Problem 3.18

Apply Equation 3.73 to the following special cases: (a) $Q = 1$; (b) $Q = H$; (c) $Q = x$; (d) $Q = p$. In each case, comment on the result, with particular reference to Equations 1.27, 1.33, 1.38, and conservation of energy (see remarks following Equation 2.21).

Solution

Equation 3.73 gives the temporal rate of change of the expectation value of an observable Q.

$$
\begin{aligned}
\frac{d}{dt}\langle Q\rangle &= \frac{d}{dt}\langle \Psi \,|\, \hat{Q} \,|\, \Psi\rangle \\
&= \frac{d}{dt}\int_{-\infty}^{\infty} \Psi^*(x,t)\hat{Q}\Psi(x,t)\,dx \\
&= \int_{-\infty}^{\infty} \frac{\partial}{\partial t}\left[\Psi^*(x,t)\hat{Q}\Psi(x,t)\right]dx \\
&= \int_{-\infty}^{\infty}\left[\frac{\partial \Psi^*}{\partial t}\hat{Q}\Psi(x,t) + \Psi^*(x,t)\frac{\partial \hat{Q}}{\partial t}\Psi(x,t) + \Psi^*(x,t)\hat{Q}\frac{\partial \Psi}{\partial t}\right]dx \\
&= \int_{-\infty}^{\infty}\left[\left(\frac{\partial \Psi}{\partial t}\right)^*\hat{Q}\Psi(x,t) + \Psi^*(x,t)\hat{Q}\frac{\partial \Psi}{\partial t}\right]dx + \int_{-\infty}^{\infty}\Psi^*(x,t)\frac{\partial \hat{Q}}{\partial t}\Psi(x,t)\,dx \\
&= \int_{-\infty}^{\infty}\left[\left(\frac{1}{i\hbar}\hat{H}\Psi(x,t)\right)^*\hat{Q}\Psi(x,t) + \Psi^*(x,t)\hat{Q}\left(\frac{1}{i\hbar}\hat{H}\Psi(x,t)\right)\right]dx + \left\langle \Psi \,\middle|\, \frac{\partial \hat{Q}}{\partial t} \,\middle|\, \Psi\right\rangle \\
&= \int_{-\infty}^{\infty}\left[\left(\frac{1}{i\hbar}\Psi(x,t)\right)^*\hat{H}^\dagger\hat{Q}\Psi(x,t) + \Psi^*(x,t)\hat{Q}\left(\frac{1}{i\hbar}\hat{H}\Psi(x,t)\right)\right]dx + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle \\
&= \int_{-\infty}^{\infty}\left[\left(\frac{1}{-i\hbar}\Psi^*(x,t)\right)\hat{H}\hat{Q}\Psi(x,t) + \frac{1}{i\hbar}\Psi^*(x,t)\hat{Q}\hat{H}\Psi(x,t)\right]dx + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle \\
&= \int_{-\infty}^{\infty}\left[\frac{i}{\hbar}\Psi^*(x,t)\hat{H}\hat{Q}\Psi(x,t) - \frac{i}{\hbar}\Psi^*(x,t)\hat{Q}\hat{H}\Psi(x,t)\right]dx + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle \\
&= \int_{-\infty}^{\infty}\frac{i}{\hbar}\Psi^*(x,t)\left[\hat{H}\hat{Q}\Psi(x,t) - \hat{Q}\hat{H}\Psi(x,t)\right]dx + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,t)\left[\hat{H}\hat{Q} - \hat{Q}\hat{H}\right]\Psi(x,t)\,dx + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,t)\left[\hat{H},\hat{Q}\right]\Psi(x,t)\,dx + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle \\
&= \frac{i}{\hbar}\left\langle \Psi \,\middle|\, \left[\hat{H},\hat{Q}\right] \,\middle|\, \Psi\right\rangle + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle \\
&= \frac{i}{\hbar}\left\langle \left[\hat{H},\hat{Q}\right]\right\rangle + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle
\end{aligned} \tag{3.73}
$$

Part (a)

If $Q = 1$, then

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

and

$$\begin{aligned}
\frac{i}{\hbar}\left\langle \left[\hat{H},\hat{Q}\right]\right\rangle + \left\langle \frac{\partial \hat{Q}}{\partial t}\right\rangle &= \frac{i}{\hbar}\left\langle \Psi \,\middle|\, \left[\hat{H},\hat{Q}\right] \,\middle|\, \Psi\right\rangle + \left\langle \Psi \,\middle|\, \frac{\partial \hat{Q}}{\partial t} \,\middle|\, \Psi\right\rangle \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty} \Psi^*(x,t)\left[\hat{H},\hat{Q}\right]\Psi(x,t)\,dx + \int_{-\infty}^{\infty} \Psi^*(x,t)\frac{\partial \hat{Q}}{\partial t}\Psi(x,t)\,dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty} \Psi^*(x,t)\left(\hat{H}\hat{Q} - \hat{Q}\hat{H}\right)\Psi(x,t)\,dx + \int_{-\infty}^{\infty} \Psi^*(x,t)\underbrace{\left[\frac{\partial}{\partial t}(1)\right]}_{=0}\Psi(x,t)\,dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty} \Psi^*(x,t)\left[\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)\hat{Q} - \hat{Q}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)\right]\Psi(x,t)\,dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty} \Psi^*(x,t)\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)1 - 1\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\right]\Psi(x,t)\,dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty} \Psi^*(x,t)\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t) - \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t)\right]dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty} \Psi^*(x,t)\left[-\cancel{\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}} + \cancel{V(x)\Psi(x,t)} + \cancel{\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}} - \cancel{V(x)\Psi(x,t)}\right]dx \\
&= 0.
\end{aligned}$$

By Equation 3.73, then,

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2\,dx = 0.$$

Integrate both sides with respect to t.

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2\,dx = C \tag{1}$$

In order to determine the integration constant, suppose that $\Psi(x,t)$ is normalized at $t = 0$.

$$1 = \int_{-\infty}^{\infty} |\Psi(x,0)|^2\,dx = C$$

Therefore, equation (1) becomes

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx = 1,$$

which means the position-space wave function $\Psi(x,t)$ remains normalized for all time if it's normalized at one instance in particular.

Part (b)

If $Q = H$, then Equation 3.73 becomes

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

which is a statement of conservation of energy for time-independent potential energy functions.

Part (c)

If $Q = x$, then Equation 3.73 becomes

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

Continue the simplification.

$$\begin{aligned}
\frac{d}{dt}\langle x\rangle &= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,t)\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)x\Psi(x,t)-x\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\Psi(x,t)\right]dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,t)\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}[x\Psi(x,t)]+\cancel{V(x)x\Psi(x,t)}+\frac{\hbar^2}{2m}x\frac{\partial^2\Psi}{\partial x^2}-\cancel{xV(x)\Psi(x,t)}\right]dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,t)\left[-\frac{\hbar^2}{2m}\left(2\frac{\partial\Psi}{\partial x}+\cancel{x\frac{\partial^2\Psi}{\partial x^2}}\right)+\cancel{\frac{\hbar^2}{2m}x\frac{\partial^2\Psi}{\partial x^2}}\right]dx \\
&= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,t)\left(-\frac{\hbar^2}{m}\right)\frac{\partial\Psi}{\partial x}\,dx \\
&= \frac{1}{m}\int_{-\infty}^{\infty}\Psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x,t)\,dx \\
&= \frac{1}{m}\int_{-\infty}^{\infty}\Psi^*(x,t)\hat{p}\Psi(x,t)\,dx \\
&= \frac{1}{m}\langle\Psi\,|\,\hat{p}\,|\,\Psi\rangle \\
&= \frac{1}{m}\langle p\rangle \\
&= \langle v\rangle
\end{aligned}$$

The derivative of the expectation value of position with respect to time is the expectation value of the velocity.

Part (d)

If $Q = p$, then Equation 3.73 becomes

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

Continue the simplification.

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

This is the result of Problem 1.7.