Dynamics of the Density Operator

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I. THE DENSITY OPERATOR

Quantum-mechanical state vectors $|\psi\rangle$ convey the maximal amount of information about a system allowed by laws of quantum mechanics. Typically, the information consists of quantum numbers associated with a set of commuting observables. Furthermore, if $|\psi_1\rangle$ and $|\psi_2\rangle$ are two possible quantum states then so is their coherent superposition

$$|\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle$$

if the coefficients c_1 and c_2 are known. If the states $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthogonal ($\langle\psi_1|\psi_2\rangle = 0$) then we must have $|c_1|^2 + |c_2|^2 = 1$. But there are frequently, in fact more often than not, situations where the state vector is not precisely known. There are, for example, cases where the system of interest is interacting with some other system, possibly a large system with which it becomes entangled. It may be possible to write state vectors for the multicomponent system but not for the subsystem of interest. As an example, consider a system of two spin-$\frac{1}{2}$ particles with the eigenstates of lets say the z-component of the spin denoted $|\uparrow\rangle$ for spin up and $|\downarrow\rangle$ for spin down. A possible state vector of the combined system is

$$|\psi\rangle = \frac{1}{\sqrt{2}}[|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2]$$

the so called singlet state (total angular momentum zero), also known as one of the Bell states. This is an example of an entangled state. An entangled state can not be factored, in any basis, into a product of states of the two subsystems i.e.

$$|\psi\rangle \neq |\text{spin }1\rangle|\text{spin }2\rangle.$$

Entanglement is, apart from the superposition principle itself, an essential mystery of quantum mechanics. Note that entanglement follows from the superposition principle and is not something imposed on the theory.

Quantum states described by state vectors are said to be pure states. States that can not be described by state vectors are said to be in mixed states. Mixed states are described by the density operator

$$\hat{\rho} = \sum_i |\psi_i\rangle p_i \langle\psi_i| = p_i \sum_i |\psi_i\rangle\langle\psi_i|$$

where the sum is over an ensemble (in the sense of statistical mechanics) where p_i is the probability of the system being in the i-th state of the ensemble $|\psi_i\rangle$ where $\langle\psi_i|\psi_i\rangle = 1$. The probabilities satisfy the obvious relations

$$0 \leq p_i \leq 1, \qquad \sum_i p_i = 1, \qquad \sum_i p_i^2 \leq 1.$$

For the special case where all p_i vanish except say the j-th one, $p_i = \delta_{ij}$ we obtain

$$\hat{\rho} = |\psi_j\rangle\langle\psi_j|$$

the density operator for the pure state $|\psi_j\rangle$. Note that the density operator for this case is just the projection operator onto the state $|\psi_j\rangle$ and for the more general case of

$$\hat{\rho} = \sum_i |\psi_i\rangle p_i \langle\psi_i| = p_i \sum_i |\psi_i\rangle\langle\psi_i|$$

the density operator is a sum of projection operators over the ensemble weighted with the probabilities of each member of the ensemble. We now introduce a complete, orthonormal, basis $\{|\varphi_n\rangle\}$ ($\sum_n |\varphi_n\rangle\langle\varphi_n| = \hat{I}$) eigenstates of some observable. Then for the i-th member of the ensemble we may write

$$|\psi_i\rangle = \sum_n \sum_n |\varphi_n\rangle\langle\varphi_n|\psi_i\rangle = \sum_n c_n^{(i)}|\varphi_n\rangle$$

where

$$c_n^{(i)} = \langle\varphi_n|\psi_i\rangle.$$

The matrix element of $\hat{\rho}$ between n and n' eigenstates is

$$\langle\varphi_n|\hat{\rho}|\varphi_{n'}\rangle = \sum_i \langle\varphi_n|\psi_i\rangle p_i \langle\psi_i|\varphi_{n'}\rangle.$$

The quantities $\langle\varphi_n|\hat{\rho}|\varphi_{n'}\rangle$ form the elements of the density matrix. Taking the trace of this matrix we get

$$\mathrm{Tr}\,\hat{\rho} = \sum_i p_i = 1.$$

Since $\hat{\rho}$ is Hermitian, the diagonal elements $\langle\varphi_n|\hat{\rho}|\varphi_n\rangle$ must be real, and it follows that

$$0 \leq \langle\varphi_n|\hat{\rho}|\varphi_n\rangle \leq 1.$$

Now lets consider the square of the density operator: $\hat{\rho}^2 = \hat{\rho}\cdot\hat{\rho}$. For a pure state where $\hat{\rho} = |\psi\rangle\langle\psi|$ it follows that

$$\hat{\rho}^2 = \hat{\rho}$$

and thus

$$\mathrm{Tr}\,\hat{\rho}^2 = \mathrm{Tr}\,\hat{\rho} = 1.$$

For a statistical mixture

$$\mathrm{Tr}\,\hat{\rho}^2 \leq \left[\sum_i p_i\right]^2 = 1.$$

The equality holds if and only if $|\langle\psi_i|\psi_j\rangle|^2 = 1$ for every pair of states $|\psi_i\rangle$ and $|\psi_j\rangle$. This is possible only if all the $|\psi_i\rangle$ are collinear in the Hilbert space i.e. equivalent up to an overall phase factor.

A. Example

Consider the superposition of the vacuum and one-photon number states

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\phi}|1\rangle)$$

where ϕ is just some phase. The density operator associated with this state is given by

$$\hat{\rho}_\psi = \frac{1}{2}[|0\rangle\langle 0| + |1\rangle\langle 1| + e^{i\phi}|1\rangle\langle 0| + e^{i\phi}|0\rangle\langle 1|].$$

On the other hand, the density operator for an equally populated mixture of vacuum and one-photon states is

$$\hat{\rho}_M = \frac{1}{2}[|0\rangle\langle 0| + |1\rangle\langle 1|].$$

The two density operators differ by the presence of the “off-diagonal” or “coherence”, terms in the former, such terms being absent in the case of the mixture. The absence of the coherence terms is of course what makes the distinction between a state exhibiting full quantum-mechanical behaviour and one that does not. It is easy to check that

$$\mathrm{Tr}\,\hat{\rho}_M^2 = \frac{1}{2}.$$

II. DYNAMICS OF THE DENSITY OPERATOR

In the absence of dissipative interactions and in the absence of explicitly time-dependent interaction, the density operator evolves unitarily according to

$$\frac{d\hat{\rho}}{dt} = \frac{i}{\hbar}[\hat{\rho}, \hat{H}]$$

which can be easily proved by using the fact that each of the states $|\psi_i\rangle$ of the ensemble satisfies the Schrödinger equation

$$i\hbar\frac{d|\psi_i\rangle}{dt} = \hat{H}|\psi_i\rangle.$$

The equation

$$\frac{d\hat{\rho}}{dt} = \frac{i}{\hbar}[\hat{\rho}, \hat{H}]$$

is known as the von Neumann equation, the quantum-mechanical analogue of the Liouville equation associated with the evolution phase-space probability distributions in statistical mechanics. The equation is sometimes written as

$$i\hbar\frac{d\hat{\rho}(t)}{dt} = [\hat{H}, \hat{\rho}(t)] \equiv \mathcal{L}\hat{\rho}(t)$$

where $\mathcal{L}$ is known as the Liouvillian superoperator.