CHAPTER 2

Schrödinger Equation and Wave Function

2.1 Write the Schrödinger equation for a particle in a potential $\sin x$.

The Schrödinger equation is

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \sin x\,\psi\ .$$

2.2 For a particle carrying a charge q in a uniform time-dependent electric field $\mathbf{E}(t)$ the force experienced by it is $\mathbf{F} = -\nabla(-q\mathbf{E}(t)\cdot\mathbf{X})$. Write the Schrödinger equation of the system.

The Schrödinger equation is

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi - (q\mathbf{E}(t)\cdot\mathbf{X})\psi\ .$$

2.3 Write the Schrödinger equation for a charged particle moving in an electromagnetic field with the Hamiltonian

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}(\mathbf{X},t)\right)^2 + q\phi(\mathbf{X},t)\ .$$

Rewrite the Schrödinger equation for $\mathbf{A} = (Bz, 0, 0)$ and $\phi = -Ez$.

The Schrödinger equation is

$$\begin{aligned}
\mathrm{i}\hbar\frac{\partial\psi}{\partial t} &= \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2\psi + q\phi\psi \\
&= \frac{1}{2m}\left(-\hbar^2\nabla^2\psi + \frac{q^2}{c^2}A^2\psi - p\left(\frac{q}{c}\mathbf{A}\psi\right) - \frac{q}{c}\mathbf{A}\cdot\mathbf{p}\psi\right) + q\phi\psi \\
&= \frac{1}{2m}\left[-\hbar^2\nabla^2\psi + 2\mathrm{i}\hbar\frac{q}{c}\mathbf{A}\cdot\nabla\psi + \mathrm{i}\hbar\frac{q}{c}\psi\nabla\cdot\mathbf{A} + \frac{q^2}{c^2}\mathbf{A}^2\psi\right] + q\phi\psi\ .
\end{aligned}$$

For $\mathbf{A} = (Bz, 0, 0)$ and $\phi = -Ez$ we have

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left[-\hbar^2\nabla^2\psi + 2\mathrm{i}\hbar\frac{q}{c}Bz\psi_z + \frac{q^2}{c^2}B^2z^2\psi\right] - qEz\psi\ .$$

2.4 What is the Schrödinger equation of a system of two particles of masses m_1 and m_2 carrying charges q_1 and q_2 respectively with $H = \frac{1}{2m_1}p_1^2 + \frac{1}{2m_2}p_2^2 + \frac{q_1q_2}{r_{12}}$ and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$?

The Schrödinger equation $\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = H\psi$ becomes

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m_1}\nabla_1^2\psi - \frac{\hbar^2}{2m_2}\nabla_2^2\psi + \frac{q_1q_2}{r_{12}}\psi\ ,$$

where

$$\nabla_i^2 = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2}, \quad i = 1, 2\ .$$

2.5 Starting from the Schrödinger equation for ψ, obtain the equation for ψ^*.

The Schrödinger equation for ψ is

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{X}, t)\psi\ .$$

Taking complex conjugate of the above equation we get

$$-\mathrm{i}\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V^*(\mathbf{X}, t)\psi^*\ .$$

This is the Schrödinger equation for ψ^*.

2.6 If E_1 and E_2 are the eigenvalues and ϕ_1 and ϕ_2 are the eigenfunctions of a Hamiltonian operator then find whether the energy corresponding to the superposition state $\phi_1 + \phi_2$ is equal to $E_1 + E_2$ or not.

We have $H\phi_1 = E_1\phi_1$ and $H\phi_2 = E_2\phi_2$. Then

$$\begin{aligned} H(\phi_1 + \phi_2) &= H\phi_1 + H\phi_2 \\ &= E_1\phi_1 + E_2\phi_2 \\ &\neq (E_1 + E_2)(\phi_1 + \phi_2)\ . \end{aligned}$$

2.7 Express the Schrödinger equation $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)\right]\psi(x,y,z) = E\psi(x,y,z)$ in the spherical polar coordinates defined by $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$ and in the parabolic coordinates defined by $\xi = r(1-\cos\theta)$, $\eta = r(1+\cos\theta)$, $\phi = \phi\cos\theta$.

In spherical polar coordinates the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + V(r,\theta,\phi)\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)\ .$$

In the parabolic coordinates the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\left[\frac{4}{\xi+\eta}\left\{\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right) + \frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right) + \frac{1}{\xi\eta}\frac{\partial^2}{\partial\phi^2}\right\} + V(\xi,\eta,\phi)\right]\psi = E\psi\ .$$

2.8 Find the condition under which both $\psi(\mathbf{X},t)$ and $\psi^*(\mathbf{X},-t)$ will be the solutions of the same time-dependent Schrödinger equation.

The Schrödinger equations for $\psi(\mathbf{X},t)$ and $\psi^*(\mathbf{X},-t)$ are given by

$$\begin{aligned} \mathrm{i}\hbar\frac{\partial\psi}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{X},t)\psi\ , \\ \mathrm{i}\hbar\frac{\partial\psi^*}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2\psi^* + V^*(\mathbf{X},-t)\psi \end{aligned}$$

respectively. The above two equations are identical if $V(\mathbf{X},t) = V^*(\mathbf{X},-t)$, that is if V is real and an even function of t.

2.9 What is the major difference between real and complex wave functions?

The probability current density $\mathbf{J}$ is given by

$$\mathbf{J} = \frac{\hbar}{2m\mathrm{i}}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]\ .$$

If ψ is real then $\mathbf{J} = 0$. If ψ is complex then $\mathbf{J}$ need not be zero.

2.10 What is the difference between the wave function $\psi_1 = \mathrm{e}^{\mathrm{i}(kx-\omega t)}$ and $\psi_2 = \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{X}-\omega t)}$?

ψ_1 is a plane (probability)wave travelling along a one-dimensional line. ψ_2 is a three-dimensional (probability)wave.

2.11 Write the Hamiltonian of a photon.

For a photon $H = E = mc^2 = mcc = pc$.

2.12 What is the physical meaning of $\langle x \rangle = 0$?

ψ is symmetric or antisymmetric with respect to $x = 0$.

2.13 Write the operator forms of kinetic energy and angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$.

The operator form of kinetic energy $mv^2/2$ is

$$(\text{K.E.})_{\text{op}} = \frac{1}{2} m \mathbf{v}^2 = \frac{\mathbf{p}^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2 .$$

For $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ we have with $\mathbf{r} = \mathbf{i}x + \mathbf{j}y + \mathbf{k}z$

$$\begin{aligned} \mathbf{L} &= \mathbf{r} \times \mathbf{p} = \begin{vmatrix} i & j & k \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \\ &= \mathbf{i}\,(yp_z - zp_y) + \mathbf{j}\,(zp_x - xp_z) + \mathbf{k}\,(xp_y - yp_x) . \end{aligned}$$

The components of $\mathbf{L}$ are

$$\begin{aligned} L_x &= \mathrm{i}\hbar \left(-y\frac{\partial}{\partial z} + z\frac{\partial}{\partial y} \right) = \mathrm{i}\hbar \left(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z} \right) , \\ L_y &= \mathrm{i}\hbar \left(-z\frac{\partial}{\partial x} + x\frac{\partial}{\partial z} \right) = \mathrm{i}\hbar \left(x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x} \right) , \\ L_z &= \mathrm{i}\hbar \left(-x\frac{\partial}{\partial y} + y\frac{\partial}{\partial x} \right) = \mathrm{i}\hbar \left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} \right) . \end{aligned}$$

2.14 Consider the one-dimensional Schrödinger equation $u(x) = -\frac{\mathrm{d}}{\mathrm{d}x} \ln \psi(x)$. Obtain the Schrödinger equation under the change of variable $u(x) = -\frac{\mathrm{d}}{\mathrm{d}x} \ln \psi(x)$.

The general transformation is $u = -\psi_x/\psi$ or $\psi_x = -u\psi$. Then $\psi_{xx} = -u_x\psi - u\psi_x$. Now, the Schrödinger equation is rewritten as (with $\lambda = 2mE/\hbar^2$ and $g = 2mV/\hbar^2$)

$$-u_x\psi - u\psi_x + (\lambda - g)\psi = 0 \quad \text{or} \quad -u_x\psi + u^2\psi + (\lambda - g)\psi = 0 .$$

That is, $u_x - u^2 - \lambda + g = 0$.

2.15 Find the conditions to be satisfied by the functions f and g such that under the transformation $\psi = f(x)F(g(x))$ the Schrödinger equation $\psi_{xx} + (E-V)\psi = 0$ can be written as

$$F_{gg} + Q(g)F_g + R(g)F(g) = 0\,. \tag{2.1}$$

Then show that

$$E - V = (g')^2\left[R - \frac{1}{2}Q_g - \frac{Q^2}{4}\right] + \left(\frac{g''}{2g'}\right)' - \left(\frac{g''}{2g'}\right)^2\,. \tag{2.2}$$

In terms of f and F the Schrödinger equation is written as

$$fF'' + 2f'F' + f''F + (E-V)fF = 0\,, \tag{2.3}$$

where prime denotes differentiation with respect to x. Since F is $F(g(x))$ we have

$$F' = F_g g'\,, \quad F'' = F_{gg}(g')^2 + F_g g''\,. \tag{2.4}$$

Then Eq. (2.3) becomes

$$F_{gg} + \left(\frac{2f'}{g'f} + \frac{g''}{g'^2}\right)F_g + \left[\frac{f''}{g'^2 f'^2} + \frac{(E-V)}{g'^2}\right]F = 0\,. \tag{2.5}$$

Comparison of Eqs. (2.1) and (2.5) gives

$$Q = \frac{2f'}{g'f} + \frac{g''}{g'^2}\,, \quad R = \frac{f''}{g'^2 f'^2} + \frac{E-V}{g'^2}\,. \tag{2.6}$$

The conditions on f and g are given by Eqs. (2.6). From Eqs. (2.6) we obtain

$$\frac{f'}{f} = \frac{g'Q}{2} - \frac{g''}{2g'} \tag{2.7a}$$

$$E - V = g'^2 R - \frac{f''}{f}\,. \tag{2.7b}$$

From (2.7a) we find f''/f and substituting it in (2.7b) we obtain

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{f'}{f}\right) = \frac{f''}{f} - \frac{f'^2}{f^2}\,. \tag{2.8}$$

That is,

$$\begin{aligned}
\frac{f''}{f} &= \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{f'}{f}\right) + \frac{f'^2}{f^2} \\
&= \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{g'Q}{2} - \frac{g''}{2g'}\right) + \left(\frac{g'Q}{2} - \frac{g''}{2g'}\right)^2 \\
&= \frac{1}{2}Q_g - \left(\frac{g''}{2g'}\right) + \frac{g'^2Q^2}{4} + \left(\frac{g''}{2g'}\right)^2\,.
\end{aligned} \tag{2.9}$$

Substituting the above in Eq. (2.7b) we obtain the Eq. (2.2).

2.16 What are the effects of addition of a constant to a potential on the time-independent Schrödinger equation and the energy levels?

The time-independent Schrödinger equation with the addition of a constant α to a potential is given by

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V + \alpha\right)\psi_n = E_n\psi_n \ .$$

This can be rewritten as

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi_n = (E_n - \alpha)\,\psi_n = E'_n\psi_n \ ,$$

where $E'_n = E_n - \alpha$. Therefore ψ_n remains the same but the energy eigenvalues of the new system are $E_n - \alpha$.

2.17 Which of the following wave functions are admissible in quantum mechanics? State the reasons.

(a) e^{-x^2}. (b) sech$x$. (c) e^{-x}. (d) tanh$x$. (e) $\sin x$, $0 < x < 2\pi$. (f) $\sin x$, $-\infty < x < \infty$. (g) $\sqrt{\mathrm{e}^{-x^2}}$. (h) $\tan x$. (i) sec$x$. (j) $x\mathrm{e}^{-x^2}$. (k) $1 - x^2$, $-1 < x < 1$.

The conditions to be satisfied by a wave function are: (i) ψ should be normalizable. (ii) It should be single-valued. (iii) It must be finite at every point. (iv) It and its first partial derivatives must be continuous.

The functions (a), (b), (e), (j) and (k) satisfy all the above conditions and hence they are admissible wave functions (verify).

The functions (c), (d), (f), (h), (i) are nonnormalizable. The function (g) is multivalued. Therefore, they are not admissible wave functions.

2.18 Normalize the wave function $\psi = N\mathrm{e}^{\mathrm{i}kx - x^2/(2\sigma^2)}$.

From the normalization condition we obtain

$$1 = \int_{-\infty}^{\infty} \psi^*\psi \,\mathrm{d}x = N^2\sigma \int_{-\infty}^{\infty} \mathrm{e}^{-y^2}\,\mathrm{d}y = N^2\sigma\sqrt{\pi} \ .$$

Thus $N = 1/\left(\sigma\sqrt{\pi}\,\right)^{1/2}$.

2.19 Find the value of N for which the wave function $\psi(x) = N$ for $|x| < a$ and 0 for $|x| > a$ is normalized.

The normalization condition gives

$$\begin{aligned} 1 &= \int_{-a}^{a} \psi^*\psi \,\mathrm{d}x = N^2 \int_{-a}^{a} \mathrm{d}x = N^2 x|_{-a}^{a} \\ &= 2aN^2 \ . \end{aligned}$$

Thus, $N = 1/\sqrt{2a}\,$.

2.20 Normalize the wave function $\psi = \mathrm{e}^{-|x|}\sin\alpha x$. It is given that $\displaystyle\int_0^\infty \mathrm{e}^{-x}\sin\alpha x\,\mathrm{d}x = \alpha^2/(1+\alpha^2)$.

The normalization condition gives

$$\begin{aligned}
1 &= N^2\int_{-\infty}^{\infty}\mathrm{e}^{-2|x|}\sin^2\alpha x\,\mathrm{d}x \\
&= N^2\int_{-\infty}^{0}\mathrm{e}^{2x}\sin^2\alpha x\,\mathrm{d}x + N^2\int_0^\infty \mathrm{e}^{-2x}\sin^2\alpha x\,\mathrm{d}x \\
&= 2N^2\int_0^\infty \mathrm{e}^{-2x}\sin^2\alpha x\,\mathrm{d}x \\
&= -\frac{N^2}{2}\mathrm{e}^{-2x}\,|_0^\infty - \frac{N^2}{2}\int_0^\infty \mathrm{e}^{-x}\cos\alpha x\,\mathrm{d}x \\
&= \frac{N^2}{2} - \frac{N^2}{2}\left[-\mathrm{e}^{-x}\cos\alpha x\,|_0^\infty - \alpha\int_0^\infty \mathrm{e}^{-x}\sin\alpha x\,\mathrm{d}x\right] \\
&= \frac{N^2}{2} - \frac{N^2}{2}\left[1 - \frac{\alpha^3}{1+\alpha^2}\right] \\
&= \frac{N^2\alpha^3}{2(1+\alpha^2)}\,.
\end{aligned}$$

That is, $N = \sqrt{2(1+\alpha^2)/\alpha^3}\,$.

2.21 A particle of mass m moves in a one-dimensional box of length L with origin as the centre. If the wave function of this particle is $\psi(x) = Nx(1-x^2)$ for $|x| < L/2$ and 0 otherwise find the factor N.

N can be determined from normalization condition. We obtain

$$\begin{aligned}
1 &= N^2\int_{-L/2}^{L/2} x^2\left(1-x^2\right)^2\,\mathrm{d}x \\
&= N^2\int_{-L/2}^{L/2}\left(x^2 - 2x^4 + x^6\right)\,\mathrm{d}x \\
&= N^2\left[\frac{L^3}{12} - \frac{L^5}{160} + \frac{L^7}{448}\right]
\end{aligned}$$

Thus,

$$N = \left[\frac{L^3}{12} - \frac{L^5}{160} + \frac{L^7}{448}\right]^{-1/2}\,.$$

If L is very small then $N \approx \sqrt{12/L^3}$.

2.22 A quantum mechanical particle moving in one-dimension has the wave function $\psi(x) = cx\mathrm{e}^{-|x|/b}$, $-\infty < x < \infty$ where c and b are constants ($b > 0$). Find the probability that the position of the particle lies in the region $-\infty < x \leq b$.

First, we normalize the wave function. We obtain

$$\begin{aligned}
1 &= \int_{-\infty}^{\infty} \psi^* \psi \,\mathrm{d}x \\
&= c^2 \int_{-\infty}^{\infty} x^2 \mathrm{e}^{-2|x|/b} \,\mathrm{d}x \\
&= c^2 \int_{-\infty}^{0} x^2 \mathrm{e}^{2x/b} \,\mathrm{d}x + c^2 \int_{0}^{\infty} x^2 \mathrm{e}^{-2x/b} \,\mathrm{d}x \\
&= 2c^2 \int_{0}^{\infty} x^2 \mathrm{e}^{-2x/b} \,\mathrm{d}x \,.
\end{aligned}$$

Substituting $2x/b = y$ in the integral, we get

$$1 = \frac{b^3 c^2}{4} \int_0^{\infty} y^2 \mathrm{e}^{-y} \,\mathrm{d}y \,.$$

Integrating by parts we get

$$1 = \frac{b^3 c^2}{2} \int_0^{\infty} y \mathrm{e}^{-y} \,\mathrm{d}y = \frac{b^3 c^2}{2} \int_0^{\infty} \mathrm{e}^{-y} \,\mathrm{d}y = \frac{b^3 c^2}{2} \,.$$

That is $c^2 = 2/b^3$ or $c = \sqrt{2/b^3}$. The probability $P(-\infty < x \leq b)$ is

$$\begin{aligned}
P &= \int_{-\infty}^{b} \psi^* \psi \,\mathrm{d}x \\
&= \frac{2}{b^3} \left[\int_{-\infty}^{0} x^2 \mathrm{e}^{2|x|/b} \,\mathrm{d}x + \int_0^b x^2 \mathrm{e}^{-2x/b} \,\mathrm{d}x \right] \\
&= \frac{2}{b^3} \frac{b^3}{8} \left[- \int_{\infty}^{0} y^2 \mathrm{e}^{-y} \,\mathrm{d}y + \int_0^b y^2 \mathrm{e}^{-y} \,\mathrm{d}y \right] \\
&= \frac{1}{4} \left[\int_0^{\infty} y^2 \mathrm{e}^{-y} \,\mathrm{d}y + \int_0^b y^2 \mathrm{e}^{-y} \,\mathrm{d}y \right]
\end{aligned}$$

Integrating by parts we get

$$P = 1 - \frac{\mathrm{e}^{-b}}{4} \left(b^2 + 2b + 2 \right) \,.$$

2.23 What is the probability current density corresponding to $\psi(x) = A\mathrm{e}^{-\alpha x}$ where A and α are constants?

The probability current density is given by

$$\mathbf{J} = \frac{\hbar}{2m\mathrm{i}}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right] .$$

Since the given ψ is real, $\psi^* = \psi$,

$$\mathbf{J} = \frac{\hbar}{2m\mathrm{i}}\left[\psi\nabla\psi - \psi\nabla\psi\right] = 0 .$$

2.24 A free particle in one-dimension is in a state described by $\psi = A\,\mathrm{e}^{\mathrm{i}(p_x x - Et)/\hbar} + B\,\mathrm{e}^{-\mathrm{i}(p_x x + Et)/\hbar}$ where p_x and E are constants. Find the probability current density.

$\mathbf{J}$ is given by

$$\begin{aligned}\mathbf{J} &= \frac{\hbar}{m}\,\mathrm{Im}(\psi^*\nabla\psi) \\ &= \frac{\hbar}{m}\,\mathrm{Im}\left\{\left[A^*\mathrm{e}^{-\mathrm{i}(p_x x - Et)/\hbar} + B^*\mathrm{e}^{\mathrm{i}(p_x x + Et)/\hbar}\right]\right. \\ &\qquad \left.\times\frac{\mathrm{i}p_x}{\hbar}\left[A\mathrm{e}^{\mathrm{i}(p_x x - Et)/\hbar} + B\mathrm{e}^{-\mathrm{i}(p_x x + Et)/\hbar}\right]\right\} \\ &= \frac{p_x}{m}\left[|A|^2 - |B|^2\right] .\end{aligned}$$

2.25 If the wave function of a particle at $t = 0$ is $\psi(x,0) = N\mathrm{e}^{-\mathrm{i}kx - (x^2/2a^2)}$ calculate the probability density and current density.

First, we normalize the given wave function. We obtain

$$1 = \int_{-\infty}^{\infty}\psi^*\psi\,\mathrm{d}x = 2N^2 a\int_0^{\infty}\mathrm{e}^{-y^2}\,\mathrm{d}y = N^2 a\sqrt{\pi} .$$

That is $N = (1/(a^2\pi))^{1/4}$. The probability density is obtained as

$$P(x) = \frac{1}{a\sqrt{\pi}}\,\mathrm{e}^{-x^2/a^2} .$$

Then the current density is determined as

$$\begin{aligned}J(x) &= \frac{\hbar}{2m\mathrm{i}}\left(\psi^*\frac{\mathrm{d}\psi}{\mathrm{d}x} - \psi\frac{\mathrm{d}\psi^*}{\mathrm{d}x}\right) \\ &= \frac{\hbar k}{m}\frac{1}{a\sqrt{\pi}}\,\mathrm{e}^{-x^2/a^2} \\ &= \frac{\hbar k}{m}P(x) .\end{aligned}$$

2.26 For the Gaussian wave function $\psi(x) = \left(\frac{1}{\sigma\sqrt{\pi}}\right)^{1/2} \mathrm{e}^{-x^2/2\sigma^2}$ calculate the probability current density.

The probability current density is given by

$$J = \frac{\hbar}{2m\mathrm{i}}\left(\psi^*\frac{\mathrm{d}\psi}{\mathrm{d}x} - \psi\frac{\mathrm{d}\psi^*}{\mathrm{d}x}\right) .$$

For any real ψ

$$\psi^*\frac{\mathrm{d}\psi}{\mathrm{d}x} - \psi\frac{\mathrm{d}\psi^*}{\mathrm{d}x} = 0 .$$

Then $J = 0$. Therefore, for the real Gaussian function $J = 0$.

2.27 Verify whether the wave function $\psi = N\mathrm{e}^{\mathrm{i}kx - x^2/(2a^2)}$ satisfies the continuity equation or not.

The continuity equation is given by $\frac{\partial\rho}{\partial t} + \frac{\mathrm{d}J}{\mathrm{d}x} = 0$. For the given function $\rho = \psi^*\psi = N^2\mathrm{e}^{-x^2/a^2}$ and $\frac{\partial\rho}{\partial t} = 0$. Further

$$\begin{aligned} J &= \frac{\hbar}{m}\mathrm{Im}\left(\psi^*\frac{\mathrm{d}\psi}{\mathrm{d}x}\right) \\ &= \frac{\hbar}{m}\mathrm{Im}\left(N^2\mathrm{e}^{-x^2/a^2}\left(\mathrm{i}k - x/a^2\right)\right) \\ &= \frac{N^2\hbar k}{m}\mathrm{e}^{-x^2/a^2} . \end{aligned}$$

Then

$$\frac{\mathrm{d}J}{\mathrm{d}x} = -2\frac{N^2\hbar k}{ma^2}x\mathrm{e}^{-x^2/a^2} .$$

Now the continuity equation becomes $x\mathrm{e}^{-x^2/a^2} = 0$ which is true only if $x = 0$. Hence, the given ψ does not satisfy the continuity equation.

2.28 The wave function of a linear harmonic oscillator with potential $V = m\omega^2x^2/2$ is $\psi = x\mathrm{e}^{-m\omega x^2/(2\hbar)}$. Find its energy.

The Schrödinger equation for a potential V is

$$\psi_{xx} + \frac{2m}{\hbar^2}(E - V)\psi = 0 .$$

For the given potential and ψ the above equation becomes

$$\frac{-3m\omega}{\hbar}x + \frac{m^2\omega^2}{\hbar^2}x^3 + \frac{2mE}{\hbar^2}x - \frac{m^2\omega^2}{\hbar^2}x^3 = 0 .$$

From the above equation we get $E = 3\hbar\omega/2$.

2.29 If $\psi = \sqrt{1/L}\cos(\pi x/(2L))$ for the system confined to the potential $V(x) = 0$ for $|x| < L$ and ∞ for $|x| > L$ then calculate E.

The Schrödinger equation for the given system is

$$\psi_{xx} + \frac{2m}{\hbar^2}E\psi = 0\ .$$

Then

$$E\psi = -\frac{\hbar^2}{2m}\psi_{xx} = \frac{\hbar^2}{2m\sqrt{L}}\left(\frac{\pi}{2L}\right)^2 \cos\frac{\pi x}{2L} = \frac{\hbar^2\pi^2}{8mL^2}\psi\ .$$

Thus. $E = \hbar^2\pi^2/(8mL^2)$.

2.30 The wave function of a particle confined to a box of length L is $\sqrt{2/L}\,\sin(\pi x/L)$ in the region $0 < x < L$ and zero everywhere else. Calculate the probability of finding the particle in the region $0 < x \le L/2$.

We obtain

$$\begin{aligned} P(0 < x \le L/2) &= \int_0^{L/2} \psi^*\psi\,\mathrm{d}x \\ &= \frac{2}{L}\int_0^{L/2} \sin^2\frac{\pi x}{L}\,\mathrm{d}x \\ &= \frac{1}{L}\int_0^{L/2}\left(1 - \cos\left(\frac{2\pi x}{L}\right)\right)\mathrm{d}x = \frac{1}{2}\ . \end{aligned}$$

2.31 Write the law of conservation of energy $H = T + V$ in terms of expectation values.

We write $\langle H\rangle = \langle T\rangle + \langle V\rangle$.

2.32 Are the wave functions

$$\psi_1 = \left(\frac{1}{\pi a_0^3}\right)^{1/2} \mathrm{e}^{-r/a_0} \ \text{and}\ \psi_2 = \left(\frac{1}{32\pi a_0^3}\right)^{1/2}\left(2 - \frac{r}{a_0}\right)\mathrm{e}^{-r/(2a_0)}$$

of the electron in hydrogen atom orthogonal?

The orthogonality integral is calculated as

$$\begin{aligned} \int_0^{\infty} \psi_1^*\psi_2\,\mathrm{d}\tau &\propto \int_0^{\infty}\left(2 - \frac{r}{a_0}\right) r^2 \mathrm{e}^{-3r/2a_0}\,\mathrm{d}r \\ &\propto 6\int_0^{\infty} y^2\mathrm{e}^{-y}\,\mathrm{d}y - 2\int_0^{\infty} y^3\mathrm{e}^{-y}\,\mathrm{d}y \\ &\propto 6\int_0^{\infty} y^2\mathrm{e}^{-y}\,\mathrm{d}y - 6\int_0^{\infty} y^2\mathrm{e}^{-y}\,\mathrm{d}y \\ &= 0\ . \end{aligned}$$

Since $\int_0^{\infty} \psi_1^*\psi_2\mathrm{d}\tau = 0$, the given two wave functions are orthogonal.

2.33 Find the potential corresponding to the following wave functions:

(a) $\psi = \dfrac{1}{\pi^{1/4}}\mathrm{e}^{-x^2/2}$, $E = \hbar\omega/2$.

(b) $\psi = A\sin(\pi x/(2L))$ for $|x| < L$ and 0 for $|x| > L$, $E = \hbar^2\pi^2/(8mL^2)$.

(c) $\psi = \alpha x\mathrm{e}^{-\beta x}\mathrm{e}^{\mathrm{i}E/\hbar}$.

(d) $\psi = (mV_0/\hbar)\mathrm{e}^{-kx}$ for $x > 0$, $(mV_0/\hbar)\mathrm{e}^{kx}$ for $x < 0$ and $E = -mV_0/(2\hbar^2)$, $k^2 = mV_0/\hbar^2$.

(a) The eigenvalue equation $H\psi = E\psi$ is

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V\psi = E\psi \quad \text{or} \quad V\psi = \frac{\hbar^2}{2m}\psi_{xx} + E\psi\,.$$

Substituting the given ψ and E in the above equation we get

$$V\psi = \frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}(-x)\psi + E\psi = \frac{\hbar^2}{2m}\left(-\psi + x^2\psi\right) + E\psi\,.$$

Then

$$V = \frac{\hbar^2}{2m}\left(-1 + x^2\right) + E = \frac{\hbar^2}{2m}\left(x^2 - 1\right) + \frac{\hbar\omega}{2}\,.$$

(b) For the given wave function we obtain

$$\begin{aligned} V\psi &= \frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}\frac{\pi}{2L}A\cos\frac{\pi x}{2L} + E\psi \\ &= -\frac{\hbar^2\pi^2}{8mL^2}\psi + E\psi \\ &= -E\psi + E\psi \\ &= 0\,. \end{aligned}$$

Therefore, $V(x) = 0$ for $|x| < L$ and ∞ for $|x| > L$.

(c) Using the given wave function we get

$$\begin{aligned} V\psi &= \frac{\hbar^2}{2m}\alpha\mathrm{e}^{\mathrm{i}E/\hbar}\frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{e}^{-\beta x} - \beta x^2\mathrm{e}^{-\beta x}\right) + E\psi \\ &= \frac{\hbar^2}{2m}\alpha\mathrm{e}^{\mathrm{i}E/\hbar}\left(-\beta\mathrm{e}^{-\beta x} - 2\beta x\mathrm{e}^{-\beta x} + \beta^2x^2\mathrm{e}^{-\beta x}\right) + E\psi \end{aligned}$$

or

$$V\alpha x\mathrm{e}^{-\beta x}\mathrm{e}^{\mathrm{i}E/\hbar} = \frac{\hbar^2}{2m}\alpha\mathrm{e}^{\mathrm{i}E/\hbar}\left(-\beta\mathrm{e}^{-\beta x} - 2\beta x\mathrm{e}^{-\beta x} + \beta^2x^2\mathrm{e}^{-\beta x}\right) + E\psi\,.$$

That is,

$$V = \frac{\hbar^2}{2m}\left(-\frac{\beta}{x} - 2\beta + \beta^2 x\right) + E\ .$$

(d) For the given wave function for $x > 0$

$$V\psi = \frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}(-k\psi) + E\psi = \frac{\hbar^2}{2m}k^2\psi + E\psi\ .$$

Then $V = \dfrac{k^2}{2}\left(\dfrac{\hbar^2}{m} - 1\right)$. Similarly, for $x < 0$ we obtain $V = \dfrac{k^2}{2}\left(\dfrac{\hbar^2}{m} - 1\right)$.

2.34 A particle of mass m is confined in the infinite square-well potential $V = 0$ for $0 < x \leq L$ and $V = \infty$ otherwise. It has the normalized stationary state eigenfunctions $\phi_n(x)$ and eigenvalues $E_n = n^2\hbar^2\pi^2/(2mL^2)$. Its wave function at time $t = 0$ is given by $\psi(x, 0) = (\phi_1(x) + \phi_2(x))/\sqrt{2}$. What is the smallest positive time τ for which $\psi(x, t)$ will be orthogonal to $\psi(x, 0)$?

The wave function $\psi(x, t)$ is

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left(\phi_1 \mathrm{e}^{-\mathrm{i}E_1 t/\hbar} + \phi_2 \mathrm{e}^{-\mathrm{i}E_2 t/\hbar}\right)\ .$$

At $t = \tau$ the condition for $\psi(x, 0)$ and $\psi(x, t)$ to be orthogonal is

$$\int_0^L \psi^*(x,\tau)\psi(x,0)\,\mathrm{d}x = 0\ .$$

We get

$$\int_0^L \left(\phi_1^* \mathrm{e}^{\mathrm{i}E_1\tau/\hbar} + \phi_2^* \mathrm{e}^{\mathrm{i}E_2\tau/\hbar}\right)(\phi_1 + \phi_2)\ \mathrm{d}x = 0\ .$$

Since $\int_0^L \phi_m\phi_n\,\mathrm{d}x = \delta_{mn}$ we get $\mathrm{e}^{\mathrm{i}E_1\tau/\hbar} + \mathrm{e}^{\mathrm{i}E_2\tau/\hbar} = 0$. That is

$$\cos\frac{E_1\tau}{\hbar} + \mathrm{i}\sin\frac{E_1\tau}{\hbar} + \cos\frac{E_2\tau}{\hbar} + \mathrm{i}\sin\frac{E_2\tau}{\hbar} = 0\ .$$

Equating the real and imaginary parts to zero separately we get

$$\cos\frac{E_1\tau}{\hbar} = -\cos\frac{E_2\tau}{\hbar}\ , \quad \sin\frac{E_1\tau}{\hbar} = -\sin\frac{E_2\tau}{\hbar}\ .$$

We rewrite the above conditions as

$$\cos\frac{E_1\tau}{\hbar} = \cos\frac{\pi + E_2\tau}{\hbar}\ , \quad \sin\frac{E_1\tau}{\hbar} = \sin\frac{\pi + E_2\tau}{\hbar}\ .$$

Thus, $\tau = \hbar\pi/(E_1 - E_2)$. Since $E_2 > E_1$ we write $\tau = \hbar\pi/(E_2 - E_1)$.

2.35 Show that $\langle xp_x + p_x x\rangle$ is real.

Consider $\langle p_x x\rangle$. We obtain

$$\begin{aligned}\langle p_x x\rangle &= \int_{-\infty}^{\infty} \psi^* p_x x\psi \, \mathrm{d}x \\ &= \int_{-\infty}^{\infty} (p_x^\dagger \psi)^* x\psi \, \mathrm{d}x \\ &= \left(\int_{-\infty}^{\infty} p_x \psi x^* \psi^* \, \mathrm{d}x\right)^* \\ &= \left(\int_{-\infty}^{\infty} \psi^* x p_x \psi \, \mathrm{d}x\right)^* \\ &= \langle xp_x\rangle^* \, .\end{aligned}$$

Now, $\langle xp_x + p_x x\rangle = \langle xp_x\rangle + \langle p_x x\rangle = \langle xp_x\rangle + \langle xp_x\rangle^* = 2\mathrm{Re}\langle xp_x\rangle$. Thus $\langle xp_x + p_x x\rangle$ is real.

2.36 Show that $\langle A^n\rangle = \langle A\rangle^n$ in its eigenstates.

Let $A\psi = \alpha\psi$. Then we obtain

$$\begin{aligned}\langle A^n\rangle &= \int_{-\infty}^{\infty} \psi^* A^n \psi \, \mathrm{d}\tau \\ &= \int_{-\infty}^{\infty} \psi^* A^{n-1} A\psi \, \mathrm{d}\tau \\ &= \alpha \int_{-\infty}^{\infty} \psi^* A^{n-1} \psi \, \mathrm{d}\tau \\ &= \alpha^n \int_{-\infty}^{\infty} \psi^* \psi \, \mathrm{d}\tau \\ &= \alpha^n \, .\end{aligned}$$

We find $\langle A\rangle = \int_{-\infty}^{\infty} \psi^* A\psi \, \mathrm{d}\tau = \alpha \int_{-\infty}^{\infty} \psi^* \psi \, \mathrm{d}\tau = \alpha$. Hence, $\langle A^n\rangle = \alpha^n = \langle A\rangle^n$.

2.37 Calculate $\langle p_x^2\rangle$ for $\psi = \sqrt{k}\mathrm{e}^{-k|x|}$.

We obtain

$$\langle p_x^2\rangle = \int_{-\infty}^{\infty} \psi^* p_x^2 \psi \, \mathrm{d}x = -\hbar^2 \int_{-\infty}^{\infty} \mathrm{e}^{-k|x|} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \mathrm{e}^{-k|x|} \, \mathrm{d}x \, .$$

The above equation can be rewritten as

$$\langle p_x^2\rangle = -\hbar^2 k \left[\int_{-\infty}^{0} \mathrm{e}^{kx} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \mathrm{e}^{kx} \, \mathrm{d}x + \int_{0}^{\infty} \mathrm{e}^{-kx} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \mathrm{e}^{-kx} \, \mathrm{d}x\right] \, .$$

Then we obtain

$$\langle p_x^2\rangle = -\hbar^2 k^3\left[\int_{-\infty}^{0} \mathrm{e}^{2kx}\,\mathrm{d}x + \int_{0}^{\infty} \mathrm{e}^{-2kx}\,\mathrm{d}x\right] = -\hbar^2 k^2 \;.$$

2.38 A particle of mass m in the one-dimensional energy well $V(x) = 0$ for $0 \le x \le L$ and ∞ otherwise is in a state whose wave function is given by $\psi(x) = Nx(L-x)$ where N is the normalization constant. Determine $\langle E\rangle$ in this state.

The normalization condition gives

$$1 = N^2\int_0^L x^2(L-x)^2\,\mathrm{d}x = \frac{N^2L^5}{30}\;.$$

That is, $N = \sqrt{30/L^5}$. Next,

$$\begin{aligned}\langle E\rangle &= \int_0^L \psi^* H\psi\,\mathrm{d}x\\ &= \int_0^L \psi\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\psi\,\mathrm{d}x\\ &= \frac{\hbar^2}{m}N^2\int_0^L \left(xL - x^2\right)\mathrm{d}x\\ &= \frac{5\hbar^2}{mL^2}\;.\end{aligned}$$

2.39 Show that $\dfrac{\mathrm{d}}{\mathrm{d}t}\langle x^2\rangle = \dfrac{2}{m}\langle xp_x\rangle - \dfrac{\mathrm{i}\hbar}{m}$.

$\langle x^2\rangle$ is given by $\langle x^2\rangle = \int_{-\infty}^{\infty}\psi^* x^2\psi\,\mathrm{d}x$. Then

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle x^2\rangle &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}\psi^* x^2\psi\,\mathrm{d}x\\ &= \int_{-\infty}^{\infty}\frac{\partial\psi^*}{\partial t}x^2\psi\,\mathrm{d}x + \int_{-\infty}^{\infty}\psi^* x^2\frac{\partial\psi}{\partial t}\,\mathrm{d}x\;.\end{aligned}$$

Using the Schrödinger equation for $\dfrac{\partial\psi}{\partial t}$ and $\dfrac{\partial\psi^*}{\partial t}$ we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle x^2\rangle &= -\frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{\infty}\left(\frac{p_x^2\psi^*}{2m} + V\psi^*\right)x^2\psi\mathrm{d}x\\ &\quad +\frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{\infty}\psi^* x^2\left(\frac{p_x^2}{2m}\psi + V\psi\right)\mathrm{d}x\\ &= \frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty}\psi^* p_x^2\left(x^2\psi\right)\,\mathrm{d}x - \frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty}\psi^* x^2 p_x^2\psi\,\mathrm{d}x\;.\end{aligned}$$

Expanding the first integral we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle x^2\rangle &= \frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty}\psi^*\left(2p\psi p_x x^2+\psi p^2 x^2\right)\,\mathrm{d}x\\ &= \frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty}\psi^*\left(-4\mathrm{i}\hbar x p_x\psi+2\psi(-\mathrm{i}\hbar)^2\right)\,\mathrm{d}x\\ &= \frac{2}{m}\langle xp_x\rangle-\frac{\mathrm{i}\hbar}{m}\,.\end{aligned}$$

2.40 Show that $\dfrac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x^2\rangle=\dfrac{2}{m^2}\langle p_x^2\rangle+\dfrac{2}{m}\langle xF\rangle$.

We have $\dfrac{\mathrm{d}}{\mathrm{d}t}\langle x^2\rangle=\dfrac{2}{m}\langle xp_x\rangle-\dfrac{\mathrm{i}\hbar}{m}$. Then

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x^2\rangle &= \frac{2}{m}\frac{\mathrm{d}}{\mathrm{d}t}\langle xp_x\rangle\\ &= \frac{2}{m}\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}\psi^*(xp_x)\psi\,\mathrm{d}x\\ &= \frac{2}{m}\int_{-\infty}^{\infty}\frac{\partial\psi^*}{\partial t}xp_x\psi\,\mathrm{d}x+\frac{2}{m}\int_{-\infty}^{\infty}\psi^* xp_x\frac{\partial\psi}{\partial t}\,\mathrm{d}x\,.\end{aligned}$$

Using the Schrödinger equation

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x^2\rangle &= \frac{\mathrm{i}}{m^2\hbar}\int_{-\infty}^{\infty}p_x^2\psi^* xp_x\psi\,\mathrm{d}x+\frac{2\mathrm{i}}{m\hbar}\int_{-\infty}^{\infty}V\psi^* xp_x\psi\,\mathrm{d}x\\ &\quad-\frac{\mathrm{i}}{m^2\hbar}\int_{-\infty}^{\infty}\psi^* xp_x^3\psi\,\mathrm{d}x-\frac{2\mathrm{i}}{m\hbar}\int_{-\infty}^{\infty}\psi^* xp_x(V\psi)\,\mathrm{d}x\\ &= \frac{\mathrm{i}}{m^2\hbar}\int_{-\infty}^{\infty}\psi^2\left[p_x(p_x xp_x\psi+xp_x^2\psi)-xp_x^3\psi\right]\,\mathrm{d}x\\ &\quad-\frac{2\mathrm{i}}{m\hbar}\int_{-\infty}^{\infty}\psi^* x\psi\left(-\mathrm{i}\hbar\frac{\mathrm{d}V}{\mathrm{d}x}\right)\,\mathrm{d}x\,.\end{aligned}$$

Substituting $F=-\mathrm{d}V/\mathrm{d}x$ we get

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x^2\rangle &= \frac{\mathrm{i}}{m^2\hbar}\int_{-\infty}^{\infty}\psi^*\left(2p_x xp_x^2\psi\right)\,\mathrm{d}x+\frac{2}{m}\langle xF\rangle\\ &= \frac{2\mathrm{i}}{m^2\hbar}\int_{-\infty}^{\infty}\psi^*(-\mathrm{i}\hbar)p_x^2\psi\,\mathrm{d}x+\frac{2}{m}\langle xF\rangle\\ &= \frac{2}{m^2}\langle p_x^2\rangle+\frac{2}{m}\langle xF\rangle\,.\end{aligned}$$

2.41 Show that $\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x^2\rangle = \langle 2Fp_x + p_xF\rangle$.

By definition $\langle p_x^2\rangle = \int_{-\infty}^{\infty}\psi^* p_x^2\psi\mathrm{d}\tau$. Then

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x^2\rangle = \int_{-\infty}^{\infty}\frac{\partial\psi^*}{\partial t}p_x^2\psi\,\mathrm{d}\tau + \int_{-\infty}^{\infty}\psi^* p_x^2\frac{\partial\psi}{\partial t}\,\mathrm{d}\tau\ .$$

Using the Schrödinger equation we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x^2\rangle &= -\frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{\infty}\left(\frac{p_x^2\psi^*}{2m} + V\psi^*\right)p_x^2\psi\,\mathrm{d}\tau \\ &\quad + \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{\infty}\psi^* p_x^2\left(\frac{p_x^2\psi}{2m} + V\psi\right)\,\mathrm{d}\tau\ .\end{aligned}$$

That is,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x^2\rangle &= \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{\infty}V\psi^* p_x^2\psi\,\mathrm{d}\tau - \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{\infty}\psi^* p_x^2\left(V\psi\right)\,\mathrm{d}\tau \\ &= -\frac{\mathrm{i}}{\hbar}\left[2\int_{-\infty}^{\infty}\psi^* p_xVp_x\psi\,\mathrm{d}\tau + \int_{-\infty}^{\infty}\psi^*\left(p_x^2V\right)\psi\mathrm{d}\tau\right] \\ &= -2\frac{\mathrm{i}}{\hbar}(-\mathrm{i}\hbar)\int_{-\infty}^{\infty}\psi^*\nabla Vp_x\psi\,\mathrm{d}\tau - \frac{\mathrm{i}}{\hbar}(-\mathrm{i}\hbar)\int_{-\infty}^{\infty}\psi^*(p_x\nabla V)\psi\,\mathrm{d}\tau \\ &= 2\int_{-\infty}^{\infty}\psi^* Fp_x\psi\,\mathrm{d}\tau + \int_{-\infty}^{\infty}\psi^* p_xF\psi\mathrm{d}\tau \\ &= \langle 2Fp_x + p_xF\rangle\ .\end{aligned}$$

2.42 Show that $\frac{\mathrm{d}}{\mathrm{d}t}\langle p_xx\rangle = \frac{1}{m}\langle p_x^2\rangle + \langle xF\rangle$.

The expectation value of p_xx is

$$\begin{aligned}\langle p_xx\rangle &= \int_{-\infty}^{\infty}\psi^* p_xx\psi\,\mathrm{d}x \\ &= -\mathrm{i}\hbar\int_{-\infty}^{\infty}\psi^*\psi\,\mathrm{d}x + \int_{-\infty}^{\infty}\psi^* xp_x\psi\,\mathrm{d}x \\ &= -\mathrm{i}\hbar + \int_{-\infty}^{\infty}\psi^* xp_x\psi\,\mathrm{d}x\ .\end{aligned}$$

Now

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle p_xx\rangle &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}\psi^* xp_x\psi\,\mathrm{d}x \\ &= \int_{-\infty}^{\infty}\frac{\partial\psi^*}{\partial t}xp_x\psi\,\mathrm{d}x + \int_{-\infty}^{\infty}\psi^* xp_x\frac{\partial\psi}{\partial t}\,\mathrm{d}x\ .\end{aligned}$$

We have

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \frac{p_x^2}{2m}\psi + V\psi \ , \quad -\mathrm{i}\hbar\frac{\partial\psi^*}{\partial t} = \frac{p_x^2}{2m}\psi^* + V\psi^* \ .$$

Using these two equations for $\partial\psi/\partial t$ and $\partial\psi^*/\partial t$ we get

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x x\rangle &= \frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty} p_x^2\psi^* x p_x\psi\,\mathrm{d}x + \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{\infty} V\psi^* x p_x\psi\,\mathrm{d}x \\
&\quad -\frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty}\psi^* x p_x^3\psi\,\mathrm{d}x - \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{\infty}\psi^* x p_x(V\psi)\,\mathrm{d}x \\
&= \frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty}\psi^* p_x^2(x p_x\psi)\,\mathrm{d}x - \frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty}\psi^* x p_x^3\psi\,\mathrm{d}x \\
&\quad + \int_{-\infty}^{\infty}\psi^* x\psi F\,\mathrm{d}x \ .
\end{aligned}$$

Then

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x x\rangle &= \frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty}\psi^* p_x^2(x p_x\psi)\,\mathrm{d}x - \frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty}\psi^* x p_x^3\psi\,\mathrm{d}x + \langle xF\rangle \\
&= \frac{\mathrm{i}}{2m\hbar}\int_{-\infty}^{\infty}\psi^* p_x x p_x^2\psi\,\mathrm{d}x + \langle xF\rangle \\
&= \frac{1}{m}\int_{-\infty}^{\infty}\psi^* p_x^2\psi\,\mathrm{d}x + \langle xF\rangle \\
&= \frac{1}{m}\langle p_x^2\rangle + \langle xF\rangle \ .
\end{aligned}$$

2.43 For a free particle show that $\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x^2\rangle = 0$ and $\frac{\mathrm{d}}{\mathrm{d}t}\langle xp_x + p_x x\rangle = \frac{2}{m}\langle p_x^2\rangle$.

We have the result

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x x\rangle = \frac{1}{m}\langle p_x^2\rangle + \langle xF\rangle \ , \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle p_x^2\rangle = \langle 2Fp_x + p_x F\rangle \ .$$

For a free particle $F = 0$ and hence

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x x\rangle = \frac{1}{m}\langle p_x^2\rangle \ , \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle p_x^2\rangle = 0 \ .$$

Consider $[x, p_x] = xp_x - p_x x = \mathrm{i}\hbar$. From this we write

$$\begin{aligned}
xp_x - p_x x + p_x x - p_x x &= \mathrm{i}\hbar \\
xp_x + p_x x - 2p_x x &= \mathrm{i}\hbar \\
xp_x + p_x x &= \mathrm{i}\hbar + 2p_x x \ .
\end{aligned}$$

Then

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle xp_x + p_x x\rangle = 2\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x x\rangle = \frac{2}{m}\langle p_x^2\rangle \ .$$

2.44 ϕ_1 and ϕ_2 are the only eigenfunctions of a system belonging to the energy eigenvalues E_0 and $-E_0$ respectively. In a measurement of the energy of the system, $\langle E\rangle$ is found to be $E_0/2$. Find the wave function of the system.

The wave function of the system is $\psi = C_1\phi_1 + C_2\phi_2$, $\quad C_1^2 + C_2^2 = 1$. Further

$$\begin{aligned}\langle E\rangle &= C_1^2 E_1 + C_2^2 E_2\\ &= C_1^2 E_0 - C_2^2 E_0\\ &= E_0\left(C_1^2 - C_2^2\right) .\end{aligned}$$

Since $\langle E\rangle = E_0/2$ we get $C_1^2 - C_2^2 = 1/2$. Solving $C_1^2 + C_2^2 = 1$ and $C_1^2 - C_2^2 = 1/2$ we get $C_1 = \sqrt{3}/2$ and $C_2 = 1/2$. Then

$$\psi = \frac{\sqrt{3}}{2}\phi_1 + \frac{1}{2}\phi_2 .$$

2.45 The H of a charged particle in uniform electric and magnetic fields is given by $H = \dfrac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 - eE_0\mathbf{k}.\mathbf{k}$ where $\mathbf{A} = B_0(-y, x, 0)/2$. Both electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$ are applied along the z-direction. Applying Ehrenfest's theorem, show that $\dfrac{\mathrm{d}}{\mathrm{d}t}\langle\mathbf{r}\rangle = \dfrac{1}{m}\langle\mathbf{p} - e\mathbf{A}\rangle$ and $\dfrac{\mathrm{d}}{\mathrm{d}t}\langle\mathbf{p} - e\mathbf{A}\rangle = eE_0\mathbf{k} + \dfrac{e}{m}\langle\mathbf{p} - e\mathbf{A}\rangle \times \nabla \times \mathbf{A}$.

$\nabla \times \mathbf{A}$ is obtained as $\nabla \times \mathbf{A} = B_0\mathbf{k}$. H is $\dfrac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 - eE_0$. Now, consider $\dfrac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle$. We obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle &= \int_{-\infty}^{\infty}\frac{\partial\psi^*}{\partial t}x\psi\,\mathrm{d}x + \int_{-\infty}^{\infty}\psi^* x\frac{\partial\psi}{\partial t}\,\mathrm{d}x\\ &= -\frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{\infty}H\psi^* x\psi\,\mathrm{d}x + \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{\infty}\psi^* xH\psi\,\mathrm{d}x\\ &= \frac{1}{\mathrm{i}\hbar}\langle[x, H]\rangle .\end{aligned}$$

Next, we find

$$\begin{aligned}
[x, H] &= \left[x, \frac{1}{2m}(\mathbf{p} - e\mathbf{A}) \cdot (\mathbf{p} - e\mathbf{A}) + eE_0\right] \\
&= \frac{1}{2m}\left[x, p_x^2\right] + \frac{1}{2m}\left[x, e^2 A^2\right] \\
&\quad -\frac{1}{2m}[x, \mathbf{p} \cdot e\mathbf{A}] - \frac{1}{2m}[x, e\mathbf{A} \cdot \mathbf{p}] + [x, eE_0] \\
&= \frac{1}{2m}\left[x, p_x^2\right] - \frac{1}{2m}(\mathrm{i}\hbar e A_x) - \frac{1}{2m}(\mathrm{i}\hbar e A_x) \\
&= \frac{\mathrm{i}\hbar}{m} p_x - \frac{\mathrm{i}\hbar}{m} e A_x \;.
\end{aligned}$$

Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{1}{\mathrm{i}\hbar}\left(\frac{\mathrm{i}\hbar}{m}p_x - \mathrm{i}\hbar\frac{eA_x}{m}\right) = \frac{1}{m}(p_x - eA_x) \;.$$

Hence,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{r}\rangle = \frac{1}{m}\langle \mathbf{p} - e\mathbf{A}\rangle \;.$$

Next,

$$\begin{aligned}
\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle \mathbf{r}\rangle &= \langle \mathbf{F}\rangle = \frac{\mathrm{d}}{\mathrm{d}t} m \frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{r}\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{p} - e\mathbf{A}\rangle \\
&= \frac{1}{\mathrm{i}\hbar}\langle[\mathbf{p} - e\mathbf{A}, H]\rangle
\end{aligned}$$

We obtain with $\mathbf{v} = \mathrm{d}\mathbf{r}/\mathrm{d}t$, $\mathbf{B} = \nabla \times \mathbf{A}$

$$\begin{aligned}
\langle \mathbf{F}\rangle &= e\mathbf{E} + \frac{e}{2m}\langle \mathbf{v} \times \mathbf{B} - \mathbf{B} \times \mathbf{v}\rangle \\
&= e\mathbf{E} + \frac{e}{2m}[(\mathbf{p} - e\mathbf{A}) \times \mathbf{B} - \mathbf{B} \times (\mathbf{p} - e\mathbf{A})] \\
&= e\mathbf{E} + \frac{e}{m}[(\mathbf{p} - e\mathbf{A}) \times \nabla \times A] \;.
\end{aligned}$$

Hence,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{p} - e\mathbf{A}\rangle = \langle \mathbf{F}\rangle = eE_0\mathbf{k} + \frac{e}{m}(\mathbf{p} - e\mathbf{A}) \times \nabla \times \mathbf{A} \;.$$

2.46 A particle of mass m enclosed in a one-dimensional box of length L such that $0 < x < L$, has energy eigenfunctions $\phi_n(x) = A\sin(n\pi x/L)$, $n = 1, 2, \cdots$ and $E_n = n^2\pi^2\hbar^2/(2mL^2)$. At $t = 0$, the particle has the wave function $\psi(x) = B\sin(2\pi x/L)\cos(\pi x/L)$ where B is a constant. (i) If the energy of the particle is measured at $t = 0$, what are the possible results of the measurement? (ii) What is the expectation value of energy?

(i) The wave function can be written as a combination of eigenfunctions as

$$\begin{aligned} \psi &= B \sin\frac{2\pi x}{L}\cos\frac{\pi x}{L} \\ &= \frac{B}{2}\left(\sin\frac{\pi x}{L} + \sin\frac{3\pi x}{L}\right) \\ &= \frac{B}{2}\left(\phi_1 + \phi_3\right) \,. \end{aligned}$$

That is, the system can have only two eigenstates ϕ_1 and ϕ_3 each with probability $B^2/4$. Further, $(B^2/4) + (B^2/4) = 1$ gives $B = \sqrt{2}$. Therefore,

$$\psi = \frac{1}{\sqrt{2}}\left(\phi_1 + \phi_3\right) \,.$$

If the energy is measured then one may get the energy as E_1 with the probability $1/2$ and E_3 with probability $1/2$.

(ii) We obtain

$$\langle E\rangle = C_1^2 E_1 + C_3^2 E_3 = \frac{1}{2}\left(E_1 + E_3\right) = \frac{5\pi^2\hbar^2}{2mL^2} \,.$$

2.47 Given the normalized ground state wave function of hydrogen atom $\psi_{100} = 1/(\pi a_0^3)^{1/2}\,\mathrm{e}^{-r/a_0}$ find the expectation value of its z-coordinate.

We obtain

$$\langle z\rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{\pi a_0^2}\mathrm{e}^{-2r/a_0} z r^2 \,\mathrm{d}r\, \sin\theta \mathrm{d}\theta\, \mathrm{d}\phi \,.$$

Substituting $z = r\cos\theta$ we get

$$\begin{aligned} \langle z\rangle &= \frac{1}{\pi a_0^3}\int_0^\infty \int_0^\pi \int_0^{2\pi} r^3 \mathrm{e}^{-2r/a_0} \sin\theta\cos\theta \,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi \\ &= -\frac{1}{2a_0^3}\cos 2\theta\big|_0^\pi \int_0^\infty r^3\mathrm{e}^{-2r/a_0}\,\mathrm{d}r \\ &= 0\,. \end{aligned}$$

2.48 If $H\phi_n(x) = E_n\phi_n(x)$ find the expectation value of the Hamiltonian operator H in the normalized superposition state $\psi(x,t) = \sum_{n=0}^{\infty} C_n\phi_n(x)\,\mathrm{e}^{-\mathrm{i}E_n t/\hbar}$.

We obtain

$$\begin{aligned}
\langle E\rangle &= \langle\psi|H|\psi\rangle \\
&= \sum_{n'}\sum_{n} C^*_{n'}C_n \mathrm{e}^{\mathrm{i}(E_{n'}-E_n)t/\hbar}\int_{-\infty}^{\infty}\phi^*_{n'}H\phi_n\,\mathrm{d}x \\
&= \sum_{n'}\sum_{n} C_n C^*_{n'}\mathrm{e}^{\mathrm{i}(E'_n-E_n)t/\hbar}\int_{-\infty}^{\infty}\phi^*_{n'}E_n\phi_n\,\mathrm{d}x \\
&= \sum_{n'}\sum_{n} C_n C^*_{n'}\mathrm{e}^{\mathrm{i}(E'_n-E_n)t/\hbar}E_n\delta_{nn'} \\
&= \sum_{n}|C_n|^2 E_n\ .
\end{aligned}$$

2.49 Consider a system in a state $\psi = (\phi_1+\phi_2)/\sqrt{2}$ where ϕ_1 and ϕ_2 are orthonormal eigenfunctions with the eigenvalues E_1 and E_2 respectively. What is the probability of finding the system in the energy E_1? What is $\langle E\rangle$?

The probability of finding the system with energy E_1 is $(1/\sqrt{2})^2 = 1/2$. Next

$$\langle E\rangle = \sum_{n=1}^{2}|C_n|^2E_n = \frac{1}{2}E_1+\frac{1}{2}E_2 = \frac{1}{2}(E_1+E_2)\ .$$

2.50 Consider a spherically symmetric potential energy function given by $V(r) = 0$, for $0 < r < a$ and ∞ for $r > a$. Given the solution $\psi(r) = A\dfrac{\sin kr}{r} + B\dfrac{\cos kr}{r}$ where $k = (2mE/\hbar^2)^{1/2}$ satisfying the Schrödinger equation, obtain the corresponding eigenvalues by applying proper boundary conditions.

As $r\to 0$, ψ must be finite. The condition $\lim_{r\to 0}\psi(r) =$ finite sets $B = 0$. So $\psi(r) = A\dfrac{\sin kr}{r}$. At $r = a$ we require $\psi = 0$. This gives $\sin ka = 0$. That is, $ka = n\pi$, $n = 1, 2, \cdots$. Hence, the energy eigenvalues are given by

$$E_n = \frac{\hbar^2k_n^2}{2m} = \frac{n^2\hbar^2\pi^2}{2ma^2}\ .$$