Lectures on Quantum Decoherence

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Lecture 1 – Basic Concepts

1.1 Introducing decoherence

Classical physics has led us to the strategy of dealing with idealised isolated systems. This has been very successful and got incorporated into quantum mechanics without much scrutiny.

But isolated quantum systems have been an obstacle in understanding the quantum-to-classical transition. We therefore require open quantum systems, not as an add-on or a 'fix', but as an essential and more complete description of many systems of interest today, from quantum optics to quantum computing, and even (possibly) quantum biology.

On locality

Quantum mechanics is a local theory (in the sense that all interactions are local and so there is no *physical* action at a distance). But, the states that can be generated by these local interactions are distinctly *non-local* due to entanglement. We talk about this in terms of non-local correlations.

Entanglement means the outside environment no longer just perturbs the system, but rather *defines* the observable physical properties of the system.

Entanglement with an environment does two things:

1. It causes irreversible loss of coherence from the quantum system

2. It limits/selects a small number of possible observables

Quantum decoherence (loss of information) is a separate process from classical dissipation (loss of energy).

For macroscopic bodies, decoherence is incredible fast, and it happens everywhere. Even the CMB will cause decoherence.

The first paper on decoherence was by Zeh [Zeh, H.D., "On the interpretation of measurement in quantum theory", *Found Phys* **1**, 69–76 (1970)]. That was over half a century ago and yet standard textbooks on quantum mechanics still largely ignore the subject, claiming (correctly) that the measurement of physical quantities (observables) are represented by Hermitian operators, but that these somehow *instantaneously* change the quantum state of the system into one of the eigenstates of that operator. We will see in these lectures that that is not the case, but rather that measurement involves several stages, and that it is a dynamical process.

> Decoherence does not destroy superpositions, it simply extends them to include the environment. So, while decoherence is something that happens to the system of interest, what is really going on is that the environment is encoding, via quantum correlations, information about the system.

1.2 Quantum entanglement

Consider a quantum system, S, described by state vector $|\Psi\rangle$. It is composed of two subsystems (so, it is called a bipartite quantum system): S_1 and S_2, with state vectors $|\Psi_1\rangle$, $|\Psi_2\rangle$, respectively.

If S cannot be split into a tensor product of the states of S_1 and S_2, i.e. if $|\Psi\rangle \neq |\psi\rangle_1 \otimes |\psi\rangle_2$, then we say that S is entangled with respect to S_1 and S_2.

[Note: we will be using the shorthand notation $|\psi\rangle_1 \otimes |\psi\rangle_2 \equiv |\psi\rangle_1 |\psi\rangle_2$.]

Consider for example that S_1 and S_2 are two spin-$\frac{1}{2}$ particles described by basis states $|0\rangle$ and $|1\rangle$.

That is, $|0\rangle_1$ corresponds to particle 1 pointing in the spin up direction with respect to some axis, say the z-axis, and $|1\rangle_1$ corresponds to particle 1 pointing spin down along the same axis. Thus,

$$\sigma_z |0\rangle = |0\rangle \qquad \text{and} \qquad \sigma_z |1\rangle = -|1\rangle \ , \tag{1.1}$$

where σ_z is the Paul spin operator. If $|\psi\rangle_1$ and $|\psi\rangle_2$ are each in a superposition of these spin states, then we can write

$$|\psi\rangle_1 = \alpha_1 |0\rangle_1 + \beta_1 |1\rangle_1 \ , \tag{1.2}$$

$$|\psi\rangle_2 = \alpha_2 |0\rangle_2 + \beta_2 |1\rangle_2 \ . \tag{1.3}$$

Note that we would normally write these two wave functions with the subscripts inside the kets (that is, $|\psi_1\rangle$ and $|\psi_2\rangle$), but I am keeping them outside for clarity later on.

If the particles are <u>not</u> initially entangled, then their combined system is

$$|\Psi\rangle = |\psi\rangle_1 |\psi\rangle_2 = \Big(\alpha_1 |0\rangle_1 + \beta_1 |1\rangle_1\Big)\Big(\alpha_2 |0\rangle_2 + \beta_2 |1\rangle_2\Big) \ . \tag{1.4}$$

Let us keep things simple and assume both particles are in 50/50 superpositions of being spin up and down. So,

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\Big(|0\rangle_1 + |1\rangle_1\Big) \cdot \frac{1}{\sqrt{2}}\Big(|0\rangle_2 + |1\rangle_2\Big) \ . \tag{1.5}$$

Clearly, here the two particles' superpositions are not entangled and they are each described by separate (uncorrelated) quantum states (wave functions). The opposite extreme is if they are *maximally entangled*. This is called a **Bell state**:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\Big(|0\rangle_1 |0\rangle_2 + |1\rangle_1 |1\rangle_2\Big) \ , \tag{1.6}$$

which says that if particle 1 is spin up, then so is particle 2, and vice versa.

Note that they could also be maximally entangled such that they always have opposite spin and the sign between them could be a plus or a minus. These would still be Bell states:

$$|\Phi\rangle_\pm = \frac{1}{\sqrt{2}}\Big(|0\rangle_1 |1\rangle_2 \pm |0\rangle_1 |1\rangle_2\Big) \ . \tag{1.7}$$

The degree of entanglement between the two particles could be anything between unentangled (Eq.(1.5)) and fully entangled (eqs.(1.6) or (1.7)).

What is the difference between these two extremes when it comes to measurement?

Answer:
If we measure the spin of particle 2 in a Bell state and find it to have spin up ($|0\rangle_2$ then this immediately tells us the spin of particle 1. But for an uncorrelated (unentangled) pair, measuring the spin of particle 2 tells us nothing about particle 1 and just leaves it in its original superposition.

Now here is the subtlety: What if the quantum states of particles 1 and 2 are each in superpositions of different basis states $\{|\psi_i\rangle\}$ and $\{|\phi_i\rangle\}$, respectively, that do not necessarily form orthonormal sets like spin states. We will assume that they are in a general entangled Bell state defined as

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\Big(|\psi_1\rangle\,|\phi_1\rangle + |\psi_2\rangle\,|\phi_2\rangle\Big)\ . \tag{1.8}$$

Consider particle 2: if $|\phi_1\rangle$ and $|\phi_2\rangle$ *are* orthogonal – for example eigenstates of an operator corresponding to some observable, A, and so macroscopically distinguishable (such as their spin in a magnetic field or their positions measured on a dial on a classical detector). Then a measurement of A would yield an eigenvalue corresponding to one or other of them: $|\phi_1\rangle$ or $|\phi_2\rangle$. This will immediately tell us the state of particle 1 because one of the two terms in Eq.(1.8) will disappear.

However, if $|\phi_1\rangle_2$ and $|\phi_2\rangle_2$ are not orthogonal – that is they have non-zero overlap – then we will only get partial information on particle 1. In fact, if they overlap completely then this means that $|\phi_1\rangle$ and $|\phi_2\rangle$ are the same and can be factorised out:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\Big(|\psi_1\rangle + |\psi_2\rangle\Big)\ |\phi_1\rangle\ , \tag{1.9}$$

and so we learn nothing about particle 1.

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.

1.3 The density matrix

For a pure state $|\Psi\rangle$, the density matrix operator (or just 'density matrix') is a very useful quantity if we wish to go beyond the unitary dynamics of the Schrödinger equation to describe open quantum systems, mixed states, ensembles and the measurement process. It is defined as

$$\hat{\rho} = |\Psi\rangle\langle\Psi| \ . \tag{1.10}$$

If $|\Psi\rangle$ is expressed as a superposition states in some orthonormal basis

$$|\Psi\rangle = \sum_i c_i \, |\psi_i\rangle \ , \tag{1.11}$$

then

$$\hat{\rho} = \sum_{ij} c_i c_j^* \, |\psi_i\rangle\langle\psi_j| \ . \tag{1.12}$$

Let us consider the simple case of $i, j = 1, 2$ (eg spin states of a spin-1/2 particle or a particle in a superposition of two energy states) then we can easily expand out the sums to get four terms:

$$\hat{\rho} = |c_1|^2 \, |\psi_1\rangle\langle\psi_1| + |c_2|^2 \, |\psi_2\rangle\langle\psi_2| + \underbrace{c_1 c_2^* \, |\psi_1\rangle\langle\psi_2| + c_1^* c_2 \, |\psi_2\rangle\langle\psi_1|}_{\text{interference terms}} \ . \tag{1.13}$$

We can see here that we can write $\hat{\rho}$ as a 2×2 matrix in the $\{|\psi_i\rangle\}$ basis (which has matrix elements $\langle\psi_i| \, \hat{\rho} \, |\psi_j\rangle$) to obtain (since $\langle\psi_i| \, \psi_j\rangle = \delta_{ij}$):

$$\begin{pmatrix} |c_1|^2 & c_1 c_2^* \\ c_1^* c_2 & |c_2|^2 \end{pmatrix}$$

In this sense you can see that the interference terms are the off-diagonal ones in the matrix. Often, we talk about decoherence (or measurement) destroying the interference terms in Eq.(1.13) or the off-diagonal elements in the matrix, leaving just the diagonal elements. We will see later that this is what is referred to as a mixed state density matrix.

Note however that whether or not there is any interference (non-zero off-diagonal elements in $\hat{\rho}$) depends on our choice of basis. **Just because a density matrix is diagonal is some basis does *not* mean the system is behaving classically.**

The Trace of $\hat{\rho}$

Unlike the above statement in bold, the *trace* of density matrix is independent of the basis chosen when we write it as an actual matrix (rather than just an operator). To see this, let's do a simple example:

Consider a state that is in a superposition of spin up and down with respect to the z-axis:

$$|\Psi\rangle = \alpha\,|0\rangle_z + \beta\,|1\rangle_z\ . \tag{1.14}$$

Clearly, our density matrix operator is similar to that in Eq.(1.13):

$$\begin{aligned}\hat{\rho} &= |\Psi\rangle\langle\Psi| \\ &= |\alpha|^2\,|0\rangle_z\,\langle 0|_z + |\beta|^2\,|1\rangle_z\,\langle 1|_z + \alpha\beta^*\,|0\rangle_z\,\langle 1|_z + \alpha^*\beta\,|1\rangle_z\,\langle 0|_z\ .\end{aligned} \tag{1.15}$$

But we can always write our two eigenvector $|0\rangle_z$ and $|1\rangle_z$ in terms of superpositions of eigenstates of σ_x:

$$|0\rangle_z = \frac{1}{\sqrt{2}}\Big(|0\rangle_x + |1\rangle_x\Big)\ , \tag{1.16}$$

$$|1\rangle_z = \frac{1}{\sqrt{2}}\Big(|0\rangle_x - |1\rangle_x\Big)\ . \tag{1.17}$$

Substituting these into Eq.(1.14),

$$|\Psi\rangle = \frac{\alpha}{\sqrt{2}}\Big(|0\rangle_x + |1\rangle_x\Big) + \frac{\beta}{\sqrt{2}}\Big(|0\rangle_x - |1\rangle_x\Big) \tag{1.18}$$

$$= \frac{1}{\sqrt{2}}\Big[(\alpha+\beta)\,|0\rangle_x + (\alpha-\beta)\,|1\rangle_x\Big] \tag{1.19}$$

and the density matrix is then

$$\begin{aligned}\hat{\rho} = |\Psi\rangle\langle\Psi| = \frac{1}{2}\Big[&|\alpha+\beta|^2\,|0\rangle_x\,\langle 0|_x + |\alpha-\beta|^2\,|1\rangle_x\,\langle 1|_x \\ &+ (\alpha+\beta)(\alpha-\beta)^*\,|0\rangle_x\,\langle 1|_x \\ &+ (\alpha+\beta)^*(\alpha-\beta)\,|1\rangle_x\,\langle 0|_x\Big]\ .\end{aligned} \tag{1.20}$$

Now let us evaluate the trace of the density matrix in the two bases:

In the basis of σ_z eigenstates, it is trivial:

$$\mathrm{Tr}(\hat{\rho}) = \langle 0|_z\,\hat{\rho}\,|0\rangle_z + \langle 1|_z\,\hat{\rho}\,|1\rangle_z = |\alpha|^2 + |\beta|^2\ . \tag{1.21}$$

And in the basis of σ_x eigenstates:

$$\begin{aligned} \mathrm{Tr}(\hat{\rho}) &= \langle 0|_x \,\hat{\rho}\, |0\rangle_x + \langle 1|_x \,\hat{\rho}\, |1\rangle_x \\ &= \frac{1}{2}|\alpha+\beta|^2 + \frac{1}{2}|\alpha-\beta|^2 \\ &= \frac{1}{2}|\alpha|^2 + \frac{1}{2}|\beta|^2 + \cancel{\frac{1}{2}\alpha\beta^*} + \cancel{\frac{1}{2}\alpha^*\beta} \\ &\quad + \frac{1}{2}|\alpha|^2 + \frac{1}{2}|\beta|^2 - \cancel{\frac{1}{2}\alpha\beta^*} - \cancel{\frac{1}{2}\alpha^*\beta} \\ &= |\alpha|^2 + |\beta|^2 \end{aligned} \tag{1.22}$$

A simpler way to see that $\mathrm{Tr}(\hat{\rho})$ is basis independent is look at what its diagonal elements represent: they are simply the probabilities of getting the different outcomes (eigenvalues) of a particular observable whose eigenstates make up that particular basis, and their sum must add up to 1. It doesn't matter what basis we choose the trace is just a sum of probabilities and we have

$$\boxed{\mathrm{Tr}(\hat{\rho}) = 1} \tag{1.23}$$

The trace as an expectation value

Consider some observable, O, with corresponding operator $\hat{O}$, and let us derive the quantity $\mathrm{Tr}(\hat{\rho}\hat{O})$. We choose an orthonormal basis for the matrix corresponding to the product $\hat{\rho}\hat{O}$ as the basis of eigenstates $\{|\psi_i\rangle\}$ of $\hat{O}$:

$$\hat{O}\,|\psi_i\rangle = \alpha_i\,|\psi_i\rangle \ . \tag{1.24}$$

Thus,

$$\begin{aligned} \mathrm{Tr}(\hat{\rho}\hat{O}) &= \sum_i \langle\psi_i|\,\hat{\rho}\hat{O}\,|\psi_i\rangle = \sum_i \langle\psi_i|\,\hat{\rho}\;\alpha_i\,|\psi_i\rangle \\ &= \sum_i \langle\psi_i|\,|\Psi\rangle\langle\Psi|\,\alpha_i\,|\psi_i\rangle = \sum_i \alpha_i |\langle\psi_i|\,|\Psi\rangle|^2 \,. \end{aligned} \tag{1.25}$$

However, imagine expanding the wave function $|\Psi\rangle$ in the basis of $|\psi_i\rangle$: ($|\Psi\rangle = \sum_i c_i\,|\psi_i\rangle$). Then the coefficients, c_i, are just the overlap amplitude $\langle\psi_i|\,|\Psi\rangle$, and $|c_i|^2$ is just the probability of finding a system described by $|\Psi\rangle$ with eigenvalue α_i (that is, in the eigenstate $|\psi_i\rangle$) if we were to measure observable O.

So we can instead write our trace as

$$\mathrm{Tr}(\hat{\rho}\hat{O}) = \sum_i \alpha_i |c_i|^2 \,. \tag{1.26}$$

But you should recall (yes, you really should) that this is simply the definition of the expectation value of an operator (the average of all the eigenvalues, each weighted by the probability of getting it on measurement).

$$\left[\langle\hat{O}\rangle = \langle\Psi|\,\hat{O}\,|\Psi\rangle = \textstyle\sum_{ij} c_i^* \,\langle\psi_i|\,\hat{O}\,c_j\,|\psi_j\rangle = \sum_{ij} c_i^* c_j \,\langle\psi_i|\,\alpha_j\,|\psi_j\rangle = \sum_i \alpha_i |c_i|^2\right].$$

We have shown the very useful relation involving the density matrix:

$$\boxed{\langle\hat{O}\rangle \;= \mathrm{Tr}(\hat{\rho}\hat{O})} \tag{1.27}$$

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Lecture 2 – Mixed States

2.1 Defining 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 don't know what this pure state is. It might be $|\Psi_1\rangle$ or it might be $|\Psi_2\rangle$ with (let us assume) equal probability (where here the probability reflects our ignorance rather than a property of the system itself). We express this ignorance as a mixed state density matrix

$$\hat{\rho} = \frac{1}{2}\underbrace{|\Psi_1\rangle\langle\Psi_1|}_{\hat{\rho}_1} + \frac{1}{2}\underbrace{|\Psi_2\rangle\langle\Psi_2|}_{\hat{\rho}_2}, \tag{2.1}$$

where the factors of $\frac{1}{2}$ are classical probabilities. This is a true mixed state density matrix (to be compared with an 'improper' mixed state density matrix we will encounter in the next lecture). Note we can also use it to describe an ensemble of systems rather than just one, where half of them are in pure state $|\Psi_1\rangle$ and other half are in pure state $|\Psi_2\rangle$.

In general, we can write a density matrix as

$$\boxed{\hat{\rho} = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|}, \tag{2.2}$$

which can now describe a mixed state. Again, this can either describe a single particle/system that is in some pure state $|\Psi_i\rangle$, but we just don't know which one (and the p_is reflect our ignorance), or of an ensemble of many particles/systems, some of which are in one pure state while others are in different pure states, where the p_is now reflect the fraction of the ensemble population in any given pure state.

Note that if $\hat{\rho}$ is a pure state density matrix then there is just one value of p that is unity and we just have $\hat{\rho} = |\Psi\rangle\langle\Psi|$ (see Eq.(1.10)).

What about the expectation value of some operator $\langle\hat{O}\rangle$ now that we are dealing with the more general case of mixed states?
That is, can we still write it as the trace of the product of a mixed density matrix and $\hat{O}$? Does Eq.(1.28) still hold for mixed states?

It turns out that the answer is yes, and this is quite straightforward to prove:

Consider the mixed state density matrix in Eq.(2.1). If it is really in state $|\Psi_1\rangle$ then the expectation value of an operator, $\hat{O}$ is

$$\langle\hat{O}\rangle_1 = \langle\Psi_1|\,\hat{O}\,|\Psi_1\rangle = \mathrm{Tr}(\hat{\rho}_1\hat{O})\ . \tag{2.3}$$

But likewise if it is actually in state $|\Psi_2\rangle$ then the expectation value is

$$\langle\hat{O}\rangle_2 = \langle\Psi_2|\,\hat{O}\,|\Psi_2\rangle = \mathrm{Tr}(\hat{\rho}_2\hat{O})\ . \tag{2.4}$$

Since we don't know which state it is in, the classical probabilities of Eq.(2.1) are reflected in the average expectation value

$$\begin{aligned}
\langle\hat{O}\rangle &= \tfrac{1}{2}\langle\hat{O}\rangle_1 + \tfrac{1}{2}\langle\hat{O}\rangle_2 \\
&= \tfrac{1}{2}\big(\mathrm{Tr}(\hat{\rho}_1\hat{O}) + \mathrm{Tr}(\hat{\rho}_2\hat{O})\big) \\
&= \mathrm{Tr}\big(\tfrac{1}{2}\hat{\rho}_1\hat{O}\big) + \mathrm{Tr}\big(\tfrac{1}{2}\hat{\rho}_2\hat{O}\big) \\
&= \mathrm{Tr}\big((\tfrac{1}{2}\hat{\rho}_1 + \tfrac{1}{2}\hat{\rho}_2)\hat{O}\big) \\
&= \mathrm{Tr}(\hat{\rho}\hat{O})\ .
\end{aligned} \tag{2.5}$$

So, yes, even though $\hat{\rho}$ here is a mixed state density matrix, the expectation value formula still works.

$\Big[$ Similarly, even for a mixed $\hat{\rho}$, $\mathrm{Tr}(\hat{\rho}) = 1$, since $\mathrm{Tr}(\hat{\rho}_1) = \mathrm{Tr}(\hat{\rho}_2) = 1.$ $\Big]$

2.2 Mixed states as ensembles

We've said that the definition of a general density matrix in Eq.(2.2) means it may have been prepared in some pure state but we just don't know which one. However, if we have an *ensemble* of identical systems (particles) with some of them prepared in pure state $|\Psi_1\rangle$ and some in pure state $|\Psi_2\rangle$, etc, then the 'p_i's are now no longer probabilities, but tell us what fraction of the ensemble is in state $|\Psi_i\rangle$. Often, this ensemble interpretation is what is assumed when we talk about density matrices.

2.3 The difference between pure and mixed states

Recall that if a system described by $|\Psi\rangle$ is made up of two entangled subsystems then we *cannot* write them as a tensor product: $|\Psi_1\rangle \otimes |\Psi_2\rangle$. Similarly, we cannot write their density matrices as $\hat{\rho}_1 \otimes \hat{\rho}_2$.

Thus, if we start off at $t = 0$ with $\hat{\rho}(0) = \hat{\rho}_1(0) \otimes \hat{\rho}_2(0)$, then we say that subsystems 1 and 2 are initially uncorrelated (not entangled). Also, both $\hat{\rho}_1(0)$ and $\hat{\rho}_2(0)$ describe pure states and the overall $\hat{\rho}(0)$ will also be a pure state. But, as systems 1 and 2 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 (wave function). However, there is no reason why the overall combined system described by $\hat{\rho}(t)$ cannot remain in a pure state.

If the combined system's state vector is expanded in some basis (repeating Eq.(1.11)):

$$|\Psi\rangle = \sum_i c_i \, |\psi_i\rangle \ , \tag{2.6}$$

then the corresponding, pure, density matrix (Eq.1.12) is

$$\hat{\rho}_{\text{pure}} = |\Psi\rangle\langle\Psi| = \sum_{ij} c_i c_j^* \, |\psi_i\rangle\langle\psi_j| \ . \tag{2.7}$$

See how the right hand side above differs from the sum in Eq.(2.2). Here we are summing over two indices and $c_i c_j^*$ is not necessarily a real probability. In fact, we can rewrite (2.7) as

$$\hat{\rho}_{\text{pure}} = \underbrace{\sum_i |c_i|^2 \, |\psi_i\rangle\langle\psi_i|}_{\text{diagonal}} + \underbrace{\sum_{j\neq i} c_i c_j^* \, |\psi_i\rangle\langle\psi_j|}_{\text{offdiagonal}} \; . \tag{2.8}$$

You can now see that 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. It is this second term that disappears during decoherence, turning a pure state (quantum) with off-diagonal elements present to a mixed state (classical) with diagonal elements only.

For a pure state

$$\hat{\rho}^2 = \big(\,|\Psi\rangle\langle\Psi|\,\big)^2 = |\Psi\rangle\langle\Psi|\,\Psi\rangle\langle\Psi| = |\Psi\rangle\langle\Psi| = \hat{\rho}\,, \tag{2.9}$$

(provided of course that $|\Psi\rangle$ is normalised).

In fact, $\boxed{\hat{\rho}^2 = \rho}$ is a definition of a pure state.

But this relation does not hold for a mixed state,

$$\rho^2 = \big(\sum_i p_i \, |\Psi_i\rangle\langle\Psi_i|\,\big)^2 = \sum_{ij} p_i p_j \, |\Psi_i\rangle\langle\Psi_i|\,\Psi_j\rangle\langle\Psi_j| \; . \tag{2.10}$$

We have two options:

(a) if $\langle\Psi_i|\,\Psi_j\rangle \neq 0$ (and why should they be orthogonal?) then Eq.(2.10) cannot be simplified and we cannot have $\hat{\rho}^2 = \rho$;

(b) Even if $\langle\Psi_i|\,\Psi_j\rangle = \delta_{ij}$ then

$$\rho^2 = \sum_i p_i^2 \, |\Psi_i\rangle\langle\Psi_i| \; , \tag{2.11}$$

which is compared with our definition from earlier:

$$\rho = \sum_i p_i \, |\Psi_i\rangle\langle\Psi_i| \; . \tag{2.12}$$

So, again, $\hat{\rho}^2 \neq \rho$

Therefore, $\boxed{\hat{\rho}^2 \neq \rho \qquad \text{for a mixed state}}$.

2.4 Quantifying 'mixedness'

There are two simple measures of purity (or mixedness) of a density matrix. Both of these quantities measure the amount of entanglement between the system and the environment as the system progressively decoheres and evolves from an initially pure state to a final mixed state:

1. **Purity**: $\zeta = \mathrm{Tr}(\hat{\rho}^2)$

   For a pure state, clearly

   $$\zeta = \mathrm{Tr}(\hat{\rho}^2) = \mathrm{Tr}(\hat{\rho}) = 1\,. \tag{2.13}$$

   The opposite extreme is a maximally mixed state of the form of Eq.(2.2) in which the different states $\{|\Psi_i\rangle\}$ form an orthonormal basis in the system's Hilbert space, then from Eq.(2.11) we see that

   $$\zeta = \sum_i^N p_i^2\,, \tag{2.14}$$

   and it can easily be shown that the minimum value the purity can be is $\frac{1}{N}$.

   Proof:

   $$\text{Since} \qquad \sum_i^N p_i = 1$$

   then for maximum mixing (minimum purity in Eq.(2.14)) we would want to distribute the probabilities equally

   $$p_1 = p_2 = p_3 = \cdots = p_N = \frac{1}{N}$$

   Therefore

   $$\zeta = N \times \left(\frac{1}{N}\right)^2 = \frac{1}{N}\,.$$

2. **Von Neumann entropy**: $S(\hat{\rho})$

This is defined as

$$\boxed{S(\hat{\rho}) = -\mathrm{Tr}\big(\hat{\rho}\log_2\hat{\rho}\big)}\,. \tag{2.15}$$

It can also be written in the form:

$$\boxed{S(\hat{\rho}) = -\sum_i \lambda_i \log_2 \lambda_i}\,, \tag{2.16}$$

where λ_i are the eigenvalues of $\hat{\rho}$. Note that this is a non-trivial statement. It follows from the fact that the trace of any matrix, A, is equal to the sum of its eigenvalues. We will not prove that here as it would take a little longer than these lectures have time for. Suffice it to say that it relies on properties of matrices involving what are called upper triangular matrices and the Schur decomposition. You can look it up if you want.

Anyway, if a pure state density matrix, $\hat{\rho} = |\Psi\rangle\langle\Psi|$, acts on the state vector $|\Psi\rangle$, then trivially

$$\hat{\rho}\,|\Psi\rangle = |\Psi\rangle\langle\Psi|\,\Psi\rangle = |\Psi\rangle\ , \tag{2.17}$$

which is an eigenvalue equation with eigenvalue of $\hat{\rho}$ being $\lambda = 1$.

Therefore

$$S(\hat{\rho}_{\text{pure}}) = -1\ \log_2 1 = 0\,. \tag{2.18}$$

That is, the von Neumann entropy of a pure state is zero.

But for the maximally mixed case, with $\{|\Psi_i\rangle\}$ forming an orthonormal set, we can see that they are the eigenvectors of $\hat{\rho}$:

$$\hat{\rho}\,|\Psi_i\rangle = \sum_j p_j\,|\Psi_j\rangle\langle\Psi_j|\,\Psi_i\rangle = p_i\,|\Psi_i\rangle\ , \tag{2.19}$$

and in this basis, $\hat{\rho}$ will be a diagonal matrix whose eigenvalues, λ_i, are just the classical probabilities, p_i:

$$\begin{pmatrix} p1 & & & & & \\ & p_2 & & \bigcirc & & \\ & & p_3 & & & \\ & \bigcirc & & \bullet & & \\ & & & & \bullet & \\ & & & & & \bullet \end{pmatrix}$$

Therefore, using the definition of the entropy in Eq.(2.16)

$$\begin{aligned} S(\hat{\rho}_{\text{mixed}}) &= -\sum_i \frac{1}{N}\log_2\left(\frac{1}{N}\right) \\ &= -N \times \frac{1}{N}\big(\log_2 1 - \log_2 N\big) = \log_2 N \,. \qquad (2.20) \end{aligned}$$

Thus the von Neumann entropy ranges from zero (for a pure state) up to a maximum of $\log_2 N$ for a mixed state. For just two mixed states, $S = 1$, for three, $S = 1.58$, for four, $S = 2$, and so on. The more states make up $\hat{\rho}$, the more scope for entanglement and the higher the entropy.

So far, we've said that the probabilities in the definition of $\hat{\rho}_{\text{mixed}}$ are just a measure of our ignorance regarding which *pure* state, $|\Psi_i\rangle$, the system is really in. But, **just writing our mixed-state density matrix in the form of Eq.(2.2) does not mean that it is actually in one of those pure states. We also need to *know* that it was indeed prepared in one of those states**.

Example

Consider a spin state that has previously been measured by a detector (prepared) along the z-axis. It is thus in a pure state of either $|0\rangle_z$ or $|1\rangle_z$. If we don't know which of the states it is in, we must describe it by a mixed state,

$$\hat{\rho} = \tfrac{1}{2}\,|0\rangle_z\,\langle 0|_z + \tfrac{1}{2}\,|1\rangle_z\,\langle 1|_z \;. \qquad (2.21)$$

But, as we said in the last lecture in Eqs.(1.16) and (1.17), each of $|0_z\rangle$ and $|1_z\rangle$ can itself be written as a linear superposition of eigenstates of σ_x. Therefore

$$\begin{aligned} \hat{\rho} &= \frac{1}{2}.\frac{1}{\sqrt{2}}\Big(|0\rangle_x + |1\rangle_x\Big).\frac{1}{\sqrt{2}}\Big(\langle 0|_x + \langle 1|_x\Big) + \frac{1}{\sqrt{2}}\Big(|0\rangle_x - |1\rangle_x\Big).\frac{1}{\sqrt{2}}\Big(\langle 0|_x - \langle 1|_x\Big) \\ &= \frac{1}{4}\Big[|0\rangle_x\,\langle 0|_x + \cancel{|0\rangle_x\,\langle 1|_x} + \cancel{|1\rangle_x\,\langle 0|_x} + |1\rangle_x\,\langle 1|_x \\ &\qquad\qquad + |0\rangle_x\,\langle 0|_x - \cancel{|0\rangle_x\,\langle 1|_x} - \cancel{|1\rangle_x\,\langle 0|_x} + |1\rangle_x\,\langle 1|_x\Big] \\ &= \frac{1}{2}\,|0\rangle_x\,\langle 0|_x + \frac{1}{2}\,|1\rangle_x\,\langle 1|_x \;. \qquad (2.22) \end{aligned}$$

This looks just like Eq.(2.21), but now it no longer reflects our ignorance of which pure state the system is in. A mixed-state density matrix can be written in any number of ways and its partition into a set of states is arbitrary. So, unless we know the physical axis along which the spin state has been prepared, then the density matrix alone can only give us probabilities of *different sets* of pure states. Thus, interpreting a mixed-state density matrix simply as a measure of our ignorance of what pure state the system is not reliable.