

4.E: Postulates and Principles of Quantum Mechanics (Exercises)

Solutions to select questions can be found online.

4.3

The function $\psi^*\psi$ has to be real, nonnegative, finite, and of definite value everywhere. Why?

Solution

If we follow the Born interpretation of wavefunctions, then $\psi^*\psi$ is a probability density and hence must follow standard probability properties including being non-negative, finite and of a definite value at any relevant point in the space of the wavefunction. Moreover, the integral of $\psi^*\psi$ over all this space must be equal to 1.

4.5

Why are the following functions not acceptable wave functions for a 1D particle in a box with length a ? N is a normalization constant.

a. $\psi = N \cos \frac{n\pi x}{L}$

b. $\psi = \frac{N}{\sin \frac{n\pi x}{a}}$

c. $\psi = N \tan \frac{\pi x}{a}$

Solution

The boundary conditions that need to be met are $\psi(0) = \psi(a) = 0$. This does not meet them. The proposed wavefunction blows up to infinity at $x = 0$ and $x = a$. Tan is not defined for $x = \frac{a}{2}$.

4.12

Show that the sets of functions: $\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$ where $n = 1, 2, 3, \dots$ is orthonormal.

Solution

Let

$$\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Because $\psi^* = \psi$ and is real, then

$$\int_0^L \psi^* \psi dx = \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \sqrt{\frac{2}{L}} \sin\left(\frac{m\pi x}{L}\right) dx$$

Letting $n = m$

$$\begin{aligned} \int_0^L \psi^* \psi dx &= \frac{2}{L} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi x}{L}\right) dx \\ &= \frac{2}{L} \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \\ &= \frac{2}{L} \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1 \end{aligned}$$

Letting $n \neq m$

$$\begin{aligned} \int_0^L \psi^* \psi dx &= \frac{2}{L} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx \\ &= \frac{2}{L} \frac{1}{2} \int_0^L \left[\cos\left(\frac{(n-m)\pi x}{L}\right) - \cos\left(\frac{(n+m)\pi x}{L}\right) \right] dx \\ &= \frac{1}{L} \left[\frac{L}{(n-m)\pi} \left[\sin\left(\frac{(n-m)\pi L}{L}\right) - \sin\left(\frac{(n-m)\pi 0}{L}\right) \right] - \frac{L}{(n+m)\pi} \left[\sin\left(\frac{(n+m)\pi L}{L}\right) - \sin\left(\frac{(n+m)\pi 0}{L}\right) \right] \right] = 0 \end{aligned}$$

and thus $\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$ ($n=1, 2, 3, \dots$) are orthonormal.

4.13

Show that $a \cdot b \cdot c = \sum_{ik} a_i b_i c_k e_k$

$$\begin{aligned} \sum_i a_i e_i \cdot \sum_j b_j e_j \cdot \sum_k c_k e_k &= \sum_{ik} a_i b_i c_k e_k \\ \sum_i \sum_j a_i b_j (e_i \cdot e_j) \cdot \sum_k c_k e_k &= \sum_{ik} a_i b_i c_k e_k \\ e_i \cdot e_j &= \delta_{ij} = 1 \end{aligned}$$

when $i = j$

$$\begin{aligned} \sum_i a_i b_i \cdot \sum_k c_k e_k &= \sum_{ik} a_i b_i c_k e_k \\ \sum_{ik} a_i b_i c_k e_k &= \sum_{ik} a_i b_i c_k e_k \end{aligned}$$

4.14

Determine if the following operators commute

$$\hat{B} = \frac{d}{dx}$$

and

$$\hat{C} = x^5$$

Solution

We must solve $[\hat{B}, \hat{C}]$, by solving for $\hat{B}\{\hat{C}f(x)\}$ and $\hat{C}\{\hat{B}f(x)\}$ for a wavefunction $f(x)$ and see if they are equal.

$$\hat{B}\{\hat{C}f(x)\} = \hat{B}\{x^5 f(x)\} = \frac{d}{dx}\{x^5 f(x)\} = 5x f(x) + x^5 f'(x)$$

$$\hat{C}\{\hat{B}f(x)\} = \hat{C}\{f'(x)\} = x^5 f'(x)$$

since

$$[\hat{B}, \hat{C}] = 5x f(x) + x^5 f'(x) - x^5 f'(x) = 5x f(x) \neq 0$$

The two operators do not commute.

4.15

Do the following combinations of angular momentum operators commute? Show work to justify the answer (do not just write "yes" or no").

- \mathbf{L}_x and \mathbf{L}_y
- \mathbf{L}_y and \mathbf{L}_z
- \mathbf{L}_z and \mathbf{L}_x

with

$$\mathbf{L}_x = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$\mathbf{L}_y = -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

$$\mathbf{L}_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

Estimate the answer to Part C based on the pattern gathered from parts A and B; no work necessary for Part C.

Solution

a.

$$\begin{aligned} [\mathbf{L}_x, \mathbf{L}_y] &= (y p_z - z p_y)(z p_x - x p_z)\Psi - (z p_x - x p_z)(y p_z - z p_y)\Psi, \\ &= (z p_x y p_z - z^2 p_x p_y - x y p_z p_z - x z p_y p_z)\Psi - (y p_z z p_x - y x p_z p_z + z^2 p_y p_x + z x p_z p_y)\Psi \\ &[\mathbf{L}_x, \mathbf{L}_y] = i\hbar \mathbf{L}_z, \end{aligned}$$

Does **not** commute, i.e., is not zero.

b.

$$\begin{aligned} [\mathbf{L}_y, \mathbf{L}_z] &= (z p_x - x p_z)(x p_y - y p_x)\Psi - (x p_y - y p_x)(z p_x - x p_z)\Psi \\ &= (x p_y z p_x - x^2 p_y p_z - y z p_x p_x - y x p_z p_x)\Psi - (z p_x x p_y - z y p_x p_x + x^2 p_z p_y + x y p_x p_z)\Psi \\ &[\mathbf{L}_y, \mathbf{L}_z] = i\hbar \mathbf{L}_x, \end{aligned}$$

Does **not** commute, i.e., is not zero.

c. This part only requires that we notice the rotation of variables and consistency of format/equations. In doing so, we better understand the relation between the parts of the angular momentum operator. The work below does not need to be shown for credit, but it may clarify things or make the solution clearer if you are still having trouble assessing and using the pattern.

$$\begin{aligned} [\mathbf{L}_z, \mathbf{L}_x] &= (x p_y - y p_x)(y p_z - z p_y)\Psi - (y p_z - z p_y)(x p_y - y p_x)\Psi \\ &= (y p_z x p_y - y^2 p_z p_x - z x p_y p_y - z y p_x p_y)\Psi - (x p_y y p_z - x z p_y p_z + y^2 p_x p_z + y z p_x p_y)\Psi \\ &[\mathbf{L}_z, \mathbf{L}_x] = i\hbar \mathbf{L}_y, \end{aligned}$$

Does not commute, i.e., is not zero.

These calculations show that you can have only one well-defined component of the angular momentum because of the uncertainty principle says the others will not be known (since they do not commute).

4.17

For two operators to commute, what property must hold? Use the operators \hat{L}^2 and \hat{L}_z as an example to show that this property holds.

Solution

The commutators when applied to a wavefunction must equal the 0 eigenfunction.

$$\begin{aligned} \hat{L}^2 \hat{L}_z \psi(x) - \hat{L}_z \hat{L}^2 \psi(x) &= 0 \\ \hat{L}^2 \hat{L}_z - \hat{L}_z \hat{L}^2 \psi(x) &= 0 \psi(x) \\ \hat{L}^2 \hat{L}_z - \hat{L}_z \hat{L}^2 &= 0 \end{aligned}$$

4.21

Show that the angular momentum and kinetic energy operators commute and therefore can be measured simultaneously to arbitrary precision.

Solution

Show that

$$[\hat{K}, \hat{L}] = 0$$

where the operators can be broken up into 3 components

$$L_x = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$L_y = -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

$$L_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

and $\hat{K}_x = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$. The same can be written for \hat{K} in the y and z directions.

$$[\hat{K}, \hat{L}] = [\hat{K}_x, \hat{L}_x] + [\hat{K}_y, \hat{L}_y] + [\hat{K}_z, \hat{L}_z]$$

For the x-direction

$$\begin{aligned} [\hat{K}_x, \hat{L}_x] &= \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}, -i\hbar \left(y \frac{d}{dz} - z \frac{d}{dy} \right) \right] \\ &= \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \left(-i\hbar \left(y \frac{d}{dz} - z \frac{d}{dy} \right) \right) - i\hbar \left(y \frac{d}{dz} - z \frac{d}{dy} \right) \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \\ &= \frac{i\hbar^3}{2m} \left(y \frac{d^3}{dx^2 dz} - z \frac{d^3}{dx^2 dy} \right) - \frac{i\hbar^3}{2m} \left(y \frac{d^3}{dx^2 dz} - z \frac{d^3}{dx^2 dy} \right) = 0 \end{aligned}$$

The process can be repeated for the y and z directions and following the same steps the commutations turn out to be 0. Therefore, kinetic energy and angular momentum commute.

4.22

Show that the position and angular momentum operator commutes. Can the position and angular momentum be measured simultaneously to a arbitrary precision?

Solution

First, we must prove that the position operator, $\hat{\mathbf{R}} = \hat{\mathbf{i}}\hat{x} + \hat{\mathbf{j}}\hat{y} + \hat{\mathbf{k}}\hat{z}$, and the angular momentum operator $\hat{\mathbf{L}} = \hat{\mathbf{i}}\hat{L}_x + \hat{\mathbf{j}}\hat{L}_y + \hat{\mathbf{k}}\hat{L}_z$, commute.

In order to prove the commutation,

$$\begin{aligned} [\hat{\mathbf{R}}, \hat{\mathbf{L}}] &= [\hat{\mathbf{i}}\hat{x} + \hat{\mathbf{j}}\hat{y} + \hat{\mathbf{k}}\hat{z}, \hat{\mathbf{i}}\hat{L}_x + \hat{\mathbf{j}}\hat{L}_y + \hat{\mathbf{k}}\hat{L}_z] \\ &= [\hat{x}, \hat{L}_x] + [\hat{y}, \hat{L}_y] + [\hat{z}, \hat{L}_z] \\ &= 0 \end{aligned}$$

where we have used the fact that

$$\hat{\mathbf{i}} \cdot \hat{\mathbf{i}} = \hat{\mathbf{j}} \cdot \hat{\mathbf{j}} = \hat{\mathbf{k}} \cdot \hat{\mathbf{k}} = 1$$

and

$$\hat{\mathbf{i}} \cdot \hat{\mathbf{j}} = \hat{\mathbf{j}} \cdot \hat{\mathbf{k}} = \hat{\mathbf{k}} \cdot \hat{\mathbf{i}} = 0$$

Now that we have proved that the two operators commute, the relationship of commutation means that the position and total angular momentum of any electrons can be measured simultaneously to arbitrary precision.

4.25

If both $|\Psi_n\rangle$ and $|\Psi_m\rangle$ satisfy the **time-independent** Schrödinger Equation (these are called *stationary states*)

$$|\Psi_n(x, t)\rangle = \Psi_n(x)e^{-iE_n t/\hbar}$$

and

$$|\Psi_m(x, t)\rangle = \Psi_m(x)e^{-iE_m t/\hbar}$$

show that any linear superposition of the two wavefunctions

$$|\Psi(x, t)\rangle = c_n|\Psi_n(x, t)\rangle + c_m|\Psi_m(x, t)\rangle$$

also satisfies the **time-dependent** Schrödinger Equation.

Solution

The time-dependent Schrödinger Equation is

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

Plug $\Psi(x, t)$ into the time-dependent equation.

$$\hat{H}c_n\Psi_n(x)e^{-iE_n t/\hbar} + c_m\Psi_m(x)e^{-iE_m t/\hbar} = i\hbar \frac{\partial}{\partial t}c_n\Psi_n(x)e^{-iE_n t/\hbar} + c_m\Psi_m(x)e^{-iE_m t/\hbar}$$

$$\hat{H}c_n\Psi_n(x)e^{-iE_n t/\hbar} + c_m\Psi_m(x)e^{-iE_m t/\hbar} = E_n c_n\Psi_n(x)e^{-iE_n t/\hbar} + E_m c_m\Psi_m(x)e^{-iE_m t/\hbar}$$

$$[\frac{\partial}{\partial t}c_n\Psi_n(x)e^{-iE_n t/\hbar} + c_m\Psi_m(x)e^{-iE_m t/\hbar}] = -[iE_n c_n\Psi_n(x)e^{-iE_n t/\hbar} + iE_m c_m\Psi_m(x)e^{-iE_m t/\hbar}]$$

combine all the constants (except for E) into c_n and c_m

$$[i\hbar [-iE_n c_n\Psi_n(x)e^{-iE_n t/\hbar} - iE_m c_m\Psi_m(x)e^{-iE_m t/\hbar}]] = E_n c_n\Psi_n(x)e^{-iE_n t/\hbar} + E_m c_m\Psi_m(x)e^{-iE_m t/\hbar}$$

$$[\text{Since } \hat{H}\Psi(x, t) \text{ and } i\hbar \frac{\partial \Psi(x, t)}{\partial t} \text{ are equal, they satisfy the time-dependent equation.}]$$

4.26

Starting with

$$\langle x \rangle = \int \psi^*(x, t)x\psi(x, t)dx$$

and the time-independent Schrödinger equation, demonstrate that

$$\frac{d\langle x \rangle}{dt} = \int \psi^* \frac{i}{\hbar} (\hat{H}x - x\hat{H})\psi dx$$

Given that

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

show that

$$\hat{H}x - x\hat{H} = -2\frac{\hbar^2}{2m} \frac{d}{dx} = -\frac{\hbar^2}{m} \frac{i}{\hbar} \hat{P}_x = -\frac{i\hbar}{m} \hat{P}_x$$

4.28

Derive the condition on operators that arises from forcing eigenvalues to be real with complex conjugates.

Solution

Starting with an eigenvalue problem with a \hat{G} as our operator we recognize

$$\hat{G}\psi = \lambda\psi$$

Solving for our eigenvalue we must multiply by our complex conjugate wavefunction and integrate both sides to see

$$\int \psi^* \hat{G}\psi d\tau = \int \psi^* \lambda\psi d\tau = \lambda \int \psi^* \psi d\tau = \lambda$$

We can repeat this calculation but with a complex conjugate of our initial eigenvalue problem

$$\hat{G}^* \psi^* = \lambda^* \psi^*$$

Solving for our eigenvalue we multiply ψ and integrate both sides to find that

$$\int \psi \hat{G}^* \psi^* d\tau = \int \psi \lambda^* \psi^* d\tau = \lambda^* \int \psi \psi^* d\tau = \lambda^*$$

Since we restricted λ to be real both eigenvalue problems return the same eigenvalue. We can then relate the operator side of both equations to know that

$$\boxed{\int \psi^* \hat{G}\psi d\tau = \int \psi \hat{G}^* \psi^* d\tau}$$

4.31

Prove that the position operator is Hermitian.

Solution

We must see if the operator satisfies the following requirement to be in Hermitian:

$$\int_{-\infty}^{\infty} (\hat{A}\psi^*)\psi dx = \int_{-\infty}^{\infty} \psi^* \hat{A}\psi dx$$

Substitute \hat{X} for \hat{A} into the above equation:

$$\int_{-\infty}^{\infty} (\hat{X}\psi^*)\psi dx = \int_{-\infty}^{\infty} \psi^* \hat{X}\psi dx$$

$$\int_{-\infty}^{\infty} (\hat{X}\psi^*)\psi dx = \int_{-\infty}^{\infty} \psi^* \hat{X}\psi dx$$

$$\int_{-\infty}^{\infty} (\hat{X}\psi)^*\psi dx = \int_{-\infty}^{\infty} \psi^* \hat{X}\psi dx$$

$$\int_{-\infty}^{\infty} \psi^* \hat{X}^* \psi dx = \int_{-\infty}^{\infty} \psi^* \hat{X}\psi dx$$

Since $\hat{X}^* \equiv \hat{X}$:

$$\int_{-\infty}^{\infty} \psi^* \hat{X}\psi dx = \int_{-\infty}^{\infty} \psi^* \hat{X}\psi dx$$

Therefore the Position Operator is Hermitian.

4.31

Prove that the momentum operator is a Hermitian

Solution

Hermitian: $\int \psi_j^* \hat{H} \psi_i dx$

Momentum Operator: $\hat{P} = -i\hbar \frac{d}{dx}$

We will first start by showing you

$$\int_{-\infty}^{\infty} \psi_j (-i\hbar \frac{d}{dx}) \psi_i dx$$

$$\frac{d\psi_i}{dx} dx = d\psi_i$$

$$\int_{-\infty}^{\infty} \psi_j (-i\hbar \frac{d}{dx}) \psi_i dx = i\hbar \int_{-\infty}^{\infty} \psi_j d\psi_i$$

Using integration by parts with $u = \psi_j^*$ and $dv = d\psi_i$

We can notice now that for a confined particle the product $\psi_j^* \psi_i$ will go to zero at each of the endpoints

We get in the end $-i\hbar \frac{d}{dx} = -i\hbar \frac{d}{dx} \rightarrow$ momentum operator

4.32

Which of the following operators are Hermitian:

- a. x ,
- b. d/dx
- c. $h d^2/dx^2$
- d. $i d^2/dx^2$

Solution

A Hermitian Operator \hat{A} satisfies

$$\langle \Psi^* | \hat{A} | \Psi \rangle = \langle \Psi | \hat{A}^* | \Psi^* \rangle$$

x

$$\int \Psi^* x \Psi dx = \int \Psi x \Psi^* dx$$

where $x^* = x$.

Operator x is Hermitian

d/dx

$$\begin{aligned} \int \Psi^* d/dx \Psi dx \\ = \int \Psi^* d\Psi \end{aligned}$$

Here we can use Integration by Parts $\int v du = uv - \int u dv$ with $v = \Psi^*$ and $dv = d\Psi$

$$= [\Psi^* \Psi] - \int \Psi d\Psi^*$$

$[\Psi^* \Psi]$ evaluated at infinity and negative infinity is 0, because of the assumption that this wavefunction approaches 0 as one extends to infinity in both directions

$$= - \int \Psi d/dx \Psi^* dx$$

Here we inserted dx/dx into the integral

$$= \int \Psi (-d/dx) \Psi^* dx$$

$d/dx^* = d/dx$, not $-d/dx$, so this operator is **not Hermitian**.

h d²/dx²

$$\begin{aligned} \int \Psi^* h (d^2/dx^2) \Psi dx \\ = h \int \Psi^* (d^2/dx^2) \Psi \end{aligned}$$

Here we can use Integration by Parts $\int v du = uv - \int u dv$ with $u = \Psi^*$ and $dv = d(d\Psi/dx)$

$$\begin{aligned} &= h [\Psi^* d\Psi/dx] - \int (d\Psi/dx) d\Psi^* \\ &= h [\Psi^* d\Psi/dx] - \int (d\Psi^*/dx) d\Psi \end{aligned}$$

$[\Psi^* d\Psi/dx]$ evaluated at infinity and negative infinity is 0, because of the assumption that this wavefunction approaches 0 as one extends to infinity in both directions. This implies that $d\Psi/dx$, for example, also approach 0.

$$= -h \int (d\Psi^*/dx) d\Psi$$

Here we can use Integration by Parts $\int v du = uv - \int u dv$ with $u = d\Psi^*/dx$ and $dv = d\Psi$

$$= -h([\Psi d\Psi^*/dx] - \int \Psi d^2\Psi^*/dx^2)$$

$[\Psi^* d\Psi/dx]$ evaluated at infinity and negative infinity is 0, because of the assumption that this wavefunction approaches 0 as one extends to infinity in both directions. This implies that that $d\Psi^*/dx$, for example, also approaches 0.

$$\begin{aligned} &= h \int \Psi (d^2\Psi^*/dx^2) dx \\ &= h \int \Psi (d^2\Psi^*/dx^2) dx \\ &= \int \Psi h (d^2/dx^2) \Psi^* dx \end{aligned}$$

$h(d^2/dx^2)^* = h(d^2/dx^2)$, so this operator is Hermitian

$i d^2/dx^2$

$$\begin{aligned} &\int \Psi^* i (d^2/dx^2) \Psi dx \\ &= i \int \Psi^* (d^2/dx^2) \Psi dx \end{aligned}$$

Here we can use Integration by Parts

$$\begin{aligned} \int v du &= uv - \int u dv \\ \text{with } u &= \Psi^* \text{ and } dv = d(d\Psi/dx) \\ &= i[\Psi^* d\Psi/dx] - \int (d\Psi/dx) d\Psi^* \\ &= i[\Psi^* d\Psi/dx] - \int (d\Psi^*/dx) d\Psi \end{aligned}$$

$[\Psi^* d\Psi/dx]$ evaluated at infinity and negative infinity is 0, because of the assumption that this wavefunction approaches 0 as one extends to infinity in both directions. This implies that that $d\Psi/dx$, for example, also approach 0.

$$= -i \int (d\Psi^*/dx) d\Psi$$

Here we can use Integration by Parts $\int v du = uv - \int u dv$ with $u = d\Psi^*/dx$ and $dv = d\Psi$

$$= -i([\Psi d\Psi^*/dx] - \int \Psi d^2\Psi^*/dx^2)$$

$[\Psi^* d\Psi/dx]$ evaluated at infinity and negative infinity is 0, because of the assumption that this wavefunction approaches 0 as one extends to infinity in both directions. This implies that that $d\Psi^*/dx$, for example, also approach 0.

$$\begin{aligned} &= i \int \Psi (d^2\Psi^*/dx^2) dx \\ &= i \int \Psi (d^2\Psi^*/dx^2) dx \\ &= \int \Psi i (d^2/dx^2) \Psi^* dx \\ i(d^2/dx^2)^* &= -i(d^2/dx^2) \end{aligned}$$

so this operator is NOT Hermitian

4.32

Determine whether the following operators are Hermitian and whether they commute:

$$\hat{A} = i \frac{d}{dx}$$

and

$$\hat{B} = i \frac{d^2}{dx^2}$$

Given that $-\infty < x < \infty$ and the operators functions are well behaved.

Solution

If the operator satisfies this condition it is *Hermitian*

$$\int_{-\infty}^{\infty} f^*(x) \hat{A} f(x) dx = \int_{-\infty}^{\infty} f(x) \hat{A} f^*(x) dx$$

A)

$$\begin{aligned} \int_{-\infty}^{\infty} f^* \left(i \frac{df}{dx} \right) dx &= i \int_{-\infty}^{\infty} f^* \frac{df}{dx} dx = i \left(\left[\int_{-\infty}^{\infty} f^* f \right] - \int_{-\infty}^{\infty} f \frac{df^*}{dx} dx \right) \\ &= -i \int_{-\infty}^{\infty} f \frac{df^*}{dx} dx = \int_{-\infty}^{\infty} f \left(-i \frac{d}{dx} \right) f^* dx \\ &= \int_{-\infty}^{\infty} f \left(i \frac{d}{dx} \right)^* f^* dx \end{aligned}$$

This operator is Hermitian

B)

$$\begin{aligned} \int_{-\infty}^{\infty} f^* \left(i \frac{d^2 f}{dx^2} \right) dx &= \left[\int_{-\infty}^{\infty} f^* i \frac{df}{dx} \right] - \int_{-\infty}^{\infty} \frac{df^*}{dx} \frac{df}{dx} dx \\ &= -i \left[\int_{-\infty}^{\infty} f \frac{df^*}{dx} \right] + i \int_{-\infty}^{\infty} f \frac{d^2 f^*}{dx^2} dx \\ &= - \int_{-\infty}^{\infty} f \frac{d^2 f^*}{dx^2} dx \end{aligned}$$

This operator is **not** Hermitian

If the operators commute they have to satisfy this condition

$$\begin{aligned} \hat{A}\hat{B}f &= \hat{B}\hat{A}f \\ \hat{A}\hat{B}f &= \frac{d}{dx} \left(\frac{d^2 f}{dx^2} \right) = \frac{d^3 f}{dx^3} \\ \hat{B}\hat{A}f &= \frac{d^2}{dx^2} \left(\frac{df}{dx} \right) = \frac{d^3 f}{dx^3} \end{aligned}$$

This pair of operators commutes.

4.34

Consider two wavefunctions

$$\psi_1(x) = A \sin(k_1 x) + B \cos(k_1 x) \quad (4.E.1)$$

and

$$\psi_2(x) = C \sin(k_2 x) + D \cos(k_2 x)$$

Given the boundary conditions are:

$$\psi(0) = 0$$

and

$$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \quad \text{at } x = 0$$

$$A + B = C, k_1(A - B) = k_2 C$$

and given a expression of

$$R = \frac{B^2}{A^2} \quad (4.E.2)$$

Derive the simplest expression of R based on the terms from the boundary conditions provided above.

Solution

Since

$$A + B = C, k_1(A - B) = k_2 C \quad (4.E.3)$$

,

$$k_1(A - B) = k_2(A + B) \quad (4.E.4)$$

$$k_1 A - k_1 B = k_2 A + k_2 B \quad (4.E.5)$$

$$(k_1 - k_2)A = (k_1 + k_2)B \quad (4.E.6)$$

Thus,

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \quad (4.E.7)$$

$$R = \frac{B^2}{A^2} = \left(\frac{B}{A}\right)^2 = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \quad (4.E.8)$$

4.34

A particle is moving in a field. Half-way through the field, there is a line that represents potential energy. To the left of the line, the potential energy is

$$x < 0$$

and to the right of the line the potential energy is

$$x > 0$$

. If the particle's energy is less than the potential energy line will the particle reflect when the its energy is greater than the Potential energy barrier height?

Solution

When

$$x < 0$$

the Schrödinger equation is as followed:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi_1}{dx^2} = E\psi_1$$

and the solution to this equation is:

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

where

$$k_1 = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$$

Region Two where $x > 0$:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_2}{dx^2} + V_0\psi_2 = E\psi_2$$

and the solution to the equation is:

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$$

and

$$k_2 = \left[\frac{2m(E - V_0)}{\hbar^2}\right]^{1/2}$$

Notice the difference between the two Schrödinger equations. Equation one does not have a potential energy component because it is before the potential energy field hence have zero potential energy. After the potential energy field, the Schrödinger equation has a potential energy component because the particle has potential energy at this moment.

When you solve the differential solutions to the Schrödinger equations you find that the amount that is reflected back of a particle by the line is equal to the amount that is transmitted after the line. This is all we can find out for the information given. However, if we solve this solution for when the Energy of the particle is greater than the potential energy line and compare the differential solutions to all four wave functions then we find that all particles will be reflected by the barrier.

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