Pure States, Mixtures and the Density Operator

Frank Rioux
Department of Chemistry
College of St. Benedict | St. John's Unversity

Calculations with polarized and un-polarized light will be used to illustrate the difference between pure states and mixtures, and to demonstrate the utility of the density operator.

In Heisenberg's matrix mechanics pure states are represented by vectors and operators by matrices. For example, light polarized at an angle θ relative to the vertical is represented by the following Dirac ket vector,

$$|\theta\rangle = \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix}$$

The matrix operator for a polarizer oriented at an angle θ relative to the vertical in Dirac notation is represented by a ket-bra product (outer product).

$$\hat{\theta} = |\theta\rangle\langle\theta| = \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} \begin{pmatrix} \cos(\theta) & \sin(\theta) \end{pmatrix} = \begin{pmatrix} \cos^2(\theta) & \cos(\theta)\sin(\theta) \\ \cos(\theta)\sin(\theta) & \sin^2(\theta) \end{pmatrix}$$

The state vector is normalized because the bra-ket product, or inner product, is unity.

$$\langle\theta|\theta\rangle = \begin{pmatrix} \cos(\theta) & \sin(\theta) \end{pmatrix} \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} = \cos^2(\theta) + \sin^2(\theta) = 1$$

Clearly the state vector is an eigenstate of the operator with unit eigenvalue.

$$\hat{\theta}|\theta\rangle = |\theta\rangle\langle\theta|\theta\rangle = |\theta\rangle$$

Un-polarized light from an incandescent bulb is incident upon a polarizing film oriented at an angle θ relative to the vertical producing θ-polarized light, $|\theta\rangle$. State preparation, such as this, is an essential first step in any quantum mechanical analysis.

As shown below, the expectation value for the passage of this θ-polarized light through a vertical polarizer is $\cos^2(\theta)$.

$$\langle V\rangle = \langle\theta|\hat{V}|\theta\rangle = \begin{pmatrix} \cos(\theta) & \sin(\theta) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix} = \cos^2(\theta)$$

We can also argue that θ-polarized light is a coherent superposition of vertically and horizontally polarized light.

$$|\theta\rangle = |v\rangle\langle v|\theta\rangle + |h\rangle\langle h|\theta\rangle = \cos(\theta)|v\rangle + \sin(\theta)|h\rangle = \cos(\theta)\begin{pmatrix}1\\0\end{pmatrix} + \sin(\theta)\begin{pmatrix}0\\1\end{pmatrix}$$

where

$$|v\rangle\langle v| + |h\rangle\langle h| = 1$$

is the identity operator. In other words, $|v\rangle$ and $|h\rangle$ are an orthonormal basis for linear polarization. Any linear polarization state can be expressed as a superposition of these basis vectors.

The probability that a θ-polarized photon will pass a vertical polarizer in this approach is the probability amplitude for that event squared, $|\langle v|\theta\rangle|^2 = \cos^2(\theta)$.

The calculation for the expectation value $\langle\theta|\hat{V}|\theta\rangle$ can also be re-cast in terms of $\hat{\theta}$ by exploiting the idempotency of $\hat{V}$.

$$\hat{V}\,\hat{V} = \hat{V}|v\rangle\langle v| = |v\rangle\langle v|v\rangle\langle v| = |v\rangle\langle v| = \hat{V}$$

Using $\hat{V} = \hat{V}\,\hat{V}$ we find

$$\langle V\rangle = \langle\theta|\hat{V}\,\hat{V}|\theta\rangle = \langle\theta|\hat{V}|v\rangle\langle v|\theta\rangle = \langle v|\theta\rangle\langle\theta|\hat{V}|v\rangle = \langle v|\hat{\theta}\,\hat{V}|v\rangle = \mathrm{Trace}\left(\hat{\theta}\,\hat{V}\right)$$

where *Trace* signifies the sum of the diagonal elements of the product matrix. By substituting $\hat{\theta}$ and $\hat{V}$ we find agreement with the previous method of calculating the expectation value.

$$\langle V\rangle = \mathrm{Trace}\left[\begin{pmatrix}\cos^2(\theta) & \cos(\theta)\sin(\theta)\\ \cos(\theta)\sin(\theta) & \sin^2(\theta)\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}\right] = \cos^2(\theta)$$

This approach, while mathematically interesting, is non-intuitive compared with the previous traditional method. One might question its utility in the face of the more direct method of calculating expectation values.

The utility of this method is apparent when one considers the calculation of the expectation values for a mixture – such as un-polarized light. Un-polarized light is an even mixture of all possible polarization states. However, it can be treated as a 50-50 mixture of any two orthogonal polarization states. Such a mixture **cannot** be represented by the wave function,

$$\left|\Psi\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\theta\right\rangle + \left|\theta + \frac{\pi}{2}\right\rangle\right)$$

because in quantum mechanical notation this represents a pure state, a coherent superposition of two orthogonal polarization states.

Rather, a mixture must be represented by a **density operator**, which is a weighted sum of the operators representing the states making up the mixture. The density operator for un-polarized light is,

$$\hat{\rho} = \frac{1}{2}\left|\theta\right\rangle\left\langle\theta\right| + \frac{1}{2}\left|\theta + \frac{\pi}{2}\right\rangle\left\langle\theta + \frac{\pi}{2}\right|$$

The expectation value for un-polarized light to pass a vertical polarizer according to the last method is

$$\left\langle V\right\rangle = \text{Trace}\left[\frac{1}{2}\left(\begin{pmatrix}\cos^2(\theta) & \cos(\theta)\sin(\theta) \\ \cos(\theta)\sin(\theta) & \sin^2(\theta)\end{pmatrix} + \begin{pmatrix}\cos^2(\theta + \frac{\pi}{2}) & \cos(\theta + \frac{\pi}{2})\sin(\theta + \frac{\pi}{2}) \\ \cos(\theta + \frac{\pi}{2})\sin(\theta + \frac{\pi}{2}) & \sin^2(\theta + \frac{\pi}{2})\end{pmatrix}\right)\begin{pmatrix}1 & 0 \\ 0 & 0\end{pmatrix}\right] = \frac{1}{2}$$

This method can be used to derive an alternative method for calculating the expectation value for a mixture.

$$\left\langle V\right\rangle = \text{Trace}\left[\hat{\rho}\,\hat{V}\right] = \left\langle v\right|\hat{\rho}\,\hat{V}\left|v\right\rangle$$

$$\left\langle V\right\rangle = \left\langle v\right|\left(\frac{1}{2}\left|\theta\right\rangle\left\langle\theta\right| + \frac{1}{2}\left|\theta + \frac{\pi}{2}\right\rangle\left\langle\theta + \frac{\pi}{2}\right|\right)\hat{V}\left|v\right\rangle = \frac{1}{2}\left\langle v|\theta\right\rangle\left\langle\theta|v\right\rangle + \frac{1}{2}\left\langle v\middle|\theta + \frac{\pi}{2}\right\rangle\left\langle\theta + \frac{\pi}{2}\middle|v\right\rangle$$

$$\left\langle V\right\rangle = \frac{1}{2}\left\langle\theta|v\right\rangle\left\langle v|\theta\right\rangle + \frac{1}{2}\left\langle\theta + \frac{\pi}{2}\middle|v\right\rangle\left\langle v\middle|\theta + \frac{\pi}{2}\right\rangle = \frac{1}{2}\left\langle\theta\right|\hat{V}\left|\theta\right\rangle + \frac{1}{2}\left\langle\theta + \frac{\pi}{2}\middle|\hat{V}\middle|\theta + \frac{\pi}{2}\right\rangle$$

$$\left\langle V\right\rangle = \frac{1}{2}\cos^2(\theta) + \frac{1}{2}\cos^2(\theta + \frac{\pi}{2}) = \frac{1}{2}$$

In general, for a mixture the expectation value is calculated as

$$\left\langle V\right\rangle = \sum_i p_i\left\langle\Psi_i\right|\hat{V}\left|\Psi_i\right\rangle$$

where p_i is the probability associated with the state $\left|\Psi_i\right\rangle$.