Density matrices

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Density matrix formulation of QM

$|\psi\rangle$: vector in Hilbert space. Describes a quantum mechanical state
(properly: state = ray in Hilbert space)

To $|\psi\rangle$ we can associate an operator, or matrix:

$$\rho_\psi = |\psi\rangle\langle\psi| \qquad (\rho_\psi)_{ij} = \langle i|\psi\rangle\langle\psi|j\rangle \quad : \text{density matrix}$$

Expectation value of operator O in state ψ:

$$\langle O\rangle_\psi = \langle\psi|O|\psi\rangle = \sum_i \langle\psi|O|i\rangle\langle i|\psi\rangle = \sum_i \langle i|\psi\rangle\langle\psi|O|i\rangle = \mathrm{Tr}(|\psi\rangle\langle\psi|O)$$

$$= \mathrm{Tr}(\rho_\psi O)$$

Time evolution of density matrix:

$$\rho(t) = U(t)\,\rho(0)\,U^+(t) \qquad \partial_t\rho = \frac{i}{\hbar}[\rho, H] \qquad (\text{"Schrödinger eqn for } \rho\text{"})$$

$$U = e^{-iHt}$$

$\rho_\psi : |\psi\rangle\langle\psi|$: pure state

We can also describe more general states, which are not pure. Eg a state that has probability $p_i \in [0,1]$ of being in state $|i\rangle$:

$$\rho = \sum_i p_i |i\rangle\langle i| \qquad \sum_i p_i = 1 \quad : \text{mixed states}$$

$$\neq |\psi\rangle\langle\psi|$$

We can distinguish pure and mixed states by their entropy:

$$S = -\sum_i p_i \log p_i = -\mathrm{Tr}(\rho\log\rho) \quad : \text{von Neumann entropy of } \rho$$

For a pure state can choose $|1\rangle = |\psi\rangle$ $\quad p_1 = 1 \quad p_{i>1} = 0 \quad \Rightarrow S_{\text{pure state}} = 0$

while for a generic mixed state $S_{\text{mixed state}} \neq 0$.

Mixed thermal state:

$$p_i = \frac{e^{-\beta E_i}}{Z} \qquad Z = \sum_i e^{-\beta E_i} \qquad \beta = \frac{1}{T}$$

$$H|i\rangle = E_i|i\rangle$$

$$\rho_\beta = \frac{1}{Z} \sum_i e^{-\beta E_i} |i\rangle\langle i| = \frac{1}{Z} e^{-\beta H}$$

Thermal expectation values:

$$\langle O \rangle_\beta = \mathrm{Tr}(\rho_\beta O) = \sum_i \frac{O_i e^{-\beta E_i}}{Z} \qquad O_i = \langle i | O | i \rangle$$