100

Controll Questions for Lectures 2 to 5

Karl Kukk

March 27, 2025

1 Question 5

20

Probability current density j expressed by formula (1), is a mathematical quantity that describes the flow of probability associated with the wave function of a particle.

$$j = \frac{i\hbar}{2M}\left(\Psi\frac{d\Psi^*}{dx} - \Psi^*\frac{d\Psi}{dx}\right) \tag{1}$$

The probability current is similar to flowing liquids in classical mechanics or electric currents in electromagnetism. For example, if electrons move through a conductor, their probability current density describes the flow of charge. Similarly, with two gaseous regions of different density, one high and one low, when particles diffuse from the higher density section to the lower one, the probability current describes how the likelihood of finding a particle changes over time.

If the wave function Psi happens to be real, then the probability current density is 0, since the complex conjugate of a real number is that very same real number.

$$\Psi = \Psi^* \tag{2}$$

And since this is the case, expression (1) transforms to

$$j = \frac{i\hbar}{2M}\left(\Psi\frac{d\Psi^*}{dx} - \Psi^*\frac{d\Psi}{dx}\right) = \frac{i\hbar}{2M}\left(\Psi\frac{d\Psi}{dx} - \Psi\frac{d\Psi}{dx}\right) = \frac{i\hbar}{2M}(0) = 0 \tag{3}$$

2 Question 11

20

Hermitian operators are used to solve the eigenvalue problem because they ensure that measurable physical quantities have real eigenvalues. This is essential because any physical measurements like energy or momentum must yield real values.

A Hermitian operator $\hat{A}$ in a Hilbert space satisfies the condition:

$$\hat{A}^\dagger = \hat{A} \tag{4}$$

where $\hat{A}^\dagger$ represents the Hermitian adjoint of $\hat{A}$. This means that for any two states $|\psi\rangle$ and $|\phi\rangle$ in the Hilbert space, the following holds:

$$\langle \psi | \hat{A}\phi \rangle = \langle \hat{A}\psi | \phi \rangle \tag{5}$$

Proving that eigenvalues of hermitian operators are real numbers: Let $\hat{A}$ be a Hermitian operator with eigenvalues a_n and eigenfunctions φ_n:

$$\hat{A}\varphi_n = a_n \varphi_n. \tag{6}$$

Taking the inner product with $\langle \varphi_n |$ gives:

$$\langle \varphi_n | \hat{A}\varphi_n \rangle = a_n \langle \varphi_n | \varphi_n \rangle. \tag{7}$$

Since $\hat{A}$ is Hermitian, we also have:

$$\langle \hat{A}\varphi_n | \varphi_n \rangle = a_n^* \langle \varphi_n | \varphi_n \rangle. \tag{8}$$

Equating these expressions,

$$(a_n - a_n^*) \langle \varphi_n | \varphi_n \rangle = 0. \tag{9}$$

Since $\langle \varphi_n | \varphi_n \rangle \neq 0$, it follows that $a_n^* = a_n$, proving eigenvalues of Hermitian operators are real.

3 Question 18

$\boxed{20}$

For a free particle in one dimension, the time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E\psi(x) \tag{10}$$

This is a simple second-order differential equation with solutions that are of the form:

$$\psi_k(x) = \frac{1}{\sqrt{L}} e^{ikx} \tag{11}$$

The wave function $\psi_k(x)$ is a plane wave that satisfies the periodic boundary conditions, meaning that:

$$\psi_k(x + L) = \psi_k(x) \tag{12}$$

This implies that the allowed wave numbers are quantized:

$$k = \frac{2\pi n}{L} \tag{13}$$

where n is any integer greater than zero.

From this, we can say that the wave functions of a free particle are:

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{i\frac{2\pi n}{L}x} \tag{14}$$

Now, to show orthogonality, we compute the inner product of two wave functions. $\psi_n(x)$ and $\psi_m(x)$, and check they equal zero when $n \neq m$. We shall define the inner product as:

$$\langle \psi_n | \psi_m \rangle = \int_0^L \psi_n^*(x)\psi_m(x)\, dx \tag{15}$$

When substituting $\psi_n(x)$ and $\psi_m(x)$, we get:

$$\langle \psi_n | \psi_m \rangle = \int_0^L \frac{1}{\sqrt{L}} e^{-i\frac{2\pi n}{L}x} \cdot \frac{1}{\sqrt{L}} e^{i\frac{2\pi m}{L}x}\, dx \tag{16}$$

$$\langle \psi_n | \psi_m \rangle = \frac{1}{L} \int_0^L e^{i\frac{2\pi(m-n)}{L}x}\, dx \tag{17}$$

$$\int_0^L e^{i\frac{2\pi(m-n)}{L}x}\, dx = \frac{L}{i2\pi(m-n)} \left[e^{i\frac{2\pi(m-n)}{L}x} \right]_0^L \tag{18}$$

Since the exponential term $e^{i\frac{2\pi(m-n)}{L}L} = e^{i2\pi(m-n)} = 1$, we get:

$$\langle \psi_n | \psi_m \rangle = \frac{1}{L}\left(L \cdot \delta_{mn} \right) = \delta_{mn} \tag{19}$$

Where δ_{mn} is the Kronecker delta, which is 1 if $m = n$ and 0 if $m \neq n$.

Therefore, the wave functions must be orthogonal.

Now let us move on with wave functions, energy and momentum for case n=3.

Using equation (14), we can show that in case number 3, equation (14) transforms to:

$$\psi_3(x) = \frac{1}{\sqrt{L}} e^{i\frac{2\pi \cdot 3}{L}x} = \frac{1}{\sqrt{L}} e^{i\frac{6\pi}{L}x} \tag{20}$$

Energy in a state is defined as:

$$E_n = \frac{\hbar^2 k^2}{2m} \tag{21}$$

Substituting k from equation (13) into the energy expression:

$$E_3 = \frac{\hbar^2}{2m}\left(\frac{6\pi}{L}\right)^2 = \frac{\hbar^2}{2m} \cdot \frac{36\pi^2}{L^2} \tag{22}$$

The momentum associated with the state is related to the wave number by:

$$p_n = \hbar k \tag{23}$$

Again, substituting equation (13) into this expression at case n=3, we get:

$$p_3 = \hbar \cdot \frac{6\pi}{L} \tag{24}$$

4 Question 27

20

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0$$

1)

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}, \quad \hat{p}_y = -i\hbar\frac{\partial}{\partial y}$$

$$[\hat{p}_x, \hat{p}_y] = \hat{p}_x\hat{p}_y - \hat{p}_y\hat{p}_x$$

$$= \left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial y}\right) - \left(-i\hbar\frac{\partial}{\partial y}\right)\left(-i\hbar\frac{\partial}{\partial x}\right) = 0$$

Thus, $\hat{p}_x$ and $\hat{p}_y$ are commutative.

2)

$$[\hat{p}_x^2, \hat{p}_y] = \hat{p}_x^2\hat{p}_y - \hat{p}_y\hat{p}_x^2$$

$$= \left((-i\hbar)^2\frac{\partial^2}{\partial x^2}\right)\left(-i\hbar\frac{\partial}{\partial y}\right) - \left(-i\hbar\frac{\partial}{\partial y}\right)\left((-i\hbar)^2\frac{\partial^2}{\partial x^2}\right)$$

$$= -i\hbar^3\left(\frac{\partial^3}{\partial x^2\partial y} - \frac{\partial^3}{\partial y\partial x^2}\right)$$

$$\frac{\partial^2}{\partial x^2}\left(\frac{\partial}{\partial y}\psi(x,y)\right) - \frac{\partial}{\partial y}\left(\frac{\partial^2}{\partial x^2}\psi(x,y)\right) = \left[\frac{\partial^2}{\partial x^2}, \frac{\partial}{\partial y}\right] = 0$$

Thus, $\hat{p}_x^2$ and $\hat{p}_y$ are commutative.

5 Question 32

20

For the case of a stepped potential barrier, we are to show that for $E > U_0$, the flux of particles moving towards the barrier (incident particles) is given by:

$$j_i = \frac{\hbar k_1 A^2}{m}, \tag{25}$$

where $k_1 = \frac{\sqrt{2mE}}{\hbar}$.

For a particle in one dimension, the time-independent Schrödinger equation is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{26}$$

where $\psi(x)$ is the wave function, E is the energy, and $V(x)$ is the potential. The probability density current j is given by expression (1).

Assuming a potential step at $x = 0$, we consider the following:

- For $x < 0$, $V(x) = 0$ (free particle region).
- For $x > 0$, $V(x) = U_0$ (potential step).

The general form of the wave function is:

- For $x < 0$ (region where $V(x) = 0$):

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x}, \tag{27}$$

where $k_1 = \frac{\sqrt{2mE}}{\hbar}$ is the wave number corresponding to the energy E of the particle. Here, A and B are constants.

- For $x > 0$ (region where $V(x) = U_0$):

$$\psi(x) = Ce^{ik_2x}, \tag{28}$$

where $k_2 = \frac{\sqrt{2m(E-U_0)}}{\hbar}$ is the wave number in the region beyond the potential step.

For the incident wave $\psi(x) = Ae^{ik_1x}$, we compute the derivatives:

$$\frac{d\psi(x)}{dx} = ik_1Ae^{ik_1x}, \tag{29}$$

$$\frac{d\psi^*(x)}{dx} = -ik_1A^*e^{-ik_1x}. \tag{30}$$

Substituting these into the expression for the probability current density:

$$j_i = \frac{\hbar}{2mi}\left(A^*e^{-ik_1x} \cdot (ik_1Ae^{ik_1x}) - Ae^{ik_1x} \cdot (-ik_1A^*e^{-ik_1x})\right). \tag{31}$$

Simplifying:

$$j_i = \frac{\hbar k_1}{m}|A|^2. \tag{32}$$

Using $k_1 = \frac{\sqrt{2mE}}{\hbar}$, we have:

$$j_i = \frac{\hbar\sqrt{2mE}}{m\hbar}A^2 = \frac{\sqrt{2mE}}{m}A^2. \tag{33}$$

Therefore, the flux of particles moving towards the potential barrier for $E > U_0$ is:

$$j_i = \frac{\hbar k_1 A^2}{m}, \tag{34}$$

where $k_1 = \frac{\sqrt{2mE}}{\hbar}$.