\Sigma_{++} + \Sigma_{--} + \Sigma_{+-} + \Sigma_{-+} = 0$. Although these relation resemble the ones satisfied by the G_{ab}s a more careful analysis shows that the matricial Σ is more like G^{-1} than G (see the discussion on the classical dynamics of the random manifold and the dependence on k; the relation between G and Σ is the same here).

In these equations, as in the classical case, $S(\omega)$ is the spectral density of the bath:

$$S(\omega) = \frac{\pi}{2} \sum_{a=1}^{N_b} \frac{c_a^2}{m_a \omega_a} \delta(\omega - \omega_a) \; , \tag{5.224}$$

that can also be taken of the form in (5.148),

$$S(\omega) = 2\gamma_0\tilde{\omega} \, \left(\frac{\omega}{\tilde{\omega}}\right)^{\alpha} \, e^{-\omega/\Lambda} \; . \tag{5.225}$$

As usual, a counterterm cancels the mass renormalization. The η and Γ kernels are independent of T and $\hbar$ and are thus identical to the classical ones, see eq. (4.28).The kernel ν does depend on T and $\hbar$. After a change of variables in the integral, in the cases in which $S(\omega) \propto \omega^{\alpha}$,

$$\nu(t) = t^{-(1+\alpha)} g\left(\frac{\beta\hbar}{t}, \Lambda t\right) \tag{5.226}$$

and

$$\lim_{\beta\hbar/t\to 0} \beta\hbar\nu(t) = 2\Gamma(t) \; . \tag{5.227}$$

The *classical limit* is realized at *high temperature* and/or *long times*.

Figure 5.5-left shows the time-dependence of the kernels ν in the quantum Ohmic case for different values of T. In the right panel of the same figure we show the dependence on α of the kernel ν.

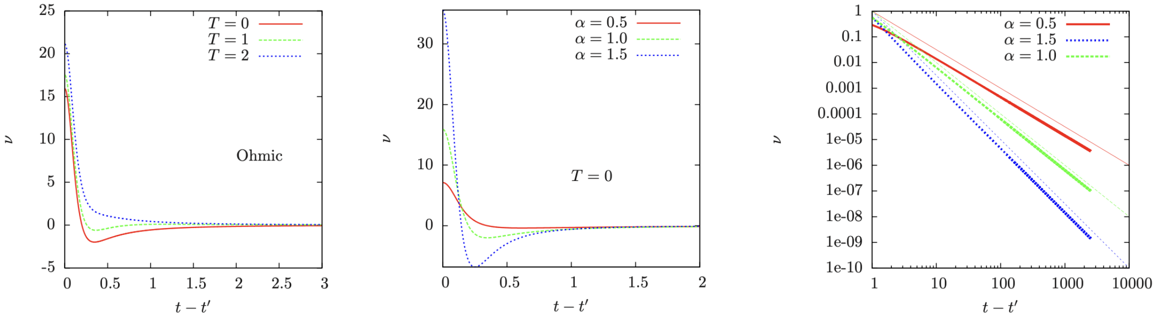

Figure 5.5: The kernel ν. (a) Ohmic $\alpha = 1$ case for different values of T ($\Lambda = 5$). (b) $T = 0$ for different values of α ($\hbar = 1 = \gamma_0 = \tilde{\omega} = 1$ and $\Lambda = 5$) in linear scale. (c) Same as (b) but in logarithmic scale.

Upper critical initial conditions for the system

Next, we have to choose an initial density matrix for the system. One natural choice, having in mind the quenching experiments usually performed in classical system, is the *diagonal density matrix*

$$\langle X| \, \hat{\rho}_S(0) \, |X'\rangle = \delta(X - X') \tag{5.228}$$

that corresponds to a random 'high-temperature' situation and that simplifies considerably the expression in (5.217). As in the classical stochastic problem, $\mathrm{Tr}\hat{\rho}_S^{\mathrm{red}}(0) = 1$ and it is trivially independent of disorder. Hence, there is no need to introduce replicas in such a quantum dynamic calculation.

Equilibrium initial conditions for the system

One might also be interested in using equilibrium initial conditions for the isolated system

$$\langle X|\,\hat{\rho}_S(0)\,|X'\rangle = Z_S^{-1}\langle X|\,e^{-\beta \hat{H}_S}\,|X'\rangle\;. \tag{5.229}$$

This factor introduces interesting real-time – imaginary-time correlations [89].

5.7.8 Transformation to 'MSR-like fields'

Newton dynamics

We use $x_\pm = x \pm (\hbar/2)\,\hat{x}$. We first study the kinetic terms:

$$\frac{\mathrm{i}}{\hbar}\int dt\,\frac{m}{2}\left(\dot{x}_+^2 - \dot{x}_-^2\right) \;=\; \frac{\mathrm{i}}{\hbar}\int dt\,\frac{m}{2}\left[\left(\dot{x}+\frac{\hbar}{2}\dot{\hat{x}}\right)^2 - \left(\dot{x}-\frac{\hbar}{2}\dot{\hat{x}}\right)^2\right] \tag{5.230}$$

expanding the squares the integrand equals $-2\hbar\,\dot{\hat{x}}\dot{x}$ and integrating by parts

$$-\int dt\; i\hat{x}\; m\ddot{x}\;. \tag{5.231}$$

The potential term

The potential term is treated similarly

$$-\frac{\mathrm{i}}{\hbar}\left[V(x_+) - V(x_-)\right] \;=\; -\frac{\mathrm{i}}{\hbar}\left[V\left(x+\frac{\hbar}{2}\hat{x}\right) - V\left(x-\frac{\hbar}{2}\hat{x}\right)\right] \tag{5.232}$$

Note that this expression is specially simple for quadratic and quartic potentials:

$$= \begin{cases} -x i\hat{x} & \text{quadratic} \qquad V(y) = y^2 \\ -4x i\hat{x}\left[x^2 - \phi_0^2 + \left(\frac{\hbar}{2}\right)^2 (\mathrm{i}\hat{x})^2\right] & \text{quartic} \qquad V(y) = (y^2 - y_0^2)^2 \end{cases}$$

The noise terms

We introduce the variables x and $i\hat{x}$ in the action terms generated by the coupling to the environment and the classical limit of the kernel ν:

$$\begin{aligned} \frac{\mathrm{i}}{\hbar}\,S_E \;=\; & -\int_0^{\mathcal{T}} dt' \int_0^{\mathcal{T}} dt''\; i\hat{x}(t')\; 2\theta(t'-t'')\frac{d\Gamma(t'-t'')}{dt'}\; 2x(t'') \\ & + \int_0^{\mathcal{T}} dt' \int_0^{\mathcal{T}} dt''\; i\hat{x}(t')\hbar\nu(t'-t'')i\hat{x}(t'') \\ =\; & 4\int_0^{\mathcal{T}} dt' \int_0^{\mathcal{T}} dt''\; i\hat{x}(t')\;\gamma(t'-t'')\;\dot{x}(t'') \\ & + \int_0^{\mathcal{T}} dt' \int_0^{\mathcal{T}} dt''\; i\hat{x}(t')\hbar\nu(t'-t'')i\hat{x}(t'')\;. \end{aligned} \tag{5.233}$$

(Apart from a border term that can be treated more carefully and check that it disappears.)

5.7.9 Classical limit

In the classical limit, $\hbar \to 0$, the Schwinger-Keldysh effective action reduces to the one in the functional representation of a Newton classical mechanics (no bath) or a Langevin process with coloured noise (bath). The kinetic term eq. (5.231) is already in the expected form with no nead to take $\hbar \to 0$. The potential term

$$-\frac{\mathrm{i}}{\hbar}\left[V(x_+) - V(x_-)\right] = -V'(x)\mathrm{i}\hat{x} + O(\hbar^2) \;\simeq\; -V'(x)\mathrm{i}\hat{x} \tag{5.234}$$

upto first order in $\hbar$. In the noise terms we just have to take the classical limit of the kernel ν:

$$\begin{aligned}\frac{\mathrm{i}}{\hbar}\,S_E \;\simeq\;& 4\int_0^{\mathcal{T}} dt' \int_0^{\mathcal{T}} dt''\; \mathrm{i}\hat{x}(t')\;\gamma(t'-t'')\;\dot{x}(t'') \\ & +2k_BT\int_0^{\mathcal{T}} dt' \int_0^{\mathcal{T}} dt''\; \mathrm{i}\hat{x}(t')\;\Gamma(t'-t'')\;i\hat{x}(t'')\end{aligned} \tag{5.235}$$

with $O(\hbar)$ corrections (apart from a border term that can be treated more carefully and check that it disappears.)

6 Chaos & localization in quantum systems

*** This section is under construction. In 2024, Davide Venturelli will give these lessons. ***

If you want to see notes on Random Matrices, check:
`https://www.lpthe.jussieu.fr/ leticia/TEACHING/Master2020/random-matrices.pdf`
`https://www.lpthe.jussieu.fr/ leticia/TEACHING/Master2019/RandomMatricesAdvances.pdf`

Intro: mention random matrices and more dynamical measurements

6.1 Chaos in classical & quantum systems

In classical Hamiltonian systems chaos is associated to the exponential divergence $\delta\vec{x}_i(t) \sim e^{\lambda_i t}$ with $\{\vec{x}_i(t)\}$ and $\{\vec{x}_i'(t)\}$ two trajectories starting from nearby initial conditions $\{\vec{x}_i(0)\}$ and $\{\vec{x}_i(0)+\delta\vec{x}_i(0)\}$. (The difference can eventually saturate.) The *Lyapunov exponent* is then defined as

$$\lambda = \lim_{t\gg t_0} \frac{1}{t} \ln \left| \frac{\partial x_i(t)}{\partial x_j(0)} \right| = \lim_{t\gg t_0} \frac{1}{t} |\{x_i(t), x_j(0)\}| \tag{6.236}$$

where the curly brackets represent the Poisson bracket. ** the above is not very precise, treat indices better ***

If one wanted to generalize the definition above to quantum systems, one will need to use the expectation values of the position operator. Indeed, nothing spectacular can happen for a state (or wave function) which follows the linear Schr|'odinger equation. But the expectation value of

$$\lambda = \lim_{t\gg t_0} \frac{1}{t} |[\hat{x}_i(t), \hat{x}_j(0)]| \tag{6.237}$$

*** Expand *** The two-point correlation function of Heisenberg operators at different times, establishing a departure from the corresponding classical correlator after a relatively short time (Shepelyanskii 1981, Shepelyansky 1983). In systems with well defined classical counterpart, this short scale corresponds to the Ehrenfest time.

6.2 Random matrices

Historically, the distribution of spacings in the energy level spectrum has been used to quantify quantum chaos. The hypothesis, well verified in a large number of systems, is that it is Poisson for integrable and satisfies the Wigner surmise for non-integrable systems. The OTOC is expected to be another measure of quantum chaos.
`https://www.lpthe.jussieu.fr/ leticia/TEACHING/Master2020/random-matrices.pdf`

6.3 Anderson Localization

6.4 Many-body localization

A Pauli operators

We recall here definitions and properties of the spin 1/2 operators.

A.1 The spin 1/2

The spin (angular momentum) is a quantum observable, which in three-dimensional Euclidean space is represented by a three component operator $\hat{\vec{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$. The states are represented by two component spinors.

The commutation relation of spin 1/2 operators are

$$[\hat{S}_i^a, \hat{S}_j^b] = i\hbar\epsilon_{abc}\hat{S}_i^c\delta_{ij} \ , \tag{A.1.1}$$

with Latin indices taking values $1, 2, 3$ and corresponding to x, y, z. We stress that spin operators acting on different sites commute.

The spin 1/2 operators have eigenvalues $\pm\hbar/2$. For instance,

$$\hat{S}_z \,|\uparrow\rangle = \frac{\hbar}{2}\,|\uparrow\rangle \qquad\qquad \hat{S}_z\,|\downarrow\rangle = -\frac{\hbar}{2}\,|\downarrow\rangle \ , \tag{A.1.2}$$

and see the Pauli subsection to identify the eigenvectors of the other two operators, $\hat{S}_x$, and $\hat{S}_y$. The states $|\uparrow\rangle$ and $|\downarrow\rangle$ are also represented as $|+\rangle$ and $|-\rangle$. In the main text we use the notation $|0\rangle$ and $|1\rangle$, respectively, for up and down.

The Hilbert space of a single spin is two-dimensional: for instance a basis is $\{|\uparrow\rangle, |\downarrow\rangle\}$, the two eigenstates of $\hat{S}_z$.

Raising and *lowering*, or *ladder* operators are defined as

$$\hat{S}_i^+ = \hat{S}_i^x + i\hat{S}_i^y \qquad\qquad \hat{S}_i^+ = \hat{S}_i^x - i\hat{S}_i^y \tag{A.1.3}$$

and act on the up and down state as

$$\begin{aligned} \hat{S}_i^+|-\rangle &= |+\rangle \qquad\qquad & \hat{S}_i^-|+\rangle &= |-\rangle \\ \hat{S}_i^+|+\rangle &= |-\rangle \qquad\qquad & \hat{S}_i^-|-\rangle &= |+\rangle \end{aligned} \tag{A.1.4}$$

Exercise A.4 Show that

$$\{\hat{S}_i^+, \hat{S}_j^-\} = \delta_{ij} \tag{A.1.5}$$

with { , } the anti-commutator.

Equations (A.1.4) are thus similar to the action of creation and annihilation spinless fermionic operators

$$\begin{aligned} \hat{c}_i^\dagger|0\rangle &= |1\rangle \qquad\qquad & \hat{c}_i|1\rangle &= |0\rangle \\ \hat{c}_i^\dagger|1\rangle &= |0\rangle \qquad\qquad & \hat{c}_i|0\rangle &= |1\rangle \end{aligned} \tag{A.1.6}$$

On different sites the spin operators commute and are then different from fermion operators.

A.2 The Pauli matrices

The spin operators are often represented by 2×2 complex *Pauli matrices* and the states by two row columnar vectors. These matrices are labeled with numbers or directions, $\sigma^1 = \sigma^x$, $\sigma^2 = \sigma^y$, $\sigma^3 = \sigma^z$, with

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{A.2.7}$$

In this representation $\hat{s}_a = \hbar/2\sigma_a$. We list below a number of important properties.

- They are Hermitian $(\sigma^a)^\dagger = \sigma^a$, for $a = 1, 2, 3$, with the $\dagger$ operation consisting in the combination of a transposition and complex conjugate operation.
- Together with the identity matrix $\mathbb{I}$ (sometimes noted σ^0) the Pauli matrices form a basis for the real vector space of 2×2 Hermitian matrices: any such matrix can be written in a unique way as a linear combination of them, with all coefficients being real numbers.
- Their inverses equal themselves, as they square to the identity, $(\sigma^a)^2 = \mathbb{I}$. In other words, they are idempotent.
- They are unitary, $(\sigma^a)^\dagger \sigma^a = \sigma^a (\sigma^a)^\dagger = \mathbb{I}$. This follows from $(\sigma^a)^2 = \mathbb{I}$ for $a = 1, 3$ the real ones and $(\sigma^2)^\dagger = (\sigma^2)$ and $(\sigma^2)^2 = \mathbb{I}$ for the one with imaginary entries.
- Their traces vanish, $\mathrm{Tr}\, \sigma^a = 0$ and their determinants are all equal, $\det \sigma^a = -1$, for $a = 1, 2, 3$.
- Consequently, their eigenvalues are ±1.
- Their normalized eigenvectors are

$$\sigma_z : \qquad |\uparrow\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |\downarrow\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{A.2.8}$$

$$\sigma_y : \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix} \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix} \tag{A.2.9}$$

$$\sigma_x : \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{A.2.10}$$

respectively.

- Their commutation relations are
$$[\sigma^a, \sigma^b] = 2\mathrm{i}\epsilon_{abc}\sigma^c \tag{A.2.11}$$
with ϵ_{abc} the Levi-Civita symbol, $\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1$, $\epsilon_{132} = \epsilon_{321} = \epsilon_{213} = -1$, and zero in all cases in which two indices are equal.
- They anti-commute: $\{\sigma^a, \sigma^b\} = 2\delta_{ab}\mathbb{I}$.
- One readily checks $\sigma^a\sigma^b = \delta^{ab} + \mathrm{i}\epsilon^{abc}\sigma^c$.
- $\sigma^x \,|\uparrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\downarrow\rangle$ and $\sigma^x \,|\downarrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle$.
- $\sigma^y \,|\uparrow\rangle = \begin{pmatrix} 0 \\ \mathrm{i} \end{pmatrix} = \mathrm{i}\,|\downarrow\rangle$ and $\sigma^y \,|\downarrow\rangle = \begin{pmatrix} -\mathrm{i} \\ 0 \end{pmatrix} = -\mathrm{i}\,|\uparrow\rangle$.

B The matrix element

Let us start recalling a number of basic properties of quantum mechanics.

The combination of exponentials of non-commuting operators is given by the *Baker-Campbell-Hausdorff formula*
$$e^{\hat{A}}\, e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]+\dots} , \tag{B.1}$$
where higher-order repeated commutators are shown by the dots.

The *Trotter product formula* applies to arbitrary $n \times n$ complex matrices or operators and it reads
$$e^{\mathrm{i}(\hat{A}+\hat{B})} = \lim_{N\to\infty} (e^{\mathrm{i}\hat{A}/N} e^{\mathrm{i}\hat{B}/N})^N \tag{B.2}$$

At least formally, the evolution operator $\hat{U}(t,0) = e^{-\mathrm{i}\hat{H}t/\hbar}$ can be expressed in terms of the eigenstates $|n\rangle$ of $\hat{H}$, $\hat{H}|n\rangle = E_n|n\rangle$,
$$\hat{U}(t,0) = e^{-\mathrm{i}\hat{H}t/\hbar} = \sum_n |n\rangle\langle n| e^{-\mathrm{i}E_n t/\hbar} . \tag{B.3}$$

In the $|x\rangle$ basis,
$$\langle x|\hat{U}(t,0)|x'\rangle = \sum_n \langle x|n\rangle\langle n|x'\rangle e^{-\mathrm{i}E_n t/\hbar} = \sum_n \psi_n(x)\psi_n^*(x') e^{-\mathrm{i}E_n t/\hbar} . \tag{B.4}$$

One can check that $U(x',t;x,0) \to \delta(x-x')$ for $t \to 0$.

Exercise B.1 Use the fact that for a free particle of mass m, the states $|n\rangle$ are just plane wave momentum states, and take the continuum limit of the sum over n (which becomes an integral over momenta) to show $U(x,t;x',0) = (m/2\pi\mathrm{i}\hbar t)^{1/2} \exp[\mathrm{i}m(x-x')^2/(2\hbar t)]$. In this case it is clear that $U(x',t;x,0) \to \delta(x-x')$ for $t \to 0$.

- Take an *orthonormal complete basis* of eigenstates, $|x\rangle$, of the position operator, $\hat{x}$, that is $\hat{x}|x\rangle = x|x\rangle$, with $\langle x'|x\rangle = \delta(x-x')$.

– Fourier transform each of these states,

$$|p\rangle = \int \frac{dx}{\sqrt{2\pi\hbar}}\, e^{\mathrm{i}xp/\hbar}\, |x\rangle \ , \tag{B.5}$$

and build another orthonormal complete basis of eigenstates, now of the momentum operator, $\hat{p}|p\rangle = p|p\rangle$. Indeed,

$$\begin{aligned} \langle p'|p\rangle &= \frac{1}{2\pi\hbar}\int dx \int dy\; e^{\mathrm{i}px/\hbar}e^{-\mathrm{i}p'y/\hbar}\; \langle y|x\rangle \\ &= \frac{1}{2\pi\hbar}\int dx \int dy\; e^{\mathrm{i}px/\hbar}e^{-\mathrm{i}p'y/\hbar}\; \delta(y-x) \\ &= \frac{1}{2\pi\hbar}\int dx\; e^{\mathrm{i}(p-p')x/\hbar} \\ &= \delta(p-p') \ . \end{aligned} \tag{B.6}$$

With these normalisations, two *resolutions of the identity* are

$$1 = \int dx\; |x\rangle\langle x| = \int dp\; |p\rangle\langle p| \ . \tag{B.7}$$

Because of the orthonormality of the elements $|x\rangle$, the bra-kets

$$\langle x|p\rangle = \frac{e^{\mathrm{i}xp/\hbar}}{\sqrt{2\pi\hbar}} \tag{B.8}$$

are *plane waves*. (As usual with Fourier transforms, there is some liberty in the placement of the $2\pi\hbar$ factor. We use this convention.)

In the rewriting of the finite time evolution function we encounter factors which are *matrix elements* of the kind

$$U(x_{k+1},t_{k+1};x_k,t_k) = \langle x_{k+1}|e^{-\mathrm{i}\,\hat{H}\frac{\delta t}{\hbar}}|x_k\rangle \ . \tag{B.9}$$

This infinitesimal evolution operator can be factorised over the time-interval $\delta t \to 0$, since one can neglect the non-commutativity of the kinetic and potential energy terms (the higher order terms are proportional to higher powers of δt, which is infinitesimal[5]), and use Trotter's formula:

$$e^{-\mathrm{i}\hat{H}\frac{\delta t}{\hbar}} \approx e^{-\mathrm{i}\,\frac{\hat{p}^2}{2m}\frac{\delta t}{\hbar}}\, e^{-\mathrm{i}\,V(\hat{x})\frac{\delta t}{\hbar}} \ . \tag{B.10}$$

Then,

$$U(x_{k+1},t_{k+1};x_k,t_k) = e^{-\mathrm{i}\,V(x_k)\frac{\delta t}{\hbar}}\; \langle x_{k+1}|e^{-\mathrm{i}\,\frac{\hat{p}^2}{2m}\frac{\delta t}{\hbar}}|x_k\rangle \ , \tag{B.11}$$

---

[5] While all this is fine for finite-dimensional matrices with finite matrix elements, it can be more delicate for operators in Hilbert space which could have large or even singular matrix elements. Still, we follow this route and neglect higher order terms in all the non-pathological cases we will deal with here.

where the operator $V(\hat{x})$ acting on the right ket gave rise to the function V evaluated at the eigenvalue x_k. The remaining factor is the *free-particle propagator*. Inserting now the identity

$$\mathbb{I} = \int dp_k \; |p_k\rangle\langle p_k| \tag{B.12}$$

we have

$$\begin{aligned} U(x_{k+1}, t_{k+1}; x_k, t_k) &= e^{-\mathrm{i}\, V(x_k)\frac{\delta t}{\hbar}} \int dp_k \; \langle x_{k+1}| e^{-\mathrm{i}\,\frac{\hat{p}^2}{2m}\frac{\delta t}{\hbar}} |p_k\rangle \; \langle p_k|x_k\rangle \\ &= e^{-\mathrm{i}\, V(x_k)\frac{\delta t}{\hbar}} \int dp_k \; e^{-\mathrm{i}\,\frac{p_k^2}{2m}\frac{\delta t}{\hbar}} \; \langle x_{k+1}|p_k\rangle \; \langle p_k|x_k\rangle \end{aligned} \tag{B.13}$$

Using now that the free-particle wave function is

$$\langle p_k|x_k\rangle = \frac{1}{\sqrt{2\pi\hbar}} \; e^{-\frac{\mathrm{i}}{\hbar}\, p_k x_k} \tag{B.14}$$

we have

$$U(x_{k+1}, t_{k+1}; x_k, t_k) = \int \frac{dp_k}{2\pi\hbar} \; e^{-\mathrm{i}\,\frac{p_k^2}{2m}\frac{\delta t}{\hbar}} \; e^{\mathrm{i} p_k \left(\frac{x_{k+1}-x_k}{\delta t}\right)\frac{\delta t}{\hbar}} \; e^{-\mathrm{i}\, V(x_k)\frac{\delta t}{\hbar}} \; . \tag{B.15}$$

(We note that one cannot evaluate this result from a Taylor series expansion in powers of δt of the exponential of the kinetic energy operator, the result is singular in the $\delta t \to 0$ limit.) The sign of the linear term in p_k in the exponential can be changed to minus, after a change of variables $p_k \to -p_k$. If one now performs the integral over the momentum p_k

$$U(x_{k+1}, t_{k+1}; x_k, t_k) = \left(\frac{-\mathrm{i}m}{2\pi\delta t\hbar}\right)^{1/2} \; e^{\mathrm{i}\,\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\delta t}\right)^2 \frac{\delta t}{\hbar} - \mathrm{i}\, V(x_k)\frac{\delta t}{\hbar}} \; . \tag{B.16}$$

The prefactor is included in the integral measure and no longer written.

C Stationary phase approximation

The stationary phase approximation extends the steepest descent of Laplace method to integrals of rapidly varying imaginary exponentials. The idea is that sinusoids with rapidly varying phase cancel under the sum over all of them.

Calling $\hbar$ the small parameter, when a function f of a single real variable x has only one extreme x^*, $f'(x^*) = 0$, the formula is

$$\lim_{\text{“}\hbar \ll f(x)\text{”}} \int dx \; e^{\mathrm{i} f(x)/\hbar} = e^{\mathrm{i} f(x^*)/\hbar} \; e^{\mathrm{i}\pi/4 \; \mathrm{sign} f''(x^*)} \; \left(\frac{2\pi\hbar}{|f''(x^*)|}\right)^{1/2} \tag{C.1}$$

The idea to prove this equation is the same as for the usual steepest descent of saddle-point approximation. One expands the function in the exponential to second order in the distance from its extreme x^*:

$$\begin{aligned} f(x) &= f(x^*) + f'(x^*)(x-x^*) + \frac{1}{2}f''(x^*)(x-x^*)^2 + \mathcal{O}((x-x^*)^3) \\ &\sim f(x^*) + \frac{1}{2}f''(x^*)(x-x^*)^2 \end{aligned} \tag{C.2}$$

The first term is a constant with respect to x and comes out of integral. The quadratic corrections remain to be integrated over

$$\lim_{\text{“}\hbar \ll f(x)\text{”}} \int dx\, e^{\mathrm{i}f(x)/\hbar} = e^{\mathrm{i}f(x^*)/\hbar} \int dx\, e^{\mathrm{i}\frac{1}{2}f''(x^*)(x-x^*)^2/\hbar}\,. \tag{C.3}$$

When $\hbar$ is small compared to $f''(x^*)$, even a small difference $x - x^*$ will lead to rapid oscillations within the integral and cancellations. Then one can integrate over x going from $-\infty$ to ∞. The result is Eq. (C.1).

If the function f has several stationary points, then one separates the integral in non-overlapping intervals and approximates the result on each of them separately in the way described above.

D Some subjects for final exam

- **Random quantum circuits**

  Random quantum circuits are quantum circuits in which the sequence of gates is chosen randomly according to certain rules or distributions. These circuits play an important role in quantum information science and quantum computing, particularly for benchmarking quantum processors and studying properties of quantum systems.

  - *Random Quantum Circuits*
    M. P. A. Fisher, V. Khemani, A. Nahum, and S. Vijay
    Annual Review of Condensed Matter Physics 14, 335 (2023)

- **Mpemba effect**

  The Mpemba effect is a counterintuitive phenomenon where, under certain conditions, hot water can freeze faster than cold water. It has been observed in various settings but remains a subject of scientific debate due to the complexity and variability of the underlying mechanisms.

  - *Multiple quantum Mpemba effect: exceptional points and oscillations*,
    A. K. Chatterjee, S. Takada, and H. Hayakawa,
    arXiv:2311.01347
  - *Quantum Mpemba effect in a quantum dot with reservoirs*,
    A. K. Chatterjee, S. Takada, and H. Hayakawa,
    arXiv:2304.02411, Phys. Rev. Lett. 131, 080402 (2023)

- **Entanglement entropy**

  Entanglement entropy is a measure of quantum entanglement in a system, quantifying how strongly a subsystem is entangled with the rest of the system. It is widely used in quantum information theory, condensed matter physics, and quantum gravity.

  - *Generalised Hydrodynamics description of the Page curve-like dynamics of a freely expanding fermionic gas*,
    M. Saha, M. Kulkarni, and A. Dhar,
    arXiv:2402.18422
  - J. Eisert, M. Cramer, and M.B. Plenio,
    Area laws for the entanglement entropy - a review
    arXiv:0808.3773, Rev. Mod. Phys. 82, 277 (2010)
  - R. Islam, R. Ma, P. M. Preiss, M. E. Tai, A. Lukin, M. Rispoli, and M. Greiner,
    Measuring entanglement entropy in a quantum many-body system
    arXiv:1509.01160, Nature **528**, 77 (2015)
  - J. I. Latorre and A. Riera,
    A short review on entanglement in quantum spin systems,
    https://arxiv.org/pdf/0906.1499, J. Phys. A **42**, 504002 (2009)
  - N. Laflorencie,
    Entanglement entropy and localization in disordered quantum chains,
    arXiv:2112.09102, Chapter book in "Entanglement in Spin Chains - From Theory to Quantum Technology Applications", Bayat, A., Bose, S., Johannesson, H. (eds)

- **Engineering symmetries in time**

  Engineering symmetries in time refers to the deliberate design or manipulation of temporal structures in physical or mathematical systems to exploit symmetry principles, akin to spatial symmetries. This concept is often applied in physics, quantum mechanics, and engineering to achieve desired dynamic behaviors, enhance performance, or simplify problem-solving.

  - *Engineering Hierarchical Symmetries*,
    Z. Fu, R. Moessner, H. Zhao, and M. Bukov,
    arXiv:2402.13519

- **OTOCs and FDT**

  The Out-of-Time-Ordered Correlation (OTOC) is a quantum mechanical measure used to characterize the growth of operator commutators and assess the scrambling of quantum information in a system. It has become a key tool in studying quantum chaos, thermalization, and the spreading of quantum entanglement.

  - N. Tsuji, T. Shitara, and M. Ueda, *Bound on the exponential growth rate of*

  out-of-time-ordered correlators, Phys. Rev. E **98**, 012216 (2018).
  - S. Pappalardi, L. Foini, and J. Kurchan,
    Quantum bounds and fluctuation-dissipation relations,
    SciPost Phys. **12**, 130 (2022).

- **Loschmidt echo**

  The Loschmidt echo is a measure of the revival occurring when an imperfect time-reversal procedure is applied to a complex quantum system.

  - T. Gorin, T. Prosen, T. H. Seligman, and M. Žnidarič,
    Dynamics of Loschmidt echoes and fidelity decay,
    Physics Reports, **435**, 33 (2006).
  - A. Goussev, R. A. Jalabert, H. M. Pastawski, and D. Wisniacki,
    Loschmidt Echo,
    arXiv:1206.6348, Scholarpedia 7, 11687 (2012).

- **Quantum Brownian motion**

  Quantum Brownian motion is a model describing the behaviour of a quantum system interacting with a large environment, where the environment induces random fluctuations and dissipation on the system, analogous to classical Brownian motion. However, unlike classical Brownian motion, quantum Brownian motion incorporates quantum effects such as coherence, superposition, and entanglement.

  - J. Bonart and L. F. Cugliandolo,
    From non equilibrium quantum Brownian motion to impurity dynamics in 1D quantum liquids,
    Phys. Rev. A **86**, 023636 (2012)

- **Dicke model**

  The Dicke model is a spin-boson model with the spin being the system and the boson the bath. On can see effects like decoherence in simple terms here.

  - D. Villaseñor, S. Pilatowsky-Cameo, J. Chávez-Carlos, M. A. Bastarrachea-Magnani, S. Lerma-Hernández, L. F. Santos, and J. G. Hirsch,
    Classical and Quantum Properties of the Spin-Boson Dicke Model: Chaos, Localization, and Scarring
    arXiv:2405.20381

- **Models of baths**

  A quantum bath is a concept from quantum mechanics and quantum statistical physics that refers to an environment or reservoir of quantum systems interacting with a primary quantum system of interest. This "bath" provides a way to model how the primary system exchanges energy, particles, or information with its surroundings, leading to effects like dissipation, decoherence, or thermalization.

- G. W. Ford, M. Kac, and P. Mazur,
  Statistical mechanics of assemblies of coupled oscillators,
  J. Math. Phys. **6**, 504 (1965).
- N. Prokof'ev and P. Stamp,
  Theory of the spin bath,
  Rep. Prog. Phys. **63**, 669 (2000).

- **Localization by an Ohmic bath**

  An Ohmic bath consists of a continuum of harmonic oscillators (e.g., phonons, photons, or other modes) with spectral density $J(\omega) = \gamma\omega$ that interact with a quantum particle under a two well potential. For $\gamma > 1$ tunnelling is inhibited and the particle remains localized in the well it was initiated.

  - A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger,
    Dynamics of the dissipative two-state system,
    Rev. Mod. Phys. **59**, 1 (1987).
  - A. J. Bray and M. A. Moore,
    Influence of Dissipation on Quantum Coherence,
    Phys. Rev. Lett. **49**, 1545 (1982).
  - A. O. Caldeira and A. J. Leggett,
    Quantum tunnelling in a dissipative system,
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