

Problem 4.1

- (a) Work out all of the **canonical commutation relations** for components of the operators \mathbf{r} and \mathbf{p} : $[x, y]$, $[x, p_y]$, $[x, p_x]$, $[p_y, p_z]$, and so on. *Answer:*

$$[r_i, p_j] = -[p_i, r_j] = i\hbar\delta_{ij}, \quad [r_i, r_j] = [p_i, p_j] = 0, \quad (4.10)$$

where the indices stand for x, y , or z , and $r_x = x$, $r_y = y$, and $r_z = z$.

- (b) Confirm the three-dimensional version of **Ehrenfest's theorem**,

$$\frac{d}{dt}\langle\mathbf{r}\rangle = \frac{1}{m}\langle\mathbf{p}\rangle, \quad \text{and} \quad \frac{d}{dt}\langle\mathbf{p}\rangle = \langle-\nabla V\rangle. \quad (4.11)$$

(Each of these, of course, stands for *three* equations—one for each component.) *Hint:* First check that the “generalized” Ehrenfest theorem, Equation 3.73, is valid in three dimensions.

- (c) Formulate **Heisenberg's uncertainty principle** in three dimensions. *Answer:*

$$\sigma_x\sigma_{p_x} \geq \hbar/2, \quad \sigma_y\sigma_{p_y} \geq \hbar/2, \quad \sigma_z\sigma_{p_z} \geq \hbar/2, \quad (4.12)$$

but there is no restriction on, say, $\sigma_x\sigma_{p_y}$.

[**TYPO: This is bad notation because i represents both $\sqrt{-1}$ and an index.**]

Solution

Part (a)

Evaluate the commutation relations, using the test function $f = f(x, y, z)$. The mixed partial derivatives of f are equal by Clairaut's theorem.

$$[\hat{x}, \hat{y}]f = (\hat{x}\hat{y} - \hat{y}\hat{x})f = (xy - yx)f = 0$$

$$[\hat{y}, \hat{z}]f = (\hat{y}\hat{z} - \hat{z}\hat{y})f = (yz - zy)f = 0$$

$$[\hat{x}, \hat{z}]f = (\hat{x}\hat{z} - \hat{z}\hat{x})f = (xz - zx)f = 0$$

$$\begin{aligned} [\hat{p}_x, \hat{p}_y]f &= (\hat{p}_x\hat{p}_y - \hat{p}_y\hat{p}_x)f = \left[\left(-i\hbar\frac{\partial}{\partial x} \right) \left(-i\hbar\frac{\partial}{\partial y} \right) - \left(-i\hbar\frac{\partial}{\partial y} \right) \left(-i\hbar\frac{\partial}{\partial x} \right) \right] f \\ &= \left(-\hbar^2\frac{\partial^2}{\partial x\partial y} + \hbar^2\frac{\partial^2}{\partial y\partial x} \right) f \\ &= -\hbar^2\frac{\partial^2 f}{\partial x\partial y} + \hbar^2\frac{\partial^2 f}{\partial y\partial x} \\ &= 0 \end{aligned}$$

Evaluate more of the commutation relations.

$$\begin{aligned}
 [\hat{p}_y, \hat{p}_z] f &= (\hat{p}_y \hat{p}_z - \hat{p}_z \hat{p}_y) f = \left[\left(-i\hbar \frac{\partial}{\partial y} \right) \left(-i\hbar \frac{\partial}{\partial z} \right) - \left(-i\hbar \frac{\partial}{\partial z} \right) \left(-i\hbar \frac{\partial}{\partial y} \right) \right] f \\
 &= \left(-\hbar^2 \frac{\partial^2}{\partial y \partial z} + \hbar^2 \frac{\partial^2}{\partial z \partial y} \right) f \\
 &= -\hbar^2 \frac{\partial^2 f}{\partial y \partial z} + \hbar^2 \frac{\partial^2 f}{\partial z \partial y} \\
 &= 0
 \end{aligned}$$

$$\begin{aligned}
 [\hat{p}_x, \hat{p}_z] f &= (\hat{p}_x \hat{p}_z - \hat{p}_z \hat{p}_x) f = \left[\left(-i\hbar \frac{\partial}{\partial x} \right) \left(-i\hbar \frac{\partial}{\partial z} \right) - \left(-i\hbar \frac{\partial}{\partial z} \right) \left(-i\hbar \frac{\partial}{\partial x} \right) \right] f \\
 &= \left(-\hbar^2 \frac{\partial^2}{\partial x \partial z} + \hbar^2 \frac{\partial^2}{\partial z \partial x} \right) f \\
 &= -\hbar^2 \frac{\partial^2 f}{\partial x \partial z} + \hbar^2 \frac{\partial^2 f}{\partial z \partial x} \\
 &= 0
 \end{aligned}$$

$$\begin{aligned}
 [\hat{x}, \hat{p}_x] f &= (\hat{x} \hat{p}_x - \hat{p}_x \hat{x}) f = \left[x \left(-i\hbar \frac{\partial}{\partial x} \right) - \left(-i\hbar \frac{\partial}{\partial x} \right) x \right] f \\
 &= -i\hbar x \frac{\partial}{\partial x} (f) + i\hbar \frac{\partial}{\partial x} (xf) \\
 &= -i\hbar x \frac{\partial f}{\partial x} + i\hbar x \frac{\partial f}{\partial x} + i\hbar f \\
 &= i\hbar f
 \end{aligned}$$

$$\begin{aligned}
 [\hat{x}, \hat{p}_y] f &= (\hat{x} \hat{p}_y - \hat{p}_y \hat{x}) f = \left[x \left(-i\hbar \frac{\partial}{\partial y} \right) - \left(-i\hbar \frac{\partial}{\partial y} \right) x \right] f \\
 &= -i\hbar x \frac{\partial}{\partial y} (f) + i\hbar \frac{\partial}{\partial y} (xf) \\
 &= -i\hbar x \frac{\partial f}{\partial y} + i\hbar x \frac{\partial f}{\partial y} \\
 &= 0
 \end{aligned}$$

$$\begin{aligned}
 [\hat{x}, \hat{p}_z] f &= (\hat{x} \hat{p}_z - \hat{p}_z \hat{x}) f = \left[x \left(-i\hbar \frac{\partial}{\partial z} \right) - \left(-i\hbar \frac{\partial}{\partial z} \right) x \right] f \\
 &= -i\hbar x \frac{\partial}{\partial z} (f) + i\hbar \frac{\partial}{\partial z} (xf) \\
 &= -i\hbar x \frac{\partial f}{\partial z} + i\hbar x \frac{\partial f}{\partial z} \\
 &= 0
 \end{aligned}$$

Evaluate more of the commutation relations.

$$\begin{aligned}
 [\hat{y}, \hat{p}_x] f &= (\hat{y}\hat{p}_x - \hat{p}_x\hat{y})f = \left[y \left(-i\hbar \frac{\partial}{\partial x} \right) - \left(-i\hbar \frac{\partial}{\partial x} \right) y \right] f \\
 &= -i\hbar y \frac{\partial}{\partial x} (f) + i\hbar \frac{\partial}{\partial x} (yf) \\
 &= -i\hbar y \frac{\partial f}{\partial x} + i\hbar y \frac{\partial f}{\partial x} \\
 &= 0
 \end{aligned}$$

$$\begin{aligned}
 [\hat{y}, \hat{p}_y] f &= (\hat{y}\hat{p}_y - \hat{p}_y\hat{y})f = \left[y \left(-i\hbar \frac{\partial}{\partial y} \right) - \left(-i\hbar \frac{\partial}{\partial y} \right) y \right] f \\
 &= -i\hbar y \frac{\partial}{\partial y} (f) + i\hbar \frac{\partial}{\partial y} (yf) \\
 &= -i\hbar y \frac{\partial f}{\partial y} + i\hbar y \frac{\partial f}{\partial y} + i\hbar f \\
 &= i\hbar f
 \end{aligned}$$

$$\begin{aligned}
 [\hat{y}, \hat{p}_z] f &= (\hat{y}\hat{p}_z - \hat{p}_z\hat{y})f = \left[y \left(-i\hbar \frac{\partial}{\partial z} \right) - \left(-i\hbar \frac{\partial}{\partial z} \right) y \right] f \\
 &= -i\hbar y \frac{\partial}{\partial z} (f) + i\hbar \frac{\partial}{\partial z} (yf) \\
 &= -i\hbar y \frac{\partial f}{\partial z} + i\hbar y \frac{\partial f}{\partial z} \\
 &= 0
 \end{aligned}$$

$$\begin{aligned}
 [\hat{z}, \hat{p}_x] f &= (\hat{z}\hat{p}_x - \hat{p}_x\hat{z})f = \left[z \left(-i\hbar \frac{\partial}{\partial x} \right) - \left(-i\hbar \frac{\partial}{\partial x} \right) z \right] f \\
 &= -i\hbar z \frac{\partial}{\partial x} (f) + i\hbar \frac{\partial}{\partial x} (zf) \\
 &= -i\hbar z \frac{\partial f}{\partial x} + i\hbar z \frac{\partial f}{\partial x} \\
 &= 0
 \end{aligned}$$

$$\begin{aligned}
 [\hat{z}, \hat{p}_y] f &= (\hat{z}\hat{p}_y - \hat{p}_y\hat{z})f = \left[z \left(-i\hbar \frac{\partial}{\partial y} \right) - \left(-i\hbar \frac{\partial}{\partial y} \right) z \right] f \\
 &= -i\hbar z \frac{\partial}{\partial y} (f) + i\hbar \frac{\partial}{\partial y} (zf) \\
 &= -i\hbar z \frac{\partial f}{\partial y} + i\hbar z \frac{\partial f}{\partial y} \\
 &= 0
 \end{aligned}$$

Evaluate the last commutation relation.

$$\begin{aligned}
 [\hat{z}, \hat{p}_z] f &= (\hat{z}\hat{p}_z - \hat{p}_z\hat{z})f = \left[z \left(-i\hbar \frac{\partial}{\partial z} \right) - \left(-i\hbar \frac{\partial}{\partial z} \right) z \right] f \\
 &= -i\hbar z \frac{\partial}{\partial z} (f) + i\hbar \frac{\partial}{\partial z} (zf) \\
 &= -i\hbar z \frac{\partial f}{\partial z} + i\hbar z \frac{\partial f}{\partial z} + i\hbar f \\
 &= i\hbar f
 \end{aligned}$$

Therefore,

$$\begin{aligned}
 [\hat{x}, \hat{y}] &= 0 & \Rightarrow & [\hat{y}, \hat{x}] = -[\hat{x}, \hat{y}] = 0 \\
 [\hat{y}, \hat{z}] &= 0 & \Rightarrow & [\hat{z}, \hat{y}] = -[\hat{y}, \hat{z}] = 0 \\
 [\hat{x}, \hat{z}] &= 0 & \Rightarrow & [\hat{z}, \hat{x}] = -[\hat{x}, \hat{z}] = 0 \\
 [\hat{p}_x, \hat{p}_y] &= 0 & \Rightarrow & [\hat{p}_y, \hat{p}_x] = -[\hat{p}_x, \hat{p}_y] = 0 \\
 [\hat{p}_y, \hat{p}_z] &= 0 & \Rightarrow & [\hat{p}_z, \hat{p}_y] = -[\hat{p}_y, \hat{p}_z] = 0 \\
 [\hat{p}_x, \hat{p}_z] &= 0 & \Rightarrow & [\hat{p}_z, \hat{p}_x] = -[\hat{p}_x, \hat{p}_z] = 0 \\
 [\hat{x}, \hat{p}_x] &= i\hbar & \Rightarrow & [\hat{p}_x, \hat{x}] = -[\hat{x}, \hat{p}_x] = -i\hbar \\
 [\hat{x}, \hat{p}_y] &= 0 & \Rightarrow & [\hat{p}_y, \hat{x}] = -[\hat{x}, \hat{p}_y] = 0 \\
 [\hat{x}, \hat{p}_z] &= 0 & \Rightarrow & [\hat{p}_z, \hat{x}] = -[\hat{x}, \hat{p}_z] = 0 \\
 [\hat{y}, \hat{p}_x] &= 0 & \Rightarrow & [\hat{p}_x, \hat{y}] = -[\hat{y}, \hat{p}_x] = 0 \\
 [\hat{y}, \hat{p}_y] &= i\hbar & \Rightarrow & [\hat{p}_y, \hat{y}] = -[\hat{y}, \hat{p}_y] = -i\hbar \\
 [\hat{y}, \hat{p}_z] &= 0 & \Rightarrow & [\hat{p}_z, \hat{y}] = -[\hat{y}, \hat{p}_z] = 0 \\
 [\hat{z}, \hat{p}_x] &= 0 & \Rightarrow & [\hat{p}_x, \hat{z}] = -[\hat{z}, \hat{p}_x] = 0 \\
 [\hat{z}, \hat{p}_y] &= 0 & \Rightarrow & [\hat{p}_y, \hat{z}] = -[\hat{z}, \hat{p}_y] = 0 \\
 [\hat{z}, \hat{p}_z] &= i\hbar & \Rightarrow & [\hat{p}_z, \hat{z}] = -[\hat{z}, \hat{p}_z] = -i\hbar.
 \end{aligned}$$

Part (b)

The governing equation for the wave function in three dimensions is

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(x, y, z, t) \Psi(x, y, z, t).$$

Divide both sides by $i\hbar$.

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \nabla^2 \Psi - \frac{i}{\hbar} V \Psi$$

Take the complex conjugate of both sides.

$$\frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m} \nabla^2 \Psi^* + \frac{i}{\hbar} V \Psi^*$$

Calculate the time-derivative of the expectation value of x_j , where x_j is x , y , or z depending if j is 1, 2, or 3, respectively.

$$\begin{aligned}
 \frac{d}{dt}\langle x_j \rangle &= \frac{d}{dt}\langle \Psi | \hat{x}_j | \Psi \rangle \\
 &= \frac{d}{dt} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi^*(x, y, z, t)(x_j)\Psi(x, y, z, t) dx dy dz \\
 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\partial}{\partial t} [\Psi^*(x, y, z, t)(x_j)\Psi(x, y, z, t)] dx dy dz \\
 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x_j \left(\frac{\partial \Psi^*}{\partial t} \Psi + \Psi^* \frac{\partial \Psi}{\partial t} \right) dx dy dz \\
 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x_j \left[\left(-\frac{i\hbar}{2m} \nabla^2 \Psi^* + \frac{i}{\hbar} V \Psi^* \right) \Psi + \Psi^* \left(\frac{i\hbar}{2m} \nabla^2 \Psi - \frac{i}{\hbar} V \Psi \right) \right] dx dy dz \\
 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x_j \left(-\frac{i\hbar}{2m} \Psi \nabla^2 \Psi^* + \frac{i\hbar}{2m} \Psi^* \nabla^2 \Psi \right) dx dy dz \\
 &= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x_j (\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*) dx dy dz \\
 &= \frac{i\hbar}{2m} \left(\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x_j \Psi^* \nabla^2 \Psi dx dy dz - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x_j \Psi \nabla^2 \Psi^* dx dy dz \right) \quad (1)
 \end{aligned}$$

Green's first identity is essentially the multidimensional integration-by-parts formula.

$$\iiint_D v \nabla^2 u dV = \oint_{\text{bdy } D} v \frac{\partial u}{\partial n} dS - \iiint_D \nabla v \cdot \nabla u dV$$

u and v are any two differentiable functions, D is the domain that these two functions are defined on, $\text{bdy } D$ is the boundary of D , and

$$\frac{\partial u}{\partial n} = \hat{\mathbf{n}} \cdot \nabla u$$

is the directional derivative of u in the outward normal direction from the boundary. For the infinite domain here, the boundary term vanishes, as Ψ and its derivatives vanish as $|\mathbf{x}| \rightarrow \infty$.

Using Green's first identity, the two integrals in equation (1) become

$$\begin{aligned}
 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x_j \Psi^* \nabla^2 \Psi dx dy dz &= 0 - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \nabla(x_j \Psi^*) \cdot \nabla \Psi dx dy dz \\
 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x_j \Psi \nabla^2 \Psi^* dx dy dz &= 0 - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \nabla(x_j \Psi) \cdot \nabla \Psi^* dx dy dz,
 \end{aligned}$$

which means

$$\begin{aligned}
 \frac{d}{dt}\langle x_j \rangle &= \frac{i\hbar}{2m} \left[- \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \nabla(x_j \Psi^*) \cdot \nabla \Psi dx dy dz + \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \nabla(x_j \Psi) \cdot \nabla \Psi^* dx dy dz \right] \\
 &= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\nabla(x_j \Psi) \cdot \nabla \Psi^* - \nabla(x_j \Psi^*) \cdot \nabla \Psi] dx dy dz.
 \end{aligned}$$

Simplify the integrand.

$$\begin{aligned}
\frac{d}{dt}\langle x_j \rangle &= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\nabla(x_j\Psi) \cdot \nabla\Psi^* - \nabla(x_j\Psi^*) \cdot \nabla\Psi] dV \\
&= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\left(\sum_{k=1}^3 \delta_k \frac{\partial}{\partial x_k} \right) (x_j\Psi) \cdot \left(\sum_{l=1}^3 \delta_l \frac{\partial}{\partial x_l} \right) \Psi^* - \left(\sum_{k=1}^3 \delta_k \frac{\partial}{\partial x_k} \right) (x_j\Psi^*) \cdot \left(\sum_{l=1}^3 \delta_l \frac{\partial}{\partial x_l} \right) \Psi \right] dV \\
&= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\sum_{k=1}^3 \delta_k \frac{\partial}{\partial x_k} (x_j\Psi) \cdot \sum_{l=1}^3 \delta_l \frac{\partial \Psi^*}{\partial x_l} - \sum_{k=1}^3 \delta_k \frac{\partial}{\partial x_k} (x_j\Psi^*) \cdot \sum_{l=1}^3 \delta_l \frac{\partial \Psi}{\partial x_l} \right] dV \\
&= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\sum_{k=1}^3 \sum_{l=1}^3 (\delta_k \cdot \delta_l) \frac{\partial}{\partial x_k} (x_j\Psi) \frac{\partial \Psi^*}{\partial x_l} - \sum_{k=1}^3 \sum_{l=1}^3 (\delta_k \cdot \delta_l) \frac{\partial}{\partial x_k} (x_j\Psi^*) \frac{\partial \Psi}{\partial x_l} \right] dV \\
&= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\sum_{k=1}^3 \sum_{l=1}^3 \delta_{kl} \frac{\partial}{\partial x_k} (x_j\Psi) \frac{\partial \Psi^*}{\partial x_l} - \sum_{k=1}^3 \sum_{l=1}^3 \delta_{kl} \frac{\partial}{\partial x_k} (x_j\Psi^*) \frac{\partial \Psi}{\partial x_l} \right] dV \\
&= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\sum_{k=1}^3 \frac{\partial}{\partial x_k} (x_j\Psi) \frac{\partial \Psi^*}{\partial x_k} - \sum_{k=1}^3 \frac{\partial}{\partial x_k} (x_j\Psi^*) \frac{\partial \Psi}{\partial x_k} \right] dV \\
&= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\sum_{k=1}^3 \left(\frac{\partial x_j}{\partial x_k} \Psi + x_j \frac{\partial \Psi}{\partial x_k} \right) \frac{\partial \Psi^*}{\partial x_k} - \sum_{k=1}^3 \left(\frac{\partial x_j}{\partial x_k} \Psi^* + x_j \frac{\partial \Psi^*}{\partial x_k} \right) \frac{\partial \Psi}{\partial x_k} \right] dV \\
&= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\sum_{k=1}^3 \left(\delta_{jk} \Psi + x_j \frac{\partial \Psi}{\partial x_k} \right) \frac{\partial \Psi^*}{\partial x_k} - \sum_{k=1}^3 \left(\delta_{jk} \Psi^* + x_j \frac{\partial \Psi^*}{\partial x_k} \right) \frac{\partial \Psi}{\partial x_k} \right] dV \\
&= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\sum_{k=1}^3 \delta_{jk} \Psi \frac{\partial \Psi^*}{\partial x_k} + \sum_{k=1}^3 x_j \frac{\partial \Psi}{\partial x_k} \frac{\partial \Psi^*}{\partial x_k} - \sum_{k=1}^3 \delta_{jk} \Psi^* \frac{\partial \Psi}{\partial x_k} - \sum_{k=1}^3 x_j \frac{\partial \Psi^*}{\partial x_k} \frac{\partial \Psi}{\partial x_k} \right) dV \\
&= \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\Psi \frac{\partial \Psi^*}{\partial x_j} - \Psi^* \frac{\partial \Psi}{\partial x_j} \right) dV \\
&= -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\Psi^* \frac{\partial \Psi}{\partial x_j} - \Psi \frac{\partial \Psi^*}{\partial x_j} \right) dV \\
&= -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} \left(\Psi^* \frac{\partial \Psi}{\partial x_j} - \Psi \frac{\partial \Psi^*}{\partial x_j} \right) dx_j \right] dA \\
&= -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x_j} dx_j - \int_{-\infty}^{\infty} \Psi \frac{\partial \Psi^*}{\partial x_j} dx_j \right) dA \\
&= -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x_j} dx_j - \underbrace{\left(\Psi \Psi^* \right) \Big|_{-\infty}^{\infty}}_{=0} - \int_{-\infty}^{\infty} \frac{\partial \Psi}{\partial x_j} \Psi^* dx_j \right] dA \\
&= -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x_j} dx_j + \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x_j} dx_j \right] dA
\end{aligned}$$

Therefore, in component form,

$$\begin{aligned}
 \frac{d}{dt}\langle x_j \rangle &= -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(2 \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x_j} dx_j \right) dA \\
 &= -\frac{i\hbar}{m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x_j} dx dy dz \\
 &= \frac{1}{m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar \frac{\partial}{\partial x_j} \right) \Psi dx dy dz \\
 &= \frac{1}{m} \langle \Psi | \hat{p}_j | \Psi \rangle \\
 &= \frac{1}{m} \langle p_j \rangle,
 \end{aligned}$$

or as a vector equation,

$$\frac{d}{dt}\langle \mathbf{r} \rangle = \frac{1}{m} \langle \mathbf{p} \rangle.$$

Now take the time-derivative of the expectation value of momentum.

$$\begin{aligned}
 \frac{d}{dt}\langle \mathbf{p} \rangle &= \frac{d}{dt} \langle \Psi | \hat{\mathbf{p}} | \Psi \rangle \\
 &= \frac{d}{dt} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi^*(x, y, z, t) (-i\hbar \nabla) \Psi(x, y, z, t) dx dy dz \\
 &= -i\hbar \frac{d}{dt} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi^*(x, y, z, t) \nabla \Psi(x, y, z, t) dx dy dz \\
 &= -i\hbar \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\partial}{\partial t} [\Psi^*(x, y, z, t) \nabla \Psi(x, y, z, t)] dx dy dz \\
 &= -i\hbar \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\left(\frac{\partial \Psi^*}{\partial t} \right) \nabla \Psi + \Psi^* \nabla \left(\frac{\partial \Psi}{\partial t} \right) \right] dx dy dz \\
 &= -i\hbar \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[\left(-\frac{i\hbar}{2m} \nabla^2 \Psi^* + \frac{i}{\hbar} V \Psi^* \right) \nabla \Psi + \Psi^* \nabla \left(\frac{i\hbar}{2m} \nabla^2 \Psi - \frac{i}{\hbar} V \Psi \right) \right] dx dy dz \\
 &= -i\hbar \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[-\frac{i\hbar}{2m} \nabla^2 \Psi^* \nabla \Psi + \frac{i}{\hbar} V \Psi^* \nabla \Psi + \frac{i\hbar}{2m} \Psi^* \nabla (\nabla^2 \Psi) - \frac{i}{\hbar} \Psi^* \nabla (V \Psi) \right] dx dy dz \\
 &= -i\hbar \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[-\frac{i\hbar}{2m} \nabla^2 \Psi^* \nabla \Psi + \cancel{\frac{i}{\hbar} V \Psi^* \nabla \Psi} + \frac{i\hbar}{2m} \Psi^* \nabla (\nabla^2 \Psi) - \frac{i}{\hbar} \Psi^* \nabla V \Psi - \cancel{\frac{i}{\hbar} \Psi^* V \nabla \Psi} \right] dx dy dz \\
 &= -i\hbar \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[-\frac{i\hbar}{2m} \nabla^2 \Psi^* \nabla \Psi + \frac{i\hbar}{2m} \Psi^* \left(\sum_{j=1}^3 \delta_j \frac{\partial}{\partial x_j} \right) \left(\sum_{k=1}^3 \frac{\partial^2 \Psi}{\partial x_k^2} \right) - \frac{i}{\hbar} \Psi^* \nabla V \Psi \right] dx dy dz \\
 &= -i\hbar \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[-\frac{i\hbar}{2m} \nabla^2 \Psi^* \nabla \Psi + \frac{i\hbar}{2m} \Psi^* \sum_{k=1}^3 \frac{\partial^2}{\partial x_k^2} \left(\sum_{j=1}^3 \delta_j \frac{\partial \Psi}{\partial x_j} \right) - \frac{i}{\hbar} \Psi^* \nabla V \Psi \right] dx dy dz
 \end{aligned}$$

As a result,

$$\begin{aligned}
 \frac{d}{dt}\langle \mathbf{p} \rangle &= -i\hbar \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[-\frac{i\hbar}{2m} \nabla^2 \Psi^* \nabla \Psi + \frac{i\hbar}{2m} \Psi^* \nabla^2 (\nabla \Psi) - \frac{i}{\hbar} \Psi^* \nabla V \Psi \right] dx dy dz \\
 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[-\frac{\hbar^2}{2m} \nabla^2 \Psi^* \nabla \Psi + \frac{\hbar^2}{2m} \Psi^* \nabla^2 (\nabla \Psi) - \Psi^* \nabla V \Psi \right] dx dy dz \\
 &= \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\Psi^* \nabla^2 (\nabla \Psi) - \nabla^2 \Psi^* \nabla \Psi] dx dy dz - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi^* \nabla V \Psi dx dy dz.
 \end{aligned}$$

Green's second identity says that

$$\iiint_D (u \nabla^2 v - v \nabla^2 u) d\mathcal{V} = \iint_{\text{bdy } D} \left(u \frac{\partial v}{\partial n} - v \frac{\partial u}{\partial n} \right) d\mathcal{S}$$

for any two functions, u and v , on a domain D . For $u = \Psi^*$ and $v = \nabla \Psi$ and D being all of space, Green's second identity becomes

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\Psi^* \nabla^2 (\nabla \Psi) - \nabla^2 \Psi^* \nabla \Psi] d\mathcal{V} = 0$$

because Ψ and its derivatives go to zero as $|\mathbf{x}| \rightarrow \infty$. Therefore,

$$\begin{aligned}
 \frac{d}{dt}\langle \mathbf{p} \rangle &= \frac{\hbar^2}{2m}(0) - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi^* \nabla V \Psi dx dy dz \\
 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi^* (-\nabla V) \Psi dx dy dz \\
 &= \langle \Psi | -\nabla V | \Psi \rangle \\
 &= \langle -\nabla V \rangle.
 \end{aligned}$$

Part (c)

Apply the generalized uncertainty principle for two observables,

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2,$$

to the results of part (a).

$$\begin{aligned} [\hat{x}, \hat{y}] = 0 & \Rightarrow \sigma_x \sigma_y \geq 0 \\ [\hat{y}, \hat{z}] = 0 & \Rightarrow \sigma_y \sigma_z \geq 0 \\ [\hat{x}, \hat{z}] = 0 & \Rightarrow \sigma_x \sigma_z \geq 0 \\ [\hat{p}_x, \hat{p}_y] = 0 & \Rightarrow \sigma_{p_x} \sigma_{p_y} \geq 0 \\ [\hat{p}_y, \hat{p}_z] = 0 & \Rightarrow \sigma_{p_y} \sigma_{p_z} \geq 0 \\ [\hat{p}_x, \hat{p}_z] = 0 & \Rightarrow \sigma_{p_x} \sigma_{p_z} \geq 0 \\ [\hat{x}, \hat{p}_x] = i\hbar & \Rightarrow \sigma_x \sigma_{p_x} \geq \frac{\hbar}{2} \\ [\hat{x}, \hat{p}_y] = 0 & \Rightarrow \sigma_x \sigma_{p_y} \geq 0 \\ [\hat{x}, \hat{p}_z] = 0 & \Rightarrow \sigma_x \sigma_{p_z} \geq 0 \\ [\hat{y}, \hat{p}_x] = 0 & \Rightarrow \sigma_y \sigma_{p_x} \geq 0 \\ [\hat{y}, \hat{p}_y] = i\hbar & \Rightarrow \sigma_y \sigma_{p_y} \geq \frac{\hbar}{2} \\ [\hat{y}, \hat{p}_z] = 0 & \Rightarrow \sigma_y \sigma_{p_z} \geq 0 \\ [\hat{z}, \hat{p}_x] = 0 & \Rightarrow \sigma_z \sigma_{p_x} \geq 0 \\ [\hat{z}, \hat{p}_y] = 0 & \Rightarrow \sigma_z \sigma_{p_y} \geq 0 \\ [\hat{z}, \hat{p}_z] = i\hbar & \Rightarrow \sigma_z \sigma_{p_z} \geq \frac{\hbar}{2} \end{aligned}$$