Mixed states

By the *mixed* state of a system we mean the probabilistic combination of the states we have discussed so far, called *pure*. (Note that formally a pure state is a special case of a mixed state). For computational reasons, mixed states are usually represented by a density matrix rather than a vector. Thus, the density matrix of a mixed state is of the form

$$\rho = \sum p_i \rho_i,$$

where p_i are non-negative numbers with sum one (i.e., discrete probability distributions) and ρ_i are density matrices. The set $\{(\rho_i, p_i)\}$ where $\sum p_i = 1$ is called an *ensemble of states*. A mixed state thus represents a situation where, in addition to the underlying quantum-mechanical uncertainty about the measurement result, there is also „ordinary" probabilistic uncertainty about what pure state the system is in. Note that we get a mixed state even if the states ρ_i are themselves mixed. This shows a fundamental advantage of this approach to mixed states: we can treat the density matrix as a single state, regardless of whether it is mixed or pure. It is easy to see that this is also true of the evolution of a system: if ρ is the density matrix of a system, then $U\rho U^\dagger$ is the density matrix of that system after applying the unitary operation U (including the appropriate probabilistic interpretation).

The previous observation can be reinforced: we can operate on a mixed state **without knowing what pure states it consists of**. Indeed, the same density matrix can arise from different sets of states. However, we noted that not knowing the „correct" decomposition of the density matrix into pure states does not prevent us from computing the evolution of the system. We now show that the same is true for measurements: the density matrix uniquely determines the results of the measurements (i.e., their probability distribution). To this end, we define a more general notion of measurement than that of projective measurement, to which we have restricted ourselves in formulating the relevant postulate.

Postulate 3' The measurement of a quantum system is given by a system of operators M_i satisfying the condition

$$\sum_i M_i^\dagger M_i = I.$$

After measuring the state $|\psi\rangle$, the system with probability $\langle\psi|M_i^\dagger M_i|\psi\rangle$ is in the state

$$\frac{M_i|\psi\rangle}{\sqrt{\langle\psi|M_i^\dagger M_i|\psi\rangle}}\,.$$

If the use of the operator M_i is associated with the measured value m_i, then the expected value of the measurement is

$$E(m) = \sum_i p_i m_i = m_i \langle\psi|M_i^\dagger M_i|\psi\rangle = \langle\psi|M|\psi\rangle\,,$$

where

$$M = \sum m_i M_i^\dagger M_i$$

is called *observable*.

Using the density matrix $\rho = |\psi\rangle\langle\psi|$ and the relation $\langle\psi|A|\psi\rangle = \mathrm{tr}(A|\psi\rangle\langle\psi|)$, we obtain the equivalent condition that the i-th state measurement ρ will occur with probability $\mathrm{tr}(M_i^\dagger M_i \rho)$ and the system will be in the state after such a measurement

$$\frac{M_i \rho M_i^\dagger}{\mathrm{tr}(M_i^\dagger M_i \rho)} .$$

The mean value of the measurement is $\mathrm{tr}(M\rho)$.

Thus, the state after the measurement can be seen as a mixed state $\sum_i M_i \rho M_i^\dagger$. From linearity we get the desired property that the above holds even if the original measured state ρ was mixed, independently of the particular set of states. Let us illustrate this fact on the expected value. If $\rho = \sum p_i \rho_i$, where ρ_i are the pure states, then the expected outcome of the measurement of the pure state ρ_i is $\mathrm{tr}(M\rho)$. Since the state ρ_i is measured with probability p_i, the mean of the mixed state measurement is

$$\sum p_i \,\mathrm{tr}(M\rho_i) = \mathrm{tr}(M \sum p_i \rho_i) = \mathrm{tr}(M\rho) .$$

Note further that while we need to know the measurement operators to compute the state of the system after the measurement, for the statistics of the results it is sufficient to know the set $\{M_i^\dagger M_i\}$, which is the decomposition of the identity into positive operators. For a one-time measurement where we are not interested in the state of the system after the measurement (e.g., this is naturally true for destructive measurements such as photon detection), it is sufficient to specify such a set E_i. A measurement defined in this way is called POVM (positive operator value measurement) in the literature.

The diagonal form of the pure state density matrix contains exactly one 1 on the diagonal. It follows that the trace of the pure, and hence of any mixed state matrix, is equal to one. Since density matrices are positive operators, their diagonal form represents a discrete probability distribution. In other words, each mixed matrix can be viewed as a probabilistic combination of projections onto some orthonormal basis.

Recall that the density matrix of a general pure qubit is of the form $\frac{1}{2}(E + xX + yY + zZ)$, where (x, y, z) is a unit vector. The mixed state of the qubit is therefore of the form

$$\frac{1}{2} \sum p_i \left(E + x_i X + y_i Y + z_i Z \right) .$$

Vector

$$\sum p_i \left(x_i, y_i, z_i \right)$$

is the weighted average (center of gravity) of the points (x_i, y_i, z_i). The convexity of the sphere implies that it is a vector less than one. Conversely, each point in the unit sphere represents a mixed state. Thus the Bloch ball represents all mixed states, with the pure states lying on the surface.

Let ρ^{AB} be the density matrix of the composite system. We define the *reduced density matrix* on system A as

$$\rho^A := \mathrm{tr}_B \left(\rho^{AB} \right) ,$$

where tr_B is the so-called *partial trace* defined by a linear extension of the relation

$$\mathrm{tr}_B(\rho_a \otimes \rho_b) = \mathrm{tr}(\rho_b)\rho_a$$

or, written in basis vectors,

$$\mathrm{tr}_B\left(|a_i\rangle\langle a_j| \otimes |b_k\rangle\langle b_\ell|\right) = \delta_{k\ell}|a_i\rangle\langle a_j|\,.$$

The reduced density matrix ρ^A has a clear and important physical meaning. It captures the properties of the system A understood in isolation. More precisely, the measurement results of the system A alone are the same for the state ρ^A as for the state ρ^{AB}. Even more precisely, the measurement of the state ρ^A given by the operators (M_j) has the same properties as the measurement results of the state ρ^{AB} given by the operators $(M_j \otimes E)$. Another physical view of the same statement is that the matrix ρ^A describes the state of system A after (any!) measurement of system B for which we do not know the outcome (this uncertainty translates into a mixed state ρ^A). Indeed, any such measurement releases system A from entanglement with system B. These two views are equivalent: if we are restricted to measurements of system A, we cannot know whether system B has been measured or not.