# Visualizing the Difference Between a Superposition and a Mixture

Frank Rioux
Department of Chemistry
College of Saint Benedict|Saint John's University
St. Joseph, MN 56374

The superposition principle, as Feynman said, is at the heart of quantum mechanics. While its mathematical expression is simple, its true meaning is difficult to grasp. For example, given a linear superposition (not normalized) of two states,

$$|\Psi\rangle = |\phi_1\rangle + |\phi_2\rangle$$

one might assume that it represents a mixture of $\phi_1$ and $\phi_2$. In other words, half of the quons [1] are in state $\phi_1$ and half in $\phi_2$. However, the correct quantum mechanical interpretation of this equation is that the system represented by $\Psi$ is simultaneously in the states $\phi_1$ and $\phi_2$, properly weighted.

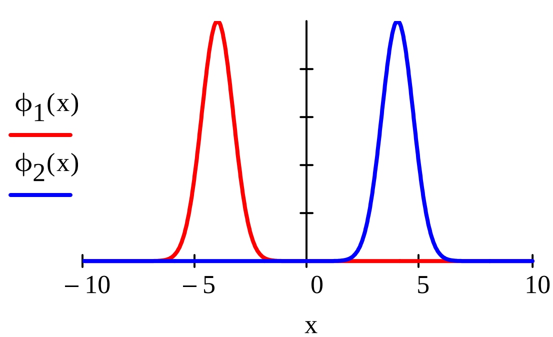
A mixture, half $\phi_1$ and half $\phi_2$, or any other ratio, cannot be represented by a wavefunction. It requires a density operator, which is a more general quantum mechanical construct that can be used to represent both pure states (superpositions) and mixtures, as shown below.

$$\hat{\rho}_{pure} = |\Psi\rangle\langle\Psi| \qquad\qquad \hat{\rho}_{mixed} = \sum p_i |\Psi_i\rangle\langle\Psi_i|$$

In the equation on the right, $p_i$ is the fraction of the mixture in the state $\Psi_i$.

To illustrate how these equations distinguish between a mixture and a superposition, we will consider a superposition and a mixture of equally weighted gaussian functions representing one-dimensional wave packets. The normalization constants are omitted in the interest of mathematical clarity. The gaussians are centered at x = +/- 4.

$$\phi_1(x) := \exp\left[-(x+4)^2\right] \qquad \phi_2(x) := \exp\left[-(x-4)^2\right]$$




To visualize how the density operator discriminates between a superposition and a mixture, we calculate its matrix elements in coordinate space for the 50-50 superposition and mixture of $\phi_1$ and $\phi_2$. The superposition is considered first.

$$\Psi(x) := \phi_1(x) + \phi_2(x)$$

The matrix elements of this pure state are calculated as follows.

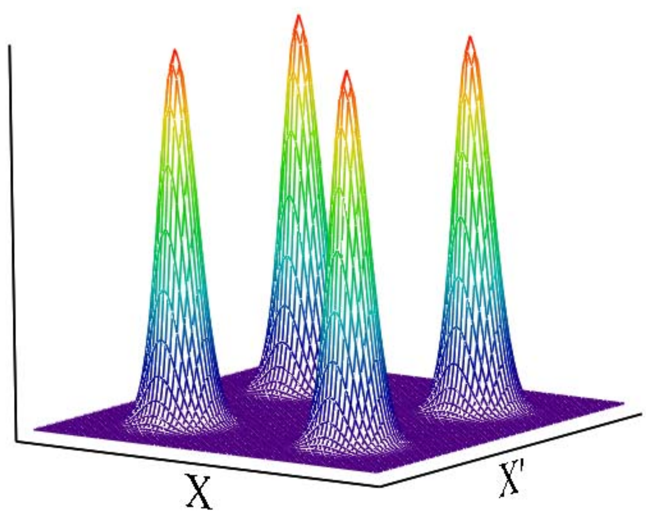
$$\rho_{pure} = \langle x | \hat{\rho}_{pure} | x' \rangle = \langle x | \Psi \rangle \langle \Psi | x' \rangle$$

Looking at the right side we see that the matrix elements are the product of the probability amplitudes of a quon in state Ψ being at x and x'. Next we display the density matrix graphically.

$$\text{DensityMatrixPure}(x, x') := \Psi(x) \cdot \Psi(x')$$

$x_0 := 8$ $\quad N := 80$ $\quad i := 0 .. N$ $\quad x_i := -x_0 + \frac{2 \cdot x_0 \cdot i}{N}$ $\quad j := 0 .. N$ $\quad x'_j := -x_0 + \frac{2 \cdot x_0 \cdot j}{N}$

$$\text{DensityMatrixPure}_{i,j} := \text{DensityMatrixPure}\left(x_i, x'_j\right)$$




DensityMatrixPure

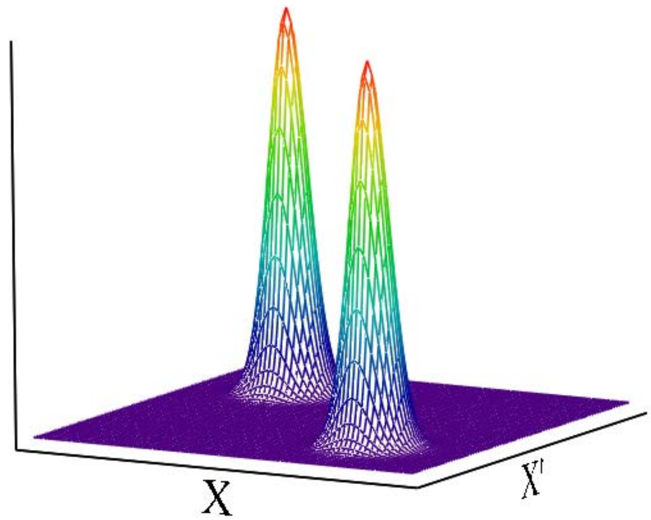
The presence of off-diagonal elements in this density matrix is the signature of a quantum mechanical superposition. For example, from the quantum mechanical perspective bi-location is possible.

Now we turn our attention to the density matrix of a mixture of gaussian states.

$$\rho_{mix} = \langle x | \hat{\rho}_{mix} | x' \rangle = \sum_i p_i \langle x | \phi_i \rangle \langle \phi_i | x' \rangle = \tfrac{1}{2} \langle x | \phi_1 \rangle \langle \phi_1 | x' \rangle + \tfrac{1}{2} \langle x | \phi_2 \rangle \langle \phi_2 | x' \rangle$$

$$\text{DensityMatrixMix}(x, x') := \frac{\phi_1(x) \cdot \phi_1(x') + \phi_2(x) \cdot \phi_2(x')}{2}$$

$$\text{DensityMatrixMix}_{i,j} := \text{DensityMatrixMix}\left(x_i, x'_j\right)$$




DensityMatrixMix

The obvious difference between a superposition and a mixture is the absence of off-diagonal elements, $\phi_1(x)\cdot\phi_2(x') + \phi_2(x)\cdot\phi_1(x')$, in the mixed state. This indicates the mixture is in a definite but unknown state; it is an example of classical ignorance.

An equivalent way to describe the difference between a superposition and a mixture, is to say that to calculate the probability of measurement outcomes for a superpostion you add the probability amplitudes and square the sum. For a mixture you square the individual probability amplitudes and sum the squares.

1. Nick Herbert (*Quantum Reality*, page 64) suggested "quon" be used to stand for a generic quantum object. "A quon is any entity, no matter how immense, that exhibits both wave and particle aspects in the peculiar quantum manner.