Quantum Mechanics

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Week 4

Quantum Mechanics

Exercise Material



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Week 3

Recap

Review

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Exercises

Quantum Mechanics

Review of Last Week

- Any questions on last week's topics?
- Feedback on the previous session?

Recap

Clarifications last week

$$[\hat{a}_-,\hat{a}_+]=1$$

They reach the same state, but scaled.

$$\hat{a}_{+}\hat{a}_{-}\psi_{n} = \sqrt{n}\hat{a}_{+}\psi_{n-1} = n\psi_{n},$$

$$\hat{a}_{-}\hat{a}_{+}\psi_{n} = \sqrt{n+1}\hat{a}_{-}\psi_{n+1} = (n+1)\psi_{n},$$

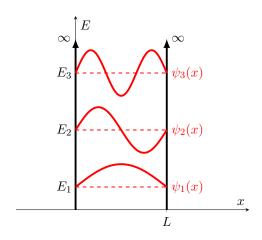
Recap

In case of a defined energy:

$$E_n \to \lambda_n \nleftrightarrow p_n$$

It is important to note:

- \bullet E_n leads to defined λ_n for standing wave patterns within the well.
- \bullet Directly relating λ_n to a precise p_n is not possible due to quantum uncertainty.
- \bullet Instead, understand λ_n as arising from an infinite superposition of traveling waves.



Commutators

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}.$$

It measures the non-commutativity of the operators.

Example:

$$[\hat{x},\hat{p}]=i\hbar$$

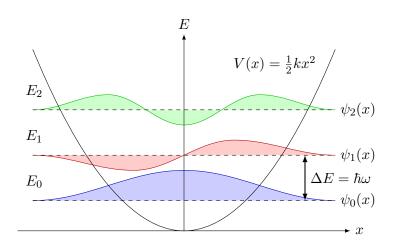
Harmonic Oscillator

The particle possesses both potential energy (V) and kinetic energy (T) at all points within its motion (except turning point where T=0)

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right), \quad E_0 = \frac{1}{2}\hbar\omega$$

$$\psi_n = \frac{1}{\sqrt{n!}} (\hat{a}_+)^n \psi_0,$$

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega,$$



Properties of the Quantum Harmonic Oscillator

- Quantized Energy Levels: The energy levels are discrete, quantized as $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$, with n being a non-negative integer.
- **Zero-Point Energy:** The ground state energy is $\frac{1}{2}\hbar\omega$. There is non-zero energy even at T=0K.
- Orthogonality: The wave functions ψ_n are orthogonal, satisfying $\int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) dx = \delta_{mn}$.
- Completeness: These wave functions form a complete basis for square-integrable functions.
- Energy Gap: The gap between successive levels is $\hbar\omega$, influenced by $\omega=\sqrt{\frac{k}{m}}$, where k is the spring constant and m is the mass.

Review

The particle can sit in infinitely many different potential shapes. For any potential, finite or infinite, the conditions for bound and scattering states are as follows:

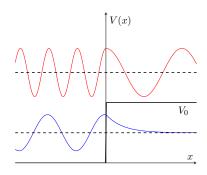
$$\begin{cases} E < V(\pm \infty) & \Rightarrow \text{ bound state} \\ E > V(\pm \infty) & \Rightarrow \text{ scattering state} \end{cases}$$

All transmission and reflection processes conserve the total energy of the system.

To solve these problems, we divide the space into regions and solve the T.I.S.E. independently for each. Then, we match the solutions at the interfaces between regions by applying boundary conditions.

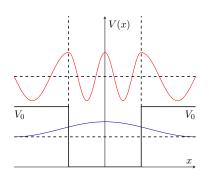
Finite Potential Step

- $E > V_0$: There is both transmission and reflection. Scattering state
- $0 < E < V_0$: The particle is reflected, and there is some penetration into the barrier. Scattering state
- $E < V_{min}$: There is no physical solution.



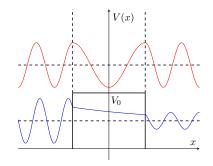
Finite Potential Well

- E > V₀: The particle experiences transmission and reflection. Scattering states.
- $0 < E < V_0$: There are bound states with some penetration into the barrier. Even if $V_0 \approx 0$, there is always at least one bound state.
- $E < V_{min}$: There is no physical solution.



Finite Potential Barrier

- $E > V_0$: The particle is transmitted and reflected. Scattering states
- $0 < E < V_0$: There is transmission and reflection, with exponential decay in the barrier. Scattering states
- $E < V_{min}$: There is no physical solution.



The wavelength of a particle's state is influenced by the potential region it occupies. The wave number in a region with potential V_0 is given by:

$$k = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} = \frac{2\pi}{\lambda}$$

In the context of quantum tunneling, the probability of tunneling occurring is given by the transmission coefficient T :

$$T \approx \frac{16E(V_0 - E)}{V_0^2} \exp\left[-2\frac{\sqrt{2m(V_0 - E)}}{\hbar}a\right]$$

Dirac's Notation

Dirac's Notation

Postulate (1)

Every physically-realizable state of the system is described in quantum mechanics by a state function $\Psi(\vec{r},t)$ that contains all accessible physical information about the system in that state.

Dirac's Notation

If Ψ is physical is **square-integrable** and **normalizable**, Ψ lives in the Hilbert Space and can also be represented by a Vector:

$$\Psi = \sum_{n=1}^{\infty} c_n f_n(\vec{r})
ightarrow egin{pmatrix} c_1 \ c_2 \ dots \ c_n \end{pmatrix}_{\psi_n} = |\Psi
angle \quad extbf{"ket"} \ \Psi^* = \sum_{n=1}^{\infty} c_n^* f_n^*(\vec{r})
ightarrow egin{pmatrix} c_1^* & c_2^* & \cdots & c_n^* \end{pmatrix}_{\psi_n} = \langle \Psi | \quad extbf{"bra"} \end{pmatrix}$$

Dirac's Notation

In the Hilbert Space we define the inner product:

$$\langle f|g\rangle = \int_a^b f(x)^* g(x) dx$$

Where functions f_n are:

Orthonormal if
$$\langle f_m|f_n\rangle=\delta_{mn}$$

Complete if
$$F(\vec{r}) = \sum_{n=1}^{\infty} c_n f_n(\vec{r})$$
 for any $F(\vec{r})$

Hermitian Operator

Postulate (2)

Every observable quantity in classical mechanics is represented in QM by a linear Hermitian operator, \hat{Q} , such taht the mean value of the observable from many identical measurements is

$$\langle Q \rangle = \int \Psi^* \hat{Q} \Psi d^3 r = \langle \Psi | \hat{Q} \Psi \rangle$$

Remark: By linearity we mean that for some functions f,g and some constants a,b \hat{Q} is linear if $\hat{Q}[af+bg]=a\hat{Q}f+b\hat{Q}g$

Hermitian Operators

An operator is Hermitian if the expectation is real, as we are measuring a physical meaningful quantity. Thus,

$$\langle Q \rangle = \langle Q \rangle^*$$

Or, using Dirac's notation:

$$\langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle$$

Properties of Hermitian Operators

• Orthogonality of Eigenstates: The eigenfunctions $|\psi_m\rangle$ and $|\psi_n\rangle$ of a Hermitian operator \hat{Q} are orthogonal if their eigenstates are non-degenerate. Thus,

$$\langle \psi_m | \psi_n \rangle = 0$$
 for $m \neq n$.

Hermitian Operators

• Completeness: The eigenstates of a Hermitian operator form a complete basis set for the Hilbert Space $\mathcal H$. Any state $|\phi\rangle$ in $\mathcal H$ can be expressed as a linear combination of these eigenstates:

$$|\Psi_{general}\rangle = \sum_{n} c_n |\psi_n\rangle$$
.

• Real Eigenvalues: The eigenvalues of a Hermitian operator are always real. If $|\psi\rangle$ is an eigenstate of \hat{Q} with eigenvalue λ , then:

$$\hat{Q}\psi=\lambda\psi,\quad ext{where}\quad \lambda\in\mathbb{R}.$$

Determinate States

Determinate States

If a system is in state Ψ that satisfies the eigenvalue equation for \hat{Q} , every measurement of \hat{Q} will yield q. This can be written in an eigenvalue equation.

$$\hat{Q}\Psi = q\Psi$$

This states Ψ are called determinate states.

ullet The spectrum of \hat{Q} encompasses all its eigenvalues, denoting the set of possible measurement outcomes for Q:

$$\mathsf{Spectrum}(\hat{Q}) = \{q_1, q_2, \dots, q_n\}.$$

Determinate States

• Degeneracy occurs when multiple distinct eigenfunctions Ψ_i and Ψ_j correspond to the same eigenvalue q:

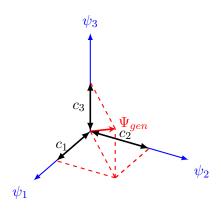
$$\hat{Q}\Psi_i=q\Psi_i$$
 and $\hat{Q}\Psi_j=q\Psi_j$ for $i
eq j.$

This states are called degenerate states.

If Ψ is not an eigenfunction of \hat{Q} , a single measurement will yield one of the eigenvalues q_n of \hat{Q} with probability $|c_n|^2$.

$$\langle Q \rangle = \sum_{n} |c_n|^2 q_n$$

Determinate States



Given $\vec{\Psi}_{gen}=c_1\vec{e}_{\psi_1}+c_2\vec{e}_{\psi_2}+c_3\vec{e}_{\psi_3}$, we define:

$$|\Psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}_{\psi_r}$$

Where, $c_n = \langle \psi_n | \Psi \rangle$, encapsulating the system's state in terms of basis vectors $\hat{\psi}_n$.

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Exercises

Exercise 1

 $\textbf{Hint:} \ \operatorname{Remember that} \ odd*even = odd$

Exercise 2

Exercise 3

Exercise 5

Questions?

THANK YOU!