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Kvantmehaanika ja spektroskoopia

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4.Show that in 3d-case the probability current density calculated by quantum equation

$$j_Q = \frac{i\hbar}{2m}\left\{\psi^*\hat{\nabla}\psi - \psi\hat{\nabla}\psi^*\right\}$$

and it classical analog $j_C = n \cdot v$ have the same measurement units.

In 3d-case we get wave functions dimensions from probability density $dP = |\psi|^2 dV$, where dP is dimensionless, dV is m^3, so ψ is $m^{-3/2}$.

Planck's constant $\hbar$ dimensions is $kg \cdot m^2 \cdot s^{-1}$ and m dimension is kg.

Taking gradient of ψ give us dimension of $m^{-5/2}$.

Putting all the dimensions together we get $\frac{(kg \cdot m^2 \cdot s^{-1})}{kg} \cdot (m^{-3/2}) \cdot (m^{-5/2})$, which gives us end result of $\frac{1}{m^2 \cdot s}$ for probability current density.

In classical mechanics $j_C = n \cdot v$, where n is number of particles per unit volume giving it a dimension of m^{-3} and v is velositi with dimensions $m \cdot s^{-1}$. Putting these dimensions together we get $\frac{1}{m \cdot s}$, which is same as quantum ones meaning they have same units of measurment.

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15. Eigenvalue problem for Hamilton operators is $\hat{H}\psi_n = E_n\psi_n$ (here ψ_n is a set of orthonormal eigenfunctions for Hamiltonian operator $\hat{H}$). How is looks like the the eigenvalue E for eigenvalue problem $\hat{H}\phi = E\phi$, here $\phi = \sum_n c_n\psi_n$. How coefficients c_n can be calculated?

Subsitude *phi* in eigenvalue problem to get $\hat{H}(\sum_n c_n\psi_n) = E(\sum_n c_n\psi_n)$.

Using the linearity of H and the fact that $H\psi_n = E_n\psi_n$, we get: $\sum_n c_n E_n \psi_n = E\sum_n c_n\psi_n$.

With ψ_n being orthonormal and lineary independant, we equate the coefficients of each ψ_n, we get $c_n E_n = E c_n$ which implies $c_n(E_n - E) = 0$

From this we get that eigenvalue E must be one of the eigenvalues E_n of the Hamiltonian, and the wavefunction ϕ must be a linear combination of the eigenfunctions ψ_n that correspond to that particular eigenvalue E.

The coefficients c_n in the expansion $\phi = \sum_n c_n\psi_n$ can be calculated using the orthonormality of the eigenfunctions ψ_n. Since $\langle\psi_m \mid \psi_n\rangle = \delta_{mn}$, we have:

$$c_n = \langle\psi_n \mid \phi\rangle = \int \psi_n^* \phi \, dV,$$

Tegelikult E= SUM(n) Cn^2*En

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24. Calculate the average ($\langle x \rangle_n, \langle p \rangle_n$) and exact ($x_n, p_n$) x-coordinate and p_x momentum for a free particle in 1d (here $n \in \mathbb{Z}$ is a quantum number of state). Were there any problems with the calculations of that four quantities? What kinds of problems? Why?

$\hat{H}\psi = E\psi$, in 1d Hamiltonian is $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x}$, giving us $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$.
Let's take $k^2 = \frac{2mE}{\hbar^2}$, we get $\frac{\partial^2\psi}{\partial x^2} = -k^2\psi$

From this differencial equasion we get $\psi(x) = C_1 e^{ikx} + C_2 e^{-ikx}$, if we take $C_2 = 0$, we simplify it to $\psi(x) = Ce^{ikx}$.

Useing periodic boundary with lenght L we get $\psi(x) = \psi(x+L)$, meaning $Ce^{ikx} = Ce^{ik(x+L)}$, from which we get $e^{ikL} = 1$, giving us $k_n = \frac{2\pi}{L}n, n \in \mathbb{Z}$

Using wave function property of it being normalized to 1, we get $C^2 \int_0^L e^{ik_n x} e^{-ik_n x} dx = 1$, from where we get $C = \frac{1}{\sqrt{L}}$, givig us $\psi_n(x) = \frac{1}{\sqrt{L}} e^{ikx}$

Looking for probapility of finding particle between x and dx, $dP(x, x + dx) = \psi\psi^* dx = \frac{1}{L}$, meaning particle is unformly likely to exist anywhere in set boundary.

The momentum operator is $\hat{p} = -i\hbar\frac{\partial}{\partial x}$. The expectation value of momentum in the state $\psi_n(x)$ is:

$$\langle p \rangle_n = \int \psi_n^*(x)\hat{p}\psi_n(x)\, dx = \hbar k_n \int |\psi_n(x)|^2\, dx = \hbar k_n$$

Meaning in this case we get avarage coordinat of x and exact momentum p_n.

We can't calculate exact x-coordinate, average location for particle in boundary is just $L/2$ (the center), which is not physically meaningful since the particle is equally likely to be found anywhere.

The position and momentum operators have fundamentally different behaviors in quantum mechanics.

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27. Operators are commute :

a.) $\hat{p}_x$ and $\hat{p}_y$?

b.) $\hat{p^2}_x$ and $\hat{p}_y$?

Operators are commute if $[A, B] = AB - BA = 0$.

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

$$[\hat{p}_x, \hat{p}_y]\psi = \hat{p}_x\hat{p}_y\psi - \hat{p}_y\hat{p}_x\psi = (-i\hbar\frac{\partial}{\partial x})(-i\hbar\frac{\partial}{\partial y})\psi - (-i\hbar\frac{\partial}{\partial y})(-i\hbar\frac{\partial}{\partial x})\psi$$

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

Meaning $\hat{p}_x$ and $\hat{p}_y$ are commute.

b)$\hat{p}_x^2 = \left(-i\hbar\frac{\partial}{\partial x}\right)^2 = -\hbar^2\frac{\partial^2}{\partial x^2}, \hat{p}_y = -i\hbar\frac{\partial}{\partial y}$

$$[\hat{p}^x, \hat{p}^y]\psi = \hat{p}^x\hat{p}^y\psi - \hat{p}^y\hat{p}^x\psi$$

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

$$= i\hbar^3\frac{\partial^3\psi}{\partial x^2\partial y} - i\hbar^3\frac{\partial^3\psi}{\partial y\partial x^2} = 0$$

Meaning $\hat{p}_x^2$ and $\hat{p}_y$ are commute.

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

Let's look at 1d-case where barrier is at $x = 0$

$$U = \begin{cases} u_0, & x < 0 \\ 0, & 0 < x < \infty \end{cases} \qquad E > u_0$$

Because system is isolated, meaning total energy stays constant, we get 2 equal energy states for left of barrier and right of barrier

$$E = \frac{1}{2}mv_1^2, \quad E = \frac{1}{2}mv_2^2 + u_0 \quad \Rightarrow \quad v_1 > v_2$$

Probapility of particle reflecting $R = [0, 1]$ and probapility of going throught the barrier $T = [0, 1]$, $\quad R + T = 1$

Using continuity contion for wave function

$$\varphi(x) = \begin{cases} \varphi_1(x), & x < 0 \\ \varphi_2(x), & 0 < x < \infty \end{cases} \qquad \begin{cases} \varphi_1(0) = \varphi_2(0) \\ \varphi_1'(0) = \varphi_2'(0) \end{cases}$$

We have Hamiltonian and flux equasions

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}, \quad j = \frac{i\hbar}{2m}\left(\varphi\hat{\nabla}\varphi^* - \varphi^*\hat{\nabla}\varphi\right)$$

From $\hat{H}\varphi_n = E_n\varphi_n$ we get

$$\hat{H}\varphi_1 = -\frac{\hbar^2}{2m}\frac{\partial^2\varphi_1}{\partial x^2} = E\varphi_1, \quad \Rightarrow \quad \frac{\partial^2\varphi_1}{\partial x^2} = -\frac{2mE}{\hbar^2}\varphi_1$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, \quad \frac{\partial^2\varphi_1}{\partial x^2} = -k_1^2\varphi_1$$

From this differencial equasion we get

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

We are only interested of reflected particles $\varphi(x) = Be^{-ik_1x}$, which we will use in flux equesion to get flux for reflected particles

$$j_R = \frac{i\hbar}{2m}B^2\left(e^{-ik_1x}ik_1e^{ik_1x} - e^{ik_1x}(-i)k_1e^{-ik_1x}\right)$$

$$= -\frac{\hbar k_1 B^2}{m}$$