State Vectors and State Operators: Superpositions, Mixed States and Entanglement

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This tutorial will use the concepts of state vector and state operator to examine superpositions and mixed states using the matrix formulation of quantum mechanics. The state vectors required are given immediately below. An unsubscripted spin arrow refers to spin in the z-direction.

$$|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix} \quad \langle\uparrow| = \begin{pmatrix}1 & 0\end{pmatrix} \quad |\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix} \quad \langle\downarrow| = \begin{pmatrix}0 & 1\end{pmatrix} \quad |\uparrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \quad \langle\uparrow_x| = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\end{pmatrix} \quad |\downarrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \quad \langle\downarrow_x| = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\end{pmatrix}$$

These same states are now defined using Mathcad syntax.

$$Szu := \begin{pmatrix}1\\0\end{pmatrix} \qquad Szd := \begin{pmatrix}0\\1\end{pmatrix} \qquad Sxu := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\1\end{pmatrix} \qquad Sxd := \frac{1}{\sqrt{2}}\cdot\begin{pmatrix}1\\-1\end{pmatrix}$$

$$Szu^T = \begin{pmatrix}1 & 0\end{pmatrix} \qquad Szd^T = \begin{pmatrix}0 & 1\end{pmatrix} \qquad Sxu^T = \begin{pmatrix}0.707 & 0.707\end{pmatrix} \qquad Sxd^T = \begin{pmatrix}0.707 & -0.707\end{pmatrix}$$

The identity and z- and x-direction spin operators (in units of h/4π) will be used.

$$I := \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} \qquad \sigma_z := \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} \qquad \sigma_x := \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$$

Dirac has said that the superposition principle is at the heart of quantum mechanics. He elaborated in *The Physical Principles of Quantum Mechanics*.

> The nature of the relationships which the superposition principle requires to exist between states of any system is of a kind that cannot be explained in terms of familiar physical concepts. One cannot in the classical sense picture a system being partly in each of two states and see the equivalence of this to the sytem being completely in some other state. There is an entirely new idea involved, to which one must get accustomed and in terms of which one must proceed to build up an exact mathematical theory, without having any detailed classical picture.

N. David Mermin [*American Journal of Physics* **71**, 29, (2003)] succinctly summarized Dirac's statement when he wrote, "Superpositions have no classical interpretation. They are sui generis, an intrinsically quantum-mechanical construct..."

We now illustrate the properties of a superposition with a specific example. A spin system with spin up in the x-direction is prepared using a Stern-Gerlach apparatus. We see from the mathematics below that this system can also be considered to be an even superposition of spin up and spin down in the z-direction.

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\left[|\uparrow\rangle + |\downarrow\rangle\right] = |\Psi\rangle \qquad \Psi := \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

Subsequent spin measurements confirm what is expressed mathematically above. If the spin system is passed through a Stern-Gerlach magnet oriented in the x-direction, the beam bends in one direction, the direction associated with spin up in the x-direction. However, if the system is passed through a Stern-Gerlach magnet oriented in the z-direction, it is split into two beams, one associated with spin up in the z-direction and one associated with spin down in the z-direction. The expectation values calculated below are consistent with these experimental results.

$$\Psi^T \cdot \sigma_x \cdot \Psi = 1 \qquad\qquad \Psi^T \cdot \sigma_z \cdot \Psi = 0$$

The state operator is a more versatile quantum construct than the mathematically simpler state vector. It is the outer product of the state vector.

$$\hat{\rho} = \left|\uparrow_x\right\rangle\left\langle\uparrow_x\right| = \frac{1}{2}\begin{pmatrix}1\\1\end{pmatrix}\begin{pmatrix}1 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix} = \left|\Psi\right\rangle\left\langle\Psi\right| \qquad \rho := \frac{1}{2}\cdot\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}$$

Expectation values can also be calculated using the state operator.

$$\left\langle\Psi\middle|\hat{A}\middle|\Psi\right\rangle = \sum_i \left\langle\Psi\middle|\hat{A}\middle|i\right\rangle\left\langle i\middle|\Psi\right\rangle = \sum_i \left\langle i\middle|\Psi\right\rangle\left\langle\Psi\middle|\hat{A}\middle|i\right\rangle = Tr\left(\hat{\rho}_\Psi \hat{A}\right) \text{ where } \sum_i \left|i\right\rangle\left\langle i\right| = Identity$$

$$\mathrm{tr}\left(\rho\cdot\sigma_x\right) = 1 \qquad\qquad \mathrm{tr}\left(\rho\cdot\sigma_z\right) = 0$$

It is not uncommon for people to look at the superposition

$$\left|\Psi\right\rangle = \frac{1}{\sqrt{2}}\left[\left|\uparrow\right\rangle + \left|\downarrow\right\rangle\right]$$

we are considering and think of it as a 50-50 mixture of spin up and spin down in the z-direction.

However, a mixture cannot be represented by a state vector. A mixture must be represented by a state operator which is a weighted sum of the outer products of the vectors contributing to the mixture, as shown below.

$$\hat{\rho}_{Mix} = \frac{1}{2}\left|\uparrow\right\rangle\left\langle\uparrow\right| + \frac{1}{2}\left|\downarrow\right\rangle\left\langle\downarrow\right| = \frac{1}{2}\left[\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0 & 1\end{pmatrix}\right] = \frac{1}{2}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} \qquad \rho_{mix} := \frac{1}{2}\cdot\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$$

Measurement of the z-direction spin gives the same results as above and might lead one to conclude that a superposition and a mixture cannot be distinguished experimentally. However, the x-direction calculation shows that a superposition is not a classical mixture of spin states, because it is in disagreement with the experimental results presented above.

$$\mathrm{tr}\left(\rho_{mix}\cdot\sigma_z\right) = 0 \qquad\qquad \mathrm{tr}\left(\rho_{mix}\cdot\sigma_x\right) = 0$$

Before moving on to composite systems and entanglement, a few additional features of the state operators for superpositions (pure states) and mixtures are illustrated.

$$\rho_{sup} := \frac{1}{2}\cdot\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix} \qquad\qquad \rho_{mix} := \frac{1}{2}\cdot\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$$

One rather obvious difference between these state operators is that the one representing a classical mixture is diagonal, while the one representing the superposition has off-diagonal elements. The presence of off-diagonal elements in a state operator is the signature of a quantum mechanical system.

All valid state operators have unit traces; the sum of the diagonal elements equals unity.

$$\mathrm{tr}(\rho_{sup}) = 1 \qquad \mathrm{tr}(\rho_{mix}) = 1$$

However, the trace of the square of the state operator distinguishes between a pure state and a mixture as shown below.

$$\mathrm{tr}(\rho_{sup}{}^2) = 1 \qquad \mathrm{tr}(\rho_{mix}{}^2) = 0.5$$

And the entropy of the pure state is 0, while the entropy of the mixed state is 1

$$S(\rho) = -\mathrm{Tr}(\rho \cdot \ln(\rho)) = -\sum_i (\lambda_i \cdot \log(\lambda_i, 2)) = \log\left[\prod_i (\lambda_i)^{-\lambda_i}, 2\right]$$

$$\lambda := \mathrm{eigenvals}(\rho_{sup}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad -\sum_{i=0}^{1} (\lambda_i \cdot \log(\lambda_i, 2)) = 0 \qquad \log\left[\prod_{i=0}^{1} (\lambda_i)^{-\lambda_i}, 2\right] = 0$$

$$\lambda := \mathrm{eigenvals}(\rho_{mix}) = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix} \qquad -\sum_{i=0}^{1} (\lambda_i \cdot \log(\lambda_i, 2)) = 1 \qquad \log\left[\prod_{i=0}^{1} (\lambda_i)^{-\lambda_i}, 2\right] = 1$$

Finally we show that ρ_{mix} cannot represent a superposition.

$$\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \neq \begin{pmatrix} a \\ b \end{pmatrix}\begin{pmatrix} a & b \end{pmatrix} = \begin{pmatrix} a^2 & ab \\ ab & b^2 \end{pmatrix}$$

Comparing the left and right sides we conclude that: $a^2 = b^2 = 1/2$ and $ab = 0$. These constraints are contradictory.

Composite two-particle entangled states are also superpositions. Below one of the Bell states is constructed. Bell states are maximally entangled superpositions of two-particle states.

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow_1\rangle \otimes |\uparrow_2\rangle + |\downarrow_1\rangle \otimes |\downarrow_2\rangle\right] = \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right] = \frac{1}{\sqrt{2}}\left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

This is an entangled state because it cannot be factored as is shown below.

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \neq \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ a_1 b_2 \\ a_2 b_1 \\ a_2 b_2 \end{pmatrix}$$

Comparing the left and right sides we conclude that: $a_1b_1 = a_2b_2 = 1/\mathrm{sqrt}(2)$ and $a_1b_2 = a_2b_1 = 0$. There are no values of a_1, a_2, b_1 and b_2 that satisfy these constraints.

Because entangled wave functions are not separable the entangled particles represented by such wave functions do not have separate identities or individual properties. However, if the spin orientation of particle 1 is learned through measurement, the spin orientation of particle 2 is also immediately known no matter how far away it may be. Entanglement suggests nonlocal phenomena which in the words of Nick Herbert are "unmediated, unmitigated and immediate."

Next we form the state operator of the two-particle entangled state.

$$|\Psi\rangle\langle\Psi| = \frac{1}{2}\left[|\uparrow_1\rangle \otimes |\uparrow_2\rangle + |\downarrow_1\rangle \otimes |\downarrow_2\rangle\right]\left[\langle\uparrow_2| \otimes \langle\uparrow_1| + \langle\downarrow_2| \otimes \langle\downarrow_1|\right]$$

$$|\Psi\rangle\langle\Psi| = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 0 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0 & 0 & 1\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\1 & 0 & 0 & 1\end{pmatrix} \qquad \rho_{ent} := \frac{1}{2}\cdot\begin{pmatrix}1 & 0 & 0 & 1\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\1 & 0 & 0 & 1\end{pmatrix}$$

The two-spin entangled state is a pure state:

$$\mathrm{tr}\left(\rho_{ent}\right) = 1 \qquad \mathrm{tr}\left(\rho_{ent}{}^2\right) = 1$$

Next we demonstrate the correlation inherent in this entangled state. Spin measurements in the z- and x-directions on the spins always yields the same result (highlighted below). Kronecker is Mathcad's command for tensor multiplication of matrices.

$$\mathrm{SzSz} := \mathrm{kronecker}\left(\sigma_z, \sigma_z\right) \quad \mathrm{tr}\left(\rho_{ent}\cdot \mathrm{SzSz}\right) = 1 \qquad \mathrm{SxSx} := \mathrm{kronecker}\left(\sigma_x, \sigma_x\right) \quad \mathrm{tr}\left(\rho_{ent}\cdot \mathrm{SxSx}\right) = 1$$

Initially the x-direction measurement result may seem strange. However, it is easy to show that writing the entangled wave function in the x-basis is identical to the z-basis version.

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \qquad \langle\uparrow_x| = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\end{pmatrix} \qquad |\downarrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \qquad \langle\downarrow_x| = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\end{pmatrix}$$

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow_{x1}\rangle \otimes |\uparrow_{x2}\rangle + |\downarrow_{x1}\rangle \otimes |\downarrow_{x2}\rangle\right] = \frac{1}{2\sqrt{2}}\left[\begin{pmatrix}1\\1\end{pmatrix}\otimes\begin{pmatrix}1\\1\end{pmatrix} + \begin{pmatrix}1\\-1\end{pmatrix}\otimes\begin{pmatrix}1\\-1\end{pmatrix}\right] = \frac{1}{2\sqrt{2}}\left[\begin{pmatrix}1\\1\\1\\1\end{pmatrix} + \begin{pmatrix}1\\-1\\-1\\1\end{pmatrix}\right] = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}$$

Inspite of the strong correlation observed when the spins of both particles are measured in the same direction, spin measurements on the individual particles are completely random.

$$\mathrm{SzI} := \mathrm{kronecker}\left(\sigma_z, I\right) \quad \mathrm{SxI} := \mathrm{kronecker}\left(\sigma_x, I\right) \quad \mathrm{ISz} := \mathrm{kronecker}\left(I, \sigma_z\right) \quad \mathrm{ISx} := \mathrm{kronecker}\left(I, \sigma_x\right)$$

$$\mathrm{tr}\left(\rho_{ent}\cdot \mathrm{SzI}\right) = 0 \quad \mathrm{tr}\left(\rho_{ent}\cdot \mathrm{SxI}\right) = 0 \quad \mathrm{tr}\left(\rho_{ent}\cdot \mathrm{ISz}\right) = 0 \quad \mathrm{tr}\left(\rho_{ent}\cdot \mathrm{ISx}\right) = 0$$

This can be confirmed by expanding the state operator in the fashion shown below, and then "tracing" over the spin states of particle 1. The terms highlighted in blue survive the trace operation.

$$|\Psi\rangle\langle\Psi| = \frac{1}{2}\left[|\uparrow_1\rangle|\uparrow_2\rangle\langle\uparrow_2|\langle\uparrow_1| + |\uparrow_1\rangle|\uparrow_2\rangle\langle\downarrow_2|\langle\downarrow_1| + |\downarrow_1\rangle|\downarrow_2\rangle\langle\uparrow_2|\langle\uparrow_1| + |\downarrow_1\rangle|\downarrow_2\rangle\langle\downarrow_2|\langle\downarrow_1|\right]$$

$$\rho_2 = \frac{1}{2}\left[\langle\uparrow_1|\Psi\rangle\langle\Psi|\uparrow_1\rangle + \langle\downarrow_1|\Psi\rangle\langle\Psi|\downarrow_1\rangle\right] = \frac{1}{2}\left[|\uparrow_2\rangle\langle\uparrow_2| + |\downarrow_2\rangle\langle\downarrow_2|\right]$$

This yields the partial state operator of particle 2 and shows that it behaves like a classical mixture, consistent with the previous results.

Now the calculations on the entangled state using the state operator will be repeated using the state vector.

$$\Psi_{ent} := \frac{1}{\sqrt{2}} \cdot (1 \ \ 0 \ \ 0 \ \ 1)^T$$

$$\Psi_{ent}{}^T \cdot SzSz \cdot \Psi_{ent} = 1 \qquad \Psi_{ent}{}^T \cdot SxSx \cdot \Psi_{ent} = 1$$

$$\Psi_{ent}{}^T \cdot SzI \cdot \Psi_{ent} = 0 \quad \Psi_{ent}{}^T \cdot ISz \cdot \Psi_{ent} = 0 \quad \Psi_{ent}{}^T \cdot SxI \cdot \Psi_{ent} = 0 \quad \Psi_{ent}{}^T \cdot ISx \cdot \Psi_{ent} = 0$$

Finally we calculate the expectation values when the spins are measured in different direction using both computational methods.

$$SzSx := \mathrm{kronecker}(\sigma_z, \sigma_x) \qquad SxSz := \mathrm{kronecker}(\sigma_x, \sigma_z)$$

$$\mathrm{tr}(\rho_{ent} \cdot SzSx) = 0 \qquad \mathrm{tr}(\rho_{ent} \cdot SxSz) = 0$$

$$\Psi_{ent}{}^T \cdot SzSx \cdot \Psi_{ent} = 0 \qquad \Psi_{ent}{}^T \cdot SxSz \cdot \Psi_{ent} = 0$$

Say the first spin is measured in the z-direction and found to be spin-up. This means the second spin is also spin-up in the z-direction, which is an even superposition of spin-up and spin-down in the x-direction, giving an over all expectation value of zero.

Ψ_{ent} is one of the Bell states. For extensive calculations on it and the other three Bell states see "Bell State Exercises."