DENSITY MATRIX

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 4.2.

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The standard probabilistic interpretation of quantum mechanical wave functions is that if you have a collection of a large number of systems all prepared in the same state, then we can calculate expectation values for the various observable quantities such as energy, spin and so on. In practice, most systems consist of a collection of various states. We can treat the statistics of such systems using a density matrix.

Suppose we have an ensemble of N sysytems, where there are n_i systems in state $|i\rangle$, so that

$$\sum_i n_i = N \tag{1}$$

We're assuming that the collection of $|i\rangle$ states form an orthonormal basis.

The density matrix is defined as

$$\rho \equiv \sum_i p_i |i\rangle \langle i| \tag{2}$$

where p_i is the probability of a single system being state $|i\rangle$. We can calculate a few properties of ρ as follows.

First, the most important property is probably the ensemble average of some observable quantity represented by an operator Ω. Within a single state, the expectation value of Ω is

$$\langle\Omega\rangle = \langle i|\Omega|i\rangle \tag{3}$$

Thus over the ensemble of systems described above, the expectation value is

$$\left\langle\bar{\Omega}\right\rangle = \sum_i p_i \langle i|\Omega|i\rangle \tag{4}$$

The angle bracket plus overbar notation indicates that two averages are occurring - an average over each individual state, represented by 3, and an ensemble average over the whole collection of systems.

This ensemble average can be expressed in terms of the density matrix, as follows.

$$\mathrm{Tr}\left(\Omega\rho\right) = \sum_j \left\langle j\left|\Omega\rho\right|j\right\rangle \tag{5}$$

$$= \sum_j \sum_i \left\langle j\left|\Omega\right|i\right\rangle p_i \left\langle i\left|j\right.\right\rangle \tag{6}$$

$$= \sum_j \sum_i \left\langle j\left|\Omega\right|i\right\rangle p_i \delta_{ij} \tag{7}$$

$$= \sum_i p_i \left\langle i\left|\Omega\right|i\right\rangle \tag{8}$$

$$= \left\langle \bar{\Omega}\right\rangle \tag{9}$$

If we want the probability of obtaining a particular eigenvalue ω of the operator Ω, then we first project out the component of the ensemble along the eigenvector $\left|\omega\right\rangle$, which we do with the projection operator $\mathbb{P}_\omega$. Thus the probability of obtaining the value ω is

$$\overline{P\left(\omega\right)} = \mathrm{Tr}\left(\mathbb{P}_\omega\rho\right) \tag{10}$$

A few other properties can be derived.

(1) From 2, we have $\rho^\dagger = \left[\sum_i p_i \left|i\right\rangle\left\langle i\right|\right]^\dagger = \sum_i p_i^* \left|i\right\rangle\left\langle i\right| = \sum_i p_i \left|i\right\rangle\left\langle i\right| = \rho$, since p_i, being a probability, is a real number.

(2) $\mathrm{Tr}\rho = \sum_j \sum_i p_i \left\langle j\left|i\right.\right\rangle\left\langle i\left|j\right.\right\rangle = \sum_j \sum_i p_i \delta_{ji}\delta_{ij} = \sum_i p_i = 1$, since probabilities must add up to 1.

(3) For a pure ensemble, there is only one state, say $\left|i\right\rangle$, in the ensemble, so $\rho = \left|i\right\rangle\left\langle i\right|$ and in this case $\rho^2 = \left|i\right\rangle\left\langle i\left|i\right.\right\rangle\left\langle i\right| = \left|i\right\rangle\left\langle i\right| = \rho$.

(4) If the ensemble is uniformly distributed over k states, then $p_i = \frac{1}{k}$ for all states in the ensemble, and $\rho = \frac{1}{k}\sum_i \left|i\right\rangle\left\langle i\right| = \frac{1}{k}I$.

(5) $\mathrm{Tr}\rho^2 = \mathrm{Tr}\sum_j \sum_i p_j p_i \left|j\right\rangle\left\langle j\left|i\right.\right\rangle\left\langle i\right| = \mathrm{Tr}\sum_j \sum_i p_j p_i \left|j\right\rangle \delta_{ij}\left\langle i\right| = \mathrm{Tr}\sum_i p_i^2 \left|i\right\rangle\left\langle i\right| = \sum_k \sum_i p_i^2 \left\langle k\left|i\right.\right\rangle\left\langle i\left|k\right.\right\rangle = \sum_i p_i^2$. Since $0 \le p_i \le 1$ and squaring a number in this range either makes it smaller (if $0 < p_i < 1$) or leaves it unchanged (if $p_i = 0$ or $p_i = 1$), and since $\sum_i p_i = 1$, we must have $\sum_i p_i^2 \le 1$, with equality only for a pure ensemble.

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