

Week ③

PHY 435 / 635 Decoherence and Open Quantum Systems

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3 Basic Formalism and Interpretation of Decoherence

In the following we want to proceed with the aim sketched in section 1: to develop a formalism that allows us to deal with the system (S) part of the models introduced in section 2 only, and find a way to effectively take into account the influence of the environment E.

For that we have to revise/ introduce the concept of...

3.1 Density matrices

3.1.1 Pure state density matrices and the trace operation

So far we are mainly used to describe a quantum system in terms of the (pure) state vector $|\Psi\rangle = \sum_n c_n |\phi_n\rangle$, where the sum denotes its decompositions in terms of some arbitrary Hilbert-space basis $\mathcal{B} = \{|\phi_n\rangle\}$. Alternatively we can write the

Density matrix/ Density operator defined as the projection

$$\hat{\rho} = |\Psi\rangle\langle\Psi| = \sum_{nm} c_n c_m^* |\phi_n\rangle\langle\phi_m|. \quad (3.1)$$

- The corresponding matrix ρ has Matrix elements $\rho_{nm} = c_n c_m^*$.
- The elements on the diagonal are $\rho_{nn} = p_n = |c_n|^2$, called populations (see QM-1/2).
- The off-diagonal element $\rho_{nm} = c_n c_m^*$ is called coherence between states n and m .

We can also formulate quantum time-evolution as in section 1.5.5 for density matrix, it is then governed by the

Von Neumann equation

$$\frac{d}{dt}\hat{\rho}(t) = -\frac{i}{\hbar}[\hat{H}(t), \hat{\rho}(t)]. \quad (3.2)$$

Examples – Coherences indicate superpositions: If the state $|\Psi\rangle$ contains a quantum superposition of basis elements $|\phi_a\rangle$ and $|\phi_b\rangle$, such as $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\phi_a\rangle + |\phi_b\rangle)$, the coherence ρ_{ab} will be nonzero (in this case $\rho_{ab} = 1/2$). Note, however, that the statement whether or not there is a superposition, and whether or not a coherence is non-zero depends on the choice of basis:

Consider the spin state: $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$, in terms of the basis $\mathcal{B} = \{|\uparrow\rangle, |\downarrow\rangle\}$

$$\rho = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} = \frac{1}{2} \left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| \right), \quad (3.3)$$

with non-vanishing coherences. We also illustrate the two notations that we intend to use: the Matrix representation of the density operator (left) and the operator form (right).

We can express $\hat{\rho}$ instead in the basis $\mathcal{B} = \{|\leftarrow\rangle, |\rightarrow\rangle\}$ (eigenstates of σ_x), we have

$$\rho = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = |\leftarrow\rangle\langle\leftarrow|, \quad (3.4)$$

with no coherences.

We also introduce the

Trace operation As known from matrices this is the sum of all diagonal elements of an operator

$$\text{Tr}[\hat{O}] \equiv \sum_k \langle \phi_k | \hat{O} | \phi_k \rangle. \quad (3.5)$$

where $\mathcal{B} = \{|\phi_n\rangle\}$ is any orthonormal basis of the Hilbertspace.

- This definition is independent of the choice of \mathcal{B} .
- We have introduced it in order to write the expectation value of an operator \hat{O} with $\hat{O}|\phi_k\rangle = o_k|\phi_k\rangle$ in a quantum state $|\Psi\rangle = \sum_n c_n|\phi_n\rangle$ as

$$\langle \hat{O} \rangle = \text{Tr}[\hat{O}\hat{\rho}] = \sum_k o_k |c_k|^2. \quad (3.6)$$

This expression is known from using state vectors $|\Psi\rangle$.

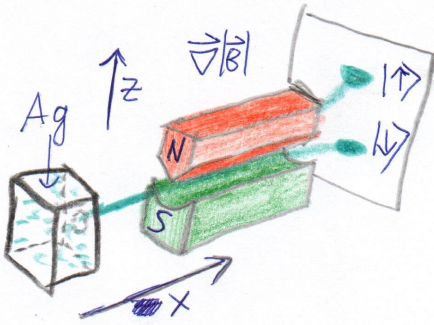
- The trace is linear $\text{Tr}[\hat{A} + \hat{B}] = \text{Tr}[\hat{A}] + \text{Tr}[\hat{B}]$ and cyclic $\text{Tr}[\hat{A}\hat{B}\hat{C}] = \text{Tr}[\hat{B}\hat{C}\hat{A}]$.

Proof of all of this: exercise.

3.1.2 Mixed state density matrices

Let us revisit the

Stern-Gerlach experiment: undertaken in 1922 to explore the quantization of angular momentum, see figure below. The Ag atom angular momentum is just given by the valence electron spin, hence $s = 1/2$. The magnetic moment of the atom due to the electron is $\hat{\boldsymbol{\mu}} = -g_s\mu_B\hat{\mathbf{S}}/\hbar$, in an inhomogeneous magnetic field this yields a Force $\hat{\mathbf{F}} = -\nabla[-\hat{\boldsymbol{\mu}} \cdot \mathbf{B}]$. With magnetic field and inhomogeneity along z we reach, all up: $F_z = -g_s\mu_B\hat{S}_z\frac{\partial}{\partial z}B_z$.



left: A beam of silver atoms is directed through a region of inhomogeneous magnetic field. The resultant different forces experienced by $|\uparrow\rangle$ and $|\downarrow\rangle$ atoms split the beam up into only two discrete spots. The device has thus demonstrated quantisation of $\hat{\mathbf{S}}$ and measured the value of \hat{S}_z for each atom.

- Importantly, the spin-component which is being measured is decided by the direction of the magnetic field and its gradient. If we had oriented the field along x , we would obtain two left-right split dots corresponding to atoms in $|\leftarrow\rangle$, $|\rightarrow\rangle$ (see section 1.5.2).
- Let us try to formally describe the situation in the figure above, where each atom from a thermal source is randomly in either the $|\uparrow\rangle$ or $|\downarrow\rangle$ state with 50% – 50% probabilities. Which state would we assign to such an atom? We could try $|\Psi\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$, which would give the correct probabilities for a measurement of \hat{S}_z (50/50).
- However what if we measure \hat{S}_x instead? We recognise the state above as $|\leftarrow\rangle$, eigenstate of \hat{S}_x . Thus if we measure \hat{S}_x instead of \hat{S}_z , we would get $+1/2$ with 100% probability. However, since we said atoms are with 50% – 50% change in $|\uparrow\rangle$ or $|\downarrow\rangle$ and $|\uparrow\rangle = (|\leftarrow\rangle + |\rightarrow\rangle)/\sqrt{2}$, $|\downarrow\rangle = (|\leftarrow\rangle - |\rightarrow\rangle)/\sqrt{2}$, we should in fact get $S_x = +1/2, -1/2$ with 50% – 50% probability for each atom. How can we write a state that describes both measurements, \hat{S}_x and \hat{S}_z correctly?
- This example points to essential differences in uncertainties in quantum mechanics and classical mechanics.

The tool to describe both types of uncertainties in one unified formalism are density matrices as in section 3.1.1, which is in fact why we introduced them.

We now define the

Mixed state density matrix

$$\hat{\rho} = \sum_n p_n |\phi_n\rangle\langle\phi_n|, \quad (3.7)$$

Here ϕ_n is an orthonormal set of states and p_n the classical probability to be in state n .

- We have $\sum_n p_n = \text{Tr}[\hat{\rho}] = 1$, expressing normalisation of our state.
- We recognize (3.1) as a special case with $p_n = \delta_{nk}$ for some k .
- Consider now the expectation value of an operator

$$\begin{aligned} \langle\hat{O}\rangle &= \text{Tr}[\hat{O}\hat{\rho}] = \sum_n \langle\phi_n|[\hat{O} \sum_m p_m |\phi_m\rangle\langle\phi_m|]|\phi_n\rangle \\ &= \sum_n p_n \langle\phi_n|\hat{O}|\phi_n\rangle \end{aligned} \quad (3.8)$$

This takes into account both, the classical and quantum mechanical formalism for uncertainties and determining an average.

Spin mixture example:

Let us apply this to the spin mixture problem discussed on the previous page. We define the state of atoms in the oven via the density matrix $\hat{\rho} = (|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)/2$, implying we simple have no knowledge of which spin state they are in, but that there is no superposition of $\uparrow + \downarrow$. Then

$$\langle\hat{S}_x\rangle = \text{Tr}[\hat{S}_x\hat{\rho}] \stackrel{\text{Eq. (3.9)}}{=} (\underbrace{\langle\uparrow|\hat{S}_x|\uparrow\rangle}_{=0} + \underbrace{\langle\downarrow|\hat{S}_x|\downarrow\rangle}_{=0})/2 = 0, \quad (3.9)$$

as required since we will find $\hat{S}_x = +1/2, -1/2$ with equal probability. Equally we also find $\langle\hat{S}_z\rangle = 0$.

- This sort of mixture is also called proper mixture, and can represent a system that **is** in a pure state, but we don't know in which. The mixture is due to our ignorance. We will learn about improper mixtures shortly.
- For this interpretation we need to know additionally that the system is in a certain set of pure states. For example we can write the density matrix in the example above equally well as $\hat{\rho} = (|\leftarrow\rangle\langle\leftarrow| + |\rightarrow\rangle\langle\rightarrow|)/2$ (exercise), which we would get when saying the system is always either in $|\leftarrow\rangle$ or $|\rightarrow\rangle$. Given only the density matrix as a mathematical object we cannot distinguish the two scenarios. This means measurements cannot distinguish between the two.

- The density matrix just introduced also plays a central role in quantum statistical physics, where we use it with $p_n = \exp[-E_n/(k_B T)]$ to describe a statistical ensemble at temperature T . Alternatively one could describe a quantum ensemble of identical systems also in a pure high-dimensional Hilbertspace (see SD 2.4.5). For ensemble averages both approaches give the same results.

Even though they have the same populations in the basis $\{|\phi_n\rangle\}$, a mixed state $\hat{\rho}$ as in (3.7) is very different from the pure state $|\Psi\rangle = \sum_n \sqrt{p_n} |\phi_n\rangle$. We have seen this in the above discussion of measurements on a state $|\leftarrow\rangle$ and on the density matrix $\hat{\rho} = (|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|)/2$.

To quantify this difference, we introduce two measures³:

Purity

$$\zeta(\hat{\rho}) = \text{Tr}[\hat{\rho}^2] \quad (3.10)$$

We can see $\zeta = 1$ if $\hat{\rho}$ is a pure state density matrix (3.1), but $\zeta < 1$ for genuine mixed states (3.7).

- For maximally mixed states $\hat{\rho} = \sum_n^N 1/N |\phi_n\rangle\langle\phi_n|$, we have $\zeta = 1/N$.
- The definition exploits that $\hat{\rho}^2 = \hat{\rho} \Leftrightarrow \hat{\rho}$ is a pure state density matrix.

An alternate measure to quantify the degree of "mixedness" of a quantum system is the

Von-Neumann Entropy defined as

$$S(\hat{\rho}) = -\text{Tr}[\hat{\rho} \log_2 \hat{\rho}] \equiv -\sum_k \lambda_k \log_2(\lambda_k). \quad (3.11)$$

The λ_k are the non-zero eigenvalues of $\hat{\rho}$. We can see $S = 0$ if $\hat{\rho}$ is a pure state density matrix (3.1), but $S > 0$ for genuine mixed states (3.7).

- For pure states only one eigenvalue is non-zero and equal to unity.
- For a maximally mixed state (see above), we have all $\lambda_k = p_k = 1/N$ and thus $S = \log_2(N)$, which is the maximum allowed value.

3.1.3 Reduced density matrices

In the previous section we saw how the density matrix concept helps us to incorporate at the same time uncertainties due to quantum effects and to classical randomness. We now see that it also is a useful tool for the objective stated at the outset of this section: To deal with S only, without E.

³many more exist

Let $\mathcal{B}_S = \{|\phi_k\rangle\}$ and $\mathcal{B}_E = \{|\varphi_l\rangle\}$ be two bases for system and environment and $\hat{O} = \hat{O}_S \otimes \mathbb{1}$ an operator that acts on the system only.

Let us denote with $|\phi_k, \varphi_l\rangle = |\phi_k\rangle \otimes |\varphi_l\rangle$ and element of the complete basis (system+environment).

Any information on the system, via measurements on it only, can be obtained from operators of that form.

Now note:

$$\begin{aligned}
\langle \hat{O} \rangle &= \text{Tr}[\hat{\rho}\hat{O}] \stackrel{\text{Eq. (3.5)}}{=} \sum_{kl} \langle \phi_k, \varphi_l | \hat{\rho}(\hat{O}_S \otimes \mathbb{1}) | \phi_k, \varphi_l \rangle \\
&= \sum_k \langle \phi_k | \left(\sum_l \langle \varphi_l | \hat{\rho} | \varphi_l \rangle \right) \hat{O}_S | \phi_k \rangle \equiv \sum_k \langle \phi_k | \text{Tr}_E[\hat{\rho}] \hat{O}_S | \phi_k \rangle \\
&\equiv \sum_k \langle \phi_k | \hat{\rho}_S \hat{O}_S | \phi_k \rangle = \text{Tr}_S[\hat{\rho}_S \hat{O}_S].
\end{aligned} \tag{3.12}$$

In the second equality we used that \hat{O} does not act on states $|\varphi_l\rangle$. Here we have introduced the

Reduced density matrix of the system

$$\hat{\rho}_S = \text{Tr}_E[\hat{\rho}], \tag{3.13}$$

where $\text{Tr}_E[\hat{O}] = \sum_l \langle \varphi_l | \hat{\rho} | \varphi_l \rangle$ is the partial trace over the environment.

- The quantity $\hat{\rho}_S$ gives all the information that we can possibly gain from measurements on the system alone. Importantly this excludes measurements that jointly determine the environmental states. We assume those are not possible.
- Let's look at some examples for a spin-spin model (section 2.3), where we chose just two environmental spins for simplicity:

Example 1: Suppose system and environment are in a separable^a state: $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \otimes \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$. States before \otimes refer to the system, after \otimes to the environment. This expands to $|\Psi\rangle = \frac{1}{2}(|\uparrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\downarrow\rangle)$, somewhat hiding the separability. We now perform the partial trace over the environment after converting this to a density matrix.

$$\hat{\rho}_S = \text{Tr}_E[\hat{\rho}] = \sum_{s_1, s_2} \langle _s_1 s_2 | \hat{\rho} | _s_1 s_2 \rangle, \tag{3.14}$$

^awrt. the system-environment splitting. The environment part is actually entangled.

Example continued: ...where in the first step spin indices s_1, s_2 run over \uparrow, \downarrow each, and we have used the "placeholder" $_$ to visualize the fact that the scalar products involving environmental spins act on the last two spin indices only.

We arrive at (exercise)

$$\hat{\rho}_S = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} = \frac{1}{2} \left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| \right), \quad (3.15)$$

which we recognise as in (3.3) as the density matrix for the pure system state $|\Psi_S\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$.

We can evaluate the purity (3.10) (exercise) and find $P = 1$ as expected.

Example 2: Now consider a state where the system is entangled with the environment: $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\uparrow\uparrow\rangle + |\downarrow\rangle \otimes |\downarrow\downarrow\rangle)$. Following the same procedure as in example 1 we reach:

$$\hat{\rho}_S = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} = \frac{1}{2} \left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| \right), \quad (3.16)$$

the mixed state already given in (3.4). The purity in this case is given by $P = 1/2$, the minimum allowed in a two-dimensional Hilbertspace.

- In the examples above we have seen that a reduced density matrix can frequently take the form of a mixed state. Unlike those in section 3.1.2 these are called improper mixtures. The interpretation is not that the system is in a pure state but we don't know which, but rather that the "system+environment" are together in a complicated entangled pure state, which is such that local measurements on the system alone are indistinguishable from the those in a proper mixed case that would be based on ignorance.
- It can be shown that, assuming a pure total state, **iff** the system and environment are separable, the reduced system state will be pure.

Example 3: Finally let's look at yet one more example: $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes (c_1|\uparrow\uparrow\rangle + c_2|\downarrow\downarrow\rangle) + |\downarrow\rangle \otimes (c_2|\uparrow\uparrow\rangle + c_1|\downarrow\downarrow\rangle))$, with $|c_1|^2 + |c_2|^2 = 1$. Note, that for $c_1 = 1, c_2 = 0$ this co-indices with example 2, and for $c_1 = c_2 = 1/\sqrt{2}$, system and environment are separable, as in example 1.

For the state in this example 3, we find

$$\hat{\rho}_S = \frac{1}{2} \begin{bmatrix} 1 & c_1 c_2^* + c_1^* c_2 \\ c_1 c_2^* + c_1^* c_2 & 1 \end{bmatrix} = \frac{1}{2} \left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + 2\text{Re}[c_1 c_2^*] (|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|) \right), \quad (3.17)$$

with purity $P = (1 + 4\text{Re}[c_1 c_2^*]^2)/2$.

Example 3 continued: Thus the purity depends on c_1 , c_2 , and in general represents a not-maximally entangled system-environment, of relevance in the following. We can get all purity values in between the maximum (1) and minimum (1/2).

3.1.4 Local Measurability of Interference and Distinguishability

We now address how the measurability of interference locally in the system depends on the structure of its entanglement with some environment. First note that the measurement of \hat{S}_x alluded to in section 3.1.2 "proves" the existence of a coherent superposition $|\Psi\rangle = c_1|\uparrow\rangle + c_2|\downarrow\rangle$ though an interference type measurement: the fraction measured in $m_{sx} = -1/2$ is $|\langle - | \Psi \rangle|^2 = |c_1 - c_2|^2 / \sqrt{2}$, vanishing only due to the coherence. For this interference to be measured, the coherences in the density matrix must be non-zero.

Consider the generic bi-partite state

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left(|\phi_1\rangle \otimes |\chi_1\rangle + |\phi_2\rangle \otimes |\chi_2\rangle \right), \quad (3.18)$$

with states $|\phi\rangle$ for the system and $|\chi\rangle$ for the environment. We do not assume the $|\chi_k\rangle$ to be mutually orthogonal. The density matrix can be written as $\hat{\rho} = \frac{1}{2} \sum_{ij} |\phi_i\rangle \langle \phi_j| \otimes |\chi_i\rangle \langle \chi_j|$.

To find the reduced density matrix of the system, we do require an orthonormal basis of the environment, let that be $\{|\varphi\rangle_n\}$. We can thus expand $|\chi_{1,2}\rangle = \sum_l c_l^{(1,2)} |\varphi_l\rangle$. Using Eq. (3.5) we obtain:

$$\begin{aligned} \hat{\rho}_S &= \text{Tr}_{\mathcal{E}} \left(\frac{1}{2} \sum_{ij} |\phi_i\rangle \langle \phi_j| \otimes |\chi_i\rangle \langle \chi_j| \right) \\ &= \frac{1}{2} \sum_{ij} |\phi_i\rangle \langle \phi_j| \sum_k \langle \varphi_k | \left(\sum_{l'} c_l^{(i)} c_{l'}^{(j)*} |\varphi_l\rangle \langle \varphi_{l'}| \right) | \varphi_k \rangle \\ &= \frac{1}{2} \sum_{ij} |\phi_i\rangle \langle \phi_j| \sum_k c_k^{(i)} c_k^{(j)*} = \frac{1}{2} \sum_{ij} |\phi_i\rangle \langle \phi_j| \langle \chi_j | \chi_i \rangle \\ &= \frac{1}{2} \left(|\phi_1\rangle \langle \phi_1| + |\phi_2\rangle \langle \phi_2| + |\phi_1\rangle \langle \phi_2| \langle \chi_2 | \chi_1 \rangle + |\phi_2\rangle \langle \phi_1| \langle \chi_1 | \chi_2 \rangle \right). \end{aligned} \quad (3.19)$$

We see several generic consequences of the bi-partite (in general entangled) state (3.18):

- If the environmental states $|\chi_{1,2}\rangle$ were fully distinguishable (orthogonal, $\langle \chi_2 | \chi_1 \rangle = 0$), then there is no coherence between $|\phi_{1,2}\rangle$ in the reduced system (see example 2).
- If they were identical ($\langle \chi_2 | \chi_1 \rangle = 1$) we had in fact a separable state and there is full coherence.
- In more general cases, the amount of coherence left in the system depends on the overlap (distinguishability) of the states $|\chi_{1,2}\rangle$ (example 3).