Kvantmehaanika, loengud 2 – 5 100

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8. **Can you show that the average value for some physical quantity A (measurable value for given quantity) i.e. ⟨A⟩ do not depend on time for stationary solution of full Schrodinger equation $i\hbar\dfrac{\partial\psi}{\partial t} = \hat{H}\psi$?** 20

   For a time-independent operator $\hat{A}$, its value in the state $\psi(\vec{r}, t)$:

$$\langle A \rangle = \int \psi^*(\vec{r}, t)\, \hat{A}\, \psi(\vec{r}, t)\, dV$$

   Stationary-state wavefunction and its complex conjugate:

$$\psi(\vec{r}, t) = e^{-iEt/\hbar}\, \psi(\vec{r}), \quad \psi^*(\vec{r}, t) = e^{iEt/\hbar}\, \psi^*(\vec{r})$$

   Substituting:

$$\implies \langle A \rangle = \int \left(e^{iEt/\hbar}\, \psi^*(\vec{r})\right)\, \hat{A}\, \left(e^{-iEt/\hbar}\, \psi(\vec{r})\right) dV = \int \psi^*(\vec{r})\, \hat{A}\, \psi(\vec{r})\, dV$$

   Final result does not depend on time.

14. **Prove that potential energy operator for harmonic oscillator is Hermitian.**

   To show that $\hat{U}(x)$ is Hermitian, it must be proven that for $\psi(x)$ and $\phi(x)$: 20

$$\langle \varphi | \hat{U} \psi \rangle = \langle \hat{U} \varphi | \psi \rangle, \quad \langle \varphi | \psi \rangle = \int_{-\infty}^{\infty} \varphi^*(x)\, \psi(x)\, dx$$

   Potential energy of harmonic oscillator:

$$\hat{U}(x) = \frac{M\omega^2 x^2}{2}$$

$$\langle \varphi | \hat{U} \psi \rangle = \int_{-\infty}^{\infty} \varphi^*(x) \left(\frac{M\omega^2 x^2}{2}\right) \psi(x)\, dx.$$

   Potential energy of harmonic oscillator has a real value, not complex:

$$\left(\frac{M\omega^2 x^2}{2}\right)^* = \frac{M\omega^2 x^2}{2}$$

$$\implies \langle \hat{U} \varphi | \psi \rangle = \int_{-\infty}^{\infty} \left[\frac{M\omega^2 x^2}{2} \varphi(x)\right]^* \psi(x)\, dx = \int_{-\infty}^{\infty} \varphi^*(x) \left(\frac{M\omega^2 x^2}{2}\right) \psi(x)\, dx$$

$$\implies \langle \varphi | \hat{U} \psi \rangle = \langle \hat{U} \varphi | \psi \rangle$$

   Potential energy operator $\hat{U}(x)$ for harmonic oscillator is Hermitian.

19. **Give a physical interpretation of the positive and negative values of the quantum number in one-dimensional periodic motion of free particle. Write expression for wavefunction, energy and momentum for state with number $n = -2$.** 20

$$\psi_n(x) = \frac{1}{\sqrt{L}} \exp\left(i\, \frac{2\pi n}{L}\, x\right) \implies \psi_{-2}(x) = \frac{1}{\sqrt{L}} \exp\left(-i\, \frac{4\pi}{L}\, x\right); \ L \text{ is the circumference, } n \in \mathbb{Z}$$

$$p_n = \hbar\, k_n = \hbar\, \frac{2\pi n}{L} \implies p_{-2} = -\frac{4\pi\hbar}{L}$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{2\pi n}{L}\right)^2 \implies E_{-2} = \frac{16\pi^2\hbar^2}{2m\,L^2}$$

Physical Interpretation:
Positive n corresponds to motion in the positive x–direction, while negative n corresponds to motion in the negative direction. The energy depends on n^2 so that states with n and $-n$ have the same energy.

29. **Operators are commute:**

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

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

a.) Commutation of $\hat{p}_x$ and $\hat{p}_y$:

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

$$[\hat{p}_x, \hat{p}_y] = \hat{p}_x\,\hat{p}_y - \hat{p}_y\,\hat{p}_x = (-i\hbar)^2\frac{\partial^2}{\partial x\partial y} - (-i\hbar)^2\frac{\partial^2}{\partial y\partial x} = 0$$

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

b.) Commutation of $\hat{p}_x$ and $\hat{x}^2$

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

Let $\psi(x)$ be an arbitrary function:

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

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

$$\implies [\hat{p}_x, \hat{x}^2]\psi(x) = -i\hbar\,(2x\,\psi(x)) = -2i\hbar\,x\,\psi(x) \implies [\hat{p}_x, \hat{x}^2] = -2i\hbar\,\hat{x} \neq 0$$

Operators $\hat{p}_x$ and $\hat{x}^2$ are not commute.

36. **What do the dependencies of *transition* and *reflection* coefficients on particle energy look like in the classical case? Why?**

- If $E < V_0$: The particle does not have enough energy to overcome the barrier. It means that particale is completely reflected:

$$R_{\text{classical}} = 1, \quad T_{\text{classical}} = 0.$$

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- If $E > V_0$: The particle has sufficient energy to pass over the barrier, so there is no reflection:

$$R_{\text{classical}} = 0, \quad T_{\text{classical}} = 1.$$

In classical case, the reflection coefficient R represents a step–like behavior: it is equal to 1 when $E < V_0$ and drops to 0 when $E > V_0$, while the transmission coefficient T is 0 for $E < V_0$ and 1 for $E > V_0$. There is no partial tunneling or partial reflection in purely classical mechanics if the particle is truly free on either side (no dissipative forces).