# Using the Trace Function to Calculate Expectation Values

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Starting with the traditional expression for the calculation of the expectation value, the identity operator is inserted between the measurement operator and the ket containing the wave function. Rearranging terms gives the trace function operating on the product of the state's density operator and the measurement operator.

$$\langle \Psi | \hat{O} | \Psi \rangle = \sum_i \langle \Psi | \hat{O} | i \rangle \langle i | \Psi \rangle = \sum_i \langle i | \Psi \rangle \langle \Psi | \hat{O} | i \rangle = Trace\left( | \Psi \rangle \langle \Psi | \hat{O} \right) \quad \text{where} \quad \sum_i | i \rangle \langle i | = Identity$$

Next this transition is carried out in detail using matrix algebra.

$$\begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \left[ \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} \right] \begin{pmatrix} a \\ b \end{pmatrix} = 2ab$$

$$\begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} + \begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 2ab$$

$$\begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 2ab$$

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

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

$$(a \;\; b) \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \end{pmatrix} \rightarrow 2 \cdot a \cdot b \qquad (a \;\; b) \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \end{pmatrix} \rightarrow 2 \cdot a \cdot b$$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot (1 \;\; 0) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot (0 \;\; 1) \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$(a \;\; b) \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot (1 \;\; 0) \cdot \begin{pmatrix} a \\ b \end{pmatrix} + (a \;\; b) \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \cdot (0 \;\; 1) \cdot \begin{pmatrix} a \\ b \end{pmatrix} \rightarrow 2 \cdot a \cdot b$$

$$(1 \;\; 0) \cdot \begin{pmatrix} a \\ b \end{pmatrix} \cdot (a \;\; b) \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + (0 \;\; 1) \cdot \begin{pmatrix} a \\ b \end{pmatrix} \cdot (a \;\; b) \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow 2 \cdot a \cdot b$$

$$\mathrm{tr}\left[ \begin{pmatrix} a \\ b \end{pmatrix} \cdot (a \;\; b) \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right] \rightarrow 2 \cdot a \cdot b \qquad \mathrm{tr}\left[ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \end{pmatrix} \cdot (a \;\; b) \right] \rightarrow 2 \cdot a \cdot b$$

The last calculation on the right is justified by the following:

$$\langle \Psi | \hat{O} | \Psi \rangle = \sum_i \langle \Psi | i \rangle \langle i | \hat{O} | \Psi \rangle = \sum_i \langle i | \hat{O} | \Psi \rangle \langle \Psi | i \rangle = Trace\left( \hat{O} | \Psi \rangle \langle \Psi | \right)$$