PHY 435 / 635 Decoherence and Open Quantum Systems
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3.2.5   What decoherence is not

There are several concepts that can mimick decoherence or are related to it, but different, that we briefly discuss at the end of this section.

I: Decoherence versus Dissipation
Dissipation is the loss of energy from the system into the environment. This happens already on a classical level, and then of course also in quantum-mechanics. We have already seen a model in section 2.2, that clearly <u>does not</u> exhibit dissipation. As stated there, this happens when $\left[\hat{H}_S, \hat{H}_{\mathrm{int}}\right] = 0$, since then $\hat{H}_S$ is a conserved observable. We have later seen, in section 3.2.3, that the model <u>does</u> exhibit decoherence though, we thus can have decoherence without dissipation

Conversely however, we will see later that whenever there is dissipation, there also will be some decoherence. The time-scales on which these two phenomena occur, are typically very different, with decoherence happening a lot faster than dissipation.

II: Decoherence versus Classical Noise/ Dephasing
Decoherence introduced above and in section 1.3.1 arises through entanglement of the system and the environment. The symptoms, vanishing coherences in a density matrix, frequently also arise when averaging over multiple noisy realisation of an ensemble. Consider the ensemble of states

$$| \Psi_k \rangle = \frac{1}{\sqrt{2}}\big(|\uparrow\rangle + e^{i\varphi_k}|\downarrow\rangle\big) \otimes |\mathcal{E}\rangle, \tag{3.36}$$

for some spin system, with environmental state $|\mathcal{E}\rangle$. This is not entangled with the environment so for each member of the ensemble we would obtain a pure reduced density matrix for the spin. However, if for whatever reason we now <u>average</u> these density matrices, we find:

$$\bar{\bar{\rho}} = \sum_k^N | \Psi_k \rangle\langle \Psi_k | = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| + \big(\frac{1}{2N}\sum_k e^{i\varphi_k}\big)|\downarrow\rangle\langle\uparrow| + \big(\frac{1}{2N}\sum_k e^{-i\varphi_k}\big)|\uparrow\rangle\langle\downarrow|. \tag{3.37}$$

The average over lots of random phases is zero, hence for $N \to \infty$ we have $\bar{\bar{\rho}} = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$, which looks just like a mixed state.

- This is also called classical noise or dephasing.

- This example is meant to caution you that you always have to be careful which exact type and source of dephasing/decoherence/noise is referred to in any work.

3.3 Some Tricks and Tools

We finish section 3 with some useful techniques for the treatment of bi-partite quantum systems (e.g. split into system+environment) and representation of quantum states.

3.3.1 The Schmidt Decomposition

Consider two systems $\mathcal{A}$ and $\mathcal{B}$ with Hilbert-spaces $\mathcal{H}_{\mathcal{A}}$ and $\mathcal{H}_{\mathcal{B}}$. For a pure state of the combined system, we then have the

> **Schmidt decomposition theorem**, that an arbitrary pure state of the composite system $\mathcal{AB}$ can be written in the form
>
> $$|\Psi\rangle = \sum_n \lambda_n |a_n\rangle |b_n\rangle, \tag{3.38}$$
>
> where $\{|a_n\rangle\}$ $[\{|b_n\rangle\}]$ form an orthonormal basis of $\mathcal{H}_{\mathcal{A}}$ $[\mathcal{H}_{\mathcal{B}}]$.

- The expansion coefficients $\lambda_n \in \mathbb{C}$ fulfill $\sum_n |\lambda_n|^2 = 1$.

- However any complex phase factors in λ_n can in fact be absorbed into the bases, such that we can chose $0 < \lambda_n \in \mathbb{R}$, hence

$$|\Psi\rangle = \sum_n \sqrt{p_n} |a_n\rangle |b_n\rangle. \tag{3.39}$$

- The Schmidt decomposition (3.39) is unique iff all the coefficients $\sqrt{p_n}$ are different from each other.

> **Proof and construction algorithm:** The Schmidt decomposition directly follows from the <u>singular value decomposition</u> (SVD) of an $N \times M$ matrix. Let $\{|\phi_n\rangle\}$ and $\{|\varphi_m\rangle\}$ be arbitrary orthonormal bases of $\mathcal{H}_{\mathcal{A}}$ and $\mathcal{H}_{\mathcal{B}}$ respectively. We then certainly can write any state $|\Psi\rangle$ in $\mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$ as
>
> $$|\Psi\rangle = \sum_n^N \sum_m^M c_{nm} |\phi_n\rangle |\varphi_m\rangle. \tag{3.40}$$
>
> We assumed $N = \dim(\mathcal{H}_{\mathcal{A}})$, and $M = \dim(\mathcal{H}_{\mathcal{B}})$. Let us interpret the coefficients c as a $N \times M$ matrix $\underline{\underline{C}}$.

Proof cont.: That matrix has a SVD

$$\underline{\underline{C}} = \underline{\underline{U}} \, \underline{\underline{\Lambda}} \, \underline{\underline{V}}, \tag{3.41}$$

with unitary matrices $\underline{\underline{U}}$ ($N \times N$), $\underline{\underline{V}}$ ($M \times M$), and a $N \times M$ matrix $\underline{\underline{\Lambda}}$ with d real and positive entries λ_k on the diagonal only.

In component notation, (3.41) becomes $c_{nm} = \sum_k^d u_{nk} \lambda_k v_{km}$, where u and v are matrix elements of $\underline{\underline{U}}$ and $\underline{\underline{V}}$.

Insertion into Eq. (3.40) gives

$$
\begin{aligned}
| \Psi \rangle &= \sum_n^N \sum_m^M \left(\sum_k^d u_{nk} \lambda_k v_{km} \right) | \phi_n \rangle | \varphi_m \rangle \\
&= \sum_k^d \lambda_k \underbrace{\left(\sum_n^N u_{nk} | \phi_n \rangle \right)}_{\equiv | a_k \rangle} \underbrace{\left(\sum_m^M v_{km} | \varphi_m \rangle \right)}_{\equiv | b_k \rangle},
\end{aligned} \tag{3.42}
$$

which takes the form (3.38) after defining the new bases $\{| a_k \rangle\}$ $[\{| b_k \rangle\}]$. This thus also gives a recipe for the construction of these.

- It can be seen from (3.38), that the reduced density matrices in systems $\mathcal{A}$ and $\mathcal{B}$ are $\hat{\rho}_{\mathcal{A}} = \sum_n p_n | a_n \rangle \langle a_n |$ and $\hat{\rho}_{\mathcal{B}} = \sum_n p_n | b_n \rangle \langle b_n |$ respectively (proof: exercise/book). We can thus also find the decomposition by determining both these reduced density matrices directly from $| \Psi \rangle$, and diagonalising them.

Example: We consider again a bi-partite spin system with state

$$| \Psi \rangle = \frac{1}{\sqrt{2}} | \downarrow\downarrow \rangle + \frac{1}{2} | \uparrow \rangle \otimes (| \uparrow \rangle + | \downarrow \rangle). \tag{3.43}$$

In terms of the basis ordering $\{| \downarrow \rangle, | \uparrow \rangle\}$ for rows and columns, this gives a matrix

$$\underline{\underline{C}} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{2} \\ 0 & \frac{1}{2} \end{bmatrix} = \underbrace{\begin{bmatrix} \frac{\sqrt{2+\sqrt{2}}}{2} & -\frac{1}{2}\sqrt{2-\sqrt{2}} \\ \frac{1}{\sqrt{2(2+\sqrt{2})}} & \frac{\sqrt{2+\sqrt{2}}}{2} \end{bmatrix}}_{=\underline{\underline{U}}} \underbrace{\begin{bmatrix} \frac{\sqrt{2+\sqrt{2}}}{2} & 0 \\ 0 & \frac{\sqrt{2-\sqrt{2}}}{2} \end{bmatrix}}_{=\underline{\underline{\Lambda}}} \underbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}}_{=\underline{\underline{V}}}, \tag{3.44}$$

where we also have already written its SVD.

Example contd.: We thus can write

$$| \Psi \rangle = \frac{\sqrt{2 + \sqrt{2}}}{2} | a_1 \rangle \otimes | b_1 \rangle + \frac{\sqrt{2 - \sqrt{2}}}{2} | a_2 \rangle \otimes | b_2 \rangle, \tag{3.45}$$

with new bases $\{| a_1 \rangle, | a_2 \rangle\} = \left\{ \frac{\sqrt{2+\sqrt{2}}}{2} | \downarrow \rangle + \frac{\sqrt{2+\sqrt{2}}}{2} | \uparrow \rangle, \ -\frac{1}{2}\sqrt{2 - \sqrt{2}} | \downarrow \rangle + \frac{\sqrt{2+\sqrt{2}}}{2} | \uparrow \rangle \right\}$
and $\{| b_1 \rangle, | b_2 \rangle\} = \left\{ \frac{1}{\sqrt{2}} | \downarrow \rangle + \frac{1}{\sqrt{2}} | \uparrow \rangle, \ -\frac{1}{\sqrt{2}} | \downarrow \rangle + \frac{1}{\sqrt{2}} | \uparrow \rangle \right\}.$
Thus even for an innocent looking example, the actual construction of (3.39) can be cumbersome.

3.3.2 The Wigner representation

Let us consider the specific example of a quantum particle moving in one dimension, e.g. the simple harmonic oscillator. The Wigner representation maps its density matrix $\hat{\rho}$ (or quantum state $| \Psi \rangle$) onto a function in phase-space $W(x, p)$.

Consider the position-space density matrix elements $\rho(x, x') = \langle x | \hat{\rho} | x' \rangle$, where $| x \rangle$ are position "eigen-states". Thus if the position-space representation of $| \Psi \rangle$ is $\Psi(x) = \langle x | \Psi \rangle$, we have $\rho(x, x') = \Psi(x)\Psi^*(x')$. Then we define the

Wigner function

$$W(x, p) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy \ e^{ipy} \ \rho(x + \frac{y}{2}, x - \frac{y}{2}) \tag{3.46}$$

where p is the momentum of the particle.

Example: Wigner function for a <u>superposition</u> of Gaussian wavepackets $\Psi(x) = \frac{\mathcal{N}}{\sqrt{2}} \left(e^{-\frac{(x-a)^2}{2\sigma^2}} + e^{-\frac{(x-b)^2}{2\sigma^2}} \right) \equiv \frac{1}{\sqrt{2}} \left(\varphi_a(x) + \varphi_b(x) \right)$, for $|a - b| \gg \sigma$, see figure below.
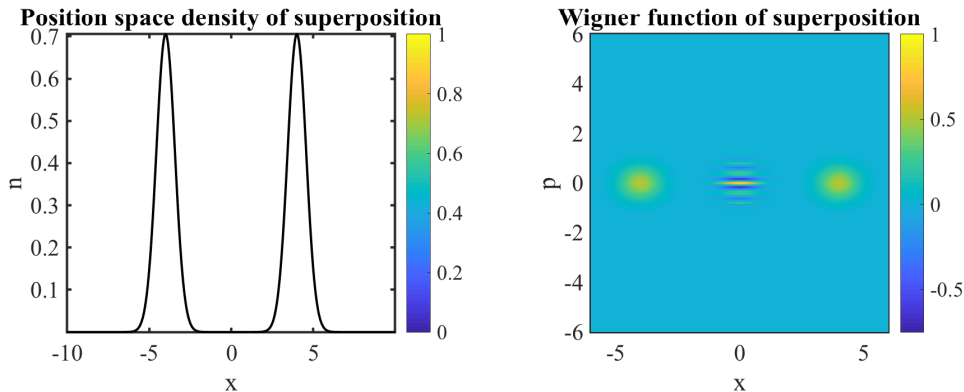
- The purpose of this is primarily to find the closest possible quantum-mechanical equivalent to the classical concept of a <u>phase-space coordinate</u>.

- Due to the uncertainty relation, we always have a distribution in phase space.

- Note, however, that $W(x, p)$ cannot be interpreted as a probability distribution, since it may take <u>negative</u> values.

- However, we can show $P(x) = \int dp\, W(x, p)$ and $P(p) = \int dx\, W(x, p)$ are the position- and momentum distributions in state ρ. For this reason, the Wigner function is called a <u>quasi-probability distribution</u>.

Example: Wigner function for a <u>mixture</u> of Gaussian wavepackets $\rho(x, x') = \varphi_a(x)\varphi_a^*(x') + \varphi_b(x)\varphi_b^*(x')$.

Position space density of mixture

Wigner function of mixture
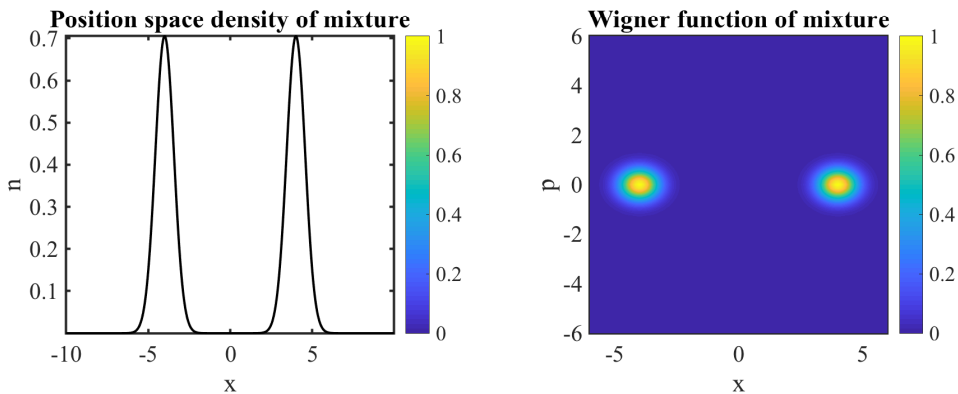
- It is typically superpositions that give rise to the negative features in the Wigner function. These are just used to pinpoint non-classical effects.

- Using the inverse of (1.20), the definition (3.46) can straightforwardly be applied to states given in the number representation $|n\rangle$.

- Similar phase space distributions for spin-states exist.

3.3.3 Purifying the Environment

In section 3.1.3 we have seen how a reduced density matrix for the system can be obtained from a pure-state density matrix for system+environment, and may then in general contain mixed features.

We can also do this in the opposite direction. Suppose you are given an <u>arbitrary</u> system density matrix, which, after diagonalization, reads $\hat{\rho}_\mathcal{S} = \sum_n p_n |\phi_n\rangle\langle\phi_n|$. This can be viewed as reduced density matrix of a <u>fictitious</u> system+environment in a <u>pure</u> state

$$|\Psi\rangle = \sum_n p_n |\phi_n\rangle |\varphi_n\rangle, \tag{3.47}$$

where $\{|\varphi_n\rangle\}$ is an arbitrary basis of the environment. (convince yourself that $\hat{\rho}_S$ is the corresponding reduced density matrix (3.13) for the system).

The main practical utility of this statement is that in all the following it makes sense to assume an initially pure state of the environment. If this was not the case we could simply enlarge the environment as above, and then do the math.

3.3.4 The operator sum formalism

The following technique is a useful tool to gain some formal insight, but typically not much use for actually solving the problem. Suppose we have a system+environment in an initial density matrix

$$\hat{\rho}(0) = \hat{\rho}(0)_S \otimes \hat{\rho}(0)_\mathcal{E}, \tag{3.48}$$

where $\hat{\rho}(0)_\mathcal{E} = \sum_k p_k |E_k\rangle\langle E_k|$ is the initial density matrix of the environment expressed in its basis $\{E_k\}$. Further assume we actually <u>know</u> the total time-evolution of system+environment given by the total time evolution operator $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$. We can then formally write the time-evolving reduced density matrix of the system as

$$\hat{\rho}(t)_S = \mathrm{Tr}_\mathcal{E}\left\{ \hat{U}(t)\left[\hat{\rho}(0)_S \otimes \sum_k p_k |E_k\rangle\langle E_k|\right] \hat{U}^\dagger(t) \right\}. \tag{3.49}$$

Using the

> **Kraus operators** defined as
>
> $$\hat{E}_{ij} = \sqrt{p_i}\langle E_j |\hat{U}(t)| E_i\rangle \tag{3.50}$$

we can rewrite (3.49) as

$$\hat{\rho}(t)_S = \sum_{ij} \hat{E}_{ij} \otimes \hat{\rho}(0)_S \otimes \hat{E}_{ij}^\dagger. \tag{3.51}$$

- Calculation and more discussion see SD 2.15.4.

- Note that the Kraus operators (3.50) act in the system only, no longer in the environment.