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8. Can you show that the average value for some physical quantity A (measurable value for given quantity) i.e. $\langle A \rangle$ do not depend on time for stationary solution of full Schrodinger equation

Suppose we have a wave function that is a stationary state: 20

$$\psi(\mathbf{r}, t) = \phi(\mathbf{r})\, e^{-iEt/\hbar},$$

where $\phi(\mathbf{r})$ is an eigenfunction of the Hamiltonian with eigenvalue E. The expectation value of an operator $\hat{A}$ is given by

$$\langle A \rangle(t) = \int \psi^*(\mathbf{r}, t)\, \hat{A}\, \psi(\mathbf{r}, t)\, d^3r.$$

Substitute the expression for $\psi(\mathbf{r}, t)$ into the formula:

$$\psi^*(\mathbf{r}, t) = \phi^*(\mathbf{r})\, e^{iEt/\hbar},$$

so we get

$$\langle A \rangle(t) = \int \left[\phi^*(\mathbf{r})\, e^{iEt/\hbar}\right] \hat{A} \left[\phi(\mathbf{r})\, e^{-iEt/\hbar}\right] d^3r.$$

Notice that

$$e^{iEt/\hbar} \cdot e^{-iEt/\hbar} = 1,$$

which means the exponential factors cancel out. Therefore, the expression simplifies to:

$$\langle A \rangle(t) = \int \phi^*(\mathbf{r})\, \hat{A}\, \phi(\mathbf{r})\, d^3r.$$

This result does not depend on time. Since the expectation value $\langle A \rangle$ does not have any time dependence, its time derivative is zero:

$$\frac{d}{dt}\langle A \rangle(t) = 0.$$

This shows that in a stationary state, the expectation value of any operator $\hat{A}$ (with no explicit time dependence) remains constant over time.

12. Why in quantum mechanics should we use Hermitian operators to solve the eigenvalue problem? Definition of Hermite operators. Show that eigenfunctions of Hermitian operators form the set of orthonormal functions.

In quantum mechanics, measurable quantities (observables) like energy, position, or momentum are represented by operators. We need the possible

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measurement results (the eigenvalues) to be real numbers. Hermitian operators have the special property that all their eigenvalues are real. This makes them the natural choice to represent observables.

An operator $\hat{A}$ is called **Hermitian** (or self-adjoint) if for any two states ϕ and ψ the following holds:

$$\langle \phi | \hat{A}\,\psi \rangle = \langle \hat{A}\,\phi | \psi \rangle.$$

This condition is equivalent to saying that

$$\hat{A} = \hat{A}^\dagger,$$

where $\hat{A}^\dagger$ is the Hermitian conjugate (adjoint) of $\hat{A}$.

Let $\hat{A}$ be a Hermitian operator and consider two of its eigenfunctions, ϕ_m and ϕ_n, corresponding to the eigenvalues a_m and a_n, respectively:

$$\hat{A}\phi_m = a_m\,\phi_m \quad \text{and} \quad \hat{A}\phi_n = a_n\,\phi_n.$$

Take the inner product of ϕ_n with the first eigenvalue equation:

$$\langle \phi_n | \hat{A}\phi_m \rangle = a_m \langle \phi_n | \phi_m \rangle.$$

Using the Hermitian property, we can write:

$$\langle \phi_n | \hat{A}\phi_m \rangle = \langle \hat{A}\phi_n | \phi_m \rangle = a_n \langle \phi_n | \phi_m \rangle.$$

Equate the two expressions:

$$a_m \langle \phi_n | \phi_m \rangle = a_n \langle \phi_n | \phi_m \rangle.$$

If $a_m \neq a_n$, then the only solution is

$$\langle \phi_n | \phi_m \rangle = 0,$$

which means ϕ_n and ϕ_m are orthogonal.

When $a_m = a_n$, the eigenfunctions belong to a degenerate subspace. In this case, one can always use a method like the Gram-Schmidt process to choose a set of orthogonal (and then normalized) eigenfunctions.

Because Hermitian operators have real eigenvalues and their eigenfunctions corresponding to different eigenvalues are orthogonal, we can always form an **orthonormal set** by normalizing these eigenfunctions. This is why we use Hermitian operators in quantum mechanics: they ensure that our measurements yield real numbers and that the state space is spanned by a complete, orthonormal set of functions.

22. Calculate the probability current density function for periodic motion of free particle in one-dimensional space. Give a physical interpretation of the result obtained.

In one-dimensional quantum mechanics, the probability current density is defined as

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$$J(x,t) = \frac{\hbar}{2mi}\left[\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}\right],$$

where $\psi(x,t)$ is the wave function of the particle. For a free particle in periodic motion, a typical solution is a plane wave:

$$\psi(x,t) = Ae^{i(kx-\omega t)},$$

with:

$$\omega = \frac{\hbar k^2}{2m},$$

where A is a (possibly complex) normalization constant, k is the wave number, and ω is the angular frequency. First, compute the spatial derivative of $\psi(x,t)$:

$$\frac{\partial\psi(x,t)}{\partial x} = ikAe^{i(kx-\omega t)} = ik\,\psi(x,t).$$

Similarly, the complex conjugate of the wave function is:

$$\psi^*(x,t) = A^*e^{-i(kx-\omega t)},$$

and its spatial derivative is:

$$\frac{\partial\psi^*(x,t)}{\partial x} = -ikA^*e^{-i(kx-\omega t)} = -ik\,\psi^*(x,t).$$

Substitute these into the expression for $J(x,t)$:

$$J(x,t) = \frac{\hbar}{2mi}\left[\psi^*(x,t)(ik\,\psi(x,t)) - \psi(x,t)(-ik\,\psi^*(x,t))\right].$$

Simplify the expression:

$$J(x,t) = \frac{\hbar}{2mi}\left[ik\,\psi^*(x,t)\psi(x,t) + ik\,\psi(x,t)\psi^*(x,t)\right].$$

Since $\psi^*(x,t)\psi(x,t) = |\psi(x,t)|^2$, this becomes:

$$J(x,t) = \frac{\hbar}{2mi}\left[2ik\,|\psi(x,t)|^2\right] = \frac{\hbar k}{m}\,|\psi(x,t)|^2.$$

The final expression for the probability current density is:

$$J(x,t) = \frac{\hbar k}{m}\,|\psi(x,t)|^2.$$

This tells us: A^2

- The current is directly proportional to the wave number k, which is related to the momentum $p = \hbar k$. Thus, a larger momentum results in a larger current.
- The probability density $|\psi(x,t)|^2$ is uniform (constant) for a normalized plane wave, meaning the probability of finding the particle is evenly distributed over space.
- A positive k indicates that the net flow of probability is in the positive x-direction, while a negative k indicates a flow in the negative x-direction.

For a free particle in periodic (plane wave) motion, the probability current is constant and reflects the steady flow of probability associated with the particle's momentum.

29. Operators are commute : a. $\hat{p}_x$ and $\hat{p}_y$ b. $\hat{p}_x$ and $\hat{x}^2$

a) Commutation of $\hat{p}_x$ and $\hat{p}_y$ The momentum operators in the x and y directions are defined as

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

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Since partial derivatives with respect to different variables commute (i.e., $\frac{\partial}{\partial x}\frac{\partial}{\partial y} = \frac{\partial}{\partial y}\frac{\partial}{\partial x}$), we have

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

Thus, the operators $\hat{p}_x$ and $\hat{p}_y$ commute.

b) Commutation of $\hat{p}_x$ and $\hat{x}^2$ We now calculate the commutator between $\hat{p}_x$ and $\hat{x}^2$:

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

Using the property of commutators for a product of operators,

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

The canonical commutation relation is

$$[\hat{x}, \hat{p}_x] = i\hbar \quad \Longrightarrow \quad [\hat{p}_x, \hat{x}] = -i\hbar.$$

Substitute this into our expression:

$$[\hat{p}_x, \hat{x}^2] = (-i\hbar)\, \hat{x} + \hat{x}\, (-i\hbar) = -2i\hbar\, \hat{x}.$$

Since $-2i\hbar\, \hat{x} \neq 0$ (in general), the operators $\hat{p}_x$ and $\hat{x}^2$ do not commute.

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

In classical mechanics, when a particle encounters a potential barrier, its behavior is completely determined by its energy relative to the barrier height V. Unlike quantum mechanics, classical mechanics does not allow for partial transmission or tunneling. The transition (transmission) coefficient T and reflection coefficient R are thus defined by a sharp threshold.

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Particle Energy $E > V$

- The particle has enough energy to overcome the barrier.
- It is always transmitted, so the **transition coefficient** is

  $$L = 1,$$

  and the **reflection coefficient** is

  $$R = 0.$$

Particle Energy $E < V$

- The particle does not have sufficient energy to cross the barrier.
- It is completely reflected, so the **transition coefficient** is

$$L = 0,$$

  and the **reflection coefficient** is

$$R = 1.$$

Reasons:

- In classical mechanics, energy is conserved, and a particle cannot overcome a barrier if its kinetic energy is insufficient.
- The outcome is deterministic. There is no probability of partial transmission or reflection as there is in quantum mechanics.
- Classical particles do not tunnel through potential barriers. The transition and reflection coefficients are therefore step functions of the energy:

$$L(E) = \begin{cases} 0 & \text{if } E < V, \\ 1 & \text{if } E > V, \end{cases} \quad \text{and} \quad R(E) = \begin{cases} 1 & \text{if } E < V, \\ 0 & \text{if } E > V. \end{cases}$$

In the classical case, the transmission and reflection coefficients change abruptly at $E = V$. For $E > V$, the particle is fully transmitted, and for $E < V$, it is completely reflected. This step-like behavior arises because classical mechanics only allows a particle to either fully overcome or not overcome the barrier, with no intermediate or probabilistic outcome.