Density Matrices and Decoherence

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Note

In what follows I will occasionally use the states $|0\rangle$ and $|1\rangle$, which are meant to be in analogy with classical bits 0, and 1. They might be referred to as **qubits**, but really they stand for the basis of any two-level system, so you may think of them as $|u\rangle$ and $|d\rangle$.

I will also work in units where $\hbar = 1$. This is a really common convention in the literature; you can imagine we've just rescaled the definition of a second so that $t/\hbar \to t$, and we're working in a quantum time scale.

1 Density Matrices

Motivation Thus far we have dealt only with probabilities as they manifest in a quantum mechanical sense. However, quantum systems can also be in indeterminate states in a purely classical sense, in the exact same way that the random variables you are used to from, say, a statistics class are in indeterminate states.

As an illustration, we could consider that your friend flips a coin, and if it's heads they prepare a qubit in some superposition

$$\text{Heads} \quad \Longrightarrow \quad |\psi_1\rangle = \frac{1}{\sqrt{2}}(|u\rangle + |d\rangle)$$

and if it's tails, they prepare it in the superposition

$$\text{Tails} \quad \Longrightarrow \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}(|u\rangle - |d\rangle)$$

After the state is prepared, you go and make a measurement of this qubit's state in the z-basis. How do we write down a state capturing the probability distribution of this system? The answer will turn out to be to write it as

$$\rho = \overbrace{\frac{1}{2}}^{p_{\text{heads}}} |\psi_1\rangle\langle\psi_1| + \overbrace{\frac{1}{2}}^{p_{\text{tails}}} |\psi_2\rangle\langle\psi_2|$$

Formal definition We can formalize the preceding consideration with the following definition:

Definition

A **density matrix** (or **density operator**), often written ρ, is an operator of Hilbert space satisfying the following properties:

- *Positive semi-definite* (non-negative eigenvalues): probabilities should be greater than zero.
- *Hermitian*: made up of projection operators, which are Hermitian.
- *Unit trace*: probabilities should sum to one.

If state $|\psi_i\rangle$ (possibly a superposition) is associated with a classical probability p_i and we have N such states, the density matrix is

$$\rho = \sum_i p_i \, |\psi_i\rangle\langle\psi_i|$$

Aside

The density matrix bears that name because in many-particle quantum mechanics one needs to integrate over ρ to get the total number of states, analogously to how one integrates over the density to get the mass.

1.1 Properties

- We can still compute the standard quantities we are able to with the density matrix. The **expectation value** of some observable A is

$$\langle A\rangle = \mathrm{tr}(\rho A)$$

Proof: For a density matrix $\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$,

$$\mathrm{tr}(\rho A) = \mathrm{tr}\left(\sum_j p_j |\psi_j\rangle\langle\psi_j| A\right) = \sum_j p_j \,\mathrm{tr}(|\psi_j\rangle\langle\psi_j| A)$$
$$= \sum_j p_j \sum_i \overbrace{\langle\psi_i|\psi_j\rangle}^{\delta_{ij}} \langle\psi_j| A |\psi_i\rangle = \underbrace{\sum_j p_j \langle\psi_j| A |\psi_j\rangle} = \langle A\rangle$$

where we've used the fact that the trace is the sum

$$\mathrm{tr}(O) = \sum_i \langle e_i| O |e_i\rangle$$

for an orthonormal basis $|e_i\rangle$ and that $|\psi_j\rangle$ is necessarily an element of some basis. From the underlined equation we see that the above definition of the density matrix makes sense because it gets us the expectation values over both the quantum probabilities and the classical probabilities. $\square$

- To **act on a state** written as a density matrix, we just notice that for a pure state

$$|\psi\rangle \to A|\psi\rangle \quad \Longrightarrow \quad |\psi\rangle\langle\psi| \to A|\psi\rangle\langle\psi| A^\dagger$$

so ρ is acted on by A as

$$\rho \to A\rho A^\dagger.$$

- ρ describes a **pure state** if and only if

$$\mathrm{tr}\big(\rho^2\big) = 1, \text{ or } \rho^2 = \mathbb{I}.$$

- We can tell if ρ contains a superposition if it has an off-diagonal:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|e_1\rangle + |e_2\rangle) \quad \Longrightarrow \quad \rho = |\psi\rangle\langle\psi| = \frac{1}{2}(|e_1\rangle\langle e_1| + |e_1\rangle\langle e_2| + |e_2\rangle\langle e_1| + |e_2\rangle\langle e_2|)$$
$$= \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}.$$

On the other hand if the matrix is entirely diagonal, it is just a classical probability distribution over definite states (not superpositions).

- **Time evolution** Using the product rule together with the Schrodinger equation $d\left|\psi\right\rangle/dt = -i\left|\psi\right\rangle/\hbar$we can find the equivalent equation of motion for the density matrix:

$$\begin{aligned}\frac{d}{dt}\left|\psi\middle\rangle\middle\langle\psi\right| &= \frac{d}{dt}\left|\psi\middle\rangle\middle\langle\psi\right| + \left|\psi\right\rangle\frac{d}{dt}\left\langle\psi\right| \\ &= -\frac{i}{\hbar}H\left|\psi\middle\rangle\middle\langle\psi\right| + \frac{i}{\hbar}\left|\psi\middle\rangle\middle\langle\psi\right|H \\ \frac{d\rho}{dt} &= -\frac{i}{\hbar}\left[H,\rho\right]\end{aligned}$$

(the relative minus sign in the second term that leads to the commutator is due to the fact that we need to take the adjoint to get to $\langle\psi|$)

We know that the time evolution of a state is $|\psi(t)\rangle = e^{iHt/\hbar}\left|\psi 0\right\rangle$, so naturally

$$\rho(t) = e^{-iHt/\hbar}\rho(t)e^{iHt/\hbar} \tag{1}$$

- **Tensor product** For two states $|\psi_1\rangle$, $|\psi_2\rangle$

$$\rho = |\psi_1\psi_2\rangle\langle\psi_1\psi_2| = |\psi_1\rangle\langle\psi_1| \otimes |\psi_2\rangle\langle\psi_2| = \rho_1 \otimes \rho_2$$

- **Examples** For an up state $|u\rangle$:

$$|u\rangle\langle u| = \begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}$$

Or for a general state $|n^+\rangle = \cos\frac{\theta}{2}\left|u\right\rangle + e^{i\phi}\sin\frac{\theta}{2}\left|d\right\rangle$

$$\left|n^+\middle\rangle\middle\langle n^+\right| = \begin{bmatrix}\cos^2\frac{\theta}{2} & \sin\theta\cos\phi\\ \sin\theta\cos\phi & \sin^2\frac{\theta}{2}\end{bmatrix} = \frac{1}{2}(\mathbb{I} + n_x\sigma_x + n_y\sigma_y + n_z\sigma_z)$$

Let's say we roll a die, and if it comes out to six we prepare a particle in an up state and if anything else we prepare the particle in a down state.

$$\rho = \frac{1}{6}\left|u\middle\rangle\middle\langle u\right| + \frac{5}{6}\left|d\middle\rangle\middle\langle d\right| = \begin{bmatrix}1/6 & 0\\ 0 & 5/6\end{bmatrix}$$

2 Coupling to an Environment

We now explicitly address a significant simplifying assumption we have heretofore been making. All of the formalism we've developed implicitly describes systems which are *closed*, i.e., isolated from and unaffected by the rest of the world. This should be clear from the fact that we've never once made mention of the quantum state of the environment the system is in. Now it is time to include these effects by incorporating the interactions the system makes with its environment; in physics parlance, we will *couple* to the environment.

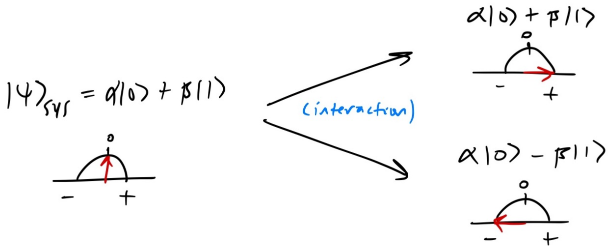

Figure 1

2.1 Quantum Channels

Toy model of POVM Generally we will consider state describing a system and an envioronment:

$$|\psi\rangle_{\text{sys}} |\phi\rangle_{\text{env}} \quad \longleftrightarrow \quad \rho_{\text{sys}} \otimes \rho_{\text{env}}$$

Now let's consider that we couple a quantum system to toy environment consisting of a pointer that can indicate 0, $+$, or $-$, and let the system interact with the pointer.

$$\begin{aligned} U: \quad & (\alpha|0\rangle + \beta|1\rangle)_{\text{sys}} \otimes |0\rangle_{\text{p}} \\ & \longrightarrow \quad (|\alpha|0\rangle + \beta|1\rangle\rangle)_{\text{sys}} \otimes |+\rangle_{\text{p}} + (\alpha|0\rangle - \beta|1\rangle)_{\text{sys}} \otimes |-\rangle_{\text{p}} \end{aligned}$$

If we are observers who come into the laboratory and look at the pointer, we collapse the pointer's state into either $|+\rangle$ or $|-\rangle$. It's clear that the pointer is entangled with the system, so we will find that the system state will be affected by our measurement. If we choose $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ we can rewrite this as

$$\begin{aligned} U: \quad & |\psi\rangle_{\text{sys}} \otimes |0\rangle_{\text{p}} \\ & \longrightarrow \quad (M^+|\psi\rangle)_{\text{sys}} \otimes |+\rangle_{\text{p}} + (M^-|\psi\rangle)_{\text{sys}} \otimes |-\rangle_{\text{p}} \end{aligned}$$

where the operators $M^\pm$ take the initial state $|\psi\rangle$ to the possible outcomes of the measurement. For a more complicated system you might have a larger set of them, $\{M_i\}$, corresponding to all the different post-measurement states of the system, which are

$$\text{Post-measurement states}: \quad \frac{M_i|\psi\rangle}{|M_i|\psi\rangle\,|}$$

these outcomes may be superpositions, they may not be orthogonal, it turns out that as long as we require $\sum_i M_i^\dagger M_i = \mathbb{I}$, the probabilities of getting an outcome i:

$$\langle\psi| M_i^\dagger M_i |\psi\rangle$$

will add to unity. We refer to these M_i (actually, to the $M_i^\dagger M_i$, since that's that provides each of the probabilities) as a **positive operator-valued measure**. $M_i^\dagger M_i$ is positive in the same sense that the density matrices were positive, and it constitutes a measure in the probability theory sense. M_i themselves are called the **Kraus operators**.

Quantum channels After interacting with our environment, if we trace out (ignore) the state of the environment[1] we'd find that the system is in some state

$$\rho' = \sum_i M_i |\psi\rangle\langle\psi| M_i^\dagger \tag{2}$$

This is referred to as a **quantum channel**. They are also referred as **completely positive, trace-preserving maps**, for the resulting state must also satisfy the defining properties of a density matrix.

A crucial property of these channels is that they need not be *unitary*, meaning they might not preserve superpositions. The evolution of the total system—the system and the environment together, will surely be unitary (in fact, one can imagine the only physically complete evolution that is truly completely unitary is the evolution of the whole universe).

The underlying mechanism is that the system gets entangled with environment, and after we ignore the environment by imagining that we are repeatedly making measurements of it, entanglement turns the superposition into a mixture. We'd only get unitary evolution if there was just one Kraus operator, because then $M_1^\dagger M_1 = \mathbb{I}$, which is the defining property of unitary operators. In, it is demonstrable that **a quantum channel is invertible if and only if it is unitary**, meaning that if the system is not closed (doesn't evolve unitarily) quantum information leaks out in an irreversible process.

2.2 Decoherence

To illustrate the power of this Kraus operator formalism we will work out a very simple example of **decoherence**. Consider a two state system interacting with a three-state environment. If the system is in the lowest energy state $|0\rangle$, the environment has an amplitude $\sqrt{p}$ of going to its first excited state, and if the system is in the excited state, the environment has a probability $\sqrt{p}$ of going to the second excited state. In both cases the system stays in its initial state.

$$\begin{aligned} U: \quad & |0\rangle_{\text{sys}} \otimes |0\rangle_{\text{env}} && \rightarrow && |0\rangle_{\text{sys}} \otimes (\sqrt{1-p}\,|0\rangle + \sqrt{p}\,|1\rangle)_{\text{env}} \\ & |1\rangle_{\text{sys}} \otimes |0\rangle_{\text{env}} && \rightarrow && |1\rangle_{\text{sys}} \otimes (\sqrt{1-p}\,|0\rangle + \sqrt{p}\,|2\rangle)_{\text{env}} \end{aligned}$$

In this case if we make a measurement on the environment there are three possibilities, $|0\rangle$, $|1\rangle$, $|2\rangle$, which is a hint that there are three Kraus operators. These turn out to be

$$M_0 = \sqrt{1-p}\mathbb{I}, \quad M_1 = \sqrt{p}\,|0\rangle\langle 0|\,, \quad M_2 = \sqrt{p}\,|1\rangle\langle 1|$$

[1] You'd use a procedure analogous to calculating the mixtures $M^{(1,2)}$ that you found in Homework 7; specifically, we carry out the partial trace with respect to the environment of the evolution operator U.

(they act on the system Hilbert space), which correspond to observing the environment in the $|0\rangle$, $|1\rangle$, and $|2\rangle$ states respectively. Let's consider the state of the system after the channel is applied; eq. (2) tells us it is

$$\rho' = \sum_{i=0}^{2} M_i \rho M_i^\dagger = \begin{bmatrix} \rho_{00} & (1-p)p_{01} \\ (1-p)\rho_{10} & \rho_{11} \end{bmatrix}$$

for the initial density matrix of the system, which we take to be arbitrary. Now, if we imagine that we apply this channel n times for n large, and that p represents a tiny amount $p = \Gamma \Delta t$ that the system is nudged into a different state for a small time step Δt, we will find that repeated application will preserve the diagonal elements but accumulate factors of $(1-p)$ in the off-diagonals:

$$\rho(n) = \begin{bmatrix} \rho_{00} & (1-p)^n p_{01} \\ (1-p)^n \rho_{10} & \rho_{11} \end{bmatrix}$$

then we say that there's some total elapsed time equal to the total number of time increments the system experiences: $t = n\Delta t$, we can use the definition of the exponent function

$$(1-p)^n = (1 - \Gamma t/n)^n \xrightarrow{n\to\infty} e^{-\Gamma t}$$

So that

$$\rho(t) = \begin{bmatrix} \rho_{00} & e^{-\Gamma t} p_{01} \\ e^{-\Gamma t} \rho_{10} & \rho_{11} \end{bmatrix} \quad \xrightarrow{t\to\infty} \quad \begin{bmatrix} \rho_{00} & 0 \\ 0 & \rho_{11} \end{bmatrix}$$

Now recall the interpretation of the off-diagonals as corresponding to a superposition, and the additional interpretation that a completely diagonal density matrix corresponds to a classical probability. What we have just shown is that coupling to an environment can lead to an exponential suppression of the superposition, such that the ultimate fate of the system is a standard classical probability, one that cannot interfere with itself a-la double-split experiment and does not require a bizarre role of the observer (the measurement problem).

3 Lindblad Equation

Above we derived an equation of motion for the density matrix (the density matrix equivalent of the Schrödinger equation), eq. (1). We can ask ourselves—can we do the same when the system is open, i.e., coupled to an environment? We've seen above such a system experiences the effect of a quantum channel through a Kraus operator M_i. This operator encodes the infinitesimal change the system undergoes during a very small time step. It turns out that if we consider the following rescaling of the Kraus operators

$$L_i = \frac{1}{\sqrt{\Delta t}} M_i, \quad i > 0$$

with the additional "zero-th" Kraus operator

$$M_0 = \mathbb{I} + (-iH + K)\Delta t, \quad H = \text{Hamiltonian} \tag{3}$$

we can construct a new equation of motion which captures the open-ness and dissipation of the system.

Aside: M_0

M_i represent the evolution of the system when environmental observations are being made that lead to some collapse in our system. M_0 plays a slightly subtler role: it corresponds to what would have been the closed evolution of the system, under the Schrödinger equation alone. This is why the Hamiltonian is there. In fact, if we consider the operator that the density matrix of a closed system evolves under and Taylor expand for a small time Δt:

$$e^{-iH\Delta t} \approx \mathbb{I} - iH\Delta t$$

we see where M_0 comes from. The presence of the K operator just makes sure that the set $M_i^\dagger M_i$ together with $M_0^\dagger M_0$ makes this a POVM.

If we apply these operators again and again like we did to derive the decoherence of a two state system above, a little elbow grease gets us the analogue of the Schrödinger equation for the density matrix of an open system. It looks like this:

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_{i>0} \left(L_i \rho L_i - \frac{1}{2} \left\{ L_i^\dagger L_i, \rho \right\} \right) \equiv \mathcal{L}[\rho]$$

This is called the **Lindblad master equation**. A few comments

- You see that the first term is just the evolution of the density matrix of a closed system. So if we set all L_i to zero, we recover a closed system.
- The sum describes the coupling to the environment as a sum over all the possible ways the system can collapse, roughly speaking.
- In the sum, the first term $L_i \rho L_i^\dagger$ is what actually induces the collapse, as it's essentially what we found above when discussing quantum channels with Kraus operators.
- The second term in the sum, $\left\{ \rho, L_i^\dagger L_i \right\}$, uses the notation $\{A, B\}$ for the **anticommutator**:

  $$\{A, B\} = AB + BA$$

  The role of that term is to keep the density matrix normalized, i.e., keep its trace unity.

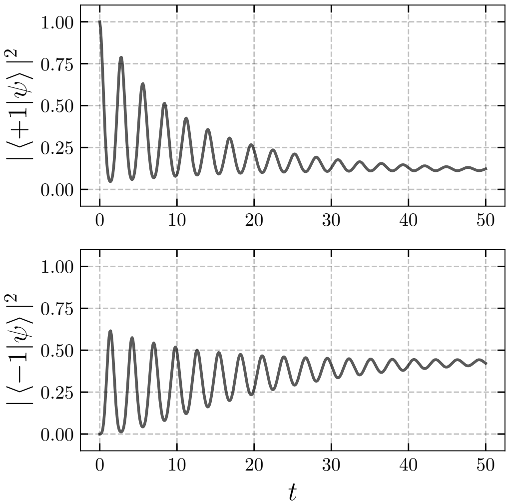

Figure 2

- L_i are called the **jump operators** or **Lindblad operators**, after Göran Lindblad, who passed almost exactly a year ago. The function $\mathcal{L}$ takes in an operator and gives you another operator according to the middle equation, and is called the **Liouvillian** or **Lindbladian**.

Simulated example You can actually simulate a density matrix evolving under the Lindblad equation without much effort. For instance, you could pick some two state system whose closed-system evolution induces an oscillation between two states; i.e., the amplitudes $|\langle\psi(t)|0\rangle|^2 \approx \cos^2 t$ and $|\langle\psi|1\rangle|^2 \approx \sin^2 t$. If we couple this system to an environment we end up seeing that the oscillations experience decoherence and gradually relax to some final final state with fixed classical probabilities (fig. 2).

3.1 Comments

We've just worked out some models wherein we see, before our very eyes, how entanglement leads to a dissipation in superposition. This is simultaneously good news and bad news. The bad news is that if we want to somehow harness the power of quantum superpositions, it's like drinking soup with a fork—the superpositions naturally tend to leak out into the environment, destroying quantum coherence. This is the main challenge of quantum computation, which is why quantum information theorists constructed all this formalism in the first place.

The prima facie good news is that now we understand the measurement problem a little better. Namely, we understand how it is that we don't see things in superpositions very commonly—the interactions with environment reduce all the quantum weirdness to classical probabilities. One might go as far as saying that this *solves* the measurement problem, but this is a little hasty. What we've shown is that superpositions tend to delocalize, so to speak, through interactions, so that entanglement spreads in a system and reduces superpositions in any subsystem to a classical probability distribution. It doesn't really answer any questions about the ultimate fate of this massive entanglement nor does it tell us what a superposition really is. In fact, sometimes it's possible to create macroscopically superposed systems which resist decoherence (don't excited about computing with these though, manipulating the states to perform computations is where things get dirty). There's sort of an analogue of Bell's inequality for such systems, called the Leggett-Garg inequality.

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