Chapter 1: The Density Matrix

I. OPEN VS. CLOSED QUANTUM SYSTEMS

The state of a closed quantum system, $|\psi\rangle$ is described by a unit vector in a Hilbert space. Observables are represented by Hermitian operators, whose expectation values can be computed according to the inner product $\langle O \rangle = \langle \psi | O | \psi \rangle$. The Hilbert state for quantum systems consisting of many particles is given by the tensor product of the single particle Hilbert spaces.

If we want to talk about open quantum systems, we are thinking about situation where we are only interested in the properties of a certain subsystem and treat the rest of the total quantum system as "the environment", i.e., a big black box. However, due to the interaction between the subsystem of interest and its environment, the quantum state of the subsystem can in general no longer be described by a vector in a Hilbert space. This can be seen from the following example of an entangled state of two particles represented by two-level systems

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle). \tag{1}$$

Suppose we are interested in the first particle only. Then, we can expand any observable $O = O_1 \otimes 1_2$ in terms of Pauli matrices using

$$O_1 = O_0\sigma_0 + O_x\sigma_x + O_y\sigma_y + O_z\sigma_z, \tag{2}$$

where σ_0 is the identity. Remarkably, we find that $\langle O \rangle = O_0$ for any choice of O, with the constant value being a direct consequence of the normalization of the quantum state. In other words, no measurement on the first particle alone can reveal any information about the quantum state. This is certainly at odds with a description in terms of a Hilbert space vector, where we can always construct Hermitian operators, to which the state is an eigenvector.

II. STATISTICAL ENSEMBLES

The most straight-forward way to describe the state of an open quantum system is to use a statistical sum (mixture) of Hilbert space vectors, giving rise to a density matrix of the

form

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \tag{3}$$

where $0 \leq p_i \leq 1$ denotes the probability to find the system in the (pure) quantum state described by the Hilbert space vector $|\psi_i\rangle$. Being probabilities, they are subject to the constraint $\sum_i p_i = 1$, resulting in $\text{Tr}\{\rho\} = 1$ while the non-existence of negative probabilities requires the density matrix to be positive-semidefinite.

Such a statistical mixture might reflect our ignorance about preparation of a quantum state, i.e., it might be pure, but we don't know which one. Or, it might also describe something more fundamental: if we have an entangled state of two subsystems, the density matrix describes the information that is in principle accessible from local measurements alone. So, how do we get from a pure state of the total system to a density operator of a subsystem? Consider a bipartite system composed of the subsystems A and B, with pure states being represented by

$$|\psi\rangle = \sum_{ij} c_{ij} |i\rangle_A |j\rangle_B \equiv \sum_{ij} c_{ij} |ij\rangle. \tag{4}$$

Then, we can define the reduced density matrix of A as the partial trace over B, given by

$$\rho_A = \text{Tr}_B\{\rho\} = \sum_{i,i'} \sum_j \langle ij|\rho|i'j\rangle |i\rangle\langle i'|. \tag{5}$$

For the pure state $\rho = |\psi\rangle\langle\psi|$, we obtain

$$\rho_A = \sum_{i,i'} \sum_j c_{ij}^* c_{i'j} |i\rangle\langle i'|. \tag{6}$$

Taking the example of the entangled state from above, we obtain for the reduced density matrix of the first particle

$$\rho_1 = \text{Tr}_2\{\rho\} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}. \tag{7}$$

Since this state is just a completely random mixture of the pure states $|0\rangle$ and $|1\rangle$. This, of course, is a direct manifestation of the fact that quantum entanglement is a nonlocal property, and therefore such a (maximally) entangled quantum state does not provide any useful information under local measurements.

As the state of the quantum system is no longer described by a Hilbert space vector, the dynamics is no longer described by the Schrdinger equation, even when ignoring the

interaction with the environment. Instead, we have

$$\frac{d}{dt}\rho = \frac{d}{dt}\sum_i p_i|\psi_i\rangle\langle\psi_i| = \sum_i p_i\left[\left(\frac{d}{dt}|\psi_i\rangle\right)\langle\psi_i| + |\psi_i\rangle\left(\frac{d}{dt}\langle\psi_i|\right)\right]$$

$$= -\sum_i p_i\frac{i}{\hbar}\left(H|\psi_i\rangle\langle\psi_i| - |\psi_i\rangle\langle\psi_i|H\right) = -\frac{i}{\hbar}\left[H,\rho\right], \tag{8}$$

which is called the Liouville-von Neumann equation. Note that this equation is analogous to the Liouville for the classical phase space density, where the commutator is replaced by Poisson brackets.

III.   VON NEUMANN ENTROPY

A very useful way to quantify the (lack of) information that can be extracted from measurements of a quantum system, is given by its von Neumann entropy, which is defined as

$$S = -\langle\log\rho\rangle = -\text{Tr}\{\rho\log\rho\} = -\sum_i p_i\log p_i. \tag{9}$$

The last equality shows that the von Neumann entropy is equivalent to the Shannon (or Gibbs) entropy used in statistical mechanics. Specifically, the entropy is maximal for the state where all probabilities are identical (the "maximally mixed state"),

$$\rho = \begin{pmatrix} 1/\Omega & & \\ & 1/\Omega & \\ & & \ddots \end{pmatrix}, \tag{10}$$

where Ω is the total Hilbert space dimension. The von Neumann entropy non-negative (it is zero if and only if ρ is pure) and it is invariant under unitary transformations and therefore does not change under Hamiltonian dynamics. Additionally, it is subadditive with respect to its subsystems, i.e.,

$$S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B), \tag{11}$$

where ρ_A and ρ_B are the density matrices of the individual subsystems A and B [1]. Consequently, by looking only at parts of the full system, we can only obtain partial information, as seen in the example above. Remarkably, for pure states of the full system, the entropies $S(\rho_A)$ and $S(\rho_B)$ are identical. This can be seen by looking at the Schmidt decomposition

[2] of the wave function of the full system,

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle |\chi_i\rangle, \tag{12}$$

which results in the reduced matrices

$$\rho_A = \sum_i |c_i|^2 |\phi_i\rangle\langle\phi_i|, \quad \rho_B = \sum_i |c_i|^2 |\chi_i\rangle\langle\chi_i|. \tag{13}$$

As the coefficients $|c_i|^2$ are identical for both subsystems, the reduced density matrices have the same nonzero eigenvalues and therefore the same entropy. Therefore, we can define an "entanglement entropy" for any pure state $|\psi\rangle$ simply as the entropy of the reduced density matrix $S(\rho_A)$. For initially mixed states, however, such an obvious measure of entanglement does not exist and the situation is much more subtle.

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[1] H. Araki and E. H. Lieb, Comm. Math. Phys. **18**, 160 (1970).

[2] M. A. Nielsen and I. L. Chuang, *Quantum computation and quantum information* (Cambridge University Press, Cambridge, 2000).