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Tutorial VI

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Reminder

EXERCISE I : Properties of the density matrix

We consider a quantum system that is in a statistical mixture of pure states $|\psi_\lambda\rangle$ (not necessarily eigenstates) with associated probabilities $\mathcal{P}_\lambda$. Recall that the density matrix (or operator) ρ is defined as

$$\rho = \sum_\lambda \mathcal{P}_\lambda \, |\psi_\lambda\rangle \, \langle\psi_\lambda|$$

1. Verify that the density matrix is hermitian (*i.e.* $\rho = \rho^\dagger$), positive (all eigenvalues of ρ are non-negative) and has unit trace $\mathrm{Tr}(\rho) = 1$.
   Reminder : the eigenvectors of ρ *are defined by* $\rho\,|\phi_i\rangle = \lambda_i\,|\phi_i\rangle$ *for eigenvalues* λ_i.
2. Show that the expectation value of a general observable $\hat{A}$ can be written $\langle\hat{A}\rangle = \mathrm{Tr}(\rho\hat{A})$.
3. Show that the $\mathrm{Tr}(\rho^2) = 1$ for a pure state. $\mathrm{Tr}(\rho^2)$ is called the 'purity' of the quantum state.

EXERCISE II : Pure and mixed states

Consider a spin-1/2 system described by the density matrix ρ, expressed using the basis $|\downarrow\rangle$, $|\uparrow\rangle$.

1. Compute the elements of the density matrix and the purity for the state $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$.

$$\begin{aligned}\rho &= \sum_\lambda \mathcal{P}_\lambda |\psi_\lambda\rangle\langle\psi_\lambda| \\ &= \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)\frac{1}{\sqrt{2}}(\langle\uparrow| + \langle\downarrow|) \\ &= \frac{1}{2}\left(|\uparrow\rangle\langle\uparrow|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\right)\end{aligned}$$

$$(\rho)_{\mathcal{B}=\{|\downarrow\rangle,|\uparrow\rangle\}} = \begin{pmatrix}\langle\downarrow|\rho|\downarrow\rangle & \langle\downarrow|\rho|\uparrow\rangle \\ \langle\uparrow|\rho|\downarrow\rangle & \langle\uparrow|\rho|\uparrow\rangle\end{pmatrix} = \begin{pmatrix}1/2 & 1/2 \\ 1/2 & 1/2\end{pmatrix}$$

$$\mathrm{Tr}(\rho^2) = \mathrm{Tr}\left[\begin{pmatrix}1/2 & 1/2 \\ 1/2 & 1/2\end{pmatrix}\right] = 1$$

2. Compute the density matrix and the purity for a state in a mixture of $|\downarrow\rangle$ and $|\uparrow\rangle$ with probabilities $\mathcal{P}_\downarrow = \mathcal{P}_\uparrow = 0.5$, and compare to the previous result.

$$|\psi_1\rangle = |\uparrow\rangle \qquad\qquad |\psi_2\rangle = |\downarrow\rangle$$

$$\rho = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$$

$$(\rho)_{\mathcal{B}=\{|\downarrow\rangle,|\uparrow\rangle\}} = \begin{pmatrix}1/2 & 0 \\ 0 & 1/2\end{pmatrix}$$

$$\mathrm{Tr}(\rho^2) = \mathrm{Tr}\left[\begin{pmatrix}1/4 & 0 \\ 0 & 1/4\end{pmatrix}\right] = \frac{1}{2}$$

Now we consider a composite quantum system consisting of two subsystems A and B. The eigenstates of the composite system can be written as as a tensor product of the eigenstates of the subsystems $|\phi_a\rangle_A |\phi_b\rangle_B$. Assume a measurement described by the observable $\hat{O}_A$ that acts only on the A subsystem. The expectation value is :

$$\langle\hat{O}_A\rangle = \mathrm{Tr}(\rho\hat{O}_A) = \sum_{a,b}\langle\phi_a|\langle\phi_b|\rho|\phi_b\rangle_B \hat{O}_A|\phi_a\rangle_A = \mathrm{Tr}(\rho_a\hat{O}_a)$$

where we have defined the reduced density matrix of the subsystem A :

$$\rho_A = \sum_b \langle\phi_b|\rho|\phi_b\rangle_B \equiv \mathrm{Tr}_B(\rho)$$

3. Assuming two spin-1/2 particles in a (pure) entangled state : $|\psi\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle_1 |\uparrow\rangle_2 - |\uparrow\rangle_1 |\downarrow\rangle_2)$. Compute the reduced density matrix ρ_1 for the first particle. How does it compare to the density matrices computed in II.1 and II.2 ?

$$\rho = \frac{1}{2}\left[|\downarrow\rangle_1 |\uparrow\rangle_2 \langle\downarrow|_1 \langle\uparrow|_2 - |\uparrow\rangle_1 |\downarrow\rangle_2 \langle\downarrow|_1 \langle\uparrow|_2 - |\downarrow\rangle_1 |\uparrow\rangle_2 \langle\uparrow|_1 \langle\downarrow|_2 + |\uparrow\rangle_1 |\downarrow\rangle_2 \langle\uparrow|_1 \langle\uparrow|_2\right]$$

$$\rho_1 = \sum_m \langle m|_2\, \rho\, |m\rangle_2 \qquad\qquad \text{with } m = \{\downarrow, \uparrow\}$$

$$\rho_1 = \begin{pmatrix} \langle\downarrow|_2\, \rho\, |\downarrow\rangle_2 & 0 \\ 0 & \langle\uparrow|_2\, \rho\, |\uparrow\rangle_2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} |\uparrow\rangle_1 \langle\uparrow|_1 & 0 \\ 0 & |\downarrow\rangle_1 \langle\downarrow|_1 \end{pmatrix}$$

This looks like a mixture state density matrix. This is then telling us that if you have an entangled system, but you only look at part of this system, then, any observable you get from this (single spin) will be indistinguishable from a mixt state.

EXERCISE III : Temporal evolution of the density matrix

We consider a quantum system that undergoes (unitary) time evolution according to the Hamiltonian H.

1. Show that the density matrix evolves according to the Liouville-von Neumann equation

$$i\hbar\frac{\mathrm{d}\rho}{\mathrm{d}t} = [H, \rho]$$

2. Assuming that H is time independent and working in a basis corresponding to the eigenvectors of H, write down an expression for the time evolution of the density matrix elements ρ_{ij}. We denote $|\phi_i\rangle$ as the eigenvectors of H with eigenvalues E_i.