Quantum Mechanics

Week 3

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Exercise Material

Webpage

Week 3

Recap

Review

Clicker Questions

Exercises

Review of Last Week

- Any questions on last week's topics?
- Feedback on the previous session?
- Additional materials you'd like to get?

Recap

Time-Dependent Schrödinger Equation (TDSE)

$$\boxed{i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t)}$$

Normalization

$$\boxed{\int_{-\infty}^{\infty} |C\cdot\Psi(x,t)|^2 dx \overset{!}{=} 1}$$

Measurements

$$\underbrace{\langle \overbrace{Q(x,p)}^{\text{Observable}} \rangle}_{\text{Expectation Value}} = \int_{-\infty}^{\infty} \Psi^* \cdot \underbrace{\hat{Q}(\hat{x},\hat{p})}_{\text{Operator}} \cdot \Psi dx$$

Uncertainty Principle

$$\sigma_x \cdot \sigma_p \geq \frac{\hbar}{2}$$

Review

Separation of Variables

We rewrite the Time-Dependent Schrödinger Equation (T.D.S.E.) and $V(x,t) \to V(x)$:

$$\boxed{i\hbar \frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t)}$$

Derivation of Separable Variables:

Assuming $\Psi(x,t) = \psi(x) \cdot \varphi(t)$, we substitute to obtain:

$$i\hbar\psi(x)\frac{\partial\varphi(t)}{\partial t} = -\frac{\hbar^2}{2m}\varphi(t)\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x)\varphi(t)$$

Separating variables yields:

$$\underbrace{i\hbar\frac{1}{\varphi(t)}\frac{\partial\varphi(t)}{\partial t}}_{\text{LHS}} = \underbrace{-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)}_{\text{RHS}} = E$$

Because each side depends on a different variable, they must equal a constant, E, the separation constant

LHS

$$i\hbar\frac{1}{\varphi}\frac{\partial\varphi}{\partial t}=E$$

$$\int\frac{\partial\varphi}{\varphi}=\frac{E}{i\hbar}\int\partial t$$

$$\ln\varphi=\frac{E}{i\hbar}t+C_1$$

With $C_2=e^{C_1}$ and $\frac{1}{i}=-i$,

$$\boxed{\varphi(t)=C_2e^{-i\frac{Et}{\hbar}}}$$

RHS (T.I.S.E.)

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2}+V=E$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=E\psi$$

With $\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V$,

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

T.I.S.E.

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

Solving the Time-Independent Schrödinger Equation (T.I.S.E.) provides us with $\psi(x)$, which, when combined with the known temporal component $\varphi(t) = e^{-\frac{iE}{\hbar}t}$, fully determines $\Psi(x,t)$.

In these separable solutions, $|\Psi|^2 = \psi^* e^{\frac{iE}{\hbar}t} \cdot \psi e^{-\frac{iE}{\hbar}t} = |\psi|^2$, they are notable for their **time-independent probability density**, characterizing them as **stationary states**.

Stationary States

In the context of separable solutions, where $\Psi(x,t) = \psi(x) \cdot \varphi(t)$, we observe that:

- The expectation value of any observable $\langle Q \rangle$ remains constant over time, i.e., $\frac{\partial \langle Q \rangle}{\partial t} = 0$.
- In particular $\frac{d\langle x \rangle}{dt} = 0 \to \langle p \rangle = 0$
- For the Hamiltonian operator, we find $\langle H \rangle = E$ and $\langle H^2 \rangle = E^2$, leading to $\sigma_H = \sqrt{\langle H^2 \rangle - \langle H \rangle^2} = 0$. Thus, energy measurements in a stationary state always return the specific value E, indicating a precisely defined total energy.

General Solutions to the T.D.S.E.

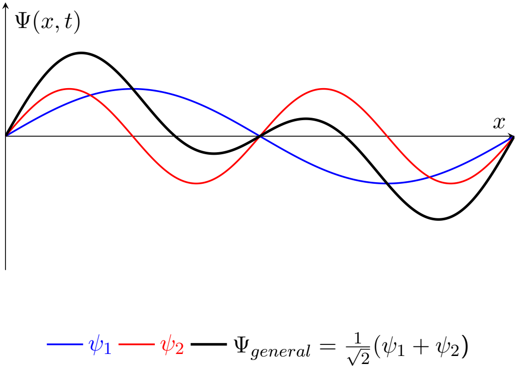
- All other T.D.S.E. solutions can be expressed via separable solutions given the linearity of the T.D.S.E.

$$\boxed{\Psi_{\text{general}}(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-\frac{iE_n}{\hbar}t}}$$

- This formula represents the general wave function as a sum of separable solutions, each with its own coefficient c_n, spatial part $\psi_n(x)$, and temporal part $e^{-\frac{iE_n}{\hbar}t}$.
- We get ψ_n and E_n by solving $\hat{H}\psi_n = E_n\psi_n$ (Eigenvalue Equation)

- $\psi_n(x)$ represents the probability amplitude when the particle has energy E_n.
- $\Psi_{\text{gen}}(x,t)$ is not a stationary state; expectation values depend on time.
- Coefficients c_n determined by the initial state $\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$.
- $|c_n|^2$ indicates the probability of measuring the energy E_n.
- Normalization condition: $\sum |c_n|^2 = 1$.

A rough sketch of what a linear combination might look like at $t = 0$.



Motion of Particle with Zero Potential

Given the time-independent Schrödinger equation (T.I.S.E.) for a particle in a region where the potential energy $V(x) = 0$:

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x),}$$

we arrive at a form analogous to the harmonic oscillator equation from classical physics:

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x),$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$ represents the wave number, related to the particle's momentum p by $k = \frac{p}{\hbar}$ and to the wavelength λ by $k = \frac{2\pi}{\lambda}$.

- **Standing Wave Solutions:** characterized by

$$\boxed{\psi_{\text{standing}}(x) = A\cos(kx) + B\sin(kx),}$$

- **Traveling Wave Solutions:** expressed as

$$\boxed{\psi_{\text{traveling}}(x) = Ce^{ikx} + De^{-ikx},}$$

Note: The distinction between standing and traveling wave solutions lies primarily in their boundary conditions.

Free Particle

A free particle is one that moves without experiencing any external forces, meaning the potential energy, $V(x)$, is zero everywhere.

Assuming a solution of the form $\psi_k(x) = Ae^{ikx}$, where $k = \pm\sqrt{\frac{2mE}{\hbar^2}}$, leads to the general solution for the wave function in both space and time:

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

with $\omega = \frac{\hbar k^2}{2m}$ representing the angular frequency of the wave. $k > 0$ defines a wave moving in positive x directions and $k < 0$ defines a wave moving in negative x directions

- Since there are no boundaries, k can take any value, allowing for any positive energy E.
- The wave function $\Psi_k(x,t)$, however, is **not normalizable** over all space, as its integral over $-\infty$ to ∞ diverges. This indicates that such states cannot represent physical particles with a definite energy.

Therefore, Quantum Mechanics states the Free Particle with a definite energy do **not** exist!

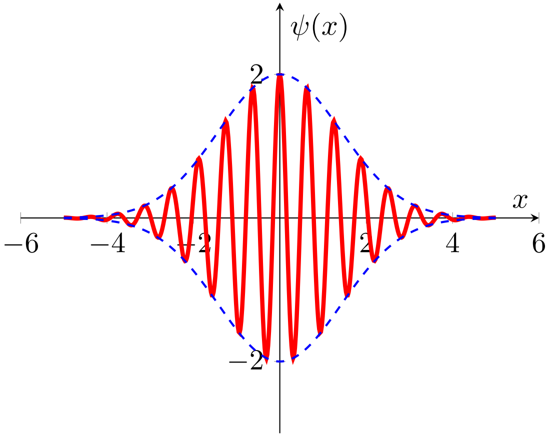
We can fix this by making a **continuous** linear combination of solutions instead of a discrete.

Wave Packets and Continuous Spectrum

To address the limitations of plane wave solutions, a more physical representation of a free particle is given by a wave packet, $\Psi_{gen}(x,t)$, a continuous superposition of plane waves:

$$\Psi_{gen}(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) \exp\left[i\left(kx - \frac{\hbar k^2}{2m}t\right)\right] dk,$$
$$\text{where } g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx$$

This approach yields a normalizable wave function that can represent a localized particle.


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

Infinite Square Well

- The Infinite Square Well (ISW) is a fundamental quantum mechanics problem illustrating quantization in a confined potential.
- It models a particle trapped in a one-dimensional box with infinitely high walls ($\psi(0) = \psi(a) = 0$).
- Potential V(x):

$$V(x) = \begin{cases} 0 & \text{for } 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}$$

- Solve $\frac{\partial^2 \psi(x)}{\partial x^2} = -k^2 \psi(x)$ using standing wave ansatz!

Wave Function and Energy Levels in ISW

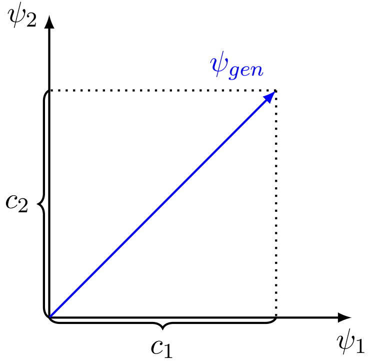
Solutions to TISE in ISW are defined by:

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

Wave Function Characteristics

- Alternating even and odd symmetries about $x = \frac{a}{2}$ (if wave centered in $x = \frac{a}{2}$).
- Increase in nodes with quantum number n.
- Orthogonality: $\langle \psi_m | \psi_n \rangle = \delta_{mn} \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n \end{cases}$, ensuring independence of states.
- Completeness allows any function $f(x)$ within the well to be expanded as a series:

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x), \quad c_n = \int_0^a \psi_n^*(x) f(x)\, dx$$



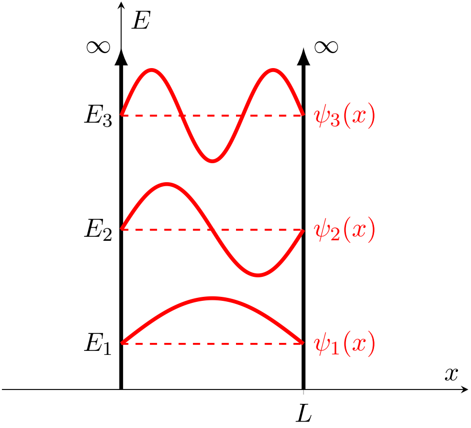
Given a general normalized function $\psi_{gen} = c_1\psi_1 + c_2\psi_2$, compute coefficients c_1, c_2 via inner (scalar) product defined in the L^2 space:

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

This illustrates, very roughly and ideal, how ψ_{gen} projects onto the basis functions ψ_1 and ψ_2, akin to vector projection in algebra.

Energy Quantization in ISW

- Energy levels are discrete: $E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$.
- The ground state (E_1) represents the lowest energy state, with $E_{n>1}$ denoting excited states.
- Energy levels scale with n^2.
- Confinement leads to higher energy: Reducing the size of the well increases the minimum energy.



E
∞
∞
E_3
$\psi_3(x)$
E_2
$\psi_2(x)$
E_1
$\psi_1(x)$
x
L

Clicker Questions

Exercises

Exercise 1

Hint: Start by expressing σ_x and σ_p using the definitions of standard deviation for position and momentum. For the nth state, evaluate the integrals for $\langle x^2 \rangle$, $\langle x \rangle^2$, $\langle p^2 \rangle$, and $\langle p \rangle^2$. Recall the uncertainty principle: $\sigma_x \sigma_p \geq \frac{\hbar}{2}$.

Exercise 2

Together

Exercise 3

Together

Questions?

THANK YOU!