PHYS-C0252 - Quantum Mechanics Part 12
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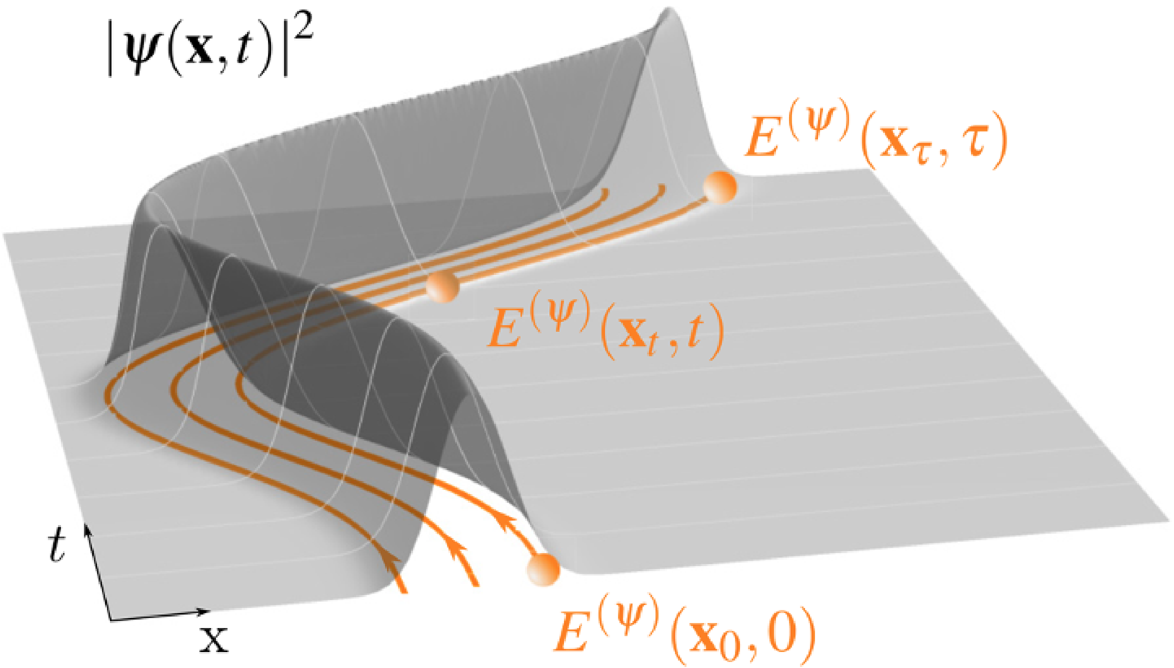

8. The Density Matrix

- The formulation of QM for systems of many degrees of freedom can also be done using the density matrix, which is an operator (in what picture?)

$$\hat{\rho}(t) \equiv |\psi(t)\rangle\langle\psi(t)|$$

Consider a general wave function expanded in orthonormal basis (e.g. energy basis)

$$\langle\psi(t)\rangle = \sum_n c_n(t)|n\rangle$$

The expectation value of an operator *A* is

$$\langle \hat{A}(t) \rangle = \sum_{n,m} c_n(t) c_m^*(t) \langle m|\hat{A}|n\rangle$$

and the elements of the density matrix can be obtained as

$$\hat{\rho}(t) = \sum_{n,m} c_n(t) c_m^*(t) |n\rangle\langle m|$$

They are defined by

$$\rho_{nm}(t) \equiv c_n(t) c_m^*(t)$$

This gives the important result that

$$\begin{aligned}\langle \hat{A}(t) \rangle &= \sum_{n,m} c_n(t) c_m^*(t) \langle m|\hat{A}|n\rangle \\ &= \sum_{n,m} \rho_{nm} \langle m|\hat{A}|n\rangle \\ &= \sum_{n,m} A_{mn} \rho_{nm}(t) \\ &= \mathrm{Tr}[\hat{A}\hat{\rho}(t)]\end{aligned}$$

Properties of the density matrix (operator):

- It is Hermitian (obviously)

- It is normalized: $\mathrm{Tr}[\hat{\rho}(t)] = 1$
- It is bound from below and above by mixed and pure states: $\mathrm{Tr}[\hat{\rho}^2(t)] = 1$ for pure states and $\mathrm{Tr}[\hat{\rho}^2(t)] < 1$ for mixed states

For mixed states, we can write in general (in a non-interacting many-particle system)

$$|\psi_i\rangle = \sum_n c_n^i |n\rangle$$

The density matrix elements are

$$\rho_{nm} = \langle n|\hat{\rho}|m\rangle = \sum_i \langle n|\psi_i\rangle\langle\psi_i|m\rangle = \sum_i \sum_{nm} c_n^i (c_m^i)^*$$

- Here the density matrix elements represent the *eigenstate coefficients averaged over the mixture*

  Diagonal elements give the probability of occupying a quantum state $|n>$ i.e. the *populations*

  Off-diagonal elements are complex (in general) and have time-dependent phase factors that describe the *evolution of coherent superpositions of the eigenstates*

8.1 Time Evolution of The Density Matrix

- Using the SE it is easy to show that (homework)

$$\frac{\partial \hat{\rho}(t)}{\partial t} = -\frac{\imath}{\hbar}[\hat{H}, \hat{\rho}]$$

which is the famous Liouville-von Neumann equation. Its formal solution is

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t)$$

where the time evolution operator (see Sec. 7.2)

$$\hat{U}(t) = e^{-\imath \int_0^t dt' \hat{H}(t')/\hbar}$$

The average of an operator can be computed either in the *Schrödinger picture* (propagating the density matrix) of in the *Heisenberg picture* (propagating the operator):

$$\langle \hat{A}(t) \rangle = \mathrm{Tr}[\hat{A}\hat{\rho}(t)] = \mathrm{Tr}[\hat{A}\hat{U}(t)\hat{\rho}(0)\hat{U}^{\dagger}(t)] = \mathrm{Tr}[\hat{A}(t)\rho(0)]$$

For a time-independent Hamiltonian the dynamics of the density matrix becomes simple as

$$\rho_{nm}(t) = \langle n|\hat{\rho}(t)|m\rangle = \langle n|\hat{U}(t)|\psi(0)\rangle\langle\psi(0)|\hat{U}^\dagger(t)|m\rangle$$

and thus for energy eigenfunctions

$$\rho_{nm}(t) = e^{-\imath(E_m - E_n)t/\hbar}\rho_{nm}(0)$$

This means that the *populations are time-independent* but the *coherences oscillate* in time with a frequency corresponding to the level splitting

8.2 Density Matrix in the Interaction Picture

- In the interaction picture we wrote (see Sec. 7.3.2)

$$\hat{H}_S = \hat{H}_S^0 + \hat{H}_S^I$$

and the evolution of the state vector is given by

$$|\psi_I(t)\rangle = e^{\imath \hat{H}_S^0 t/\hbar} |\psi_S(t)\rangle \equiv \hat{U}_0^\dagger(t) |\psi_S(t)\rangle$$

This means that the density matrix in the IP can be written as

$$\hat{\rho}_I(t) = \hat{U}_0^\dagger(t) \rho_S \hat{U}_0(t)$$

In analogy to the Schrödinger picture case, the equation of motion then becomes

$$\frac{\partial \hat{\rho}_I(t)}{\partial t} = -\frac{\imath}{\hbar}[\hat{H}_I(t), \hat{\rho}_I(t)]$$

where $\hat{H}_I(t) = \hat{U}_0^\dagger(t)\hat{H}_S\hat{U}_0(t)$