Chapter 4 Lectures — Noah

Postulates of Quantum Mechanics

"exact" = no violations found in experiment, the implementation is approximate

I. The state of any physical system is represented by a vector in a linear Space of infinite dimensions (Hilbert space) $|\Psi\rangle$
- Any linear combination of states is a state $|\Psi\rangle = \alpha|\Psi_1\rangle + \beta|\Psi_2\rangle$
- If Ψ_1, Ψ are normalized, $\langle\Psi_1|\Psi\rangle$ is the probability amplitude of finding it in state Ψ_1.

II. The physical observables are represented by Hermetian operators. The eigenvalues for the Hermitian are the results of observation of the corresponding observables. (real values).

$$\Omega|\omega_i\rangle = \omega_i|\omega_i\rangle$$

- When action is on the order of $\hbar$, you can't make a measurement without disturbing the system. (Classical mech. comes from Q mech)
- The eigenvectors are complete: $c_j = \omega_j|\Psi\rangle = \sum_i c_i \langle\omega_j|\omega_i\rangle = c_j\delta_{ij}$

Expand the state: $|\Psi\rangle = \sum_i c_i|\omega_i\rangle = \sum_i \langle\omega_i|\Psi\rangle|\omega_i\rangle = \sum_i |\omega_i\rangle\langle\omega_i|\Psi\rangle$ (expansion coef.)

Projection of Ψ along ω_i: $\tilde{P}_{\omega_i} = |\omega_i\rangle\langle\omega_i| \rightarrow \tilde{P}_\omega|\omega_i\rangle$ where $\sum_i P_{\omega_i} = 1$

III. - Given an ensemble of identically prepared in one state all we can predict is the probability of measuring value ω_i

$$P_{\omega_i} = \langle\Psi|\tilde{P}_{\omega_i}|\Psi\rangle = \langle\Psi|\omega_i\rangle\langle\omega_i|\Psi\rangle = |\langle\omega_i|\Psi\rangle|^2$$

- The state of system changes from $|\Psi\rangle$ to $|\omega_i\rangle$ as result of measurement.

IV. The Schrodinger Equation determines the dynamics. If you know state at time t_i can predict state at later time.

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle$$

Lagrangian $\mathcal{L}(q_i, \dot{q}_i)$ now x and p_x are operators. $p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$

Canonical Quantization: $[q_i, p_i] = i\hbar\delta_{ij}$ $[q_i, q_j] = 0$ $[p_i, p_j] = 0$

Spin has no classical counterpart.

Constructing Operators

Commutation X, P_x

Spinless particle moves x-axis (x, p_x)
$P_x = \hbar k$

$\langle x | x' \rangle = \delta(x-x')$

$\langle x | X | x' \rangle = x\,\delta(x-x')$ $\quad \langle x | P_x | x' \rangle = -i\hbar\,\delta'(x-x')$ $\Rightarrow [X, P_x] = i\hbar$

What are the eigenvectors of P_x ?

$P_x|p\rangle = p|p\rangle$ continuous unless box-coord.

$\langle p | p' \rangle = \delta(p-p')$

$\langle x | p \rangle$ = projection of eigenfunction p along the x component $= \delta(\hbar(k-k')) = \frac{1}{\hbar}\delta(k-k')$

$\langle k | k' \rangle = \delta(k-k')$

$\langle x | P_x | \psi \rangle = \int \underbrace{\langle x | P_x | x' \rangle}_{-i\hbar\delta'(x-x')} \underbrace{\langle x' | \psi \rangle}_{\psi(x')} dx' = -i\hbar \frac{\partial \psi}{\partial x} \Rightarrow \boxed{p_x = -i\hbar\frac{\partial}{\partial x}}$

eigenftn $|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} = \frac{1}{\sqrt{2\pi}} e^{ikx}$

$\langle x | X | \psi \rangle = x \langle x | \psi \rangle = x\,\psi(x)$ in the x-rep.

$x = +i\hbar\frac{\partial}{\partial p}$ in the p-representation

The form of the operator depends on what representation you chose.

<u>Energy Basis</u>

$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2$ harmonic oscillator take $\hbar\omega(n+\frac{1}{2})$ as basis states

$H|n\rangle = \hbar\omega(n+\frac{1}{2})|n\rangle$

$\langle n | H | m' \rangle = \hbar\omega(n+\frac{1}{2})\,\delta_{nm'}$

$\langle n | X | m' \rangle = \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{m'+1}\,\delta_{m'+1,n} + \sqrt{m'}\,\delta_{m'-1,n}\right.$

$\langle n | P_x | m' \rangle =$

<u>X-Basis is most Common</u>

$H = \frac{p_x^2}{2m} + V(x) \qquad i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$

$i\hbar\frac{\partial}{\partial t}\langle x|\psi\rangle = \langle x|\frac{p_x^2}{2m} + V(x)|\psi\rangle = i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\langle x|\psi(x,t)\rangle + V(x)\langle x|\psi(x,t)\rangle$

show that P II P II gives rise to

Abstract Representation → time dependence

$H|E\rangle = E|E\rangle$

$|\psi\rangle^{E} = \sum_i |E_i\rangle\langle E_i|\psi\rangle$ the eigenvectors of any observable (here energy) form a complete set (assuming they are discrete)

$H|E_n\rangle = E_n|E_n\rangle$ $\quad P(E_n) = |\langle E_n|\psi\rangle|^2$ $\quad |\psi\rangle = \sum_n |E_n\rangle\langle E_n|\psi\rangle$

$= \sum_{\alpha=1}^{d} |\langle E_{n,\alpha}|\psi\rangle|^2$

$i\hbar \frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$ suppose ψ is one of the eigenvectors

$i\hbar \frac{\partial}{\partial t}|E_n\rangle = H|E_n\rangle = E_n|E_n\rangle$

$\frac{\partial}{dt}|E_n\rangle = \frac{E_n}{i\hbar}|E_n\rangle = -\frac{i E_n}{\hbar}|E_n\rangle$ where $|E_n(t)\rangle$ is an arbitrary ket vector

$\frac{d\langle\circ|E_n\rangle}{\langle\circ|E_n\rangle} = -\frac{iE_n}{\hbar}\,dt \Rightarrow \boxed{|E_n(t)\rangle = C e^{-iE_n t/\hbar}}$ within a phase factor

Simple Time Dependence $\langle x|E_n(t)\rangle = \langle x|E_n(0)\rangle e^{iE_n t/\hbar} \Rightarrow |E_n(t)\rangle = |E_n(0)\rangle e^{-iE_n t/\hbar}$

Many Ways to Represent a State

$\langle p|p'\rangle = \delta(p-p')$ $\quad \langle x|x'\rangle = \delta(x-x')$ $\quad \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}$ $\quad \langle p|\psi\rangle = \phi(p,t)$

the coordinate representation is the fourier tranform of the momentum representation of the same state

$e^{i(k-k')x}$ from x $-\infty$ to $+\infty$ rapidly oscillates

Limiting procedure to normalize

$\lim_{\substack{L\to\infty \\ \Delta\to\infty}} \frac{1}{\Delta}\int_L^{L+\Delta} e^{i(k-k')x}$ and $\lim_{\substack{L\to-\infty \\ \Delta\to-\infty}} \frac{1}{\Delta}\int_L^{L+\Delta} e^{i(k-k')x}$

Box normalization $L\to\infty$ periodic boundary conditions

$\psi(x) = \int dp\, \langle x|p\rangle\langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int dp\, e^{ipx/\hbar}\phi(p,t)$ fourier tranform

1. Normalize by $\langle\psi|\psi\rangle = 1$

or

2. Normalize by dirac delta function eg a cubical box all eigenfunctions are periodic in L (periodic boundary conditions)

normalized state $= \frac{1}{\sqrt{L}} e^{ipx/\hbar} = \psi_p(x) = \psi_p(x+L) \Rightarrow e^{ipx/\hbar} = e^{ip(x+L)/\hbar} \Rightarrow e^{ipL/\hbar} = 1$

$\therefore p = n\left(\frac{2\pi\hbar}{L}\right)$

Generalize to Any Dimension

$\psi_{p_x,p_y,p_z}(x,y,z) = \frac{1}{\sqrt{L^3}} e^{i\vec{p}\cdot\vec{x}/\hbar}$ $\Rightarrow$ $p_i = n_i\left(\frac{2\pi\hbar}{L}\right)$ $p_i = \hbar k_i$ wave vector

$k_i = n_i \frac{2\pi}{L}$ discrete eigenstates

$L \to \infty$

$\langle p|p'\rangle = \delta_{pp'}$ $\Omega|\omega_1\rangle = \omega|\omega_1\rangle$ $\Omega|\omega_2\rangle = \omega|\omega_2\rangle$ can use G.S. to make orthonormal

Expectation Values in Different Representations

ABSTRACT

expansion of state vector $|\psi\rangle = \sum_i |\omega_i\rangle\langle\omega_i|\psi\rangle \Rightarrow P_{\omega_i} = |\langle\omega_i|\psi\rangle|^2$

for an ensemble of identically prepared systems:

$$\bar{\Omega} = \langle\Omega\rangle = \sum_i p(\omega_i)\omega_i = \sum_i |\langle\omega_i|\psi\rangle|^2\omega_i = \sum_i \omega_i\langle\psi|\omega_i\rangle\langle\omega_i|\psi\rangle = \sum_i \langle\psi|\Omega|\omega_i\rangle\langle\omega_i|\psi\rangle$$

$\langle\psi|\omega_i|\omega_i\rangle$ $\Omega|\omega_i\rangle = \omega_i|\omega_i\rangle$

$$= \cancel{\sum_i}\langle\psi|\Omega\,\mathbb{I}|\psi\rangle = \langle\psi|\Omega|\psi\rangle$$

In order to calculate, you need a representation $|\psi\rangle = x$-rep $|\phi\rangle = p$-rep

$$\langle\psi|x|\psi\rangle = \iint dx\,dx'\,\langle\psi|x\rangle\langle x|X|x'\rangle\langle x'|\psi\rangle = \iint dx\,dx'\,\psi^*(x)\,x\,\delta(x-x')\,\psi(x')$$

$$= \int x\psi^*\psi\,dx = i\hbar\int\phi^*(p)\frac{d\phi(p)}{dp}dp$$

integration limits must contain x

$\langle p|X|p'\rangle = i\hbar\delta'(p-p')$ $\langle p|\psi\rangle = \phi(p)$

$$\langle\psi|P_x|\psi\rangle = \iint dx\,dx'\,\langle\psi|x\rangle\underbrace{\langle x|P_x|x'\rangle}_{-i\hbar\delta'(x-x')=}\langle x'|\psi\rangle = -i\hbar\int dx\,\psi^*\underbrace{\int dx'\,\psi(x')\,\delta'(x-x')}_{d\psi/dx}$$

$$= -i\hbar\int dx\,\psi^*\frac{d\psi}{dx} = \int\phi^*\,p\,\phi(p)\,dp$$

Uncertainty Relation

$[X, P_x] = i\hbar\,\mathbb{I}$

$\Rightarrow (\Delta x)(\Delta p_x) \geq \hbar/2$

in general:

$$\langle\Omega\rangle = \frac{\langle\psi|\Omega|\psi\rangle}{\langle\psi|\psi\rangle}$$

$(\Delta A)^2 = (A - \bar{A})^2$

$$(\Delta\Omega)^2 = \langle(\Omega - \langle\Omega\rangle)^2\rangle = \langle\psi|\Omega^2 - 2\Omega\langle\Omega\rangle + \langle\Omega\rangle^2|\psi\rangle$$

$$= \langle\psi|\Omega^2|\psi\rangle - 2\langle\Omega\rangle\langle\psi|\Omega|\psi\rangle + \langle\Omega\rangle^2\underbrace{\langle\psi|\psi\rangle}_{1}$$

$$= \langle\Omega^2\rangle - 2\langle\Omega\rangle\langle\Omega\rangle + \langle\Omega\rangle^2$$

$$= \langle\Omega^2\rangle - \langle\Omega\rangle^2$$

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Compatible and Incompatible Variables

$\Omega|\omega\rangle = \omega|\omega\rangle$ $\Lambda|\lambda\rangle = \lambda|\lambda\rangle$ the result of measurement is disturbance
was ↗ measure ↑ jumps to another state

But, if it is an eigenstate of both variables, it remains in that state, make no disturbance

$\Omega|\omega,\lambda\rangle = \omega|\omega,\lambda\rangle$ and $\Lambda|\omega,\lambda\rangle = \lambda|\omega,\lambda\rangle$

$\Omega\Lambda|\omega,\lambda\rangle = \Omega\lambda|\omega,\lambda\rangle = \lambda\Omega|\omega,\lambda\rangle = \lambda\omega|\omega,\lambda\rangle$

$\Lambda\Omega|\omega,\lambda\rangle = \Lambda\omega|\omega,\lambda\rangle = \omega\Lambda|\omega,\lambda\rangle = \omega\lambda|\omega,\lambda\rangle$

$(\Omega\Lambda - \Lambda\Omega)|\omega,\lambda\rangle = |0\rangle$

There are two possible ways: ① The state made it true (could be true even if they don't commute
② $[\Omega, \Lambda] = \Omega\Lambda - \Lambda\Omega = 0$

$[X, P_x] = i\hbar \mathbb{I}$ $(XP_x - P_xX)|\psi\rangle = i\hbar|\psi\rangle$ ∴ can never be a $|0\rangle$ $\Delta x \Delta p \geq \hbar/2$

$[J_x, J_y] = i\hbar J_z \Rightarrow \Delta J_x \Delta J_y \geq \hbar/2 \langle J_z\rangle$ if $J_z = 0$ then $J_x = J_y = 0$

What happens if they are degenerate?

if 1 eigenvector has 1 eigenvalue: $|\psi\rangle = \sum_{\omega\lambda} |\omega\lambda\rangle\langle\omega\lambda|\psi\rangle$ $P(\omega,\lambda) = |\langle\omega\lambda|\psi\rangle|^2$ the probability of getting λ after ω is 1 if non-degenerate

Degenerate if λ is measured, then the state is in a linear combination of the two $|\lambda\omega_1\rangle$, ~~and~~ $|\lambda\omega_2\rangle$

$|\psi\rangle = \alpha|\omega_1\lambda\rangle + \beta|\omega_2\lambda\rangle$ $\alpha^2 + \beta^2 = 1$

measure ω 1st then you know both states

Third Observable: All commute

$[\Omega, \Lambda] = [\Omega, \Gamma] = [\Gamma, \Lambda] = 0$ you need all three state
complete set of commuting observables
the state is completely specified

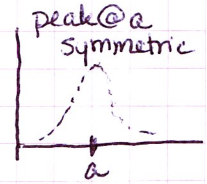
example: H, L^2, L_z energy, orbital ang. mom,

Normalization Example in Book – Math Trick

$\langle x|\psi\rangle = Ae^{-(x-a)^2/2\Delta^2}$

$\langle\psi|\psi\rangle = 1 = \int\langle\psi|x\rangle\langle x|\psi\rangle dx = \int\psi^*\psi\, dx = |A|^2\int e^{-(x-a)^2/\Delta^2}dx$

easily integrated with this substitution



$y = \frac{x-a}{\Delta} \quad \frac{dx}{\Delta} = dy$

$1 = |A|^2\Delta\int_{-\infty}^{\infty}e^{-y^2}dy = |A|^2\Delta\sqrt{\pi} \Rightarrow |A|^2 = \frac{1}{\Delta\sqrt{\pi}} \Rightarrow A = \frac{1}{\Delta^{1/2}\pi^{1/4}}$ within a phase constant

$\psi(x) = \langle x|\psi\rangle = \frac{1}{\sqrt{\Delta}\,\pi^{1/4}}e^{-(x-a)^2/2\Delta^2}$

Expectation Values

$\langle\psi|x|\psi\rangle = \int_{-\infty}^{\infty}\psi^* x\psi\, dx = a \qquad \langle x^2\rangle = a^2 + \Delta^2/2$

$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 = a^2 - a^2 + \Delta^2/2 = \Delta^2/2 \Rightarrow \Delta x = \Delta/\sqrt{2}$ also $\Delta P_x = \hbar/\sqrt{2}\Delta$

$(\Delta x)(\Delta P_x) = \left(\frac{\Delta}{\sqrt{2}}\right)\left(\frac{\hbar}{\sqrt{2}\Delta}\right) = \frac{\hbar}{2}$

$\boxed{\text{SHO}}$

Note: The Gaussian wavefunction is the ground state of 1D SHO
It is the Hermite polynomial = 1

$H = \frac{p_x^2}{2m} + \frac{m\omega^2}{2}x^2$ symmetric in x and p_x

the ground state energy is minimum $\neq 0 \Rightarrow E_{min} = \hbar/2$

$\boxed{\text{Many Particle System}}$

Particle 1 = $[x_1, x_2 x_3]$ $\quad [x_i, p_j] = i\hbar\delta_{ij} \quad [x_i, x_j] = 0 \quad [p_i, p_j] = 0$
Particle 2 = $[x_4, x_5, x_6]$
etc.

$\langle x_1 x_2 x_3 \ldots x_n|x_1' x_2' x_3' \ldots x_n'\rangle = \delta(x_1 - x_1')\delta(x_2 - x_2')\ldots$

$X_i|x_1, x_2, \ldots, x_i, \ldots, x_n\rangle = x_i|x_1, x_2, \ldots, x_i, \ldots, x_n\rangle$

$\langle x_1, x_2, \ldots, x_i, \ldots, x_n|X_i|\psi\rangle = x_i\langle x_1, x_2, \ldots, x_n|\psi\rangle = x_i\,\psi(x_1, x_2, \ldots, x_n)$

$\langle x_1, x_2, \ldots, x_i, \ldots, x_n|P_i|\psi\rangle = -i\hbar\frac{\partial}{\partial x_i}\psi(x_1, x_2, \ldots, x_i, \ldots, x_n)$

$\langle\psi|\Omega|\psi\rangle = \sum_{ij}\langle\psi|i\rangle\langle i|\Omega|j\rangle\langle j|\psi\rangle = \sum_{ij}\langle i|\psi\rangle^*\Omega_{ij}\langle j|\psi\rangle$

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Matrix Representation

$$|\psi\rangle = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2} \end{pmatrix} \quad \langle\psi|\psi\rangle = \sum_i \langle\psi|i\rangle\langle i|\psi\rangle = \sum_i \langle i|\psi\rangle^* \langle i|\psi\rangle = \begin{pmatrix} 1/2 & 1/2 & 1/\sqrt{2} \end{pmatrix}\begin{pmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2} \end{pmatrix} = 1$$

$$L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad L_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Rightarrow$$ experimental values are $\{0, 1\}$
degeneracy = 2 means 2 eigen~~values~~ vectors have same eigenvalue

$$|\psi\rangle = \sum_i |i\rangle \underbrace{\langle i|\psi\rangle}_{\text{scalar product of } \psi \text{ with eigen bra vector}}$$

$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ in this basis of L_z^2 these are the eigenvectors

$$\langle 1|\psi\rangle = (1\ 0\ 0)\begin{pmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2} \end{pmatrix} = 1/2 \quad \langle 2|\psi\rangle = (0\ 1\ 0)\begin{pmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2} \end{pmatrix} = 1/2 \quad \langle 3|\psi\rangle = (0\ 0\ 1)\begin{pmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2} \end{pmatrix} = 1/\sqrt{2}$$

$$|\psi\rangle = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2} \end{pmatrix} = 1/2\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + 1/2\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + 1/\sqrt{2}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

normalization constant within a phase factor

for $L_z^2 = 1$ $\quad |\psi'(L_z^2 = 1)\rangle = \left[1/2\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\right]\alpha = \frac{2}{\sqrt{3}}\left[1/2\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + 1/\sqrt{2}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\right]$

$P(1) = 1/3 \quad P(-1) = 2/3$

Read pg 141: Measurement → disturbance → state
Can prepare a system in a different state
Can only normalize overall phase factor

$$|\psi\rangle = \frac{e^{i\delta_1}}{2}|L_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}}|L_z = 0\rangle + \frac{e^{i\delta_3}}{3}|L_z = -1\rangle = e^{i\delta_1}\left(\frac{1}{2}|1\rangle + \frac{e^{i(\delta_2-\delta_1)}}{\sqrt{2}}|2\rangle + \frac{e^{i(\delta_3-\delta_1)}}{2}|3\rangle\right)$$

relative phase factors are important

Non-Relativistic Approximation

basis: $\langle x_1 x_2 \ldots x_N|P_i|\psi\rangle = -i\hbar\frac{\partial}{\partial x_i}\langle x_1 x_2 \ldots x_N|\psi\rangle = -i\hbar\frac{\partial}{\partial x_i}\psi(x_1 x_2 \ldots x_N)$

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x,y,z) \qquad i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$$

$$i\hbar\frac{\partial}{\partial t}|\psi(x,y,z,t)\rangle = \left(\frac{p_x^2 + p_y^2 + p_z^2}{2m}\right)|\psi(x,y,z,t)\rangle + V(x,y,z)|\psi(x,y,z,t)\rangle$$

take the scalar product:

$$i\hbar\frac{\partial}{\partial t}\underbrace{\langle x,y,z}_{\text{eigenvalues}}|\psi(t)\rangle = \frac{1}{2m}\langle x\,y\,z|p_x^2 + p_y^2 + p_z^2|\psi\rangle + \langle xyz|V(x,y,z)|\psi\rangle$$

Show that: $\langle xyz|P_x^2|\psi(t)\rangle = -\frac{\hbar^2\partial^2}{\partial x^2}\psi(x,y,z,t) \longrightarrow$

coordinate representation of time-dependent Schrodinger equation:

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

momentum representation:

$$\langle p_x\, p_y\, p_z | \Psi\rangle = \phi(p_x, p_y, p_z) \qquad X \to i\hbar\frac{\partial}{\partial x}$$

$$i\hbar \frac{\partial \phi(p_x,p_y,p_z,t)}{\partial t} = \frac{p_x^2 + p_y^2 + p_z^2}{2m}\phi(p_x,p_y,p_z,t) + V\left(i\hbar\frac{\partial}{\partial p_x}, i\hbar\frac{\partial}{\partial p_y}, i\hbar\frac{\partial}{\partial p_z}\right)\phi(p_x,p_y,p_z,t)$$

Ⓐ $V = \frac{1}{2}m\omega^2(X^2+Y^2+Z^2) \longrightarrow X \to i\hbar\frac{\partial}{\partial x} \longrightarrow -\frac{\hbar^2}{2}m\omega^2\left(\frac{\partial^2}{\partial p_x^2} + \frac{\partial^2}{\partial p_y^2} + \frac{\partial^2}{\partial p_z^2}\right)$ in momentum basis

$$\langle p_x, p_y, p_z | X | \Psi\rangle = i\hbar\frac{\partial}{\partial p_x}\phi(p_x,p_y,p_z,t)$$

Ⓑ $V(x) = \frac{1}{\cosh^2(x)}$ how do you write this in the momentum representation?

1) Do a taylor's expansion
2) $X \to i\hbar\frac{\partial}{\partial p}$

Ⓒ $H = \frac{p_x^2}{2m} - fx \Rightarrow$ x-basis: $i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) - fx\Psi(x,t)$

$P_x|p\rangle = p|p\rangle$ p-basis: $i\hbar\frac{\partial}{\partial t}\phi(p,t) = \frac{p^2}{2m}\phi(p,t) - f\, i\hbar\frac{\partial}{\partial p}\phi(p,t)$

Time Evolution

How do you find the time-evolution of a wavefunction generally?

Any state vector can be expanded by the basis vectors of any observable.

$$|\Psi(t=0)\rangle = \sum_E |E\rangle\underbrace{\langle E|\Psi(t=0)\rangle}_{a_E(0)} \qquad |\Psi(t)\rangle = \sum_E |E\rangle\underbrace{\langle E|\Psi(t)\rangle}_{a_E(t)} = \sum_E a_E(t)|E\rangle$$

assumes non-degenerate eigenstates or you need another coefficient for linear independence

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

$$i\hbar\frac{\partial}{\partial t}\sum a_E(t)|E\rangle = \sum_E a_E(t)\,E\,|E\rangle$$

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time-evolution continued...

$$\sum_E \left(i\hbar \frac{da_E}{dt} - a_E(t)E \right) |E\rangle = 0$$

$$i\hbar \frac{da_E}{dt} = E a_E(t)$$

$$\int \frac{da_E}{a_E} = \frac{E}{i\hbar} \int dt$$

$$\ln a_E = \left(\frac{E}{i\hbar}\right) t + C$$

$$a_E(t) = e^{Et/i\hbar + C} = \alpha e^{-(i/\hbar)Et} \qquad \alpha = a_E(0) = \langle E | \Psi(0) \rangle$$

$$a_E(t) = a_E(0) e^{-(i/\hbar)Et}$$

$$|\Psi(t)\rangle = \sum_E a_E(0) e^{-iEt/\hbar} |E\rangle = \sum_E e^{-iEt/\hbar} |E\rangle\langle E|\Psi(0)\rangle$$

** $\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0$

$$\int \frac{\partial \rho}{\partial t} d^3x + \int \vec{\nabla} \cdot \vec{j} \, d^3x \Rightarrow \frac{\partial}{\partial t} \int \rho \, d^3x = -\oint \vec{j}_m \cdot d\vec{A}$$

very large surface

$j_m \to 0$ faster than $dA \to \infty$ so it vanishes

$$\frac{d}{dt} \int \rho \, d^3x = 0$$

$$\int \rho \, d^3x = \text{constant}$$

assumes that a particle can't be created or destroyed

in general, suppose this is possible

$$|\Psi(t)\rangle = U(t,0)|\Psi(0)\rangle \qquad \text{where } U(t,0) = \sum_E e^{-iEt/\hbar} |E\rangle\langle E|$$

or $U(t,0) = e^{-iHt/\hbar}$

- so long as H is time independent
- this is a power series in $iH/\hbar$
- looks like unitary op $|\Psi(t)\rangle = U(t,0)|\Psi(0)\rangle$

can define $U^\dagger(t,0) = e^{+iHt/\hbar}$ where $U^\dagger(t,0)U(t,0) = I$

$$\langle \Psi(t)|\Psi(t)\rangle = \langle \Psi(0)|U^\dagger(t,0)\,U(t,0)|\Psi(0)\rangle = \langle \Psi(0)|\Psi(0)\rangle$$

time-dependent Schrödinger equation for 3-D particle moving in a potential field

V: real and time-independent: (V can depend on time, but if V is complex, H isn't Hermitian)

$$i\hbar \frac{\partial}{\partial t} \Psi(x,y,z,t) = -\hbar^2/2m \, \nabla^2 \Psi(x,y,z,t) + V(x,y,z)\Psi(x,y,z,t) \Rightarrow i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

$\Psi(x,y,z,t) = \langle xyz|\Psi(t)\rangle$

probability amplitude of finding coord with coord(x,yz)

$$P(x,y,z,t)\,dxdydz = |\langle xyz|\Psi(t)\rangle|^2 dxdydz = |\Psi|^2 dxdydz$$

$\int P(x,y,z,t)\,dx\,dy\,dz = 1$ always

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = -\hbar^2/2m \, \nabla^2 \Psi^* + V\Psi \Rightarrow i\hbar\left(\Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t}\right) = \frac{\hbar^2}{2m}\left[\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*\right]$$

$$\therefore i\hbar \frac{\partial \Psi^* \Psi}{\partial t} = -\frac{\hbar^2}{2m} \vec{\nabla} \cdot \left[\Psi^* \vec{\nabla}\Psi - \Psi \vec{\nabla}\Psi^*\right]$$

$$\vec{J} = \frac{\partial}{\partial t}\Psi^*\Psi = \frac{i\hbar}{2m} \vec{\nabla} \cdot \left[\Psi^* \vec{\nabla}\Psi - \Psi \vec{\nabla}\Psi^*\right] \Rightarrow \vec{j} = -\frac{i\hbar}{2m}\left(\Psi^* \vec{\nabla}\Psi - \Psi \vec{\nabla}\Psi^*\right) \quad \frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot \vec{j}$$

local conservation of charge density **

Chapter 5 Lecture Notes

Free Particle in One Dimension (non-relativistic)

$H = \frac{p_x^2}{2m} \qquad p_x|p\rangle = p|p\rangle \quad \langle p|p'\rangle = \delta(p-p') \quad \int dp\,|p\rangle\langle p| = \mathbb{I}$

$\Rightarrow H|p\rangle = \frac{p_x^2}{2m}|p\rangle = \frac{p_x}{2m}\,p_x|p\rangle = \frac{p_x}{2m}\,p|p\rangle = \frac{p^2}{2m}|p\rangle$ also an eigenstate of the Hamiltonian

two eigenvalues give you the same energy: $+p, -p$

$E^2 = \frac{p^2}{2m} \qquad -\infty < p < \infty$

$$U(t,0) = \sum_E e^{-iEt/\hbar}|E\rangle\langle E| = \int dp\, e^{-ip^2t/2m} \underbrace{|p\rangle\langle p|}_{\text{abstract operator}}$$

but, we really need the matrix element in x-basis:

in x-space U is known as the propagation function: $\langle x|U(t,0)|x'\rangle = U(xt, x'0)$

The definition of the propagation function: $|\psi(t)\rangle \equiv U(t,0)|\psi(0)\rangle$

$$\langle x|\psi(t)\rangle = \langle x|U(t,0)|\psi(0)\rangle$$

use the identity operator to get the complete set $\mathbb{I} = \int dx'|x'\rangle\langle x'|$

Now we can see the usefulness of $U(t,0)$

$\langle x|\psi(t)\rangle = \int \langle x|U(t,0)|x'\rangle\langle x'|\psi(0)\rangle dx'$

$\psi(x,t) = \int dx'\, U(xt, x'0)\,\psi(x',0)$

$$U(xt, x'0) = \langle x|U(t,0)|x'\rangle = \int dp\, e^{-ip^2t/2m\hbar} \underbrace{\langle x|p\rangle}_{\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}} \underbrace{\langle p|x'\rangle}_{\frac{1}{\sqrt{2\pi\hbar}}e^{-ip_x x'/\hbar}} = \frac{1}{2\pi\hbar}\int dp\, e^{-ip^2t/2m\hbar}\, e^{ip(x-x')/\hbar}$$

easy to integrate, complete squares + integrate using $\int e^{-y^2}dy = \sqrt{\pi} \qquad \int e^{-\alpha y^2}dy = \sqrt{\pi/\alpha}$ do as an exercise

$$\boxed{U(xt, x'0) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x')^2/2\hbar t}}$$

Example on p. 153 $\quad \psi(x',0) = \dfrac{e^{ip_0x'/\hbar}\, e^{-x'^2/2\Delta^2}}{(\pi\Delta^2)^{1/4}}$

Show it is normalized $\quad \int \psi^*(x',0)\psi(x',0)\,dx' = 1 = \frac{1}{(\pi\Delta^2)^{1/2}}\int_{-\infty}^{\infty} e^{-x'^2/\Delta^2}dx' = \left(\frac{1}{\pi\Delta^2}\right)^{1/2}\sqrt{\pi}\,\Delta = 1$

Now calculate $\Psi(x,t)$ using this result:

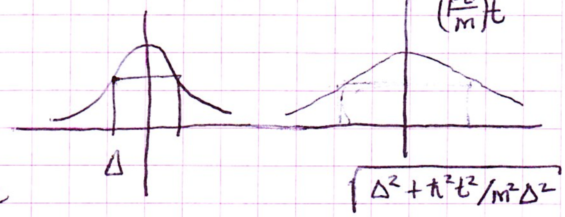
$$\Psi(x,t) = \int dx' \underbrace{\left(\frac{m}{2\pi \hbar i t}\right)^{1/2} e^{im(x-x')^2/2\hbar t}}_{U(xt,x'0)} \frac{e^{ip_0 x'/\hbar}\, e^{-x'^2/2\Delta^2}}{(\pi\Delta^2)^{1/4}}$$

$$\Rightarrow \Psi(x,t) = \pi^{1/2}\left(\Delta + \frac{i\hbar t}{m\Delta}\right)^{-1/2} e^{-(x-p_0 t/m)^2/2\Delta^2(1+\hbar t/m\Delta^2)}$$

Now calculate $\langle p \rangle$ and time evolution of wave packet:

$$\langle \Psi(x',0) | p_x | \Psi'(x',0)\rangle = \int \Psi^*(x,0)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x',0)\,dx' = p_0$$

$$P(x',0) = \Psi^*(x',0)\Psi(x,0) = \frac{e^{-x^2/\Delta^2}}{\sqrt{\pi\Delta^2}}$$



velocity is constant $= \frac{p_0}{m}$ and $x = \left(\frac{p_0}{m}\right)t$

Δ = error of position of object = uncertainty

The increase in width is given by $\left(\frac{\hbar^2 t^2}{m^2\Delta^2}\right) = \frac{(1.055\cdot 10^{-34}\,Js)^2\cdot t^2}{(10^{-6}\,kg^2)(10^{-6}\,m)^2} \approx 10^{-56}\,t^2$ ridiculously small
(luckily $\hbar$ is very small)

General Requirements of Wavefunction

$$\Psi(x,t) = \Psi(x)\,e^{-iEt/\hbar} \quad \text{and} \quad -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi = E\Psi$$

$$\frac{d^2\Psi}{dx^2} = \frac{2m}{\hbar^2}\left[V(x) - E\right]\Psi(x)$$

$$\frac{d\Psi}{dx} = \frac{2m}{\hbar^2}\int\left[V(x) - E\right]\Psi(x)\,dx$$

① Continuous in x: $\Psi = \int \frac{d\Psi}{dx}dx$

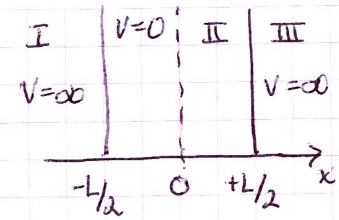
② Finite so long as V is continuous or has finite discontinuity

If V has infinite discontinuity then Ψ is continuous but Ψ' is not continuous.

If V is continuous or has finite discontinuity then Ψ and Ψ' are continuous.

Caveat:
Sometimes $V(x)$ has infinite discontinuity but the discontinuity is finite in the integral, so Ψ is still continuous.

Infinite Well In One-Dimension



with our choice of coordinate system $V(x)=V(-x)$

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

and

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

linear combination is also a solution $\Rightarrow$ $\Psi_e=\frac{\Psi(x)+\Psi(-x)}{2}$

$$\Psi_o=\frac{\Psi(x)-\Psi(-x)}{2}$$

in I, III $\Psi=0$

in II $-L/2\le x\le L/2$ $\quad -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}=E\Psi \Rightarrow \frac{d^2\Psi}{dx^2}+k^2\Psi=0 \quad \left(k^2=\frac{2mE}{\hbar^2}\right)\Rightarrow \Psi_o(x)=\sin kx$, $\Psi_e(x)=\cos kx$

BC's at $-L/2, +L/2$: $\Psi(-L/2)=\Psi(L/2)=0$ continuous

$\cos\left(k\frac{L}{2}\right)=0 \Rightarrow \frac{kL}{2}=(2n+1)\frac{\pi}{2}$ $\quad k=(2n+1)\pi/L \quad n=0,1,2,3,\ldots$

$$E=\frac{\hbar^2k^2}{2m}=(2n+1)^2\frac{\hbar^2\pi^2}{2mL^2}=(1^2,3^2,5^2,\ldots)\frac{\hbar^2\pi^2}{2mL^2}$$

the corresponding eigenfunctions $\Psi_n(x)=A\cos\left[(2n+1)\left(\frac{\pi x}{L}\right)\right]$

$$\int_{-L/2}^{L/2}\Psi_n^*(x)\Psi(x)\,dx=1=|A|^2\int_{-L/2}^{L/2}\cos^2\left[(2n+1)\frac{\pi x}{L}\right]dx=\frac{1}{2}|A|^2\int_{-L/2}^{L/2}\left\{1+\cos\left[(2n+1)\frac{2\pi}{L}x\right]\right\}dx=|A|^2\frac{L}{2}$$

$\therefore$ $A=\sqrt{\frac{2}{L}}$ within a phase factor

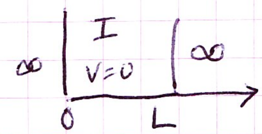
$\therefore$ $\Psi_n(x)=\sqrt{\frac{2}{L}}\cos\left[(2n+1)\frac{\pi x}{L}\right]$ $\quad$ similarly odd functions $\quad \Psi_n(x)=\sqrt{\frac{2}{L}}\sin(kx)$ $\quad \frac{kL}{2}=n\pi \quad n=1,2,3,\ldots$

$$k=\frac{2n\pi}{L} \quad E_n=\frac{\hbar^2k^2}{2m}=\frac{2\hbar^2\pi^2n^2}{mL^2}$$

$$\langle p_x\rangle=\int_{-L/2}^{L/2}\Psi_n^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi_n(x)\,dx=0 \qquad \frac{\langle p_x^2\rangle_n}{2m}=E_n \qquad (\Delta p_x)^2=\langle p_x^2\rangle-\langle p_x\rangle^2\sim\frac{\hbar^2}{L}$$

$\langle p_x^2\rangle/2m\sim\hbar^2/2mL^2$ not zero for this problem.

A better choice of coordinate system:



$\Psi=A\cos(kx)+B\sin(kx)$

$\Psi(x=0)=0=\Psi(x=L)$ $\therefore A=0$ $\quad B\sin(kL)=0\Rightarrow kL=n\pi\Rightarrow k=\left(\frac{n\pi}{L}\right)$ $n=1,2,3\ldots$

$E\neq0$ at ground state $\quad k^2=\frac{2mE}{\hbar^2}\Rightarrow E=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2\pi^2n^2}{2mL^2}$

$\sin(\theta)=-\sin(-\theta)$

$\therefore n>0$

$n=0\Rightarrow\Psi=0$ everywhere

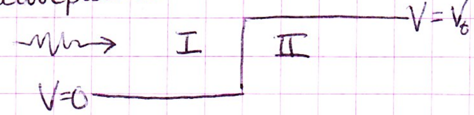
non-degenerate and all real

$$\Psi_n=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

Single Step Potential

Can solve it exactly!

wavepacket incident from the left



the center of a wave packet moves classically
the packet spreads as it moves
in extreme limit it becomes a plane wave.

I.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = E\psi_I$$

$$\psi_I'' + k^2\psi_I = 0$$

$$k^2 = \frac{2mE}{\hbar^2} \qquad \psi_I = Ae^{ikx} + Be^{-ikx}$$

~~trans~~ incident goes $+x$ — reflected goes $-x$

II.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} + V_0\psi_{II} = E\psi_{II}$$

$$\psi_{II}' + k'^2\psi_{II} = 0$$

$$k'^2 = \frac{2m}{\hbar^2}(E - V_0) \qquad \psi_{II} = Ce^{ik'x} + \cancel{De^{-ik'x}} \rightarrow 0$$

transmitted $+x$ — $-x$

Reflection and Transmission Coefficients

$$\vec{j} = \left(\frac{\hbar}{2mi}\right)(\psi^*\nabla\psi - \psi\nabla\psi^*) \qquad R = \frac{J_I^{ref}}{J_I^{inc}} \qquad T = \frac{J_{II}^{trans}}{J_I^{inc}}$$

probability current density

$$\vec{j}^{inc} = \frac{\hbar}{2mi}\left[A^*e^{-ikx}ikAe^{ikx} - Ae^{ikx}A^*(-ik)e^{-ikx}\right] = \frac{\hbar k}{m}|A|^2$$

$$j^{ref} = \frac{\hbar}{2mi}\left[B^*e^{ikx}(-ik)Be^{-ikx} - Be^{-ikx}(ik)B^*e^{ikx}\right] = +\frac{\hbar k}{m}|B|^2$$

$$j^{tran} = \frac{\hbar}{2mi}\left[C^*e^{-ik'x}C(ik')e^{ik'x} - Ce^{ik'x}(-ik')C^*e^{-ik'x}\right] = \frac{\hbar k'}{m}|C|^2$$

$$R = \frac{j^{ref}}{j^{inc}} = \frac{|B|^2}{|A|^2} \qquad T = \frac{j^{trans}}{j^{inc}} = \frac{k'|C|^2}{k|A|^2}$$

Boundary Conditions determine A, B, C $\quad \psi_I(\text{step}) = \psi_{II}(\text{step}) \quad \psi_I'(\text{step}) = \psi_{II}'(\text{step})$

$$\begin{aligned} A + B &= C \\ ik(A - B) &= ik'C \end{aligned} \Rightarrow \frac{ik(A-B)}{A} = \frac{ik'(A+B)}{A} \Rightarrow \frac{B}{A} = \frac{k-k'}{k+k'}$$

$$A + \left(\frac{k-k'}{k+k'}\right)A = C \Rightarrow \frac{C}{A} = \frac{2k}{k+k'}$$

$$\therefore \quad T = \frac{4k^2}{(k+k')^2}\frac{k'}{k} = \frac{4kk'}{(k+k')^2}$$

Theorem I: In 1-D Bound states, all bound states are non-degenerate we can chose them to be real.

Proof: Consider Finite Potential Well, it has two solutions ψ_1 and ψ_2 for same eigenvalue E: (degenerate)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + V\psi_1 = E\psi_1 \quad \text{and} \quad -\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V\psi_2 = E\psi_2$$

multiply the 1ST by ψ_2 and 2ND by ψ_1, then take the difference:

$$-\frac{\hbar^2}{2m}\left[\psi_2\psi_1'' - \psi_1\psi_2''\right] = 0$$

$$\frac{d}{dx}\left[\psi_2\psi_1' - \psi_1\psi_2'\right] = 0$$

$$\frac{d\psi}{\cancel{\psi_1}} \quad \psi_2\psi_1' - \psi_1\psi_2' = \text{constant} = 0$$ since $\psi_1, \psi_2 \to 0$ as $x \to \infty$ and it has to be true everywhere

$$\frac{d\psi_1}{\psi_1} = \frac{d\psi_2}{\psi_2} \Rightarrow \ln\psi_1 = \ln\psi_2 + C \Rightarrow \psi_1 = e^{cnst}\psi_2 = \bar{C}\psi_2$$

since they are not independent, there is only one state that works in 1-D

But $E = \frac{p^2}{2m}$ $\quad e^{ipx/\hbar} \quad e^{-ipx/\hbar}$ unbound states can be degenerate

Theorem II: A 1-D bound state energy eigenfunction can always be chosen to be real.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x) \qquad -\frac{\hbar^2}{2m}\frac{d^2\psi^*}{dx^2} + V(x)\psi^* = E\psi^*$$

if ψ is a solution then ψ^* is also a solution with the same eigenvalue

$$\psi_r = \frac{\psi + \psi^*}{2} \qquad \psi_i = \frac{\psi - \psi^*}{2i}$$ are also solutions

$\psi_i = C\psi_r$ because they can't be independent

$$\psi = \psi_r + i\psi_i = \psi_r + iC\psi_r = (1 + iC)\psi_r$$

within a phase factor, we can chose the wave function to be real.