Quantum Mechanics

Week 4

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Exercise Material

Webpage

Week 3

Recap

Review

Exercises

Review of Last Week

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

Recap

Separation of variables

$$\boxed{\Psi(x,t) = \psi(x) \cdot \varphi(t) = \psi(x) \cdot e^{-i\frac{Et}{\hbar}}}$$

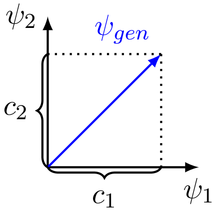
TISE $\rightarrow$ Eigenvalue Problem

$$\boxed{\hat{H}\psi = E\psi}$$

Superposition of stationary states

$$\Psi_{general}(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) \cdot e^{-i\frac{E_n t}{\hbar}}$$

- Measuring energy of particle $\hat{H}$ in $\Psi_{general}$ will obtain one of the values E_n with probability $|c_n|^2$, then the wave will "collapse" $\Psi_{general}$ into one of the ψ_n eigenstates.



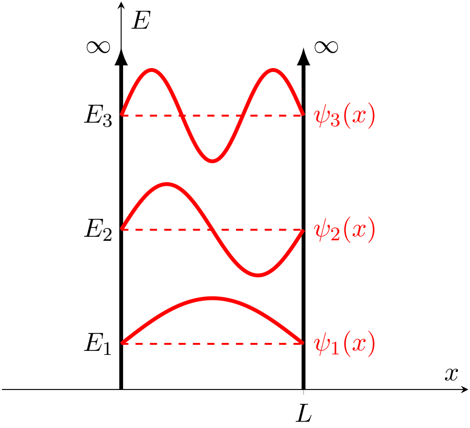
$$c_n = \int \psi_{gen}(x)\psi_n(x)dx,$$

Infinite Square Well

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \quad n \in \mathbb{Z}^+$$

- Solutions are mutually orthogonal: $\int \psi_m^* \psi_n \, \mathrm{d}x = \delta_{mn} \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases}$
- Solutions form a complete set: $f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$

Superposition of stationary states



Free Particle

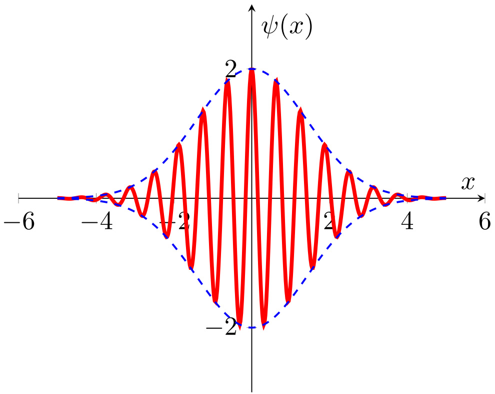
$$\boxed{\Psi_k(x,t) = Ae^{i(kx-\omega t)},}$$

- Separable Solutions are not normalizable $\rightarrow$ Free particles with a **definite** energy do not exist
- We have to do a continuous superposition of different dk waves.

$$\Psi_{gen}(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) \exp\left[i\left(kx - \frac{\hbar k^2}{2m}t\right)\right] dk,$$

$$\text{where } g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx$$

- The function $\Psi_{gen}(x,t)$ represents a **wave packet**, which is a superposition of plane waves of different wavelengths.
- The wave packet contains range of k, which correspond to different momenta $p = \hbar k$ and energies $E = \frac{\hbar^2 k^2}{2m}$.


$\psi(x)$
x
2
-2
-6
-4
-2
2
4
6

Review

Commutators

Commutators tell us whether the order of the operators applied matters. The commutator of two operators $\hat{A}$ and $\hat{B}$ is defined as:

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

It measures the non-commutativity of the operators, with $\left[\hat{A}, \hat{B}\right] = 0$ indicating that $\hat{A}$ and $\hat{B}$ commute, thus the order in which we apply the operators does not matter.

Example: Given the position operator $\hat{x}$ and the momentum operator $\hat{p} = -i\hbar\frac{\partial}{\partial x}$, the commutator $[\hat{x}, \hat{p}]$ is defined as:

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

Substituting $\hat{p}$ into the equation gives:

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

Applying the operators to a test function $f(x)$:

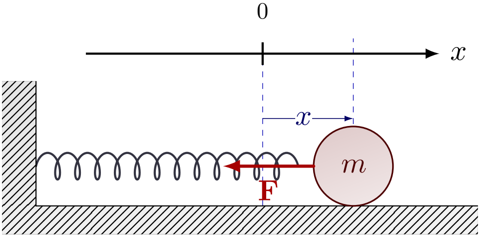
$$
\begin{aligned}
[\hat{x}, \hat{p}]f(x) &= \hat{x}(-i\hbar\frac{\partial f(x)}{\partial x}) - (-i\hbar\frac{\partial}{\partial x})(\hat{x}f(x)) \\
&= -i\hbar x\frac{\partial f(x)}{\partial x} + i\hbar\frac{\partial}{\partial x}(xf(x)) \\
&= -i\hbar x\frac{\partial f(x)}{\partial x} + i\hbar\left(f(x) + x\frac{\partial f(x)}{\partial x}\right) \\
&= i\hbar f(x)
\end{aligned}
$$

Since this operation was performed on an arbitrary function $f(x)$, we can conclude that:

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

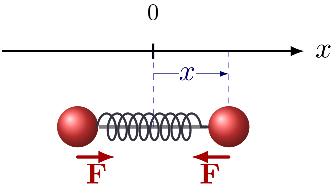
Harmonic Oscillator

In classical mechanics



We define this potential as being $V(x) = \frac{1}{2}kx^2$.

In quantum Mechanics



The harmonic oscillator is modeled by a particle in a quadratic potential well and is given by: $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$, where k is the spring constant, m is the mass of the particle, and $\omega = \sqrt{\frac{k}{m}}$ is the angular frequency of the oscillator. A typical example is the vibrations of diatomic molecules

Creation and Annihilation Operators

The quantum harmonic oscillator is elegantly analyzed using creation (raising) and annihilation (lowering) operators, denoted by $\hat{a}_+$ and $\hat{a}_-$, respectively. These operators are defined as:

$$\boxed{\begin{aligned} \hat{a}_+ &= \frac{1}{\sqrt{2\hbar m\omega}}\left(-i\hat{p} + m\omega x\right), \\ \hat{a}_- &= \frac{1}{\sqrt{2\hbar m\omega}}\left(i\hat{p} + m\omega x\right), \end{aligned}}$$

A crucial property of these operators is their non-commutativity, given by the relation $[\hat{a}_-, \hat{a}_+] = 1$.

Operational Impact on Energy Levels

The action of the creation and annihilation operators on the energy eigenstates is described by:

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

highlighting their role in "moving up or down the ladder".

Hamiltonian and Quantum States

The Hamiltonian of the harmonic oscillator, incorporating these operators, is:

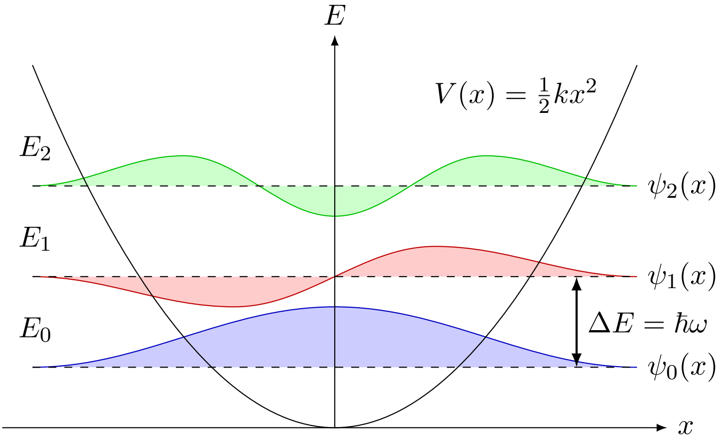
$$\boxed{\hat{H} = \hbar\omega\left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right) = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right),}$$

representing the total energy. This formalism facilitates deriving the ground state solution by solving $\hat{a}_-\psi_0 = 0$, yielding:

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

Extending this, the energy and wave function of the nth quantum state are obtained through the repeated application of $\hat{a}_+$, leading to:

$$\boxed{\begin{aligned} \psi_n &= \frac{1}{\sqrt{n!}}(\hat{a}_+)^n \psi_0, \\ E_n &= \left(n + \frac{1}{2}\right)\hbar\omega, \end{aligned}}$$


E
$V(x) = \frac{1}{2}kx^2$
E_2
$\psi_2(x)$
E_1
$\psi_1(x)$
E_0
$\Delta E = \hbar\omega$
$\psi_0(x)$
x

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 $T = 0K$.
- **Wave Function Symmetry:** Ground state wave functions are Gaussian, and higher states are Hermite-Gaussian, with $\langle x \rangle$ often zero.
- **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.

- **Existence Outside Potential Well:** There's a non-zero probability of finding a particle outside the potential well, illustrating quantum penetration into classically forbidden regions.

- **Classical Turning Points:** Comparing the quantum oscillator to its classical counterpart involves examining classical turning points where kinetic energy is zero.

- **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.

Exercises

Exercise 1

Hint: Always apply the commutators to some function $[\hat{A}, \hat{B}]f(x)$

Exercise 2

For deeper understanding

Exercise 3

Hint: $\psi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n\psi_0$ for $n = 1 \rightarrow \psi_1 = \frac{1}{\sqrt{1!}}(\hat{a}_+)^1\psi_0$ Answer MUST be normalized!

Questions?

THANK YOU!