# Loengud 2-5 Vastused 80

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## 4. Show that in the 3D case, the probability current density calculated by the quantum equation and its classical analog have the same measurement units.

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The quantum probability current density is:

$$\mathbf{j}_Q = \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right) \tag{1}$$

The classical probability current density is:

$$\mathbf{j}_C = n\mathbf{v} \tag{2}$$

The wave function $\psi$ has units:

$$\psi = \frac{1}{\sqrt{\mathrm{m}^3}} \tag{3}$$

The gradient operator $\nabla$ has:

$$\nabla = \frac{1}{\mathrm{m}} \tag{4}$$

The reduced Planck's constant $\hbar$ has units:

$$\hbar = \mathrm{J}\cdot\mathrm{s} = \frac{\mathrm{kg}\cdot\mathrm{m}^2}{\mathrm{s}} \tag{5}$$

Mass $m$ has units:

$$m = \mathrm{kg} \tag{6}$$

$\frac{\hbar}{m}$ has units:

$$\frac{\hbar}{m} = \frac{\mathrm{kg}\cdot\mathrm{m}^2/\mathrm{s}}{\mathrm{kg}} = \frac{\mathrm{m}^2}{\mathrm{s}} \tag{7}$$

The $\psi\nabla\psi^*$ has units:

$$[\psi\nabla\psi^*] = \left(\frac{1}{\sqrt{\mathrm{m}^3}}\right)\cdot\left(\frac{1}{\mathrm{m}^{7/2}}\right) = \frac{1}{\mathrm{m}^4} \tag{8}$$

So $\mathbf{j}_Q$ has :

$$\left(\frac{\mathrm{m}^2}{\mathrm{s}}\right) \cdot \left(\frac{1}{\mathrm{m}^4}\right) = \frac{1}{\mathrm{m}^2 \cdot \mathrm{s}} \tag{9}$$

For the classical case:
Number density $n$ has units:

$$n = \frac{1}{\mathrm{m}^3} \tag{10}$$

Velocity v has units:

$$\mathbf{v} = \frac{\mathrm{m}}{\mathrm{s}} \tag{11}$$

And so $\mathbf{j}_C$ has units:

$$\left(\frac{1}{\mathrm{m}^3}\right) \cdot \left(\frac{\mathrm{m}}{\mathrm{s}}\right) = \frac{1}{\mathrm{m}^2 \cdot \mathrm{s}} \tag{12}$$

Since both $\mathbf{j}_Q$ and $\mathbf{j}_C$ have the same units:

$$\frac{1}{\mathrm{m}^2 \cdot \mathrm{s}} \tag{13}$$

**The quantum and classical probability current densities share the same measurement units.**

## 15. Eigenvalue problem for Hamilton operator is.... How is looks like the eigenvalue E for eigenvalue problem? How can coefficients be calculated?

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The eigenvalue problem for the Hamiltonian operator $\hat{H}$ is given by:

$$\hat{H}\psi_n = E_n\psi_n, \tag{14}$$

where:

- $\psi_n$ are the eigenfunctions of the Hamiltonian $\hat{H}$,
- $E_n$ are the corresponding eigenvalues.

Now, consider a general function $\phi$ that can be expanded in terms of the eigenfunctions $\psi_n$:

$$\phi = \sum_n c_n\psi_n. \tag{15}$$

Applying the Hamiltonian $\hat{H}$ to both sides:

$$\hat{H}\phi = \hat{H}\sum_n c_n\psi_n. \tag{16}$$

Using the linearity of $\hat{H}$:

$$\sum_n c_n \hat{H} \psi_n = \sum_n c_n E_n \psi_n. \tag{17}$$

Since $\phi$ is also an eigenfunction with eigenvalue $E$, we have:

$$\hat{H}\phi = E\phi. \tag{18}$$

Substituting the expansion:

$$\boxed{\sum_n c_n E_n \psi_n = E \sum_n c_n \psi_n.} \tag{19}$$

Comparing both sides, we obtain: see on suur küsimus

$$\boxed{E c_n = E_n c_n.} \tag{20}$$

Thus, the eigenvalues $E$ are determined by the eigenvalues $E_n$ weighted by the coefficients $c_n$.

To determine the coefficients $c_n$, we use the orthonormality of the eigenfunctions:

$$\int \psi_m^* \psi_n \, dV = \delta_{mn}. \tag{21}$$

Multiplying both sides of the expansion by $\psi_m^*$ and integrating:

$$\int \psi_m^* \phi \, dV = \sum_n c_n \int \psi_m^* \psi_n \, dV. \tag{22}$$

Using orthonormality:

$$\int \psi_m^* \phi \, dV = \sum_n c_n \delta_{mn} = c_m. \tag{23}$$

Thus the coefficients are given by:

$$c_n = \int \psi_n^* \phi \, dV. \tag{24}$$

**This equation allows us to compute the coefficients $c_n$ when $\phi$ is known.**

**17. The task for free one-dimensional motion of a particle is stationary? Why? Write the corresponding Schrödinger equation for this task. Find the solution of it (wavefunction and energy of a free particle). What gives the periodic boundary conditions (quantum number aka the physical state number)? Give the mathematical representation for it. Normalize the wavefunction. Calculate the probability density function. Does it depend on coordinate $x$? Give the physical interpretation of the answer and its relation to the Heisenberg uncertainty principle.**

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A free particle in one dimension is described by the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x). \tag{25}$$

Rearranging, we obtain:

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0, \tag{26}$$

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

The general solution of this equation is:

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

where $A$ and $B$ are constants determined by boundary conditions.

For a particle in a box of length $L$ with periodic boundary conditions:

$$\psi(x + L) = \psi(x). \tag{28}$$

Applying this condition to the general solution gives the quantization of wave vectors:

$$k_n = \frac{2\pi n}{L}, \quad n \in Z. \tag{29}$$

The energy levels corresponding to these wave vectors are:

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{(2\pi n)^2\hbar^2}{2mL^2}. \tag{30}$$

To normalize the wavefunction:

$$\int_0^L |\psi(x)|^2 dx = 1. \tag{31}$$

For a plane wave solution:

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}. \tag{32}$$

The probability density function is:

$$|\psi_n(x)|^2 = \frac{1}{L}, \tag{33}$$

which is independent of $x$. This implies that the particle has an equal probability of being found anywhere.

This result relates to the Heisenberg uncertainty principle:

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{34}$$

Since the wavefunction is completely delocalized over $L$, the uncertainty in position $\Delta x$ is large. Consequently, the momentum $p = \hbar k_n$ is well-defined, leading to minimal uncertainty in momentum $\Delta p$. This demonstrates the fundamental wave-particle duality.

## 28. Operators are commute:

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**(a) $\hat{p}_x$ and $\hat{y}$?**
**(b) $\hat{p}_x$ and $\hat{p}_y$?**

To determine whether two operators commute we calculate their commutator:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{35}$$

**(a) $\hat{p}_x$ and $\hat{y}$**

The momentum operator in the $x$-direction is:

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}. \tag{36}$$

The position operator $\hat{y}$ simply multiplies by $y$, so:

$$[\hat{p}_x, \hat{y}] = \hat{p}_x \hat{y} - \hat{y} \hat{p}_x. \tag{37}$$

Applying these operators to a test function $f(x, y)$:

$$\hat{p}_x(\hat{y} f) = -i\hbar \frac{\partial}{\partial x}(y f) = -i\hbar y \frac{\partial f}{\partial x}. \tag{38}$$

Similarly,

$$\hat{y}(\hat{p}_x f) = y(-i\hbar \frac{\partial f}{\partial x}) = -i\hbar y \frac{\partial f}{\partial x}. \tag{39}$$

Since both terms are equal, the commutator is:

$$[\hat{p}_x, \hat{y}] = 0. \tag{40}$$

**Thus, $\hat{p}_x$ and $\hat{y}$ commute.**

**(b) $\hat{p}_x$ and $\hat{p}_y$**

The momentum operators in the $x$- and $y$-directions are:

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}, \quad \hat{p}_y = -i\hbar\frac{\partial}{\partial y}. \tag{41}$$

Computing their commutator:

$$[\hat{p}_x, \hat{p}_y] = \hat{p}_x\hat{p}_y - \hat{p}_y\hat{p}_x. \tag{42}$$

Applying to a function $f(x, y)$:

$$\hat{p}_x\hat{p}_y f = (-i\hbar\frac{\partial}{\partial x})(-i\hbar\frac{\partial}{\partial y}f) = -\hbar^2\frac{\partial^2 f}{\partial x\partial y}. \tag{43}$$

$$\hat{p}_y\hat{p}_x f = (-i\hbar\frac{\partial}{\partial y})(-i\hbar\frac{\partial}{\partial x}f) = -\hbar^2\frac{\partial^2 f}{\partial y\partial x}. \tag{44}$$

Since mixed partial derivatives commute:

$$\frac{\partial^2 f}{\partial x\partial y} = \frac{\partial^2 f}{\partial y\partial x}, \tag{45}$$

we get:

$$[\hat{p}_x, \hat{p}_y] = 0. \tag{46}$$

**Thus, $\hat{p}_x$ and $\hat{p}_y$ also commute.**

## 33. Show that for a potential barrier ($E > U_0$), the flux for reflected particles (reflected from the barrier) is $j_R = \frac{\hbar k_1 B^2}{m}$, where $k_1 = \frac{\sqrt{2mE}}{\hbar}$. 20

For a free particle approaching a potential barrier, the time-independent wavefunction in Region I (before the barrier) is:

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}, \tag{47}$$

where:

$$k_1 = \frac{\sqrt{2mE}}{\hbar}. \tag{48}$$

The probability current density is given by:

$$j = \frac{\hbar}{2mi}\left(\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right). \tag{49}$$

For the reflected wave $\psi_R = Be^{-ik_1x}$, we compute:

$$\frac{d\psi_R}{dx} = (-ik_1B)e^{-ik_1x}, \tag{50}$$

$$\psi_R^* = B^*e^{ik_1x}. \tag{51}$$

Multiplying these terms:

$$\psi_R^* \frac{d\psi_R}{dx} = B^* e^{ik_1 x}(-ik_1 B e^{-ik_1 x}) = -ik_1 B^* B, \tag{52}$$

$$\psi_R \frac{d\psi_R^*}{dx} = B e^{-ik_1 x}(ik_1 B^* e^{ik_1 x}) = ik_1 B B^*. \tag{53}$$

Thus, the probability current density for the reflected wave is:

$$j_R = \frac{\hbar}{2mi} \left( -ik_1 B^* B - ik_1 B B^* \right). \tag{54}$$

Since $B^* B = |B|^2$, this simplifies to:

$$j_R = \frac{\hbar}{2mi} \cdot (-2ik_1 |B|^2). \tag{55}$$

Finally,

$$j_R = \frac{\hbar k_1 B^2}{m}, \tag{56}$$

which proves the given result.