Problem 1.7

Calculate $d\langle p\rangle/dt$. *Answer*:

$$\frac{d\langle p\rangle}{dt} = \left\langle -\frac{\partial V}{\partial x}\right\rangle. \tag{1.38}$$

This is an instance of **Ehrenfest's theorem**, which asserts that *expectation values obey the classical laws.*[19]

Solution

Note the Schrödinger equation and take the complex conjugate of both sides.

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V(x,t)\Psi(x,t) \tag{1}$$

$$\frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V(x,t)\Psi^*(x,t) \tag{2}$$

According to Ehrenfest's theorem,

$$\langle p\rangle = m\langle v\rangle = m\frac{d\langle x\rangle}{dt}. \tag{3}$$

Start by determining the expectation value of x.

$$\begin{aligned}\langle x\rangle = \frac{\int_{-\infty}^{\infty} x|\Psi(x,t)|^2\,dx}{\int_{-\infty}^{\infty}|\Psi(x,t)|^2\,dx} = \frac{\int_{-\infty}^{\infty} x|\Psi(x,t)|^2\,dx}{1} &= \int_{-\infty}^{\infty} x|\Psi(x,t)|^2\,dx \\ &= \int_{-\infty}^{\infty} x\Psi(x,t)\Psi^*(x,t)\,dx \\ &= \int_{-\infty}^{\infty} \Psi^*(x,t)(x)\Psi(x,t)\,dx\end{aligned}$$

Differentiate both sides with respect to t.

$$\begin{aligned}\frac{d\langle x\rangle}{dt} &= \frac{d}{dt}\int_{-\infty}^{\infty} \Psi^*(x,t)(x)\Psi(x,t)\,dx \\ &= \int_{-\infty}^{\infty} \frac{\partial}{\partial t}[\Psi^*(x,t)(x)\Psi(x,t)]\,dx \\ &= \int_{-\infty}^{\infty} x\frac{\partial}{\partial t}[\Psi^*(x,t)\Psi(x,t)]\,dx \\ &= \int_{-\infty}^{\infty} x\left(\frac{\partial \Psi^*}{\partial t}\Psi + \Psi^*\frac{\partial\Psi}{\partial t}\right)dx\end{aligned}$$

[19]Some authors limit the term to the pair of equations $\langle p\rangle = m\,d\langle x\rangle/dt$ and $\langle -\partial V/\partial x\rangle = d\langle p\rangle/dt$.

Substitute equations (1) and (2) for the time derivatives.

$$\begin{aligned}
\frac{d\langle x\rangle}{dt} &= \int_{-\infty}^{\infty} x\left[\left(-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}+\frac{i}{\hbar}V\Psi^*\right)\Psi+\Psi^*\left(\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2}-\frac{i}{\hbar}V\Psi\right)\right]dx \\
&= \int_{-\infty}^{\infty} x\left(-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\Psi+\cancel{\frac{i}{\hbar}V\Psi^*\Psi}+\frac{i\hbar}{2m}\Psi^*\frac{\partial^2\Psi}{\partial x^2}-\cancel{\frac{i}{\hbar}V\Psi^*\Psi}\right)dx \\
&= \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2}-\frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)dx \\
&= \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\left[\left(\frac{\partial\Psi^*}{\partial x}\frac{\partial\Psi}{\partial x}+\Psi^*\frac{\partial^2\Psi}{\partial x^2}\right)-\left(\frac{\partial^2\Psi^*}{\partial x^2}\Psi+\frac{\partial\Psi^*}{\partial x}\frac{\partial\Psi}{\partial x}\right)\right]dx \\
&= \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\left[\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)-\frac{\partial}{\partial x}\left(\frac{\partial\Psi^*}{\partial x}\Psi\right)\right]dx \\
&= \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)dx \\
&= \frac{i\hbar}{2m}\left[\underbrace{x\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)\Bigg|_{-\infty}^{\infty}}_{=0}-\int_{-\infty}^{\infty}\underbrace{\frac{\partial}{\partial x}(x)}_{=1}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)dx\right] \\
&= \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left(\frac{\partial\Psi^*}{\partial x}\Psi-\Psi^*\frac{\partial\Psi}{\partial x}\right)dx \\
&= \frac{i\hbar}{2m}\left(\int_{-\infty}^{\infty}\frac{\partial\Psi^*}{\partial x}\Psi\,dx-\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx\right) \\
&= \frac{i\hbar}{2m}\left(\underbrace{\Psi^*\Psi\Big|_{-\infty}^{\infty}}_{=0}-\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx-\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx\right) \\
&= -\frac{i\hbar}{m}\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx
\end{aligned}$$

Multiply both sides by m

$$m\frac{d\langle x\rangle}{dt} = -i\hbar\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx$$

and use equation (3).

$$\begin{aligned}
\langle p\rangle &= -i\hbar\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx \\
&= \int_{-\infty}^{\infty}\Psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi\,dx
\end{aligned}$$

Differentiate both sides with respect to t to get $d\langle p\rangle/dt$, the desired quantity.

$$\begin{aligned}
\frac{d\langle p\rangle}{dt} &= -i\hbar\frac{d}{dt}\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx \\
&= -i\hbar\int_{-\infty}^{\infty}\frac{\partial}{\partial t}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)dx \\
&= -i\hbar\int_{-\infty}^{\infty}\left[\frac{\partial\Psi^*}{\partial t}\frac{\partial\Psi}{\partial x}+\Psi^*\frac{\partial}{\partial t}\left(\frac{\partial\Psi}{\partial x}\right)\right]dx
\end{aligned}$$

Use Clairaut's theorem to switch the order of differentiation and then substitute equations (1) and (2) for the time derivatives.

$$\begin{aligned}
\frac{d\langle p\rangle}{dt} &= -i\hbar\int_{-\infty}^{\infty}\left[\left(\frac{\partial\Psi^*}{\partial t}\right)\frac{\partial\Psi}{\partial x}+\Psi^*\frac{\partial}{\partial x}\left(\frac{\partial\Psi}{\partial t}\right)\right]dx\\
&= -i\hbar\int_{-\infty}^{\infty}\left[\left(-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}+\frac{i}{\hbar}V\Psi^*\right)\frac{\partial\Psi}{\partial x}+\Psi^*\frac{\partial}{\partial x}\left(\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2}-\frac{i}{\hbar}V\Psi\right)\right]dx\\
&= -i\hbar\int_{-\infty}^{\infty}\left[-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\frac{\partial\Psi}{\partial x}+\frac{i}{\hbar}V\Psi^*\frac{\partial\Psi}{\partial x}+\frac{i\hbar}{2m}\Psi^*\frac{\partial^3\Psi}{\partial x^3}-\frac{i}{\hbar}\Psi^*\frac{\partial}{\partial x}(V\Psi)\right]dx\\
&= -i\hbar\int_{-\infty}^{\infty}\left(-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\frac{\partial\Psi}{\partial x}+\cancel{\frac{i}{\hbar}V\Psi^*\frac{\partial\Psi}{\partial x}}+\frac{i\hbar}{2m}\Psi^*\frac{\partial^3\Psi}{\partial x^3}-\frac{i}{\hbar}\frac{\partial V}{\partial x}\Psi^*\Psi-\cancel{\frac{i}{\hbar}V\Psi^*\frac{\partial\Psi}{\partial x}}\right)dx\\
&= -i\hbar\left[-\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\frac{\partial^2\Psi^*}{\partial x^2}\frac{\partial\Psi}{\partial x}\,dx+\int_{-\infty}^{\infty}\left(\frac{i\hbar}{2m}\Psi^*\frac{\partial^3\Psi}{\partial x^3}-\frac{i}{\hbar}\frac{\partial V}{\partial x}\Psi^*\Psi\right)dx\right]\\
&= -i\hbar\left[-\frac{i\hbar}{2m}\left(\underbrace{\frac{\partial\Psi^*}{\partial x}\frac{\partial\Psi}{\partial x}\bigg|_{-\infty}^{\infty}}_{=0}-\int_{-\infty}^{\infty}\frac{\partial\Psi^*}{\partial x}\frac{\partial^2\Psi}{\partial x^2}\,dx\right)+\int_{-\infty}^{\infty}\left(\frac{i\hbar}{2m}\Psi^*\frac{\partial^3\Psi}{\partial x^3}-\frac{i}{\hbar}\frac{\partial V}{\partial x}\Psi^*\Psi\right)dx\right]\\
&= -i\hbar\left[\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\frac{\partial\Psi^*}{\partial x}\frac{\partial^2\Psi}{\partial x^2}\,dx+\int_{-\infty}^{\infty}\left(\frac{i\hbar}{2m}\Psi^*\frac{\partial^3\Psi}{\partial x^3}-\frac{i}{\hbar}\frac{\partial V}{\partial x}\Psi^*\Psi\right)dx\right]\\
&= -i\hbar\left[\frac{i\hbar}{2m}\left(\underbrace{\Psi^*\frac{\partial^2\Psi}{\partial x^2}\bigg|_{-\infty}^{\infty}}_{=0}-\int_{-\infty}^{\infty}\Psi^*\frac{\partial^3\Psi}{\partial x^3}\,dx\right)+\int_{-\infty}^{\infty}\left(\frac{i\hbar}{2m}\Psi^*\frac{\partial^3\Psi}{\partial x^3}-\frac{i}{\hbar}\frac{\partial V}{\partial x}\Psi^*\Psi\right)dx\right]\\
&= -i\hbar\left[-\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\Psi^*\frac{\partial^3\Psi}{\partial x^3}\,dx+\int_{-\infty}^{\infty}\left(\frac{i\hbar}{2m}\Psi^*\frac{\partial^3\Psi}{\partial x^3}-\frac{i}{\hbar}\frac{\partial V}{\partial x}\Psi^*\Psi\right)dx\right]\\
&= -i\hbar\int_{-\infty}^{\infty}\left(\cancel{-\frac{i\hbar}{2m}\Psi^*\frac{\partial^3\Psi}{\partial x^3}}+\cancel{\frac{i\hbar}{2m}\Psi^*\frac{\partial^3\Psi}{\partial x^3}}-\frac{i}{\hbar}\frac{\partial V}{\partial x}\Psi^*\Psi\right)dx\\
&= i^2\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial x}\Psi^*\Psi\right)dx\\
&= -\int_{-\infty}^{\infty}\left(\frac{\partial V}{\partial x}\Psi^*\Psi\right)dx\\
&= \int_{-\infty}^{\infty}\Psi^*\left(-\frac{\partial V}{\partial x}\right)\Psi\,dx\\
&= \left\langle-\frac{\partial V}{\partial x}\right\rangle
\end{aligned}$$