Review of Pure States

• *Definition:* A pure state is a vector $\Psi = |\,\psi\,\rangle$ in a Hilbert space $\mathcal{H}$.
• *Observables:* Operators $\hat{A} : \mathcal{H} \to \mathcal{H}$ that are self-adjoint (if the corresponding classical observable is real). The possible outcomes of observations are its eigenvalues, with the corresponding states being the eigenvectors. The expectation value of an observable $\hat{A}$ in a given state Ψ is

$$\langle \hat{A} \rangle = \int \mathrm{d}^3q_1 ... \,\mathrm{d}^3q_N \,\psi^*(q)\,\hat{A}\,\psi(q) = \langle\,\psi\,|\hat{A}|\,\psi\,\rangle\ .$$

• *New notation:* Given any state Ψ, define the operator $\rho = |\,\psi\,\rangle\,\langle\,\psi\,|$; in terms of a c.o.n.s., if $\Psi = \sum_\nu c_\nu\,\Psi_\nu$, then $\rho_{\nu\nu'} = c^*_\nu c_{\nu'}$. This operator (assuming that Ψ is normalized) satisfies $\rho^2 = \rho$, $\rho^\dagger = \rho$, and $\mathrm{tr}\,\rho = 1$; it is a projection operator. The expectation value of an observable $\hat{A}$ can then be written also as $\langle\hat{A}\rangle = \mathrm{tr}\,\rho\hat{A}$.

Mixed States

• *Definition:* A mixed state is an operator $\rho : \mathcal{H} \to \mathcal{H}$ satisfying $\rho^\dagger = \rho$, and $\mathrm{tr}\,\rho = 1$ (not necessarily $\rho^2 = \rho$).
• *Observables:* As usual, a quantum observable is an operator on the Hilbert space of the system, usually taken to be self-adjoint (if the corresponding classical observable is real-valued). In this case, the expectation value of an observable $\hat{A}$ is written as

$$\langle\hat{A}\rangle = \mathrm{tr}\,\rho\hat{A}\ .$$

• *Interpretation:* Since we can use any basis to calculate a trace, choose a basis of eigenvectors of an observable $\hat{A}$, labelled by ν. Then for any mixed state ρ,

$$\langle\hat{A}\rangle = \textstyle\sum_\nu \rho_{\nu\nu}\lambda_\nu\ ,$$

consistently with the fact that $\rho_{\nu\nu} = |c_\nu|^2$ is the probability that the system will be found in state ν if a measurement of $\hat{A}$ is made. In the mixed states used to represent equilibrium systems in statistical mechanics, the phase information is washed out and only the probabilities remain.

Example: Mixed State for an Electron

• *Mean value of spin:* Suppose the spin degree of freedom of an electron is described by a state with a 50% probability of the z-component being "up", and 50% of it being "down"; one pure state which gives these values is $|\,\psi\,\rangle = 2^{-1/2}(|\!\uparrow\rangle + |\!\downarrow\rangle)$. Write down a mixed state representing the situation and, using the general formalism, first check that the mean value of S_z vanishes in both states, then calculate the mean value of S_x in both states; why is the result reasonable?
• *Fluctuation of spin:* Calculate the variances $(\Delta S_z)^2$ and $(\Delta S_x)^2$ for the same two operators, and compare the results for the pure state and the mixed state; what is going on?

State Evolution

• *For a pure state:* Time evolution is governed by the Schrödinger equation,

$$\hat{H}\,\psi(x) = \mathrm{i}\hbar\,\frac{\partial\psi(x)}{\partial t}\ .$$

• *For a mixed state:* Start by working in the Schrödinger picture, and derive the time evolution of ρ from that of a pure state by taking a time derivative. If ρ is of the form $|\psi\rangle\langle\psi|$, or $\rho(x,x') = \psi^*(x)\,\psi(x')$, then

$$\frac{\partial}{\partial t}\,\rho(x,x') = \frac{1}{\mathrm{i}\hbar}\Big(\frac{\partial\psi^*(x)}{\partial t}\,\psi(x') + \psi^*(x)\,\frac{\partial\psi(x')}{\partial t}\Big) = \frac{1}{\mathrm{i}\hbar}\,[\hat{H},\rho]\ .$$

This operator acting on ρ is sometimes called the Liouvillian.
• *Remark:* Add to Schwabl the proof that the expression for the expectation value in terms of a density matrix does what we want.

Related Sections: Phys 731; Chandler; Halley, first half of Ch 2; Reif; Schwabl, Sec 1.3-1.4.