Density Operator

Another way to describe quantum mechanics is through the use of *density operators* or *density matrices*. Density operators is a operator description of an ensemble of *pure states* $p_i, |\psi_i>$ for a quantum system, where $|\psi_i>$ are the states, and p_i are their respective probabilities. Density operators are defined as below,

$$\rho = \Sigma_i p_i |\psi_i >< \psi_i|.$$

Furthermore, the postulates of quantum mechanics can be reformulated in the language of density operators.

Postulate 1: Each isolated physical system is a complex vector space that satisfies inner product (thus, an Hilbert space). Such space is defined as the *state space*. Such system is described by its *density operator*, which is a positive operator ρ with a trace of one, acting on the state space of the system. Furthermore, for a quantum system in a state ρ_i with probability p_i, the density operator for system is then $\Sigma_i p_i \rho_i$, where $\rho_i = \Sigma_{ij} p_{ij} |\psi_{ij} >< \psi_{ij}|$.

Postulate 2: Each closed quantum system evolves from time t_1 to time t_2 through a *unitary transformation U*. Hence, for a state ρ at t_1, it evolves to ρ' at t_2 through

$$\rho' = U \rho U^\dagger$$

Proof: In a closed quantum system, if the initial state is ψ_i with a probability of p_i, the state of the system evolves to $U\psi_i$ with probability of p_i for some unitary operator U. Thus, the evolution of the density operator is derived as

$$\rho' = \Sigma_i p_i U |\psi_i >< \psi_i| U^\dagger = U \rho U^\dagger$$

Postulate 3: Measurements of quantum systems are described by a collection of *measurement operators* M_m. Index *m* refers to the possible measurement outcome in an experiment. Further, for a quantum system in an initial state ρ before measurement, after measurement, the probability that index *m* occurs is

$$p(m) = tr(M_m^\dagger M_m \rho),$$

and the state of system after measurement is

$$\frac{M_m \rho M_m^\dagger}{\sqrt{tr(M_m^\dagger M_m \rho)}},$$

where the measurement operators satisfy the *completeness equation,*

$$\Sigma_m M_m^\dagger M_m = I$$

Proof: Suppose the initial state is $|\psi_i>$, then the probability of measuring *m* is

$$p(m|i) =< \psi_i|M_m^\dagger M_m|\psi_i >= tr(M_m^\dagger M_m|\psi_i >< \psi_i|),$$

and by total probability, the probability of measuring *m* is

$$p(m) = \Sigma_i p(m|i)p_i$$

$$= \Sigma_i p_i tr(M_m^\dagger M_m|\psi_i >< \psi_i|)$$

$$= \Sigma_i tr(M_m^\dagger M_m \rho).$$

And to describe the density operator of the system after measuring m, we first observe that for an initial state $|\psi_i >$, then the state after measuring m is

$$|\psi_i^m >= \frac{M_m|\psi_i>}{\sqrt{<\psi_i|M_m^\dagger M_m|\psi_i>}}.$$

This yields an ensemble of states $|\psi_i^m >$, with respective probabilities $p(i|m)$, which is constructed into the corresponding density operator ρ_m,

and by elementary probability theory, where $p(i|m) = p(m,i)/p(m) = p(m|i)p_i/p(m)$, and substitution, we have

$$\rho_m = \Sigma_i p_i \frac{M_m|\psi_i><\psi_i|M_m^\dagger}{tr(M_m^\dagger M_m \rho}$$

$$= \frac{M_m \rho M_m^\dagger}{\sqrt{tr(M_m^\dagger M_m \rho)}}$$

Postulate 4: A composite physical system's state space is described through the tensor product of each individual state space combined in the composite physical system. Such system is described below, where we have systems numbered 1, 2, …., n, and system i is prepared in state $|\rho_i >$, then the composite system is composed as

$$|\rho_1 > \otimes|\rho_2 > \otimes\ldots\otimes |\rho_n >$$

Furthermore, any operator defined as a density operator has the following characterization,

Theorem of Characterization of density operators: An operator ρ is defined as a density operator for a corresponding ensemble $p_i, |\psi_i>$ if and only if

(1) ρ has trace equal to one

(2) ρ is a positive operator

An important property, which shows that different ensembles can make up the same density matrix (which also means that the eigenvectors and eigenvalues of the density matrix do not necessarily relate to the ensemble) is stated in the theorem below.

Theorem for Unitary freedom in the ensemble for density matrices:{$|\tilde{\psi}_i>$} and {$|\tilde{\phi}_i>$} generate the same density matrix if and only if

$$|\tilde{\psi}_i>=\Sigma_j u_{ij}|\tilde{\phi}_j>,$$

in which u_{ij} is a unitary matrix of complex integer values, indexed with i and j.

Reduced density operator

The most useful application of density operator is in the study of subsystems of composite systems. This leads to the use of *reduced density operators*, which is described as such: for physical systems A and B, described by density operator ρ^{AB}, the reduced density operator for A is defined as

$$\rho^A = tr_B(\rho^{AB})$$

which performs a partial trace on B,

$$tr_B(|a_1><a_2| \otimes |b_1><b_2|) = |a_1><a_2| tr(|b_1><b_2|)$$

where $|a_1>, |a_2> \epsilon A$ and $|b_1>, |b_2> \epsilon B$, and $tr_B(|b_1><b_2|) =<b_1|b_2>$.

Other important tools for studying composite systems are *Schmidt decomposition* and *purification*.