The State Function and Expectation Values

From Section 3.3: "The third postulate of quantum mechanics establishes the existence of the state function and its relevance to the properties of a system: The state of a system at any instant in time may be represented by a state or wave function ψ which is continuous and differentiable. All information regarding the state of the system is contained in the wavefunction."

State Function - $\psi(\vec{r},t)$ - from the state function, we know everything about the system.

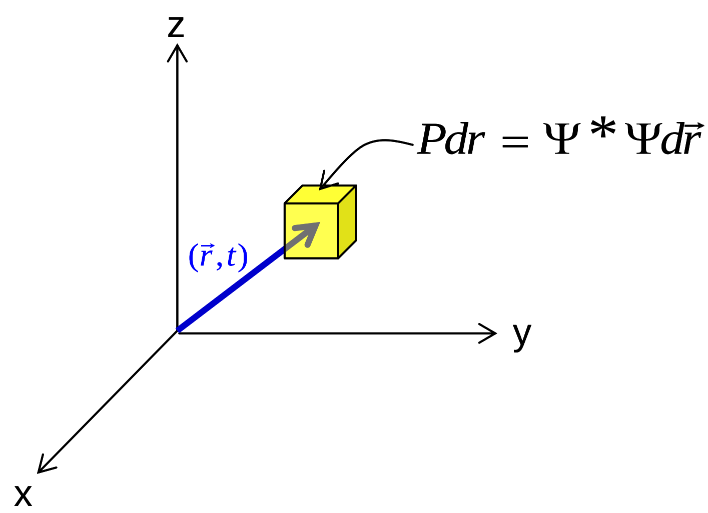
Expectation value – the value one expects to obtain in any given measurement. Generally:

$$\text{Average value:} \quad \bar{v} = \int_{-\infty}^{\infty} \Pr v\,dx$$

$$\text{Expectation value:} \quad \langle A \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{\mathbf{A}} \Psi dx$$

Example: We only know the average location, not the actual position.

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\hat{\mathbf{x}}\Psi(x,t)dx = \int_{-\infty}^{\infty} \frac{x\Psi^*\Psi dx}{|\Psi|^2}$$



Mean-Square Deviation

$$(\Delta c)^2 = \left\langle (c - \langle c \rangle)^2 \right\rangle = \left\langle c^2 - 2\langle c \rangle c + \langle c \rangle^2 \right\rangle = \langle c^2 \rangle - \langle c \rangle^2$$

Example Of Computations Using a Specific Wavefunction

Dr. Shen spent most of today's lecture time discussing the specific example on page 78-80. Portions of the homework problem 3.11 were done in class.

$$\psi(x,t) = A\underbrace{\exp\left[\frac{-(x-x_0)^2}{4a^2}\right]}_{\text{Position}}\underbrace{\exp\left(\frac{ip_0x}{\hbar}\right)}_{\text{Momentum}}\underbrace{\exp(-i\omega_0 t)}_{\text{Quantum Phase}}$$

To solve problem 3.11, we need to calculate Δx and Δp. To get the mean square deviation, we need to find <x>, <x^2>, <p> and <p^2>.

Normalization is shown in the book, introduces some dummy variables:

$$A^2 = \frac{1}{a\sqrt{2\pi}}$$

introduce dummy vari ables η and η_0

$$\eta = \frac{(x-x_0)}{a}$$

$$x = a(\eta + \eta_0)$$

$$\eta_0 = \frac{x_0}{a}$$

Computing <x>

$$\begin{aligned}
\langle x\rangle &= \int_{-\infty}^{\infty} \psi * \hat{x}\psi\, dx \\
&= \int_{-\infty}^{\infty} \psi * x\psi\, dx \\
&= A^2a^2 \int_{-\infty}^{\infty} (\eta + \eta_0) e^{-\eta^2/2}\, d\eta \\
&= \cancelto{0}{A^2a^2 \int_{-\infty}^{\infty} \eta e^{-\eta^2/2}\, d\eta} + A^2a^2\eta_0 \int_{-\infty}^{\infty} e^{-\eta^2/2}\, d\eta \\
&= 0 + A^2a^2\eta_0\sqrt{2\pi} \\
&= a\eta_0 \\
&= x_0
\end{aligned}$$

The book shows that $\langle x^2 \rangle = a^2 + x_0{}^2$ because Δx is the square root of the variance of the Gaussian function is a. Dr. Shen wrote the result and referred us to the book for details.

Computing <x^2> [Note: This part wasn't done in class, but I added it for completeness]

$$\begin{aligned}
\langle x^2 \rangle &= \int_{-\infty}^{\infty} \psi * \hat{x}\hat{x}\psi \, dx \\
&= \int_{-\infty}^{\infty} \psi * x^2 \psi \, dx \\
&= A^2 a^3 \int_{-\infty}^{\infty} (\eta + \eta_0)^2 \, e^{-\eta^2/2} \, d\eta \\
&= A^2 a^3 \int_{-\infty}^{\infty} \eta^2 e^{-\eta^2/2} \, d\eta + 2A^2 a^3 \eta_0 \cancelto{0}{\int_{-\infty}^{\infty} \eta e^{-\eta^2/2} \, d\eta} + A^2 a^3 \eta_0{}^2 \int_{-\infty}^{\infty} e^{-\eta^2/2} \, d\eta \\
&= A^2 a^3 \sqrt{2\pi} + 0 + A^2 a^3 \eta_0{}^2 \sqrt{2\pi} \\
&= A^2 a^3 \frac{1}{A^2 a} + a^2 \eta_0{}^2 \\
&= a^2 + x_0{}^2
\end{aligned}$$

Computing $\langle p \rangle$ (Dr. Shen's way)

First find:

$$\begin{aligned}
\frac{\partial}{\partial x}\psi(x,t) &= A\left\{\frac{-2(x-x_0)}{4a^2}\right\}\exp\left[\frac{-(x-x_0)^2}{4a^2}\right]\exp\left(\frac{ip_0 x}{\hbar}\right)\exp(-i\omega_0 t) \\
&\quad + A\left\{\frac{ip_0}{\hbar}\right\}\exp\left[\frac{-(x-x_0)^2}{4a^2}\right]\exp\left(\frac{ip_0 x}{\hbar}\right)\exp(-i\omega_0 t) \\
&= \left(\frac{-2(x-x_0)}{4a^2} + \frac{ip_0}{\hbar}\right)\psi(x,t)
\end{aligned}$$

$$\begin{aligned}
\langle p \rangle &= \int_{-\infty}^{\infty} \psi * \hat{p}\psi \, dx = \int_{-\infty}^{\infty} \psi * \left(-i\hbar \frac{\partial}{\partial x}\right)\psi \, dx \\
&= (-i\hbar)\int_{-\infty}^{\infty} \psi * \psi \left(\frac{-2(x-x_0)}{4a^2} + \frac{ip_0}{\hbar}\right) dx \\
&= (-i\hbar)\int_{-\infty}^{\infty} \psi * \psi \cancelto{0}{\left(\frac{-2(x-x_0)}{4a^2}\right)} dx + (-i\hbar)\frac{ip_0}{\hbar}\int_{-\infty}^{\infty} \psi * \psi \, dx \\
&= p_0
\end{aligned}$$

Carrying out the math a little more… [Note: This part wasn't done in class, but I added it for completeness]

$$\langle p\rangle = \int_{-\infty}^{\infty}\psi * \hat{p}\,\psi dx = \int_{-\infty}^{\infty}\psi * \left(-i\hbar\frac{\partial}{\partial x}\right)\psi dx$$

$$= \int_{-\infty}^{\infty}\psi * (-i\hbar)\left(\frac{-2(x-x_0)}{4a^2}+\frac{ip_0}{\hbar}\right)\psi dx$$

$$= \int_{-\infty}^{\infty}(-i\hbar)\left(\frac{-2(x-x_0)}{4a^2}+\frac{ip_0}{\hbar}\right)A^2\exp\left[\frac{-2(x-x_0)^2}{4a^2}\right]dx$$

$$= (-i\hbar)A^2\int_{-\infty}^{\infty}\left(\frac{-2(x-x_0)}{4a^2}+\frac{ip_0}{\hbar}\right)\exp\left[\frac{-2(x-x_0)^2}{4a^2}\right]dx$$

$$= (-i\hbar)A^2\int_{-\infty}^{\infty}\left(\frac{-2(x-x_0)}{4a^2}\right)\exp\left[\frac{-2(x-x_0)^2}{4a^2}\right]dx + (-i\hbar)A^2\int_{-\infty}^{\infty}\left(\frac{ip_0}{\hbar}\right)\exp\left[\frac{-2(x-x_0)^2}{4a^2}\right]dx$$

the first integral is zero because it is an odd function over all space,
for second integral, change variables to $u=(x-x_0)/a$ to $du = dx/a$

$$= (-i\hbar)A^2\left(\frac{ip_0}{\hbar}\right)\int_{-\infty}^{\infty}\exp\left[\frac{-u^2}{2}\right]a\,du$$

$$= A^2 a p_0\int_{-\infty}^{\infty}\exp\left[\frac{-u^2}{2}\right]du$$

$$= A^2 a p_0\sqrt{2\pi}$$

$$= p_0$$

The book uses a change in variables:

$$\langle p\rangle = \int_{-\infty}^{\infty}\psi * \hat{p}\,\psi dx = \int_{-\infty}^{\infty}\psi * \left(-i\hbar\frac{\partial}{\partial x}\right)\psi dx = A^2 a\int_{-\infty}^{\infty}\left(p_0+\frac{i\hbar}{2a}\eta\right)e^{-\eta^2/2}\,d\eta$$

$$= p_0 A^2 a\int_{-\infty}^{\infty}e^{-\eta^2/2}\,d\eta = p_0 A^2 a\sqrt{2\pi} = p_0$$

Back to class lecture notes…

Computing $\langle p^2 \rangle$ (Dr. Shen outlined a way and gave us the answer)

$$\hat{\mathbf{p}}^2 = \hat{\mathbf{p}}\hat{\mathbf{p}} = \left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right) = \left(\hbar^2\frac{\partial^2}{\partial x^2}\right)$$

$$\frac{\partial^2}{\partial x^2}\psi(x,t) = \frac{\partial}{\partial x}\left(\frac{-(x-x_0)}{2a^2} + \frac{ip_0}{\hbar}\right)\psi(x,t)$$
$$= \underbrace{\frac{-1}{2a^2}\psi - \frac{-(x-x_0)}{2a^2}\frac{\partial}{\partial x}\psi}_{\Rightarrow \frac{\hbar^2}{4a}} + \underbrace{\left(\frac{ip_0}{\hbar}\right)\frac{\partial}{\partial x}\psi}_{\Rightarrow p_0^2}$$

☼ **Homework: 3.11.**

Heisenberg's uncertainty principle

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Hints for homework problem:

$$\langle p \rangle = p_0$$

$$\langle p \rangle^2 = p_0^2$$

$$\langle p^2 \rangle = \frac{\hbar^2}{4a^2} + p_0^2$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\frac{\hbar^2}{4a^2} + p_0^2 - p_0^2} = \frac{\hbar}{2a}$$

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{a^2 + x_0^2 - x_0^2} = a$$

$$\Delta x \Delta p = a\frac{\hbar}{2a} = \frac{\hbar}{2}$$

Time Dependent Schrödinger Equation

This is the way to write the time dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)=\hat{H}\Psi(\vec{r},t)$$

The Hamiltonian operator is:

$$\hat{H}=\frac{p^2}{2m}+V(\vec{r},t)$$

In general, if the potential is a function of time, the problem is too complicated to solve. So, we confine ourselves to the domain of problems in which:

$$\hat{H}=\frac{p^2}{2m}+V(\vec{r})$$

Solve by using product form of wavefunction for separation of variables:

$$\Psi(\vec{r},t)=\varphi(\vec{r})T(t)$$

Put into the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\varphi(\vec{r})T(t)=\hat{H}\varphi(\vec{r})T(t)$$

$$i\hbar\varphi(\vec{r})\frac{\partial}{\partial t}T(t)=T(t)\hat{H}\varphi(\vec{r})$$

$$\frac{i\hbar\frac{\partial}{\partial t}T(t)}{T(t)}=\frac{\hat{H}\varphi(\vec{r})}{\varphi(\vec{r})}=E$$

This can be separated into two different equations, one in time and one in space. Start with time – it is easy to solve:

$$i\hbar\frac{\partial}{\partial t}T(t)=ET(t)$$

$$T(t)=A\exp\left(\frac{-iEt}{\hbar}\right)$$

The space part is the eigenvalue equation:

$$\hat{\mathbf{H}}\varphi(x)=E\varphi(x)$$

The solution to the time dependent Schrödinger equation is written this way with *n* being the quantum number (each solution has a quantum number.):

$$\Psi_n(\vec{r},t)=A\exp\left(\frac{-iEt}{\hbar}\right)\varphi_n(\vec{r})$$

$$\hat{\mathbf{H}}\varphi_n(x)=E_n\varphi_n(x)$$

Consider the free particle – V(x) = 0

Another way to write the eigenfunction plane wave in x-direction:

$$\varphi_k = A\exp(ikx)$$

$$E_k = \frac{\hbar^2 k^2}{2m} = \hbar\omega$$

$$\varphi_k(x,t) = A\exp^{i(kx-\omega t)}$$

$$f(x,t) = f(x - vt)$$

$$v = \frac{\omega}{k} = \frac{p}{2m} = \frac{\text{classical particle velocity}}{2}$$

In classical mechanics, the position is known. In quantum mechanics, different positions have the same probability.