## Classical Physics

particle in 1D, $F(x,t)$ }
initial conditions } $\Rightarrow$ position at any $t$

$x(t)$ , $v$, $p$, $T = \frac{1}{2}mv^2$

$$\underbrace{H}_{\text{Hamiltonian}} = \underbrace{T}_{\text{Kinetic energy}} + \underbrace{V}_{\text{potential energy}}$$

## Quantum Mechanics

we have: particle's wavefunction $\Psi$

$\Psi(x,t)$

Schrödinger eq.

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

operator

$$\hat{H}\Psi = \hat{T}\Psi + \hat{V}\Psi$$

$$\hat{H} \rightarrow i\hbar\frac{\partial}{\partial t} \qquad \hat{T} \rightarrow \frac{\hat{p}^2}{2m} = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

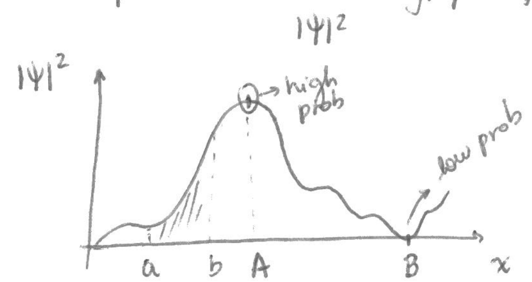
particle $\rightarrow$ localized in space } how to reconcile the two?
$\Psi(x,t) \rightarrow$ spread }
↳ represents the state of particle

### Born's statistical interpretation of $\Psi$

$|\Psi(x,t)|^2$ – prob. of finding particle at point $x$ at time $t$

$\int_a^b |\Psi(x,t)|^2 dx$ { prob. of finding particle between $a$ and $b$ at $t$

prob – area under graph of $|\Psi|^2$




$\Psi$ is complex

QM is intrinsically probabilistic

can't predict with certainty the outcome of experiments

disturbing to { physicists / philosophers } (Einstein: God does not play dice)

measurement problem

after measurement particle is at C

where was right before?

⇒ realist (Einstein) { particle was at C

QM is incomplete

$\Psi$ is not the whole story, additional information (hidden variables) }

But Bell's inequality rules out local hidden variables interpretations

non-local remain (Bohm)

⇒ orthodox { particle was nowhere

act of measurement forces it to take a stand

Copenhagen interpretation (Bohr) }

⇒ agnostic { refuses to answer

can't ask before measuring → metaphysics }

Orthodox

after measurement → $\Psi$ collapses ⇒ { repeated measurements

particle always at C }

Parenthesis . . .

## Probability – discrete variables

$N(14) = 1$ $\longrightarrow \sum_{j=0}^{\infty} N(j) = N = 14$

$N(15) = 1$

$N(16) = 3$ $\longrightarrow P(j) = \dfrac{N(j)}{N}$ $\begin{cases} P(15) = 1/14 \\ P(16) = 3/14 \end{cases}$

$N(22) = 2$

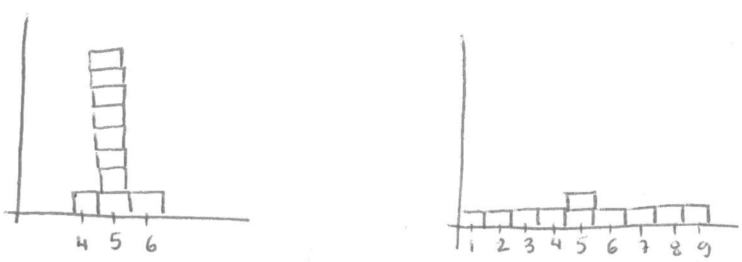
$N(24) = 2$

$N(25) = 5$ $\longrightarrow \sum_{j=0}^{\infty} P(j) = 1$

$$\langle j \rangle = \frac{\sum_{j=0}^{\infty} j\, N(j)}{N} = \sum_{j=0}^{\infty} P(j)\, j$$

$$\langle j^2 \rangle = \sum_{j=0}^{\infty} j^2 P(j)$$

$$\langle f(j) \rangle = \sum_{j=0}^{\infty} f(j)\, P(j)$$



$N = 10$

$\langle j \rangle = 5$

different distributions

$$\Delta j = j - \langle j \rangle \Rightarrow \langle \Delta j \rangle = \sum (j - \langle j \rangle) P(j) = \underbrace{\sum j P(j)}_{\langle j \rangle} - \langle j \rangle \underbrace{\sum P(j)}_{1} = 0$$

$\langle |\Delta j| \rangle$

chosen $\longrightarrow$ $\langle (\Delta j)^2 \rangle = \sum (j - \langle j \rangle)^2 P(j) = \sum j^2 P(j) - 2\langle j \rangle \underbrace{\sum j P(j)}_{\langle j \rangle} - \langle j \rangle^2 \sum P(j) = \langle j^2 \rangle - \langle j \rangle^2$

$\langle (\Delta j)^4 \rangle$

$\Rightarrow$ VARIANCE $\quad \sigma^2 \equiv \langle (\Delta j)^2 \rangle = \langle j^2 \rangle - \langle j \rangle^2$

$\Rightarrow$ STANDARD DEVIATION $\quad \sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}$

continuous variables - classical phys.

infinitesimal intervals $\rho(x)$: probability density

$$P_{ab} = \int_a^b \rho(x)\, dx$$ prob. that variable lies between a and b

$\rho(x)\, dx$ prob. to lie between $x$ and $x + dx$

$$\int_{-\infty}^{\infty} \rho(x)\, dx = 1 \qquad \langle x \rangle = \int_{-\infty}^{\infty} \rho(x)\, x\, dx$$

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)\, \rho(x)\, dx$$

$$\sigma^2 \equiv \langle x^2 \rangle - \langle x \rangle^2$$

back to QM ...

$|\Psi(x,t)|^2$ - prob. density

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx = 1 \longrightarrow$$ normalization condition

$\Psi$ normalized at $t = 0$, $\Psi$ remains normalized at any $t$

$$\underbrace{\frac{d}{dt}}_{\text{total derivative}} \int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx = 0$$

$$\underbrace{\frac{d}{dt}}_{\text{total derivative}}\int_{-\infty}^{\infty}|\Psi(x,t)|^2\,dx = \int_{-\infty}^{\infty}\underbrace{\frac{\partial}{\partial t}}_{\text{partial derivative}}\underbrace{|\Psi(x,t)|^2}_{\Psi^*\Psi}\,dx = \int_{-\infty}^{\infty}\left(\frac{\partial\Psi^*}{\partial t}\Psi + \Psi^*\frac{\partial\Psi}{\partial t}\right)dx =$$

$$\left.\begin{cases} i\hbar\dfrac{\partial\Psi}{\partial t} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\Psi}{\partial x^2} + V\Psi \longrightarrow \dfrac{\partial\Psi}{\partial t} = \dfrac{i\hbar}{2m}\dfrac{\partial^2\Psi}{\partial x^2} - i\dfrac{V}{\hbar}\Psi \\ -i\hbar\dfrac{\partial\Psi^*}{\partial t} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\Psi^*}{\partial x^2} + V\Psi^* \longrightarrow \dfrac{\partial\Psi^*}{\partial t} = -\dfrac{i\hbar}{2m}\dfrac{\partial^2\Psi^*}{\partial x^2} + i\dfrac{V}{\hbar}\Psi^* \end{cases}\right\}$$ REAL potential

$$= \int_{-\infty}^{\infty}\left[\left(-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \cancel{\frac{iV}{\hbar}\Psi^*}\right)\Psi + \Psi^*\left(\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \cancel{\frac{iV}{\hbar}\Psi}\right)\right]dx$$

$$= \int_{-\infty}^{\infty}\frac{i\hbar}{2m}\underbrace{\left(-\frac{\partial^2\Psi^*}{\partial x^2}\Psi + \Psi^*\frac{\partial^2\Psi}{\partial x^2}\right)}_{\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)}dx = \frac{i\hbar}{2m}\left(\underbrace{\Psi^*\frac{\partial\Psi}{\partial x}\Big|_{-\infty}^{\infty}}_{0} - \underbrace{\frac{\partial\Psi^*}{\partial x}\Psi\Big|_{-\infty}^{\infty}}_{0}\right) = \boxed{0}$$

$$\underbrace{\Psi(\pm\infty,t),\ \Psi^*(\pm\infty,t) \to 0}_{\text{otherwise we couldn't guarantee that } \int_{-\infty}^{\infty}|\Psi|^2dx = 1}$$

## Problem 1.14

$$\frac{dP_{ab}}{dt} = J(a,t) - J(b,t) \qquad P_{ab} = \int_a^b |\Psi(x,t)|^2\,dx$$

probability current $\quad J(x,t) = \dfrac{i\hbar}{2m}\left(\Psi\dfrac{\partial\Psi^*}{\partial x} - \Psi^*\dfrac{\partial\Psi}{\partial x}\right)$

} change in time of the probability in region $a \le x \le b$ is equal to the rate at which probability flows into the region (what enters in a minus what leaves in b)

→ continuity equation (C.E.) $\xrightarrow[\text{with}]{\text{associated}}$ conservation laws

→ conservation of
- mass $\xrightarrow{\text{C.E.}}$ fluid dynamics
- charge $\xrightarrow{\text{C.E.}}$ electromagnetism
- probability $\xrightarrow{\text{C.E.}}$ quantum mechanics

## Problem 1.15

unstable particle - decays
$\tau$ - lifetime
$P(t)$ - not constant $\Longrightarrow$ $\boxed{V = V_0 - i\Gamma}$ ← REAL and IMAGINARY parts

$V(x,t)$ is real only when there is conservation of probability

Show that

$$\frac{dP}{dt} = -\frac{2\Gamma}{\hbar} P$$

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx = \int \left( \frac{\partial \Psi^*}{\partial t}\Psi + \Psi^* \frac{\partial \Psi}{\partial t} \right) dx =$$

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + (V_0 - i\Gamma)\Psi \longrightarrow \frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V_0 \Psi - \frac{\Gamma}{\hbar}\Psi$$

$$\longrightarrow \frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V_0 \Psi^* - \frac{\Gamma}{\hbar}\Psi^*$$

$$= \int_{-\infty}^{\infty} \Bigg( \underbrace{-\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2}\Psi + \cancel{\frac{i}{\hbar} V_0 \Psi^*\Psi} - \frac{\Gamma}{\hbar}\Psi^*\Psi + \frac{i\hbar}{2m}}_{\frac{\partial}{\partial x}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \cancel{\frac{i}{\hbar} V_0 \Psi^*\Psi} - \frac{\Gamma}{\hbar}\Psi^*\Psi \Bigg) dx$$

$$= \frac{i\hbar}{2m}\cancel{\left( \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi \right)\Bigg|_{-\infty}^{\infty}} - \frac{2\Gamma}{\hbar}\int |\Psi|^2\, dx = -\frac{2\Gamma}{\hbar} P$$

$$\frac{dP}{dt} = -\frac{2\Gamma}{\hbar} P \Longrightarrow \boxed{P(t) = e^{-2\Gamma t/\hbar} P(0)} \rightarrow \boxed{P(t) = e^{-t/\tau} P(0)}$$

lifetime: $\boxed{\tau = \hbar / 2\Gamma}$

HW

| to do | to know | in class |
|---|---|---|
| 1.4 | 1.9 | 1.15 |
| 1.5 | 1.17 | |
| 1.7 | | |
| 1.14 | | |
| 1.18 | | |

## Expectation Values

$$\langle x\rangle = \int_{-\infty}^{\infty} x\,|\Psi(x,t)|^2\,dx$$

ensemble of particles all prepared in the same initial state

$\langle x\rangle \to$ average of measured results

$\hookrightarrow$ expectation value of $x$

after measurement, $\Psi$ collapses $\to$ get always the same result

integration by parts

$$\int_a^b f\frac{dg}{dx}\,dx = fg\Big|_a^b - \int_a^b \frac{df}{dx}g\,dx$$

$$\int_a^b \frac{df}{dx}g\,dx = fg\Big|_a^b - \int_a^b f\frac{dg}{dx}\,dx$$

$$\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{\infty} x\frac{\partial}{\partial t}|\Psi(x,t)|^2\,dx = \int_{-\infty}^{\infty} x\left(\frac{\partial\Psi^*}{\partial t}\Psi + \Psi^*\frac{\partial\Psi}{\partial t}\right)dx =$$

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \longrightarrow \frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{iV}{\hbar}\Psi$$

$$\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{iV}{\hbar}\Psi^*$$

$V$ is REAL

$$= \int_{-\infty}^{\infty} x\left(-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\Psi + \cancel{\frac{iV}{\hbar}\Psi^*\Psi} + \frac{i\hbar}{2m}\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \cancel{\frac{iV}{\hbar}\Psi^*\Psi}\right)dx = \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)dx$$

$$\underset{\substack{\uparrow\\ \text{integration}\\ \text{by parts}}}{=} \frac{i\hbar}{2m}\left[\cancel{x\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\Big|_{-\infty}^{\infty}} - \int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)dx\right] = -\frac{i\hbar}{2m}\,2\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx$$

by parts

$$\int_{-\infty}^{\infty}\frac{\partial\Psi^*}{\partial x}\Psi\,dx = \cancel{\Psi^*\Psi\Big|_{-\infty}^{\infty}} - \int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx$$

$$\langle v\rangle = \frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{m}\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx \longleftarrow$$ velocity of the expectation value of $v$

NOT the velocity of the particle

expectation value of $v$

prob. density of velocity – later chapter

$\langle p \rangle = m \langle v \rangle$

$$\boxed{\langle x \rangle = \int \Psi^* \overset{\hat{x}}{x} \, \Psi \, dx}$$

sandwich

$$\boxed{\langle p \rangle = \int \Psi^* \underbrace{\frac{\hbar}{i} \frac{\partial}{\partial x}}_{\hat{p}} \Psi \, dx}$$

$$\hat{T} = \frac{\hat{p}^2}{2m} \implies \langle T \rangle = -\frac{\hbar^2}{2m} \int \Psi^* \frac{\partial^2}{\partial x^2} \Psi \, dx$$

$$Q(\hat{x}, \hat{p}) \longrightarrow \langle Q(x,p) \rangle = \int \Psi^* \, Q(\hat{x}, \hat{p}) \, \Psi \, dx$$

Ehrenfest's theorem

expectation values obey classical laws

| class | quant |
|---|---|
| $v = \frac{dx}{dt}$ | $\langle v \rangle = \frac{d\langle x \rangle}{dt}$ |
| $p = m \frac{dx}{dt}$ | $\langle p \rangle = m \frac{d\langle x \rangle}{dt}$ |
| $\underbrace{\frac{dp}{dt}}_{F} = -\frac{\partial V}{\partial x}$ | $\underbrace{\frac{d\langle p \rangle}{dt} = \left\langle -\frac{\partial V}{\partial x} \right\rangle}_{\text{Problem 1.7}}$ |

Problem 1.7

$$\langle p\rangle = \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i}\frac{\partial \psi}{\partial x}\, dx$$

$$\frac{d\langle p\rangle}{dt} = \frac{\hbar}{i}\left[\int \frac{\partial \psi^*}{\partial t}\frac{\partial \psi}{\partial x}\, dx + \int \psi^* \frac{\partial}{\partial x}\frac{\partial \psi}{\partial t}\, dx\right] =$$

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

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

$$= \frac{\hbar}{i}\left[\int_{-\infty}^{\infty}\left(-\frac{i\hbar}{2m}\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial \psi}{\partial x} + \frac{iV}{\hbar}\psi^*\frac{\partial \psi}{\partial x} + \frac{i\hbar}{2m}\psi^*\frac{\partial^3\psi}{\partial x^3} - \frac{i}{\hbar}\psi^*\frac{\partial}{\partial x}(V\psi)\right) dx\right]$$

$$= \frac{\hbar}{i}\frac{i\hbar}{2m}\int\left(\underbrace{\psi^*\frac{\partial^3\psi}{\partial x^3}}_{\text{by parts}} - \frac{\partial^2\psi^*}{\partial x^2}\frac{\partial \psi}{\partial x}\right) dx + \frac{\hbar}{i}\frac{i}{\hbar}\int\underbrace{\left(V\psi^*\frac{\partial \psi}{\partial x} - \psi^*\frac{\partial(V\psi)}{\partial x}\right)}\, dx = -\int_{-\infty}^{\infty}\psi^*\frac{\partial V}{\partial x}\psi\, dx$$

$$\cancel{\psi^*\frac{\partial^2\psi}{\partial x^2}\Big|} - \underbrace{\int \frac{\partial \psi^*}{\partial x}\frac{\partial^2\psi}{\partial x^2}}_{\text{by parts}}$$

$$\cancel{-\frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x}\Big|} + \int \frac{\partial^2\psi^*}{\partial x^2}\frac{\partial \psi}{\partial x}$$

cancel

$$\cancel{V\psi^*\frac{\partial \psi}{\partial x}} - \psi^*\frac{\partial V}{\partial x}\psi - \cancel{\psi^* V\frac{\partial \psi}{\partial x}}$$

$$\frac{d\langle p\rangle}{dt} = \left\langle -\frac{\partial V}{\partial x}\right\rangle$$

## Uncertainty Principle.

in any **wave** → duality phenomenon

$$\begin{cases} \text{know } \lambda, \text{ don't know } x \\ \text{know } x, \text{ don't know } \lambda \end{cases}$$

pulse

↓ also appear in QM

### in QM

$\lambda$ ⟶ $p$

wavelength

de Broglie formula: $\lambda = \frac{h}{p}$ , $p = \frac{h}{\lambda} \to p = \frac{\hbar 2\pi}{\lambda}$

$$\Rightarrow \boxed{\sigma_x \sigma_p \geq \hbar/2}$$ Heisenberg uncertainty principle

### Problem 1.9

important to know

Gaussian integral $\boxed{\int_{-\infty}^{\infty} e^{-Ax^2} dx = \sqrt{\frac{\pi}{A}}}$ $\Rightarrow \begin{cases} \int_{-\infty}^{\infty} \overset{\text{odd}}{x} \, \overset{\text{even}}{e^{-Ax^2}} dx = 0 \\ \int_{-\infty}^{\infty} x^2 e^{-Ax^2} dx = \frac{1}{2A}\sqrt{\frac{\pi}{A}} \end{cases}$

$$= -\frac{d}{dA}\int_{-\infty}^{\infty} e^{-Ax^2} dx = -\frac{d}{dA}\pi^{1/2}A^{-1/2} = \frac{1}{2}\pi^{1/2}A^{-3/2}$$

$$= \left(\int_{-\infty}^{\infty} e^{-Ax^2} dx \int_{-\infty}^{\infty} e^{-Ay^2} dy\right)^{1/2} = \left(\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-A(x^2+y^2)} dx\, dy\right)^{1/2} \Rightarrow$$

polar coordinates $\begin{cases} x = r\cos\theta \\ y = r\sin\theta \end{cases}$ $\begin{vmatrix} \partial x/\partial r & \partial x/\partial\theta \\ \partial y/\partial r & \partial y/\partial\theta \end{vmatrix} = \begin{vmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{vmatrix} = r(\cos^2\theta + \sin^2\theta) = r$

$$\Rightarrow \iint dx\, dy\, e^{-A(x^2+y^2)} =$$

$dx\, dy = r\, dr\, d\theta$

$$= \int_0^{2\pi} d\theta \int_0^{\infty} r\, dr\, e^{-Ar^2} = 2\pi \int_0^{\infty} \frac{dq}{2} e^{-Aq} = \pi \int_0^{\infty} e^{-Aq} dq = \pi \left.\frac{e^{-Aq}}{(-A)}\right|_0^{\infty} = \frac{\pi}{A}$$

$q = r^2$

$dq = 2r\, dr$

Chapter 2

# Time - Independent Schrödinger Equation

how to get $\Psi(x,t)$ ? we need to solve

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \qquad \text{for a specified potential}$$

Let us assume V independent of t

↳ method of separation of variables $\left\{ \begin{array}{l} \text{look for solutions of the form} \\ \Psi(x,t) = \psi(x)\varphi(t) \end{array}\right.$

$$\underbrace{\frac{\partial \Psi}{\partial t}}_{\substack{\text{partial} \\ \text{derivative}}} = \psi \underbrace{\frac{d\varphi}{dt}}_{\substack{\text{ordinary} \\ \text{derivative}}} \qquad \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2\psi}{dx^2}\varphi$$

Schröd eq $\quad i\hbar \psi \frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\varphi + V\psi\varphi$

Divide by $\psi\varphi$ $\quad \underbrace{i\hbar \frac{1}{\varphi}\frac{d\varphi}{dt}}_{\substack{\text{function} \\ \text{of } t}} = \underbrace{-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V}_{\substack{\text{function of} \\ x}}$ $\Rightarrow$ both sides have to be a constant E

Separation of variables $\Rightarrow$ partial differential eq. becomes two ordinary differential equations

$$\frac{i\hbar}{\varphi}\frac{d\varphi}{dt} = E \Rightarrow \boxed{\frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi} \Rightarrow \varphi(t) = e^{-iEt/\hbar}$$

(const absorbed into normalization of $\psi$)

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E \Rightarrow \boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi}$$

→ time indep. Schröd. eq.

need V(x) to solve it

Before solving the time $\underline{\text{indep}}$ Schröd eq

let us discuss some properties of the solutions to the time $\underline{\text{dep}}$ Schröd. eq as given by the separation of variables

$$\Psi(x,t) = \psi(x)\,\varphi(t)$$

1.) They are <u>stationary</u> <u>states</u>

$$\Psi(x,t) = \psi(x)\, e^{-iEt/\hbar} \qquad \text{deps on } t$$

but the <u>probability density</u> DOES <u>NOT</u>

$$|\Psi(x,t)|^2 = \Psi^* \Psi = \psi^* e^{-iEt/\hbar}\, \psi\, e^{iEt/\hbar} = |\psi(x)|^2$$

<u>nor</u> does the <u>expectation values</u>

$$\langle Q(x,p)\rangle = \int \Psi^* Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi\, dx = \int \psi^*(x)\, Q\left(x, \frac{\hbar}{i}\frac{d}{dx}\right)\psi(x)\, dx$$

$\hookrightarrow$ $\langle x \rangle$ is CONSTANT $\Rightarrow$ $\boxed{\langle p\rangle = 0}$

2.) They have <u>definite</u> <u>total</u> <u>energy</u> $\left\{\begin{array}{l}\text{the variance of } H \text{ is zero, there is no spread} \\ \text{given a } \Psi(x,t) \text{ we get always the same energy}\end{array}\right.$

class phys: total energy is the <u>Hamiltonian</u>

$$H(x,p) = \frac{p^2}{2m} + V(x)$$

quant mech: $\hat{H}$ is an <u>operator</u> $\quad \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

$$\left.\begin{array}{l}\text{time indep} \\ \text{Schröd. eq}\end{array}\right\} \quad \boxed{\hat{H}\psi(x) = \underset{\text{(energy)}}{E}\,\psi(x)} \quad \left\{\begin{array}{l} \langle H\rangle = \int \psi(x)\, \underbrace{\hat{H}\psi(x)}_{E\psi(x)}\, dx = E\int |\psi(x)|^2 dx = E \\ \langle H^2\rangle = \int \psi(x)\, \underbrace{\hat{H}\,(\underbrace{\hat{H}\psi}_{E\hat{\psi}})}_{E^2\hat{\psi}}\, dx = E^2 \int |\psi(x)|^2 dx = E^2 \end{array}\right.$$

$$\Rightarrow \sigma_H^2 = \langle H^2\rangle - \langle H\rangle^2 = \boxed{0}$$

3) General solution is a linear combination of separable solutions

$$\text{time indep Schrod eq} \xrightarrow[\text{to various solutions}]{\text{leads}} \psi_1(x),\ \psi_2(x),\ \psi_3(x) \ldots$$

$$\downarrow \quad \downarrow \quad \downarrow$$

each associated with a seperation const (energy) $E_1 \quad E_2 \quad E_3 \ldots$

For each allowed energy there is a different wave function

$$\Psi_1(x,t) = \psi_1(x)\, e^{-iE_1t/\hbar}$$

$$\Psi_2(x,t) = \psi_2(x)\, e^{-iE_2t/\hbar}$$

$$\vdots$$

Any linear combination is a solution of the time dep Schröd. eq.

General solution:

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_nt/\hbar}}$$

→ the consts $c_n$ are fit according to the initial conditions

RECIPE
STRATEGY

Given $V(x)$ (potential) and $\Psi(x,0)$ (initial condition)

⇒ First: Use time indep. Schröd eq. to find set of solutions $\psi_1(x), \psi_2(x), \ldots$ each associated with energies $E_1, E_2, \ldots$

⇒ Second: Write down the general linear combination to fit $\Psi(x,0)$

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

⇒ Finally: Solution to time dep Schröd. eq. is simply

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_nt/\hbar}$$

CAREFUL (!)

Each separable solution $\Psi_n(x,t) = \psi_n(x)\, e^{-iE_n t/\hbar}$ is a stationary state

so probabilities and expectation values are indep. of time

BUT

the GENERAL solution is NOT a stationary state

$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_n t/\hbar}$ is NOT a stationary state

Example 2.1

$$\Psi(x,0) = c_1 \psi_1(x) + c_2 \psi_2(x)$$ assume $c_n$ and $\psi_n(x) \to$ real

$\hookrightarrow \Psi(x,t) = c_1 \psi_1(x)\, e^{-iE_1 t/\hbar} + c_2 \psi_2(x)\, e^{-iE_2 t/\hbar}$

while $|\Psi_1(x,t)|^2 = |\psi_1(x)|^2$ and $|\Psi_2(x,t)|^2 = |\psi_2(x)|^2$ do not dep on time

we see that

$$|\Psi(x,t)|^2 = \left(c_1 \psi_1(x)\, e^{iE_1 t/\hbar} + c_2 \psi_2(x)\, e^{iE_2 t/\hbar}\right)\left(c_1 \psi_1(x)\, e^{-iE_1 t/\hbar} + c_2 \psi_2(x)\, e^{-iE_2 t/\hbar}\right) =$$

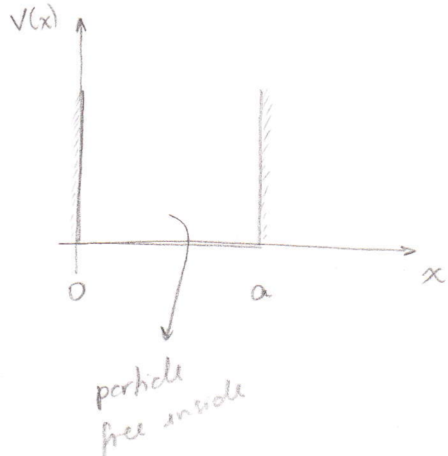
$$= c_1^2 \psi_1^2 + c_1 c_2 \psi_1 \psi_2\, e^{-i(E_2-E_1)t/\hbar} + c_1 c_2 \psi_1 \psi_2\, e^{i(E_2-E_1)t/\hbar} + c_2^2 \psi_2^2$$

$$\boxed{= c_1^2 \psi_1^2 + c_2^2 \psi_2^2 + 2 c_1 c_2 \psi_1 \psi_2 \cos\left[(E_2-E_1)t/\hbar\right]}$$

- prob. density oscillates sinusoidally at an angular frequency $(E_2-E_1)/\hbar$
- it is NOT a stationary state

# Infinite Square Well

$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$




$$\begin{cases} \text{outside}^{\text{well}} & \psi(x) = 0 \quad (\text{zero probability}) \\ \text{inside}^{\text{well}} & V = 0 \end{cases}$$

Inside:

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

$$\frac{d^2\psi}{dx^2} = -\left(\frac{2mE}{\hbar^2}\right)\psi \qquad \frac{2mE}{\hbar^2} \to k^2$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

finding roots $\lambda^2 + k^2 = 0$ → $\lambda_1 = +ik$, $\lambda_2 = -ik$

$$\psi(x) = A\sin kx + B\cos kx$$

to find A and B → boundary conditions

$$\psi(0) = 0 \Rightarrow \boxed{B = 0}$$

$$\psi(a) = 0 \Rightarrow A\sin ka = 0 \Rightarrow ka = 0, \pm\pi, \pm 2\pi, \ldots$$

$k = 0$ → bad choice ⇒ $\psi(x) = 0$

$\oplus$ or $\ominus$ → just a global phase

⇒ $ka = \pi, 2\pi, 3\pi, \ldots$ ⇒ $\boxed{k_n = \frac{n\pi}{a}}$

2-2-02

$$k^2 = \frac{2mE}{\hbar^2} \Rightarrow E_n = \frac{\hbar^2 k_n^2}{2m}$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \boxed{\frac{n^2 \pi^2 \hbar^2}{2ma^2}} \longrightarrow \text{energy is } \underline{\text{quantized}}$$

how about A ?

↳ from normalization

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = 1 \Rightarrow \int_0^a |A|^2 \sin^2(kx)\, dx = 1$$

$$\left( \begin{array}{l} \cos 2x = \cos^2 x - \sin^2 x = 1 - 2\sin^2 x \\ \Rightarrow \sin^2 x = (1 - \cos 2x)/2 \end{array} \right)$$

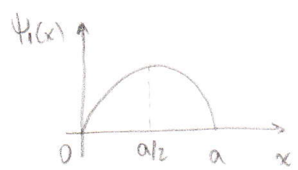
$$|A|^2 \int_0^a \left( \frac{1}{2} - \frac{\cos 2kx}{2} \right) dx = |A|^2 \left( \frac{a}{2} - \cancel{\frac{\sin(2kx)}{2(2k)}\Big|_0^a} \right) = A^2 \frac{a}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

$$\boxed{\Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left( \frac{n\pi}{a} x \right)} \longleftarrow \text{\underline{infinite} set of solutions for the time \underline{indep} Schröd. eq.}$$

$$\left\{ \begin{array}{l} \Psi_1 \to \text{ground state} \\ \Psi_{2,3,\ldots} \to \text{excited states} \end{array} \right.$$

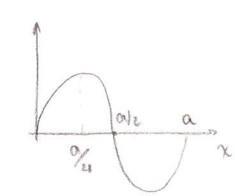
__Properties__

1) They are alternately __even__ and odd with respect to __center__ of well




$\Psi_1(x) = \sqrt{\frac{2}{a}} \sin\left( \frac{\pi x}{a} \right)$

(__even__ with respect to $a/2$)




$\Psi_2(x) = \sqrt{\frac{2}{a}} \sin\left( \frac{2\pi x}{a} \right)$

(__odd__ with respect to $a/2$)

2) Go up in energy $\Rightarrow$ one more <u>node</u>

3.) They are <u>orthonormal</u>

orthogonal + normalized

$$\int \psi_n^* \psi_n \, dx = 1$$

$$\int \psi_m^*(x) \psi_n(x) \, dx = 0 \quad \text{whenever } m \neq n$$

$$\frac{2}{a}\int_0^a \sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right)dx = \frac{2}{a}\int_0 \frac{\left[\cos\left((m-n)\frac{\pi x}{a}\right) - \cos\left((m+n)\frac{\pi x}{a}\right)\right]}{2}dx =$$

$\cos(a+b) = \cos a \cos b - \sin a \sin b$

$\cos(a-b) = \cos a \cos b + \sin a \sin b$

$$= \frac{1}{a}\left\{\frac{\sin[(m-n)\pi x/a]}{(m-n)\pi/a} - \frac{\sin[(m+n)\pi x/a]}{(m+n)\pi/a}\right\}\Bigg|_0^a = \boxed{0}$$

$$\boxed{\int \psi_m^*(x)\psi_n(x)\,dx = \delta_{mn}}$$

<u>Kronecker delta</u>

$$\delta_{mn} \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n \end{cases}$$

4) They are <u>complete</u>

= any function $f(x)$ can be written as a linear combination of them

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a}x\right)$$

<u>Fourier series</u> of $f(x)$

Use orthonormality to find coefficients $c_n$

multiply both sides by $\psi_m^*(x)$ and integrate

$$\int \psi_m^*(x)\, f(x)\, dx = \sum_n c_n \underbrace{\int \psi_m^*(x)\, \psi_n(x)\, dx}_{\delta_{nm}} = \boxed{c_m}$$

$$\boxed{c_n = \int \psi_n^*(x)\, f(x)\, dx}$$

1st property - valid when V is symmetric
2nd - universal
3rd, 4th - very general

⇒) Stationary states of the infinite square well

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$$

⇒) Most general solution

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$$

⇒) $$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a}x\right) \underbrace{\Psi(x,0)}_{\text{initial condition}} dx$$

With $\Psi(x,t)$ can find any dynamical quantity
any observable in time

Example 2.2

Particle in the infinite square well has the initial wave function

$$\Psi(x,0) = Ax(a-x) \qquad 0 \le x \le a$$

Find $\Psi(x,t)$

1st) find A

2nd) find $c_n$, given $\Psi(x,0)$

3rd) find $\Psi(x,t)$

$$\Rightarrow \int_0^a |A|^2 (ax - x^2)^2\, dx = \int_0^a |A|^2 (a^2x^2 - 2ax^3 + x^4)\, dx = |A|^2 \underbrace{\left(a^2 \frac{a^3}{3} - 2a\frac{a^4}{4} + \frac{a^5}{5}\right)}_{a^5 \underbrace{\left(\frac{1}{3} - \frac{1}{2} + \frac{1}{5}\right)}_{\frac{10-15+6}{30} = \frac{1}{30}}} = |A|^2 \frac{a^5}{30}$$

$$\boxed{A = \sqrt{\frac{30}{a^5}}}$$

$$\Rightarrow c_n = \int \psi_n^*(x)\, \Psi(x,0)\, dx = \sqrt{\frac{2}{a}}\sqrt{\frac{30}{a^5}} \int_0^a \sin\left(\frac{n\pi x}{a}\right) x(a-x)\, dx$$

$$= \frac{2\sqrt{15}}{a^3}\left\{ a\int_0^a x \sin\left(\frac{n\pi x}{a}\right) dx - \int_0^a x^2 \sin\left(\frac{n\pi x}{a}\right) dx \right\} = \boxed{\begin{cases} 0 & \text{if } n \text{ is even} \\ \frac{8\sqrt{15}}{n^3\pi^3} & \text{if } n \text{ is odd} \end{cases}}$$

(by parts)

$$\Rightarrow \Psi(x,t) = \sum_{n=1}^{\infty} \frac{8\sqrt{15}}{n^3\pi^3} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-iE_nt/\hbar}$$

$$\boxed{\Psi(x,t) = \sqrt{\frac{30}{a}} \left(\frac{2}{\pi}\right)^3 \sum_{n=1}^{\infty} \frac{1}{n^3} \sin\left(\frac{n\pi x}{a}\right) e^{-in^2\pi^2\hbar t/2ma^2}}$$

For orthonormal solutions $\int \psi_m^*(x)\, \psi_n(x)\, dx = \delta_{mn}$,

we have

① $$\boxed{\sum_{n=1}^{\infty} |c_n|^2 = 1}$$

② $$\boxed{\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n}$$

$\Big\{$ $|c_n|^2$ is the probability of getting $E_n$ when you measure energy

① ↳ follows from normalization

$$\int |\Psi(x,t)|^2 dx = 1 \longrightarrow \boxed{\sum_{n=1}^{\infty} |c_n|^2 = 1}$$

$$\int \left( \sum_{m=1}^{\infty} c_m^* \psi_m^* e^{+iE_m t/\hbar} \right) \left( \sum_{n=1}^{\infty} c_n \psi_n e^{-iE_n t/\hbar} \right) dx$$

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n e^{-i(E_n - E_m)t/\hbar} \underbrace{\int \psi_m^*(x)\, \psi_n(x)\, dx}_{\delta_{mn}} = \sum_{n=1}^{\infty} |c_n|^2$$

② ↳ time indep Schröd eq $\hat{H}\psi = E\psi$

$H\psi_n = E_n \psi_n$

$$\langle H \rangle = \int \Psi^* H \Psi\, dx = \int \left( \sum c_m^* \psi_m^*(x) \right) H \left( \sum c_n \psi_n(x) \right) dx$$

$$= \sum_m \sum_n c_m^* E_n c_n \underbrace{\int \psi_m^* \psi_n\, dx}_{\delta_{mn}} = \sum |c_n|^2 E_n$$

$$\Rightarrow \boxed{\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n}$$

expectation value of $H$ is indep. of time $\Rightarrow$ conservation of energy

# Section 23 . Harmonic Oscillator

- classical harmonic oscillator


Hooke's law

$$F = -kx = m\frac{d^2x}{dt^2}$$

$$m\frac{d^2x}{dt^2} = -kx \Rightarrow \frac{d^2x}{dt^2} = -\omega^2 x \qquad \boxed{\omega = \sqrt{\frac{k}{m}}}$$

solution: (see NOTES)

$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$

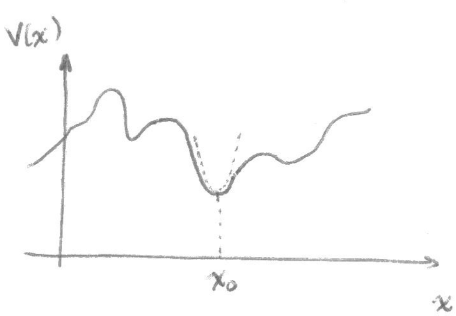
$\omega$ is the angular frequency of oscillations

Potential energy

$$\boxed{V(x) = \frac{1}{2}kx^2} \qquad \text{where } F = -\frac{dV}{dx}$$

is parabolic

- any potential is approximately parabolic in the neighborhood of a local minima




Taylor series about the minimum $x_0$

$$V(x) = V(x_0) + V'(x_0)(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 + \dots$$

$\left\{\begin{array}{l}\text{subtract } V(x_0) \\ V'(x_0) = 0 \quad (x_0 \text{ is minimum}) \\ \text{drop higher orders}\end{array}\right.$

it describes simple harmonic oscillations about $x_0$ with spring constant $V''(x_0) = k$ $\leftarrow$ $\boxed{V(x) \cong \frac{V''(x_0)}{2}(x-x_0)^2}$

- Quantum harmonic oscillator

$$\boxed{V(x) = \frac{1}{2} m \omega^2 x^2}$$

time-independent Schrödinger equation:

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi}$$

two ways to solve it

- power series method ← mathematical Physics course
- algebraic technique – ladder operators

$$\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$$

$$\boxed{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)\, e^{-\xi^2/2}} \longleftrightarrow \boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega}$$

$\boxed{n = 0, 1, 2, \ldots}$ → quantization of energy

Hermite polynomials

$H_0 = 1$

$H_1 = 2\xi$

$H_2 = 4\xi^2 - 2$

$H_3 = 8\xi^3 - 12\xi$

$\vdots$

$E_0 = \frac{\hbar\omega}{2}$ → ground state energy (or zero-point energy)

(NOT zero)

↳ no rest even at absolute zero temperature

Stationary states of the harmonic oscillator are orthonormal

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx = \delta_{mn}$$

⇒ given $\Psi(x,0)$, we can find $c_n$ and therefore $\Psi(x,t)$

•) Use Mathematica ... items a-g

Print plot

$|\psi_n(x)|^2$ and V

$\boxed{QM}$

① energies are quantized

② odd states - prob. at center is zero

③ higher n ⇒ more bumps ⇒ shorter $\lambda$ ⇒ ⇒ higher momentum ⇒ higher energy

•) Classical Harmonic oscillator

$$E = T + V$$

classically allowed region

turning points: $T = 0 \Rightarrow E = V \Rightarrow \frac{1}{2} m\omega^2 x^2 = E \Rightarrow \pm x_0 = \pm\sqrt{\frac{2E}{m\omega^2}}$

amplitude of oscillation: $\sqrt{\frac{2E}{m\omega^2}}$

$\boxed{QM}$

④ prob. for finding the particle outside the classically allowed range is NOT zero (tunneling)

↳ for energy $E_n$

↳ $P = 2\int_{x_0}^{\infty} |\psi_n|^2\, dx$

•) Distribution function for the classical harmonic oscillator

↳ calculated from the time the oscillator spends in ≠ regions

$dt = \frac{dx}{v}$ → $E = T + V \Rightarrow \frac{1}{2} m v^2 = E - \frac{1}{2} m\omega^2 x^2 \Rightarrow v = \pm\sqrt{\frac{2E}{m} - \omega^2 x^2}$

⇓

$\Downarrow$

$$P_{clas} = \frac{Norm}{v}$$

Normalization: $\displaystyle\int_{-x_0}^{x_0} \frac{Norm}{v}\,dx = 1 \Rightarrow Norm = \frac{1}{\int_{-x_0}^{x_0} \frac{dx}{v}}$

$$\boxed{P_{clas} = \frac{v^{-1}}{\int_{-x_0}^{x_0} v^{-1}\,dx}}$$

$$P_{clas} = \frac{\left(2E/m - \omega^2 x^2\right)^{-1/2}}{\int_{-x_0}^{x_0} \left(2E/m - \omega^2 x^2\right)^{-1/2} dx}$$

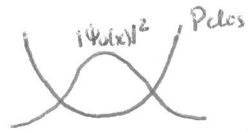
$x_0 \rightarrow$ amplitude $= \sqrt{\frac{2E}{m\omega^2}}$

Use mathematica... (h-k)

⑤ $P_{clas}$ vs. $|\psi_n(x)|^2$

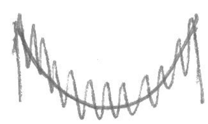
$n=0 \Rightarrow P_{clas}(x) = \dfrac{A_0}{\sqrt{\frac{2E_0}{m} - \omega^2 x^2}}$ vs. $|\psi_0|^2$

n=0




$n=100 \Rightarrow P_{clas}(x) = \dfrac{A_{100}}{\sqrt{\frac{2E_{100}}{m} - \omega^2 x^2}}$ vs. $|\psi_{100}|^2$

$n \to \infty$



$n \to \infty$ : quantum prob. resembles the classical case

Correspondence Principle:

tendency to approach the classical behavior for high quantum numbers

Good site

http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hosc.html

*TOPIC for ORAL PRESENTATION: Zero point energy

(Sc. Am. 1985 pp 70-78)

## ▪ Quantum Harmonic Oscillator

Let us assume:

m=1

ℏ=1

ω=2

and write the stationary states, the energy levels, and the potential for the harmonic oscillator as:

```
m = 1;
ℏ = 1;
ω = 2;
ξ = Sqrt[m ω / ℏ] x;
psi[nn_] := ((m ω) / (Pi ℏ)) ^ (1 / 4) 1 / Sqrt[2 ^ nn nn !] HermiteH[nn, ξ] Exp[-ξ ^ 2 / 2];
En[nn_] := (nn + 1 / 2) ℏ ω;
V = (1 / 2) m ω ^ 2 x ^ 2;
```

a) Verify that the first four stationary states are indeed normalized.

Verify that the first three stationary states are indeed orthogonal.

b) Plot the first four stationary states psi[nn] (use different colours for each plot).

c) Plot the first four probability densities Abs[psi[nn]]^2 (use different colours for each plot).

d) Plot the potential and the first four energy levels all in the same graph.

e) Add to the plot in item (d) the functions En[nn]+psi[nn] for nn=0,1,2,3.

f) Add to the plot in item (d) the functions En[nn]+Abs[psi[nn]]^2 for nn=0,1,2,3.

g) Blow up the graph from item (f) and print it for analysis.

## ▪ Comparison with the Classical Harmonic Oscillator

It is interesting to compare the distribution function for the quantum mechanical harmonic oscillator to the distribution function for a classical harmonic oscillator. For the classical oscillator, the probability distribution function can be calculated from the time the oscillator spends in the various regions. The probability function will be larger in regions where the oscillator spends more time.

h) The classical allowed region for a classical oscillator of energy E extends from -Sqrt[(2E)/(mω^2)] to Sqrt[(2E)/(mω^2)], which are the "classical turning points". The amplitude of the oscillations is then A=Sqrt[(2E)/(mω^2)]. In the ground state of the quantum harmonic oscillator, what is the probability of finding the particle outside the classically allowed region?

i) Evaluate the amplitude of the classical oscillator corresponding to the energy of the first three stationary states of the quantum mechanical harmonic oscillator and note that the amplitude is increasing with energy.

j) What is the velocity v of the classical particle as a function of position (use E=T+V)?
Given that the amount of time the particle spends in an interval *dx* around position *x* is *dx/v*, find the probability function of finding the classical particle on the interval (*-A,A*).
Plot the classical and quantum probability distribution functions for the lowest energy state *n=0*. Why does the classical probability distribution function have sharp maxima at the points of maximum displacement, and the quantum probability does not? Give a qualitative answer.

k) There is a principle of correspondence which states that in the limit of large energy and large objects, the predictions of quantum theory must be the same as predictions from classical dynamics. We know that the macroscopic world of large objects that we can observe is well described by classical dynamics. We say that we reach the 'classical limit' when the energy is large enough that the spacing between the energy levels is insignificant. Show with a plot how the probability distribution of a quantum harmonic oscillator reaches the classical limit as *n* becomes large.

## Algebraic Method

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi = E\psi$$

Let's study the operators:

$$a_+ \equiv \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x) \qquad a_- \equiv \frac{1}{\sqrt{2\hbar m\omega}}(+ip + m\omega x)$$

Motivation: trying to factor the Hamiltonian

$$H = \frac{1}{2m}\left[p^2 + (m\omega x)^2\right]$$

for numbers
$u^2 + v^2 = (iu+v)(-iu+v)$
but operators ~~do~~ may not commute

$$a_+ a_- = \frac{1}{2\hbar m\omega}(-ip + m\omega x)(+ip + m\omega x) =$$

$$= \frac{1}{2\hbar m\omega}\left[p^2 + (m\omega x)^2 + im\omega\underbrace{(xp - px)}\right]$$

commutator of $x$ and $p$

$$\boxed{[A,B] \equiv AB - BA}$$

$xp - px = [x,p]$ → test function

$$[x,p]f(x) = x\frac{\hbar}{i}\frac{df}{dx} - \frac{\hbar}{i}\frac{d}{dx}(xf) = \frac{\hbar}{i}\left(x\cancel{\frac{df}{dx}} - x\cancel{\frac{df}{dx}} - f\right) = \hbar i f$$

↳ $\boxed{[x,p] = i\hbar}$ canonical commutation relation

this result is at the heart of QM

$$a_+ a_- = \frac{1}{\hbar\omega} \underbrace{\frac{1}{2m}\left[p^2 + (m\omega x)^2\right]}_{H} + \frac{i}{2\hbar} \underbrace{[x, p]}_{i\hbar}$$

$$a_+ a_- = \frac{H}{\hbar\omega} - \frac{1}{2}$$

common notation

$$\begin{cases} a_+ = a^\dagger & \text{(a dagger)} \\ a_- = a & \end{cases}$$

$$\boxed{H = \hbar\omega\left(a_+ a_- + \frac{1}{2}\right)}$$

Verify that $\boxed{H = \hbar\omega\left(a_- a_+ - \frac{1}{2}\right)}$ (see book)

Therefore

$$[a_-, a_+] = a_- a_+ - a_+ a_- = \frac{H}{\hbar\omega} + \frac{1}{2} - \frac{H}{\hbar\omega} + \frac{1}{2} = 1$$

$$\boxed{[a_-, a_+] = 1}$$

Let's prove that

given $H\psi = E\psi$

$(a_+\psi)$ and $(a_-\psi)$ are also solutions of the Schröd eq.

with energy $\Downarrow (E + \hbar\omega)$ $\Downarrow (E - \hbar\omega)$

$(a_+ \psi)$

$$H(a_+\psi) = \hbar\omega\left(a_+a_- + \frac{1}{2}\right)(a_+\psi)$$

$$= \hbar\omega\left(a_+a_-a_+ + \frac{1}{2}a_+\right)\psi = a_+\hbar\omega\left(a_-a_+ + \frac{1}{2}\right)\psi$$

$a_-a_+ = a_+a_- + 1$

$$= a_+\hbar\omega\left(a_+a_- + \frac{1}{2} + 1\right)\psi$$

$$= a_+(H + \hbar\omega)\psi = a_+(E+\hbar\omega)\psi = (E+\hbar\omega)(a_+\psi)$$

$$H(a_-\psi) = \hbar\omega\left(a_-a_+ - \frac{1}{2}\right)(a_-\psi)$$

$$= \hbar\omega\left(a_-a_+a_- - \frac{1}{2}a_-\right)\psi = a_-\hbar\omega\left(a_+a_- - \frac{1}{2}\right)\psi$$

$a_-a_+ - 1$

$$= a_-\hbar\omega\left(a_-a_+ - \frac{1}{2} - 1\right)\psi$$

$$= a_-(H - \hbar\omega)\psi = a_-(E-\hbar\omega)\psi = (E-\hbar\omega)(a_-\psi)$$

ladder operators $\left\{ \begin{array}{l} a_+ \rightarrow \text{raising operator} \\ a_- \rightarrow \text{lowering operator} \end{array} \right\}$ generate new solutions

Ground state $\psi_0$

$$a_- \psi_0 = 0$$

$$\Rightarrow \frac{1}{\sqrt{2\hbar m\omega}} \underbrace{\left( ip + m\omega x \right)}_{\left( \hbar \frac{d}{dx} + m\omega x \right)} \psi_0 = 0$$

$$\left( \hbar \frac{d}{dx} + m\omega x \right) \psi_0 = 0 \Rightarrow \frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar} x \psi_0$$

$$\int \frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar} \int x\, dx \Rightarrow \ln \psi_0 = -\frac{m\omega x^2}{2\hbar} + \text{const}$$

$$\psi_0 = A e^{-\frac{m\omega x^2}{2\hbar}}$$

normalization $\quad |A|^2 \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar} dx = 1 \Rightarrow |A|^2 \sqrt{\frac{\pi\hbar}{m\omega}} = 1$

$$A = (m\omega/\pi\hbar)^{1/4}$$

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

$$\hbar\omega \left( a_+ \cancel{a_-} + \frac{1}{2} \right) \psi_0 = E_0 \psi_0$$

$$\Rightarrow \boxed{E_0 = \frac{\hbar\omega}{2}}$$

To generate all excited ~~ea~~ states:

$$\boxed{\psi_n(x) = A_n (a_+)^n \psi_0(x)}$$

$A_n$: from normalization

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

energy increases by $\hbar\omega$ at each step

$$\boxed{H\psi_n = E\psi_n} \rightarrow \hbar\omega\left(a_+a_- + \tfrac{1}{2}\right)\psi_n = \hbar\omega\left(n+\tfrac{1}{2}\right)\psi_n$$

$$\Downarrow$$

$$\boxed{a_+a_-\psi_n = n\,\psi_n}$$

## Normalization

$$a_+\psi_n = c_n\psi_{n+1} \qquad\qquad a_-\psi_n = d_n\psi_{n-1}$$

$$\rightarrow \int_{-\infty}^{\infty}\psi_m^*\left(a_\pm\psi_n\right)dx = \int_{-\infty}^{\infty}\left(a_\mp\psi_m\right)^*\psi_n\,dx$$

$a_-$ is the hermitian conjugate of $a_+$

$a_+$ " of $a_-$

$$= \frac{1}{\sqrt{2\hbar m\omega}}\int_{-\infty}^{\infty}\psi_m^*\left(\mp\hbar\frac{d}{dx} + m\omega x\right)\psi_n\,dx$$

$$\int\psi_m^*\frac{d\psi_n}{dx}dx = \cancel{\psi_m^*\psi_n\Big|} - \int\frac{d\psi_m^*}{dx}\psi_n$$

$$= \frac{1}{\sqrt{2\hbar m\omega}}\int_{-\infty}^{\infty}\left(\pm\hbar\frac{d}{dx} + m\omega x\right)\psi_m^*\,\psi_n\,dx = \int_{-\infty}^{\infty}\left(a_\mp\psi_m\right)^*\psi_n\,dx$$

$$\rightarrow \int_{-\infty}^{\infty}(a_+\psi_n)^*(a_+\psi_n)\,dx = \int\left(a_-a_+\psi_n\right)^*\psi_n\,dx \overset{[a_-,a_+]=1}{=} \int\left(a_+a_- + 1\right)\psi_n^*\,\psi_n\,dx$$

$$\underset{a_+a_-\psi_n = n\psi_n}{=} (n+1)\int|\psi_n|^2dx = (n+1)$$

$$|c_n|^2\int|\psi_n|^2dx = |c_n|^2$$

$$|c_n|^2 = n+1 \qquad \boxed{c_n = \sqrt{n+1}}$$

$$\int_{-\infty}^{\infty} (a_- \psi_n)^* (a_- \psi_n)\, dx = \int (a_+ a_- \psi_n)^* \psi_n \, dx = n$$

$$\| \qquad \boxed{d_n = \sqrt{n}}$$

$$|d_n|^2$$

$$\boxed{a_+ \psi_n = \sqrt{n+1}\; \psi_{n+1}} \longrightarrow \psi_{n+1} = \frac{1}{\sqrt{n+1}} a_+ \psi_n \Rightarrow$$

$$= \frac{1}{\sqrt{(n+1)(n)}} (a_+)^2 \psi_{n-1} = \frac{1}{\sqrt{(n+1)n(n-1)}} (a_+)^3 \psi_{n-2} = \dots$$

$$\boxed{a_- \psi_n = \sqrt{n}\; \psi_{n-1}}$$

$$= \frac{1}{\sqrt{(n+1)!}} (a_+)^{n+1} \psi_0$$

$$\Rightarrow \psi_1 = a_+ \psi_0 , \qquad \psi_2 = \frac{1}{\sqrt{2}} a_+ \psi_1 = \frac{1}{\sqrt{2}} (a_+)^2 \psi_0$$

$$\psi_3 = \frac{1}{\sqrt{3}} a_+ \psi_2 = \frac{1}{\sqrt{3.2}} (a_+)^2 \psi_1 = \frac{1}{\sqrt{3.2.1}} (a_+)^3 \psi_0$$

$$\psi_4 = \frac{1}{\sqrt{4.3.2.1}} (a_+)^4 \psi_0 \quad \dots$$

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{n!}} (a_+)^n \psi_0} \longleftrightarrow \boxed{E_n = \left(n + \tfrac{1}{2}\right) \hbar\omega}$$

---

Orthonormality $\int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx = \delta_{mn}$

$$\int_{-\infty}^{\infty} \psi_m^* (a_+ a_-) \psi_n \, dx = n \int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx$$

$$= \int_{-\infty}^{\infty} (a_- \psi_m)^* (a_- \psi_n)\, dx = \int_{-\infty}^{\infty} (a_+ a_- \psi_m)^* \psi_n \, dx = m \int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx$$

unless $m = n$, then $\int \psi_m^* \psi_n \, dx = 0$

(Probls. 2.12 and Example 2.5)

Find $\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$, $\langle p^2 \rangle$, $\langle T \rangle$, and $\langle V \rangle$ for the n-th stationary state

$$a_+ = \frac{1}{\sqrt{2\hbar m\omega}}\left(-ip + m\omega x\right) \qquad a_- = \frac{1}{\sqrt{2\hbar m\omega}}\left(ip + m\omega x\right)$$

$$2m\omega x = \sqrt{2\hbar m\omega}\,(a_+ + a_-)$$

$$\boxed{x = \sqrt{\frac{\hbar}{2m\omega}}\,(a_+ + a_-)}$$

$$\rightarrow \langle x \rangle = \int_{-\infty}^{\infty} \psi_n^* \sqrt{\frac{\hbar}{2m\omega}}\,(a_+ + a_-)\,\psi_n\,dx =$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\int \psi_n^*\psi_{n+1}\,dx + \sqrt{n}\int \psi_n^*\psi_{n-1}\,dx\right) = \boxed{0}$$

$$\rightarrow \langle x^2 \rangle = \frac{\hbar}{2m\omega}\int_{-\infty}^{\infty} \psi_n^*\left(\cancel{(a_+)^2} + a_+a_- + a_-a_+ + \cancel{(a_-)^2}\right)\psi_n\,dx =$$

$a_-\psi_n = \sqrt{n}\,\psi_{n-1}$

$a_+\psi_{n-1} = \sqrt{n}\,\psi_n$

$a_+\psi_n = \sqrt{n+1}\,\psi_{n+1}$

$a_-\psi_{n+1} = \sqrt{n+1}\,\psi_n$

$$= \frac{\hbar}{2m\omega}\left[n\int|\psi_n|^2\,dx + (n+1)\int|\psi_n|^2\,dx\right] =$$

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

$\boxed{2.3\text{-}14}$

$\rightarrow)\ \langle p \rangle = m \frac{d\langle x \rangle}{dt} = \boxed{0}$

$$2ip = \sqrt{2\hbar m w}\,(a_- - a_+)$$

$$\boxed{p = i\sqrt{\frac{\hbar m w}{2}}\,(a_+ - a_-)}$$

$\rightarrow)\ \langle p^2 \rangle = -\frac{\hbar m w}{2} \int \psi_n^* \left(a_+^2 - a_+ a_- - a_- a_+ + a_-^2\right) \psi_n \, dx$

$a_- \psi_n = \sqrt{n}\, \psi_{n-1}$

$a_+ \psi_{n-1} = \sqrt{n}\, \psi_n$

$$= \frac{\hbar m w}{2}(n + n + 1) = \boxed{\left(n + \frac{1}{2}\right) \hbar m w}$$

$\rightarrow)\ \langle T \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{1}{2}\left(n + \frac{1}{2}\right) \hbar w$

$\rightarrow)\ \langle V \rangle = \frac{1}{2} m w^2 \langle x^2 \rangle = \frac{1}{2}\left(n + \frac{1}{2}\right) \hbar w$

$\rightarrow)\ \sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\left(n + \frac{1}{2}\right) \frac{\hbar}{m w}}$ $\qquad \sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\left(n + \frac{1}{2}\right) \hbar m w}$

$$\boxed{\sigma_x \sigma_p = \left(n + \frac{1}{2}\right) \hbar} \geq \frac{\hbar}{2}$$

# Free particle

$V(x) = 0$

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

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \qquad\qquad k = \frac{\sqrt{2mE}}{\hbar}$$

$$E = \frac{\hbar^2 k^2}{2m}$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

$$\psi(x) = A e^{ikx} + B e^{-ikx}$$

$$\Psi(x,t) = A e^{ikx} e^{-iEt/\hbar} + B e^{-ikx} e^{-iEt/\hbar}$$

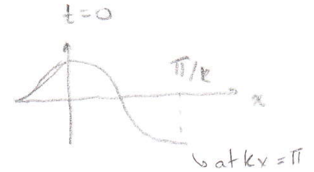
$$= A e^{ikx} e^{-i\hbar k^2 t/2m} + B e^{-ikx} e^{-i\hbar k^2 t/2m}$$

$$= A e^{ik\left(x - \underbrace{\frac{\hbar k}{2m}}_{v_{ph}} t\right)} + B e^{-ik\left(x + \underbrace{\frac{\hbar k}{2m}}_{v_{ph}} t\right)}$$

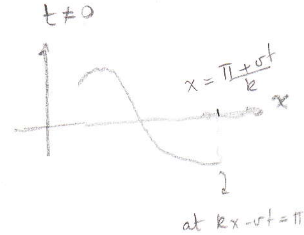
$x \pm v_{ph} t$ → shape does not change

Example $\left\{\begin{array}{l}\text{moving to the right} \\ \cos(kx - vt)\end{array}\right.$

$t = 0$




$t \neq 0$




$A e^{ik(x - v_{ph} t)}$ → wave moving to the right with $v_{ph}$

$B e^{-ik(x + v_{ph} t)}$ → wave moving to the left with $v_{ph}$

$$= A e^{ik\left(x - \frac{\hbar k}{2m} t\right)} \quad \left\{\begin{array}{l} k \oplus \rightarrow \text{left} \\ k \ominus \rightarrow \text{right}\end{array}\right.$$

(plane wave)

$$\boxed{v_{ph} = v_{quantum} = \frac{\hbar k}{2m}}$$ (speed of wave)

**BUT** $$\boxed{v_{clas} = \frac{\hbar k}{m}}$$

$$\Uparrow$$

$$\left.\begin{array}{l} E = \frac{1}{2} m v^2 \\ E = \frac{\hbar^2 k^2}{2m} \end{array}\right\} \quad v = \sqrt{\frac{2E}{m}} = \sqrt{\frac{2\hbar^2 k^2}{2m^2}}$$

→) Free particle cannot exist in a stationary state

→) Each stationary state is NOT physically realizable

↓

is NOT normalizable

$$\int_{-\infty}^{\infty} \Psi_k^* \Psi_k \, dx = |A|^2 \int_{-\infty}^{\infty} dx = |A|^2 \infty \quad (!)$$

→) but stationary states form a complete set

general solution of time dep. Schröd. eq. - linear combination of $\Psi_k(x,t)$

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \, e^{ik\left(x - \frac{\hbar k}{2m} t\right)} \, dk}$$ → WAVE PACKET

↓

$\int$ because $k, p \to$ continuous

$\left(p = \frac{h}{\lambda}, \ k = \frac{2\pi}{\lambda} \Rightarrow p = \hbar k\right)$

$\frac{\phi(k)}{\sqrt{2\pi}} \longleftrightarrow c_n$

$v_{ph} \to$ phase velocity / velocity of each wave

$v_{clas} = v_g \to$ group velocity / velocity of the group of waves / same velocity of the particle

$$v_{ph} = \frac{\omega}{k} \qquad v_g = \frac{d\omega}{dk}$$

Modern Physics example

$$\sin(kx - \omega t) + \sin\big((k+dk)x - (\omega + d\omega)t\big)$$

$$\propto \underbrace{\sin(kx - \omega t)}_{\text{}} \ \underbrace{\cos\left(\frac{dk}{2} x - \frac{d\omega}{2} t\right)}_{\text{envelope}}$$

↳ group velocity

infinite square well

$\Psi(x,0) = \sum c_n \psi_n(x) \Rightarrow \int \psi_m^* \Psi(x,0)\,dx = \sum c_n \underbrace{\int \psi_m^* \psi_n\,dx}_{\delta_{nm}}$

$\delta_{nm}$ → Kronecker delta → discrete

a) To find $\phi(k)$ we need $\Psi(x,0)$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{ikx}\, dk$$

$$\frac{1}{\sqrt{2\pi}} \int e^{-ik'x}\, \Psi(x,0)\, dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, \phi(k) \int_{-\infty}^{\infty} dx\, e^{ix(k-k')}$$

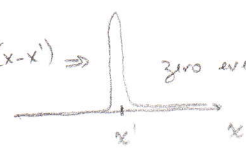
$\delta(k-k')$ ← delta function

continuous analogue of Kronecker delta

delta function

$$\boxed{\begin{aligned} \delta(x-x') &= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{iu(x-x')}\, du \\ f(x') &= \int_{-\infty}^{\infty} \delta(x-x')\, f(x)\, dx \end{aligned}}$$

$\delta(x-x') \Rightarrow$




zero everywhere, except at $x = x'$

$$\int_{-\infty}^{\infty} \delta(x)\, dx = 1$$

$$\int_{x'-\epsilon}^{x'+\epsilon} \delta(x-x')\, f(x)\, dx = f(x')$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik'x}\, \Psi(x,0)\, dx = \int_{-\infty}^{\infty} dk\, \phi(k)\, \delta(k-k') = \phi(k')$$

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

Fourier transform

$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk$ → $f(x)$ is the inverse Fourier transform of $F(k)$

$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx$ → $F(k)$ is the Fourier transform of $f(x)$

Example 2.6 Free particle is initially localized

$$\Psi(x,0) = \begin{cases} A & -a < x < a \\ 0 & \text{otherwise} \end{cases}$$

Find $\Psi(x,t)$ $\left\{ \begin{array}{l} \text{1st) normalization (find A)} \\ \text{2nd) given } \Psi(x,0)\text{, find } \phi(k) \\ \text{3rd) write } \Psi(x,t) \end{array} \right.$

$$|A|^2 \int_{-a}^{a} dx = 1 \implies |A|^2\, 2a = 1 \implies A = \frac{1}{\sqrt{2a}}$$

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

$$= \frac{1}{2\sqrt{a\pi}} \frac{e^{-ika} - e^{+ika}}{(-ik)} = \frac{1}{\sqrt{a\pi}} \frac{1}{k} \frac{\left(e^{ika} - e^{-ika}\right)}{2i} = \frac{1}{\sqrt{\pi a}} \frac{\sin ka}{k}$$

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2a}\,\pi} \int_{-\infty}^{\infty} \frac{\sin ka}{k}\, e^{ik\left(x - \frac{\hbar k}{2m} t\right)}\, dk}$$

can only solve numerically

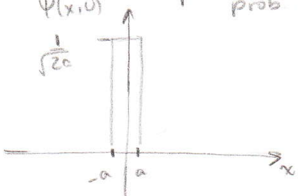
limiting cases

a) a is very small

$$\Psi(x,0) = \frac{1}{\sqrt{2a}}$$

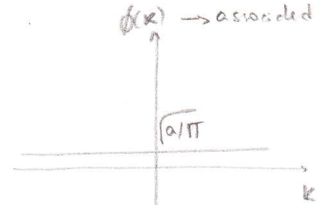
$$\frac{\sin ka}{k} \sim \frac{ka}{k} = a \implies \phi(k)\ \frac{a}{\sqrt{\pi a}} \implies \boxed{\phi(k) = \sqrt{\frac{a}{\pi}}}$$

$\Psi(x,0) \longrightarrow$ associated with prob for position



(peaked)

$\phi(k) \longrightarrow$ associated with prob for momentum



(flat)

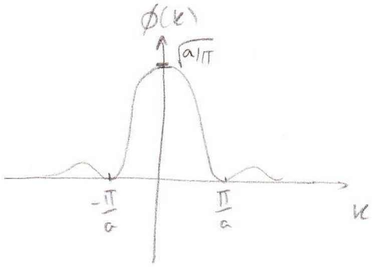
} spread in position is small $\implies$ spread in momentum is large

2.4-5

∘) a is very large

$$\frac{\sin Ka}{Ka} \begin{cases} \text{at } Ka = 0 \rightarrow \text{maximum} \\ \text{at } Ka = \pm\pi \rightarrow \text{zero} \end{cases}$$

$$\phi(K) = \frac{\sin Ka}{Ka}\sqrt{\frac{a}{\pi}}$$



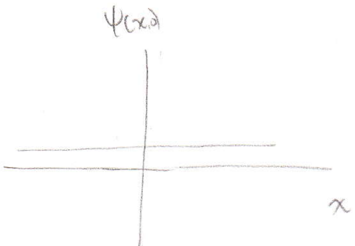

$\rightarrow$) $Ka \sim 0$

$\Downarrow$

$$\boxed{\phi(K) = \sqrt{a/\pi}}$$

$\rightarrow$) $Ka = \pm\pi$

$$\boxed{\phi(K) = 0}$$




$$\psi(x,0) = \frac{1}{\sqrt{2a}}$$

momentum is localized
position is spread

---

$v_{ph}$ may be $\neq$ from $\frac{p}{m}$

$v_{ph} \rightarrow$ phase velocity $\rightarrow$ velocity of $\psi_k$

$\frac{p}{m} \rightarrow$ group velocity $\rightarrow$ velocity of the wave packet

group velocity = to the speed of the particle it represents

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{ik\left(x - \frac{\hbar k}{2m} t\right)}\, dk$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i(kx - \omega t)}\, dk \quad \longrightarrow \quad \boxed{v_{phase} = \frac{\omega}{k}}$$

$$\boxed{\omega = \frac{\hbar k^2}{2m}} \longleftarrow \text{dispersion relation}$$

Assume

$\phi(k)$ peaked around $k_0$

$$\omega(k) \simeq \omega_0 + \omega_0' (k - k_0)$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i(kx - \omega_0 t - \omega_0'(k-k_0)t)}\, dk$$

$k - k_0 = s$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k_0 + s)\, e^{i(k_0 x + s x - \omega_0 t - \omega_0' s t)}\, ds$$

$$= \frac{1}{\sqrt{2\pi}}\, e^{i(-\omega_0 t + k_0 \omega_0' t)} \int \phi(k_0 + s)\, e^{i(k_0 + s)(x - \omega_0' t)}\, ds$$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int \phi(k_0 + s)\, e^{i(k_0 + s)x}\, ds$$

$$\Psi(x,t) = \underbrace{e^{-i(\omega_0 t - k_0 \omega_0' t)}}_{\text{phase factor}}\, \Psi(x - \omega_0' t, 0) \quad \longrightarrow \quad \boxed{v_{group} = \frac{d\omega}{dk}}$$

$$\boxed{v_{phase} = \frac{\omega}{k}}$$

$$\omega = \frac{\hbar k^2}{2m} \Longrightarrow \quad v_{particle} = v_{group} = \frac{\hbar k}{m} = 2\, v_{phase}$$

Prob. 2.22 Free particle with initial wave function
$\Psi(x,0) = A e^{-ax^2}$

a) $\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = 1 \Rightarrow |A|^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = |A|^2 \sqrt{\frac{\pi}{2a}} \Rightarrow A = \left(\frac{2a}{\pi}\right)^{1/4}$

b) Find $\Psi(x,t)$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i(kx - \frac{k^2\hbar}{2m}t)}\, dk$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2}\, e^{-ikx}\, dx$$

complete the square

trying to put in the form $(x^2 + 2Bx + B^2) = (x+B)^2$

$$-ax^2 - ikx = -a\left(x^2 + \frac{2ikx}{2a}\right) = -a\left(x^2 + \frac{2ikx}{2a} - \frac{k^2}{4a^2}\right) - \frac{k^2}{4a}$$

$$= -a\left(x + \frac{ik}{2a}\right)^2 - \frac{k^2}{4a}$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{2a}{\pi}\right)^{1/4} e^{-a(x+ik/2a)^2}\, e^{-k^2/4a}\, dx$$

$s = x + ik/2a$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{2a}{\pi}\right)^{1/4} e^{-as^2}\, e^{-k^2/4a}\, ds = \frac{1}{\sqrt{2\cancel{\pi}}} \left(\frac{2a}{\pi}\right)^{1/4} \sqrt{\frac{\cancel{\pi}}{a}}\, e^{-k^2/4a}$$

$$= \frac{1}{(2a\pi)^{1/4}}\, e^{-k^2/4a}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \frac{1}{(2a\pi)^{1/4}} \int_{-\infty}^{\infty} e^{-k^2/4a} \, e^{i\left(kx - \frac{k^2\hbar}{2m}t\right)} \, dk$$

$$-\left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right) \underbrace{\left[k^2 - \frac{2}{2} \frac{ikx}{\left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right)} - \frac{x^2}{4\left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right)^2}\right]}_{\left(\underbrace{k - \frac{ix}{2\left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right)}}_{s}\right)^2} - \frac{x^2}{4\left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right)}$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{(2a\pi)^{1/4}} \int_{-\infty}^{\infty} e^{-\left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right)s^2} \, e^{-\frac{x^2}{\left(\frac{1}{a} + \frac{i2\hbar t}{m}\right)}} \, ds$$

$$= \underbrace{\frac{1}{\sqrt{2\pi}} \frac{1}{(2a\pi)^{1/4}} \underbrace{\frac{\sqrt{\pi}}{\sqrt{\frac{1}{4a} + \frac{i\hbar t}{2m}}}}_{\frac{2\sqrt{a}}{\sqrt{1 + \frac{2ia\hbar t}{m}}}}}_{\left(\frac{16}{4 \cdot 2}\right)^{1/4} \left(\frac{1}{\pi}\right)^{1/4} \left(\frac{a^2}{a}\right)^{1/4} \frac{1}{\sqrt{1 + \frac{2ia\hbar t}{m}}}} \; \underbrace{e^{-x^2/\left(\frac{1}{a} + \frac{i2\hbar t}{m}\right)}}_{e^{-ax^2/\left(1 + 2i\frac{a\hbar t}{m}\right)}}$$

$$\boxed{= \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{1 + \frac{2ia\hbar t}{m}}} \exp\left(\frac{-ax^2}{1 + \frac{2ia\hbar t}{m}}\right)}$$

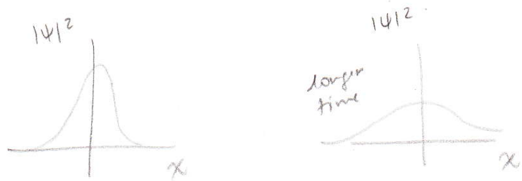
c) $|\Psi(x,t)|^2$

$$= \left(\frac{2a}{\pi}\right)^{1/2} \frac{1}{\sqrt{\left(1+\frac{4a^2\hbar^2t^2}{m^2}\right)}} \; e^{\frac{-ax^2(1+2ia\hbar t/m) - ax^2(1-2ia\hbar t/m)}{(1+4a^2\hbar^2t^2/m^2)}}$$

$$w = \sqrt{\frac{a}{1+(2\hbar a t/m)^2}} \implies 1 + (2\hbar a t/m)^2 = \frac{a}{w^2}$$

$$= \left(\frac{2\cancel{a}}{\pi}\right)^{1/2} \frac{w}{\sqrt{\cancel{a}}} \; e^{-2ax^2\frac{w^2}{a}} = \boxed{\sqrt{\frac{2}{\pi}}\, w\, e^{-2w^2x^2}}$$

$t$ increases $\Rightarrow$ $w$ decreases $\Rightarrow$ $|\Psi|^2$ decreases and broadens



# Delta Function Potential

Up to now: two kinds of solutions to time-indep. Schrö'd. eq.

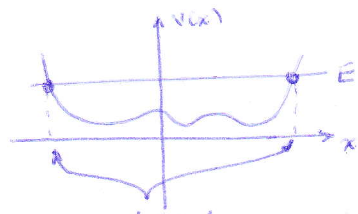
(I) Infinite square well, Harmonic Oscillator } normalizable, labeled by ~~with~~ discrete index n (physically realizable)

(II) Free particle } non-normalizable, labeled by continuous variable k (not physically realizable)

Both cases: general solution to time-dep Schröd. eq. → linear combination of stationary states
↓
(I) sum over n
(II) integral over k

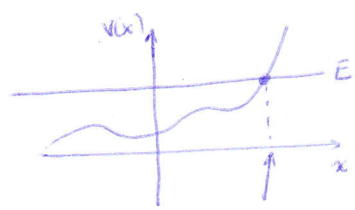
Compare with classical mechanics

if V > E on either side particle is "stuck" in between the turning points
⇒ bound state




classical turning points

if E > V on either side particle comes from infinity, slows down, and returns to infinity
⇒ scattering state




classical turning point

→) Equivalently in quantum mechanics

harm. oscill. and infinite square well } bound state $(E<V)$

free particle } scattering state $(E>V)$

What is surprising here:

- particle can leak through FINITE potential barrier (like in the case of the harm. oscill.)

⇓

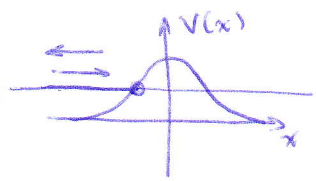
tunneling $(E<V_{(\pm\infty)})$

- particle can scatter even when $E>V(\pm\infty)$

Examples

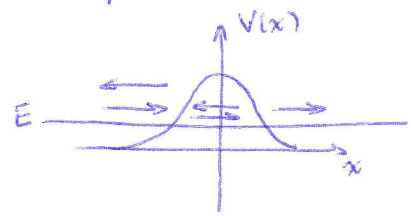
classically

Particle coming from $-\infty$

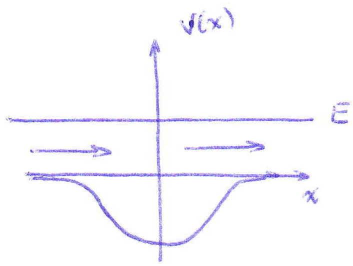



particle is reflected
transmission = 0

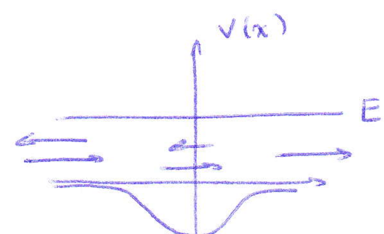
quantum mechanically




there is reflection and transmission (tunneling)




particle is transmitted
reflection = 0




there is reflection and transmission

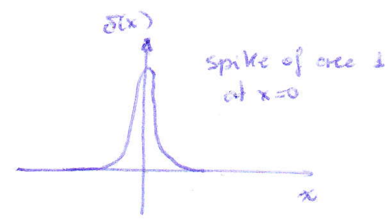
In Q.M. particle can "leak" through finite potential → tunneling

For potentials that go to zero at infinity

$$\begin{cases} E < V(\pm\infty) = 0 \Rightarrow \text{bound state} \\ E > V(\pm\infty) = 0 \Rightarrow \text{scattering state} \end{cases}$$

Dirac delta function

$$\delta(x) \equiv \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases} \xrightarrow{\text{with}} \int_{-\infty}^{\infty} \delta(x)\, dx = 1$$




$$\int_{-\infty}^{\infty} f(x)\,\delta(x-a)\,dx = f(a)$$

↓ picks out the value of f(a) at point a

also → $$\int_{a-\varepsilon}^{a+\varepsilon} f(x)\,\delta(x-a)\,dx = f(a)$$

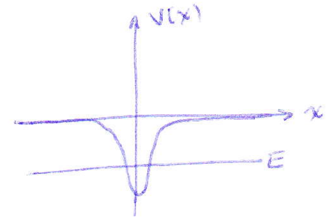
↓ domain of integration includes a

Consider

$$\boxed{V(x) = -\alpha\,\delta(x)} \qquad \alpha > 0$$

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

it yields $\begin{cases} \text{bound states } (E<0) \\ \text{and} \\ \text{scattering states } (E>0) \end{cases}$




Bound states $\boxed{E<0}$

→) $x<0 \Rightarrow V(x)=0$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = (+)K^2\psi$$

$$K = \frac{\sqrt{-2mE}}{\hbar} \qquad E<0 \Rightarrow K\ (+)$$

$$\psi(x) = A e^{-Kx} + B e^{Kx}$$

↓

blows up at $x\to-\infty \Rightarrow A=0$

$$\psi(x) = B e^{Kx} \qquad (x<0)$$

→) $x>0 \Rightarrow V(x)=0$

$$\psi(x) = F e^{-Kx} + G e^{Kx}$$

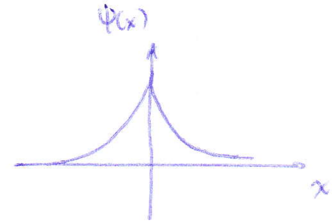
↓ blows up at $x\to+\infty$

$$\psi(x) = F e^{-Kx} \qquad (x>0)$$

How to connect the two solutions using boundary conditions at $x=0$...

1.) $\psi$ is always continuous

$$\psi(x) = \begin{cases} B e^{Kx} & (x \le 0) \\ B e^{-Kx} & (x \ge 0) \end{cases}$$




$K = ?$

Integrate Schröd. eq. around zero (from $-\epsilon$ to $+\epsilon$ with $\epsilon \to 0$)

$$-\frac{\hbar^2}{2m} \int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx^2}\, dx + \int_{-\epsilon}^{\epsilon} V(x)\,\psi(x)\, dx = \underbrace{E \int_{-\epsilon}^{\epsilon} \psi(x)\, dx}_{=0}$$

$$\Downarrow$$

$$\underbrace{\left.\frac{d\psi}{dx}\right|_{+\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon}}_{\lim_{\epsilon \to 0}} = \frac{2m}{\hbar^2} \int_{-\epsilon}^{\epsilon} (-\alpha)\,\delta(x)\,\psi(x)\, dx$$

$$\Downarrow$$

$$\Delta \frac{d\psi}{dx} = -\frac{2m\alpha}{\hbar^2}\,\psi(0)$$

$(x > 0)$ $\quad \frac{d\psi}{dx} = -BK e^{-Kx} \longrightarrow \left.\frac{d\psi}{dx}\right|_{+} = -BK$

$(x < 0)$ $\quad \frac{d\psi}{dx} = BK e^{Kx} \longrightarrow \left.\frac{d\psi}{dx}\right|_{-} = +BK$ $\qquad$ and $\underline{\psi(0) = B}$

$$\Rightarrow -2\cancel{B}K = -\frac{2m\alpha}{\hbar^2}\cancel{B} \quad \Rightarrow \boxed{K = \frac{m\alpha}{\hbar^2}}$$

$$E = -\frac{\hbar^2 K^2}{2m} = \boxed{-\frac{m\alpha^2}{2\hbar^2}}$$ allowed energy

Normalize $\psi$

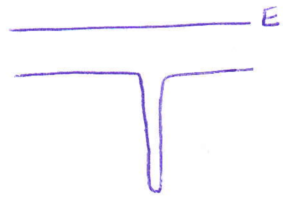
$$\int_{-\infty}^{\infty} |\psi(x)|^2\, dx = 2|B|^2 \int_0^{\infty} e^{-2Kx}\, dx =$$

$$= 2|B|^2 \left.\frac{e^{-2Kx}}{-2K}\right|_0^{\infty} = \frac{2|B|^2}{2K} = 1$$

$$B = \sqrt{K} = \frac{\sqrt{m\alpha}}{\hbar}$$

$$\boxed{\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}\, e^{-\frac{m\alpha|x|}{\hbar^2}} \quad ; \quad E = \frac{-m\alpha^2}{2\hbar^2}}$$

## Scattering States $E > 0$




$x < 0$ $(E > 0)$

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

$x > 0$ $(E > 0)$

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

$$\boxed{k^2 = \frac{2mE}{\hbar^2}} \rightarrow \boxed{E = \frac{\hbar^2 k^2}{2m}}$$

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}$$

continuity of $\psi(x)$ at $x=0$

$$\boxed{A + B = F + G}$$

can't use continuity of $\frac{d\psi}{dx}$ at $x=0$, because at this point V is infinite

so integrate Schröd. eq. from $-\epsilon$ to $\epsilon$ with $\epsilon \to 0$

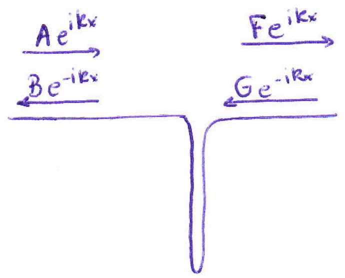
$$-\frac{\hbar^2}{2m}\left(\frac{d\psi}{dx}\bigg|_{\epsilon+} - \frac{d\psi}{dx}\bigg|_{\epsilon-}\right) - \alpha\psi(0) = E\underbrace{(\psi(+\epsilon) - \psi(-\epsilon))}_{0}$$

$$ik(F-G) - ik(A-B) = -\frac{2m\alpha}{\hbar^2}(A+B)$$

$$(F-G) = \underbrace{\frac{2m\alpha}{\hbar^2 k}}_{\beta} i(A+B) + (A-B) \longrightarrow \boxed{F - G = A(1+2i\beta) - B(1-2i\beta)}$$

! 2 equations and 5 unknowns

physically




A : amplitude of a wave coming from the left $(-\infty)$

B : " " returning to $-\infty$

G : " " coming from the right $(+\infty)$

F : " " returning to $+\infty$

particles are fired from one direction

<u>Assume</u> from the left $\Rightarrow$ scattering from the left $\Big\}$ $\boxed{G=0}$

A is the amplitude of the <u>incident</u> wave

B is the amplitude of the <u>reflected</u> wave

F is the amplitude of the <u>transmitted</u> wave

$$\left\{\begin{array}{l} A+B=F \\ F=A(1+2i\beta)-B(1-2i\beta) \end{array}\right\} \Rightarrow B=\frac{i\beta}{1-i\beta}A \quad , \quad F=\frac{1}{1-i\beta}A \qquad *$$

<u>Reflection coefficient</u>

$$R=\frac{|B|^2}{|A|^2}$$

$$\boxed{R=\frac{\beta^2}{1+\beta^2}}$$

prob. that incident particle is reflected back

Transmission coefficient

$$T=\frac{|F|^2}{|A|^2}$$

$$\boxed{T=\frac{1}{1+\beta^2}}$$

prob. that incident particle is transmitted

$$\boxed{R+T=1}$$

$$R = \frac{1}{1 + \frac{2\hbar^2 E}{m\alpha^2}} \qquad T = \frac{1}{1 + \frac{m\alpha^2}{2\hbar^2 E}} \qquad (**)$$

higher energy $\Rightarrow$ greater prob. of transmission (larger T)

smaller energy $\Rightarrow$ greater R

---

(*)

$$\left.\begin{aligned} A + B &= F \\ F &= A(1+2i\beta) - B(1-2i\beta) \end{aligned}\right\} \Rightarrow \cancel{A} - \cancel{A} - A2i\beta + B + B - B2i\beta = 0$$

$$2B(1 - i\beta) = 2i\beta A$$

$$\boxed{B = \frac{i\beta}{1-i\beta} A}$$

$$F = \frac{\cancel{(1-i\beta)}A}{(1-i\beta)} + \frac{\cancel{i\beta} A}{(1-i\beta)} \qquad \boxed{F = \frac{1}{1-i\beta} A}$$

---

(**)

$$\left.\begin{aligned} R &= \frac{\beta^2}{1+\beta^2} \\ \beta &= \frac{m\alpha}{\hbar^2 k} \\ E &= \frac{\hbar^2 k^2}{2m} \\ T &= \frac{1}{1+\beta^2} \end{aligned}\right\}$$

$$\beta = \frac{m\alpha \cancel{\hbar}}{\hbar^{\cancel{2}}\sqrt{2mE}}$$

$$\beta = \frac{\alpha}{\hbar}\sqrt{\frac{m}{2E}}$$

$$R = \frac{\alpha^2}{\cancel{\hbar^2}} \frac{m}{\cancel{2E}} \frac{\cancel{\hbar^2 2E}}{(\hbar^2 2E + m\alpha^2)}$$

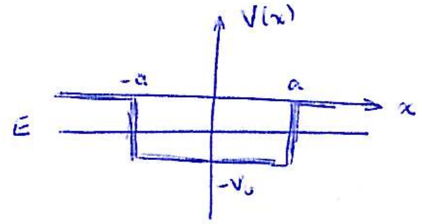
$$\boxed{R = \frac{1}{1 + \frac{2\hbar^2 E}{m\alpha^2}}} \leftarrow R = \frac{1}{(1 + 1/\beta^2)}$$

$$\boxed{T = \frac{1}{1 + \frac{m\alpha^2}{2\hbar^2 E}}}$$

## Finite Square Well

$$V(x) = \begin{cases} -V_0 & -a \le x \le a \\ 0 & |x| > a \end{cases}$$

→ **Bound State** $(E<0)$




classically the particle would be confined in the region $-a<x<a$ but in Q.M. it can be found in $x>a$ or $x<-a$

a) $x<-a$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

$$\boxed{K = \frac{\sqrt{-2mE}}{\hbar}} \longrightarrow K \oplus \text{ and real, since } E \ominus$$

$$\frac{d^2\psi}{dx^2} = K^2\psi$$

$$\psi(x) = Ae^{-Kx} + Be^{Kx}$$

$Ae^{-Kx}$ blows up at $-\infty$ $\Rightarrow A=0$

$\longrightarrow$) $\psi(x) = Be^{Kx}$ for $x<-a$

there is a probability to find the particle at $x<-a$, but it decays as $x$ approaches $-\infty$ (exponentially)

•) $-a < x < a \qquad V(x) = -V_0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \qquad \frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E+V_0)\psi$$

$$l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

$$\frac{d^2\psi}{dx^2} = -l^2\psi$$

$E$ is ⊖ , but $E+V_0$ is ⊕

$\Rightarrow$ $l$ is real and ⊕

$\longrightarrow$) $\psi(x) = C\sin(lx) + D\cos(lx)$ , for $-a < x < a$

•) $x > a$

$$\psi(x) = Fe^{-kx} + \cancel{Ge^{kx}}$$

$G=0$ because $e^{kx}$ blows up at $+\infty$

$\longrightarrow$ $\psi(x) = Fe^{-kx}$ , for $x > a$

•) To find $\cancel{A}, \underbrace{B, C, D, F}, \cancel{G}$ we use the boundary conditions

$\psi(x)$ and $\frac{d\psi}{dx}$ } are continuous at $-a$ and $+a$

**NOTE ①** — Conditions on the wave function: (Remember $|\Psi(x,t)|^2$ is the prob. density)

1.) It must be twice differentiable (⇒ Schröd. eq.)

⇓

$\psi(x)$ and $\frac{d\psi}{dx}$ must be continuous

$\frac{d\psi}{dx}$ → continuous except at points where the potential is infinite

2.) To be normalizable, it must approach zero as $x$ approaches infinity

**NOTE ②**

Here $V(x)$ is an even function

$$\boxed{V(x) = V(-x)}$$

⇓

solutions are either

even $\quad \psi(x) = \psi(-x)$

or

odd $\quad \psi(x) = -\psi(-x)$

Proof: $\psi(x)$ is a solution, ~~change~~

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

·) change $x \to -x$, we know that $V(x) = V(-x)$, for even $\psi(x)$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} + V(-x)\psi(-x) = E\psi(-x) \Rightarrow \psi(-x) \text{ is also a solution}$$

·) change $x \to -x$, $V(x) = V(-x)$, for odd $\psi(x)$

$$+\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} - V(-x)\psi(-x) = -E\psi(-x) \Rightarrow \psi(-x) \text{ is also a solution}$$

Since $V(x) = V(-x)$ <u>even</u>

we can study just one side, for example $x \geq a$
and use

$$\psi(-x) = \pm \psi(x)$$

*) let us start with the <u>even</u> solution

$$\psi(x) = \psi(-x)$$

keep the <u>cos</u>

$$\psi(x) = \begin{cases} F e^{-Kx} & x > a \\ D \cos(lx) & 0 < x < a \\ \psi(-x) & x < 0 \end{cases}$$

continuity at $x = a$

$$\begin{array}{lcl} \psi(x) \text{ at } x=a & \longrightarrow & F e^{-Ka} = D \cos(la) \\ d\psi/dx \text{ at } x=a & \longrightarrow & -K F e^{-Ka} = -l D \sin(la) \end{array}$$

$\div$ both $\Rightarrow$ $K = l \tan(la)$

$$\tan(la) = \frac{K}{l}$$

$\tan(la) = \frac{K}{l}$  $K = \frac{\sqrt{-2mE}}{\hbar}$  $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

introduce

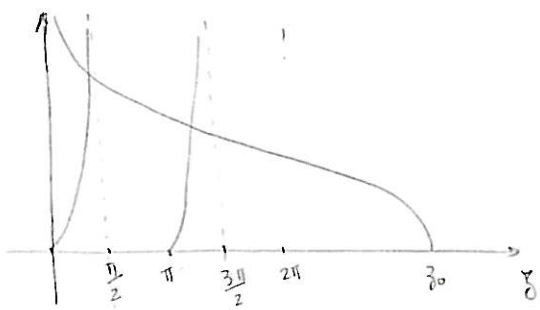
$z_0 = \frac{\sqrt{2mV_0}}{\hbar} a$ and $z = la$

$\tan(z) = \frac{Ka}{la}$  $Ka = \sqrt{z_0^2 - l^2a^2} = \sqrt{z_0^2 - z^2}$

$$\boxed{\tan(z) = \sqrt{(z_0/z)^2 - 1}}$$

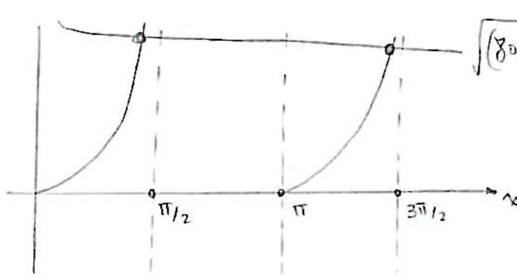
from here we find the energies

we know that
$K, l$ are real $\oplus \Rightarrow$ we only
look at $\tan(la) > 0$




limits

1) wide, deep  $a, V_0 \to$ large $\Rightarrow z_0 \to$ large




$\sqrt{(z_0/z)^2 - 1} \sim z_0/z$  and $z_0$ is very large

$\Downarrow$

$z_n \sim \frac{n\pi}{2}$  (n is odd) half of the solutions

$\Rightarrow la = \frac{n\pi}{2} \Rightarrow l^2 = \frac{n^2\pi^2}{(2a)^2} \Rightarrow \boxed{E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}}$ $\to$ infinite square well energies

2.) shallow narrow   $a, V_0$ — small, $z_0$ — very small

in the limit $z_0 < \pi/2 \rightarrow$ only one even state remain

↳ there is always ONE bound state no matter how weak the well becomes

#) odd solution

$$\psi(x) = -\psi(x)$$

→ keep sin

$$\psi(x) = \begin{cases} F e^{-Kx} & x > a \\ C \sin(lx) & 0 < x < a \\ -\psi(-x) & x < 0 \end{cases}$$

$$\begin{cases} F e^{-Ka} = C \sin(la) \\ -K F e^{-Ka} = l C \cos(la) \end{cases}$$

$$l \cot an(la) = -K$$

$$\boxed{-\cot an(la) = \frac{K}{l}}$$

$$z_0 = \frac{\sqrt{2mV_0}\,a}{\hbar}$$

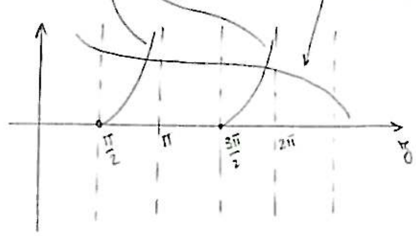
$$z = la$$

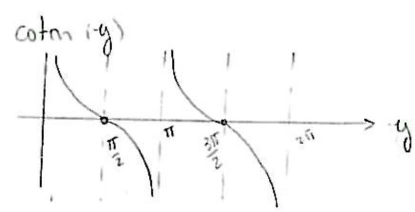
$$Ka = \sqrt{z_0^2 - z^2}$$

$$-\cot an(z) = \frac{Ka}{la} = \frac{\sqrt{z_0^2 - z^2}}{z}$$

$$\boxed{-\cot an(z) = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}}$$

⇒



Limits

1.) Wide deep

$z \sim \frac{n\pi}{2}$ n even → the other half of the solutions

$$\boxed{E_n + V_0 = \frac{n^2 \pi^2 \hbar^2}{2m\,(2a)^2}}$$

2.) Shallow, narrow

$z_0 < \pi/2 \Rightarrow$ no odd solution, so only ONE even solution remains

Therefore the solutions are:

$$\psi(x) = \begin{cases} F e^{-Kx} & x > a \\ D\cos(lx) & 0 < x < a \\ \psi(-x) & x < 0 \end{cases} \quad \text{AND} \quad \psi(x) = \begin{cases} F e^{-Kx} & x > a \\ D\sin(lx) & 0 < x < a \\ -\psi(-x) & x < 0 \end{cases}$$

normalizing to find D and F

$$1 = 2\int_0^{\infty} |\psi|^2\,dx = 2\int_0^{a} |D|^2 \cos^2(lx)\,dx + 2\int_a^{\infty} |F|^2 e^{-2Kx}\,dx$$

$\cos^2 x \longrightarrow \cos 2x = \cos^2 x - \sin^2 x = 2\cos^2 x - 1 \Rightarrow \cos^2 x = \frac{1+\cos 2x}{2}$

$$= \cancel{2}\,|D|^2 \left( \frac{a}{\cancel{2}} + \frac{\sin 2lx}{\cancel{4}_2 l}\Big|_0^a \right) + \cancel{2}\,|F|^2 \frac{e^{-2Ka}}{\cancel{2}K} \Rightarrow |D|^2 \left( a + \frac{\sin 2la}{2l} \right) + \frac{|F|^2 e^{-2Ka}}{K} = 1$$

but $F = D e^{Ka} \cos(la)$ (from continuity)

$$\Rightarrow |D|^2\left(a+\frac{\sin 2la}{2l}\right)+\frac{|D|^2\cos^2 la}{K}=1 \qquad \text{use} \quad \underline{K=l\tan(la)}$$

$$|D|^2\left(a+\frac{\sin la\cos la}{l}+\frac{\cos^3 la}{l\sin(la)}\right)=1$$

$$|D|^2\left(a+\frac{\cos la\,(\sin^2 la+\cos^2 la)}{l\sin(la)}\right)=1$$

$$|D|^2\left(a+\frac{1}{l\tan(la)}\right)=1 \Rightarrow |D|^2\left(a+\frac{1}{K}\right)=1$$

$$\boxed{D=\frac{1}{\sqrt{a+1/K}}}$$

$$\boxed{F=\frac{e^{Ka}\cos(la)}{\sqrt{a+1/K}}}$$

## ⇝ Scattering States $(E > 0)$

we don't use symmetry anymore

scattering problem is inherently asymmetric

waves come from one side only

∘) $x < -a$ $\quad V(x) = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad , \quad \frac{d^2\psi}{dx^2} = -k^2\psi \quad , \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi(x) = \underbrace{Ae^{ikx}}_{\text{comes from } -\infty} + \underbrace{Be^{-ikx}}_{\text{reflected to } -\infty}$$

∘) $-a < x < a$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \quad , \quad \frac{d^2\psi}{dx^2} = -l^2\psi \quad , \quad l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

$$\psi(x) = C\sin(lx) + D\cos(lx)$$

∘) $x > a$

there is no incoming wave, only transmission

$$\psi(x) = Fe^{ikx}$$

A → amplitude of the incident wave

B → amplitude of the reflected wave

F → amplitude of the transmitted wave

$$R = \frac{|B|^2}{|A|^2}$$ reflection coefficient
(prob that an incident particle is reflected)

$$T = \frac{|F|^2}{|A|^2}$$ transmission coefficient
(prob of transmission)

$$\boxed{R + T = 1}$$

boundary conditions

at $x=-a$
$$\begin{cases} Ae^{-ika} + Be^{+ika} = -C\sin(la) + D\cos(la) \\ ik\left(Ae^{-ika} - Be^{ika}\right) = l\left(C\cos(la) + D\sin(la)\right) \end{cases}$$

at $x=a$
$$\begin{cases} C\sin(la) + D\cos(la) = Fe^{ika} \\ l\left(C\cos(la) - D\sin(la)\right) = ikFe^{ika} \end{cases}$$

$$T = \frac{|F|^2}{|A|^2}$$

$$T = \frac{(2kl)^2}{\cos^2(2la)\,(2kl)^2 + (k^2+l^2)^2\sin^2(2la)}$$

$$B = i\frac{\sin(2la)}{2kl}(l^2-k^2)F$$

$$T = \frac{(2kl)^2}{(2kl)^2 + (k^2-l^2)^2\sin^2(2la)}$$

$T = 1$ when $\overline{2la = n\pi}$

$$F = \frac{e^{-2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}\sin(2la)}$$

$$R + T = \left(+\frac{\sin^2(2la)}{(2kl)^2}(l^2-k^2)^2 + 1\right)\frac{1}{\cos^2(2la) + \frac{(k^2+l^2)^2}{(2kl)^2}\sin^2(2la)}$$

$$= \frac{+\sin^2(2la)(l^4-2l^2k^2+k^4) + (2kl)^2}{(2kl)^2\cos^2(2la) + \sin^2(2la)(k^4+2l^2k^2+l^4)} = \frac{+\overbrace{(l^4-2l^2k^2+k^4) + (2kl)^2}^{2l^2k^2} - \cos^2(2la)(l^4-2l^2k^2+k^4)}{+(l^4+2l^2k^2+k^4) - \cos^2(2la)\left[\underbrace{k^4+2l^2k^2+l^4-(2kl)^2}_{-2l^2k^2}\right]}$$

$$= \boxed{1}$$

# Formalism

Formalism of QM is based on

- $\psi$ wave functions (don't measure $\psi$; $|\psi|^2$ - prob dens) — represented by (state of a system)
- operators (don't measure operators in the lab - access to expectation values) — represented by (observables)

mathematically: VECTORS — MATRICES

Operators act on the vectors as linear transformations

language of QM is linear algebra

## VECTORS

∘) real space $\vec{r} = 2\hat{\imath} + 3\hat{\jmath}$, where $\hat{\imath}$ and $\hat{\jmath}$ → ORTHONORMAL BASIS

using the notation $\hat{\imath} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\hat{\jmath} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$\vec{r} = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$

→) components are real numbers

→) up to 3D

VECTORS in QM
- → complex numbers
- → no restriction for dimensions

$\psi = |\alpha\rangle$

↳ Ket (Dirac notation)

$$|\alpha\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \vdots \end{pmatrix}$$

$\alpha_1, \alpha_2, \alpha_3, \ldots$ components of $|\alpha\rangle$ in a certain ORTHONORMAL basis

Example
1000 → $|\phi_1\rangle$
0100 → $|\phi_2\rangle$
0010 → $|\phi_3\rangle$
0001 → $|\phi_4\rangle$

$|\alpha\rangle = \alpha_1|\phi_1\rangle + \alpha_2|\phi_2\rangle + \alpha_3|\phi_3\rangle + \alpha_4|\phi_4\rangle$

orthonormal $\underbrace{(1\,0\,0\,0)}_{\phi_1} \cdot \underbrace{\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}}_{\phi_2} = 0$

$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ etc $\qquad |\alpha\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{pmatrix}$

→ Vector space: set of vectors with a set of scalars which is CLOSED [= operations are well defined, don't carry you out of the vector space]

under two operations:

- vector addition $|\alpha\rangle + |\beta\rangle = |\gamma\rangle$

  commutative $|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle$

  associative $|\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle$

  zero vector $|\alpha\rangle + |0\rangle = |\alpha\rangle$

  inverse vector $-|\alpha\rangle \Rightarrow |\alpha\rangle + (-|\alpha\rangle) = |0\rangle$

- scalar multiplication $a|\alpha\rangle = |\gamma\rangle$

  distributive, associative

→) linear combinations

$$a|\alpha\rangle + b|\beta\rangle + c|\gamma\rangle + \dots = |\Omega\rangle$$

$$\Psi(x) = \sum c_n \psi_n(x)$$

→) linearly independent

$|\lambda\rangle$ is L.I. of $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$ if it cannot be written as a linear comb. of them

Ex: $\hat{k}$ is L.I. of $\hat{i}$ and $\hat{j}$ { any vector in xy plane is L. Dependent on $\hat{i}$ and $\hat{j}$

→) SPAN

a set of vectors is said to SPAN the space if every vector can be written as a linear combination of this set } set also called COMPLETE

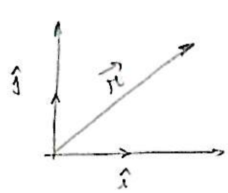
Ex: in 2D $\hat{i}$ and $\hat{j}$ SPAN the space

→) BASIS

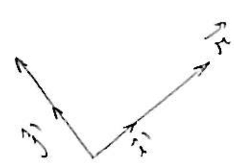
a set of L.I. vectors that SPAN the space { the number of vectors in any basis is the DIMENSION of the space

→) COMPONENTS

in a certain basis, any vector is uniquely represented by its components




$\vec{r} = 2\hat{i} + 3\hat{j}$



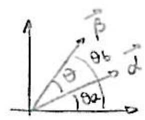

$\vec{r} = \sqrt{13}\,\hat{i}'$

the vector is always the same

but its components change according to the basis

→ Inner product

( dot product : $\vec{\alpha}\cdot\vec{\beta} = \alpha\,\beta\cos\theta$



decompound in an orthonormal basis $\hat{i}, \hat{j}$ $\begin{cases} \hat{i}\cdot\hat{j} = 0 \\ \|\hat{i}\| = 1 \\ \|\hat{j}\| = 1 \end{cases}$

$\vec{\alpha}\cdot\vec{\beta} = \alpha\beta\cos\theta = \alpha\beta\cos(\theta_b - \theta_a) = \alpha\beta\,(\cos\theta_b\cos\theta_a + \sin\theta_b\sin\theta_a)$

$= \alpha\beta\left(\frac{b_x\,a_x}{\alpha\beta} + \frac{b_y\,a_y}{\alpha\beta}\right) = a_x b_x + a_y b_y$

$\vec{\alpha}\cdot\vec{\beta} = \underbrace{(a_x \quad a_y)}_{\substack{\text{row}\\\text{vector}\\ \langle\alpha|}} \underbrace{\begin{pmatrix} b_x \\ b_y \end{pmatrix}}_{\substack{\text{column vector}\\ |\beta\rangle}} = \langle\alpha|\beta\rangle = a_x b_x + a_y b_y$ )

$\langle\alpha|\beta\rangle$

COMPONENTS

$|\beta\rangle = b_1|e_1\rangle + b_2|e_2\rangle + b_3|e_3\rangle + \dots$

BASIS

$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + a_3|e_3\rangle + \dots$

$\Longrightarrow \langle\alpha| = \langle e_1|\,a_1^* + \langle e_2|\,a_2^* + \langle e_3|\,a_3^* + \dots$

bra

bracket

$\langle\alpha|\beta\rangle = a_1^* b_1 \langle e_1|e_1\rangle + a_1^* b_2 \langle e_1|e_2\rangle + a_1^* b_3 \langle e_1|e_3\rangle + \dots$

BUT, if the basis is ORTHONORMAL ⟷ $\boxed{\langle e_i|e_j\rangle = \delta_{ij}}$

then

$$\boxed{\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + a_3^* b_3 + \dots}$$

← very convenient

$\hookrightarrow \underbrace{(a_1^* \quad a_2^* \quad a_3^* \dots)}_{\text{(row vector)}} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix}$ (column vector) } because basis is orthonormal most of the vectors we encounter in QM are functions and they live in

infinite – dimensional spaces

The collection of all functions of $x$ constitutes a vector space

But to represent a possible physical state it must be normalized

$$\int |\psi|^2 dx = 1$$

→) The set of all square-integrable functions on an interval

$f(x)$ such that $\int_a^b |f(x)|^2 dx < \infty$

constitutes a vector space called

**HILBERT SPACE**

In a infinite dim space, we define the inner-product as

$$\boxed{\langle f|g\rangle \equiv \int_a^b f(x)^* g(x)\, dx}$$

Properties:

- $\langle g|f\rangle = \langle f|g\rangle^*$
- $\langle f|f\rangle \geq 0$
- NORM: $\| f \| \equiv \sqrt{\langle f|f\rangle}$
- If $\| f \| = 1$ → vector / function is normalized

  Ex: $\| \alpha \| = \sqrt{\langle \alpha|\alpha\rangle} = 1 \Rightarrow \boxed{|a_1|^2 + |a_2|^2 + |a_3|^2 + \dots = 1}$
- $\langle f|g\rangle = 0$ ← orthogonal ; $\langle f_m|f_n\rangle = \delta_{mn}$ ← orthonormal
- set is complete if any function (in Hilbert space) can be expressed as linear comb

  $f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$ (orthonorm.) $\boxed{c_n = \langle f_n|f\rangle}$

**MATRICES** $\longrightarrow$ operators

multiply vectors by a scalar
rotate vectors

linear transformations $T$

$$\hat{T}|\alpha\rangle = |\alpha'\rangle$$

∘) transpose $\tilde{T}$

symmetric: $T = \tilde{T}$ antisym: $\tilde{T} = -T$

∘) complex conjugate $T^*$

real: $T^* = T$ imagin: $T^* = -T$

$\Rightarrow$) hermitian conjugate (or ADJOINT)

$$\boxed{T^{\dagger} = \tilde{T}^*}$$

a square matrix is hermitian (or self-adjoint) if it is equal to its $T^\dagger$

$\boxed{T = T^\dagger}$

$$(|\alpha\rangle)^{\dagger} = \langle\alpha|$$

bra is the hermitian conjugate of the ket (and vice-versa)

**OBSERVABLES are represented by hermitian operators**

$$\begin{cases} \langle w|v\rangle \overset{|v\rangle = T|u\rangle}{=} \langle w|T|u\rangle \\ \langle w|v\rangle^* = \langle v|w\rangle \underset{\langle v| = \langle u|T^\dagger}{=} \langle u|T^\dagger|w\rangle \end{cases}$$

# Expectation value of an OBSERVABLE

$$\langle T\rangle = \int \psi^* \hat{T}\, \psi\, dx = \langle \psi | T | \psi \rangle$$

$$\langle T\rangle = \overset{\langle\psi|T\psi\rangle}{\langle \psi | T | \psi \rangle}$$

(see next page)

$$\langle \psi | T\psi\rangle^* = \langle T\psi|\psi\rangle \overset{\downarrow}{=} \langle \psi | T^\dagger|\psi\rangle$$

$$\langle T\rangle^* = (\langle\psi|T|\psi\rangle)^* = \langle\psi|T^\dagger|\psi\rangle$$

since the outcome of a measurement has to be real

$$\Downarrow$$

$$\langle T\rangle = \langle T\rangle^*$$

$$\Downarrow$$

$$\boxed{T = T^\dagger}$$

a square matrix T is hermitian (or self-adjoint) if it is equal to $T^\dagger$

$$\boxed{\text{OBSERVABLES are represented by hermitian operators}}$$

Is momentum a hermitian operator?

$$\langle p\rangle = \langle\psi|p|\psi\rangle = \int \psi^* \frac{\hbar}{i}\frac{d\psi}{dx}\, dx$$

$$\langle p\rangle^* = \langle\psi|p|\psi\rangle^* = \int\left(\psi^*\frac{\hbar}{i}\frac{d\psi}{dx}\right)^* dx = \underbrace{\int \psi\left(-\frac{\hbar}{i}\frac{d\psi^*}{dx}\right) dx}$$

by parts $\cancel{-\frac{\hbar}{i}\psi\psi^*\Big|_{-\infty}^{\infty}} + \frac{\hbar}{i}\int\frac{d\psi}{dx}\psi^*\, dx = \int\psi^*\frac{\hbar}{i}\frac{d\psi}{dx}\, dx$

or $\langle p\rangle - \langle p\rangle^* = \int\frac{\hbar}{i}\frac{d}{dx}(\psi^*\psi)\, dx = \frac{\hbar}{i}\psi^*\psi\Big|_{-\infty}^{\infty} = 0$

$$\Rightarrow \langle p\rangle = \langle p\rangle^* \Rightarrow \boxed{\hat{p} = \hat{p}^\dagger}$$

more generally, a hermitian operator satisfies

$$\boxed{\langle \psi_1 | T\psi_2 \rangle = \langle T\psi_1 | \psi_2 \rangle}$$

which is equivalent to

$$\boxed{T = T^+}$$

because

$$\langle T\psi_1 | \psi_2 \rangle = \langle \psi_1 | T^+ | \psi_2 \rangle$$

Showing that

$$\langle T\psi_1 | \psi_2 \rangle = \langle \psi_1 | T^+ | \psi_2 \rangle$$

with matrices

$$|T\psi_1\rangle = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \overset{\text{column}}{\begin{pmatrix} t_{11} a_1 + t_{12} a_2 \\ t_{21} a_1 + t_{22} a_2 \end{pmatrix}} \Rightarrow \langle T\psi_1 | = \left( |T\psi_1\rangle \right)^+ = \overset{\text{row}}{\begin{pmatrix} t_{11}^* a_1^* + t_{12}^* a_2^* & t_{21}^* a_1^* + t_{22}^* a_2^* \end{pmatrix}}$$

$$\langle \psi_1 | T^+ = \begin{pmatrix} a_1^* & a_2^* \end{pmatrix} \begin{pmatrix} t_{11}^* & t_{21}^* \\ t_{12}^* & t_{22}^* \end{pmatrix} = \begin{pmatrix} a_1^* t_{11}^* + a_2^* t_{12}^* & a_1^* t_{21}^* + a_2^* t_{22}^* \end{pmatrix} \leftarrow (=)$$

$$\Downarrow$$

$$\boxed{\langle T\psi_1 | = \langle \psi_1 | T^+}$$

Showing that momentum is a hermitian operator

$$\langle f | p g \rangle = \int f^* \frac{\hbar}{i} \frac{dg}{dx} \, dx = \cancel{\frac{\hbar}{i} f^* g \Big|_{-\infty}^{\infty}} - \frac{\hbar}{i} \int \frac{df^*}{dx} g \, dx = \int \left( \frac{\hbar}{i} \frac{df}{dx} \right)^* g \, dx$$

$$= \boxed{\langle p f | g \rangle}$$

•) matrix multiplication is not, in general, commutative

commutator: $[S,T] = ST - TS$

•) transpose of product is transpose of each in reverse order

$$\widetilde{(ST)} = \tilde{T}\,\tilde{S}$$

$$\widetilde{(ST)}_{ki} = (ST)_{ik} = \sum_j S_{ij} T_{jk} = \sum_j T_{jk} S_{ij} = \sum_j (\tilde{T})_{kj} (\tilde{S})_{ji} = (\tilde{T}\tilde{S})_{ki}$$

$$\underbrace{A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \qquad \tilde{A} = \begin{pmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{pmatrix}}$$

$$A_{12} = \tilde{A}_{21}$$

$$a_{12} = a_{12}$$

$$\Rightarrow \widetilde{(ST)} = \tilde{T}\,\tilde{S}$$

•) hermitian conjugate

$$(ST)^{+} = T^{+} S^{+}$$

$$(ST)^{+} = \widetilde{(ST)}^{*} = (\tilde{T}\,\tilde{S})^{*} = T^{+} S^{+}$$

•) unit matrix

$$\mathbb{1} = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & 1 \ldots \end{pmatrix}$$

o) inverse of a square matrix

$$T^{-1}\,T = T\,T^{-1} = \mathbb{1}$$

$$\boxed{T^{-1} = \frac{1}{\det T}\,\tilde{C}}$$

transpose matrix of cofactors

$C_{11} = d(-1)^2 \quad C_{12} = c(-1)^3$

$C_{21} = b(-1)^3 \quad C_{22} = a(-1)^4$

$\Rightarrow \tilde{C} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Rightarrow \det A = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = \boxed{ad - bc}$$

$$\boxed{A^{-1} = \frac{1}{(ad-bc)}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}}$$

$$A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \Rightarrow \det A = \underbrace{\underbrace{a\begin{vmatrix} e & f \\ h & i \end{vmatrix}}_{\substack{C_{11} \\ \parallel \\ a(-1)^{1+1}|\;|}} \underbrace{- b\begin{vmatrix} d & f \\ g & i \end{vmatrix}}_{\substack{C_{12} \\ \parallel \\ b(-1)^{1+2}|\;|}} \underbrace{+ c\begin{vmatrix} d & e \\ g & h \end{vmatrix}}_{\substack{C_{13} \\ \parallel \\ c(-1)^{1+3}|\;|}}}_{\text{cofactors for one row or one column}}$$

<u>cofactor</u> $C_{ij} = (-1)^{i+j}\underbrace{|M_{ij}|}_{}$

$(n-1)\times(n-1)$ matrix that results from deleting i-th row and j-th column of original matrix

⇒) unitary matrix

$$\boxed{U^{\dagger} = U^{-1}}$$

evolution operator of a <u>CLOSED</u> syst is unitary

# EIGENVALUES and EIGENVECTORS

3D – special vectors where rotation $\Rightarrow$ $T|\alpha\rangle = |\alpha\rangle$
(vector along the rotation axis)

$\Rightarrow$ $T|\alpha\rangle = -|\alpha\rangle$
(vector along $\perp$ axis and $\theta = 180°$)

In complex vector space – also find such special vector

$$T|\alpha\rangle = \underbrace{\lambda}_{\text{eigenvalues (complex numbers)}} \underbrace{|\alpha\rangle}_{\text{eigenvectors}}$$

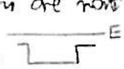
- spectrum of a matrix / operator – collection of all its eigenvalues
- if 2 or more eigenvectors share the same eigenvalue $\rightarrow$ the spectrum is DEGENERATE

$\rightarrow$) Time-indep. Schröd. eq.

$$\boxed{H\psi = \underbrace{E}_{\text{eigenval.}}\,\underbrace{\psi}_{\text{eigenvect. / eigenfunctions}}}$$

$\rightarrow$) spectrum can be DISCRETE or CONTINUOUS

(1) discrete : eigenvalues are separated from one another $\Rightarrow$ eigenfunctions lie in Hilbert space and are physically realizable states
↓
Example : H.O. (discrete and infinite dimensional spectrum), infinite square well, delta potential $E<0$
spin chain with $L$ sites (discrete and finite dimensional spectrum)

(2) continuous : eigenvalues fill out an entire range $\Rightarrow$ eigenfunctions are not normalizable [but linear combinations may be normalizable]
Example : free particle, delta potential well with $E>0$, 

(!) important

~~DISCRETE~~

DISCRETE

Normalizable eigenfunctions of a $\boxed{\text{hermitian}}$ operator have the properties $\boxed{H\psi = E\psi}$

o) Eigenvalues are REAL (as E in $H\psi = E\psi$)

hermitian operators $\Leftrightarrow$ $\langle T\rangle = \langle T\rangle^*$

$$\langle \psi | T\psi\rangle = \langle T\psi | \psi\rangle$$
$$t\langle\psi|\psi\rangle = t^*\langle\psi|\psi\rangle$$
$$t = t^*$$

$\langle T\rangle = \langle T\rangle^*$

$$\langle T\rangle = \langle \psi | T | \psi\rangle \underset{\substack{\uparrow \\ T|\psi\rangle = t|\psi\rangle}}{=} t\langle\psi|\psi\rangle \underset{\substack{\uparrow \\ \text{norm}}}{=} t$$

$$\langle T\rangle^* = \langle \psi | T | \psi\rangle^* = t^*$$

$\langle T\rangle = \langle T\rangle^* \Rightarrow \boxed{t = t^*}$

o) Eigenfunctions belonging to distinct eigenvalues are ORTHOGONAL

as $\langle \psi_m | \psi_n\rangle = 0$ in infinite square well

$$T\psi_1 = t_1\psi_1 \qquad T\psi_2 = t_2\psi_2$$

T is hermitian

$$\langle \psi_1 | T\psi_2\rangle = \langle T\psi_1 | \psi_2\rangle$$
$$t_2\langle\psi_1|\psi_2\rangle \qquad t_1^*\langle\psi_1|\psi_2\rangle$$

$\Vert$ ← from above

$$t_1\langle\psi_1|\psi_2\rangle$$

since $t_1 \neq t_2$ by assumption

$$\hookrightarrow \langle\psi_1|\psi_2\rangle = 0$$

o) finite-dim → eigenvectors of a hermitian matrix SPAN the space

$\Rightarrow$ any vector can be expressed as a linear comb of them

take it as an AXIOM for infinite-dim

(= proposition assumed without proof)

$$\Psi(x,t) = \sum c_n \psi_n(x) e^{-iE_nt/\hbar}$$ → for $\hat{H}$

# DISCRETE SPECTRUM and FINITE DIMENSIONAL

## How to find eigenvectors

$$T|\alpha\rangle = \lambda|\alpha\rangle$$

$$(T - \mathbb{1}\lambda)|\alpha\rangle = 0 \leftarrow \text{zero matrix}$$

if it had inverse $\underbrace{(T-\lambda\mathbb{1})^{-1}(T-\lambda\mathbb{1})}_{\mathbb{1}}|\alpha\rangle = 0 \Rightarrow |\alpha\rangle = 0$

but assume $|\alpha\rangle \neq 0$

$$\Rightarrow \det(T-\lambda\mathbb{1}) = 0 \iff (T-\lambda\mathbb{1}) \text{ has no inverse}$$

$$\Downarrow$$

$$\boxed{\text{characteristic equation}}$$

Example:

$$M = \begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}$$

$$\det(M-\lambda\mathbb{1}) = \begin{vmatrix} 2-\lambda & 0 & -2 \\ -2i & i-\lambda & 2i \\ 1 & 0 & -1-\lambda \end{vmatrix} = (2-\lambda)(i-\lambda)(-1-\lambda) + 2(i-\lambda) = 0$$

$$\Rightarrow (2-\lambda)(-i-i\lambda+\lambda+\lambda^2) + 2i - 2\lambda = -\cancel{2i} - 2i\lambda + \cancel{2\lambda} + 2\lambda^2 + \lambda i + i\lambda^2 - \lambda^2 - \lambda^3 + \cancel{2i} - \cancel{2\lambda}$$

$$= -\lambda^3 + (1+i)\lambda^2 - i\lambda = 0$$

$$\left\{ \begin{array}{l} \lambda_1 = 0 \\ \lambda_2 = 1 \\ \lambda_3 = i \end{array} \right\} \quad -\lambda\left(\lambda^2 - (1+i)\lambda + i\right) = 0 \rightarrow \lambda = 0$$

$$\lambda = \frac{(1+i) \pm \sqrt{(\cancel{1}+2i-\cancel{1}) - 4i}}{2}$$

$$-\lambda^3 + (1+i)\lambda^2 - i\lambda = 0$$

$$\Rightarrow -\lambda\left(\lambda^2 - (1+i)\lambda + i\right) = 0$$

$$\lambda^2 - (1+i)\lambda + i = 0 \Rightarrow \lambda = \frac{(1+i) \pm \sqrt{(\cancel{1} + 2i - \cancel{1}) - 4i}}{2}$$

$$\lambda = \frac{(1+i) \pm \sqrt{-2i}}{2} = \frac{(1+i) \pm i\sqrt{2}\sqrt{i}}{2} = \frac{(1+i) \pm i\cancel{\sqrt{2}}(1+i)/\cancel{\sqrt{2}}}{2}$$

$$\sqrt{i} = \frac{1+i}{\sqrt{2}}$$

$$\lambda = \frac{1+i \pm (i-1)}{2} \begin{array}{l} \nearrow i \\ \searrow 1 \end{array}$$

$$\boxed{\lambda = \begin{cases} 0 \\ 1 \\ i \end{cases}}$$

For $\lambda_1 = 0$

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = 0\begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\left.\begin{cases} 2x - 2z = 0 & \Rightarrow x = z \\ -2ix + iy + 2iz = 0 & \\ x - z = 0 & \Rightarrow x = z \end{cases}\right\} \Rightarrow y = 0 \Rightarrow |\alpha\rangle = \begin{pmatrix} x \\ 0 \\ x \end{pmatrix}$$

from $\langle\alpha|\alpha\rangle = 1 \Rightarrow (x^* \;\; 0 \;\; x^*)\begin{pmatrix} x \\ 0 \\ x \end{pmatrix} =$

$\Rightarrow |x|^2 = 1/2$

$\boxed{\lambda_1 = 0}$ and $\boxed{|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}}$ //

$$\begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 1 \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\begin{cases} 2x - 2z = x & \longrightarrow \quad x = 2z \Rightarrow \overline{z = x/2} \\ -2ix + iy + 2iz = y & \longrightarrow \quad -2ix + ix = y - iy \\ x - z = z & \end{cases}$$

$$-ix = y(1-i)$$

$$\underline{\overline{y = \frac{i}{(i-1)} x}}$$

$$\lambda_2 = 1 \longrightarrow \Psi_2 = \begin{pmatrix} x \\ \frac{i}{(i-1)} x \\ x/2 \end{pmatrix}$$

$$-(i+1)(i-1) = -(-1-1)$$

$$\Psi_2^* \Psi_2 = \begin{pmatrix} x^* & \frac{-i}{(-i-1)} x^* & \frac{x^*}{2} \end{pmatrix} \begin{pmatrix} x \\ \frac{i}{(i-1)} x \\ \frac{x}{2} \end{pmatrix} = 1$$

$$|x|^2 \left(1 + \frac{1}{2} + \frac{1}{4}\right) = |x|^2 \frac{7}{4} = 1 \longrightarrow x = \frac{2}{\sqrt{7}}$$

$$\overline{\underline{\lambda_2 = 1}} \Longrightarrow \Psi_2 = \frac{2}{\sqrt{7}} \begin{pmatrix} 1 \\ \frac{i}{(i-1)} \\ \frac{1}{2} \end{pmatrix} = \frac{2}{\sqrt{7}} \begin{pmatrix} 1 \\ \frac{1-i}{2} \\ \frac{1}{2} \end{pmatrix} = \boxed{\frac{1}{\sqrt{7}} \begin{pmatrix} 2 \\ 1-i \\ 1 \end{pmatrix}}$$

$$\frac{i}{i-1} = \frac{i(i+1)}{(-1-1)} = \frac{-1+i}{-2} = \frac{1-i}{2}$$

$\lambda_3 = i$ <u>etc</u>

## Changing Basis

$$M = \begin{pmatrix} 2 & 0 & -2 \\ -2i & i & 2i \\ 1 & 0 & -1 \end{pmatrix} \quad \text{and} \quad M' = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{pmatrix}$$

Same matrices but written in different basis } similar matrices

$M$ uses $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$M'$ uses $\psi_1, \psi_2, \psi_3$

while the elements may look very $\neq$ in the new basis

det and trace don't change

$\downarrow$

(sum of diagonal elements)

$\rightarrow$) check trace of $M$, $M'$

$\rightarrow$) check det

how numbers change as we change basis

$\downarrow$

in vector

in matrix

Vector

$$\boxed{|\alpha^f\rangle = S|\alpha^e\rangle}$$

Matrix

$$|\alpha'^e\rangle = T^e|\alpha^e\rangle \quad \text{and} \quad |\alpha'^f\rangle = T^f|\alpha^f\rangle$$

$$|\alpha'^f\rangle = S|\alpha'^e\rangle = S\,(T^e\underbrace{|\alpha^e\rangle}_{S^{-1}|\alpha^f\rangle}) = ST^eS^{-1}|\alpha^f\rangle$$

$\shortparallel$

$|T^f|\alpha^f\rangle$

$$\boxed{T^f = ST^eS^{-1}}$$

S – similarity matrix that effects the diagonalization is constructed by using the normalized eigenvectors as the columns of $S^{-1}$

$$S^{-1} = \begin{pmatrix} \psi_1 & \psi_2 & \psi_3 \\ \vdots & \vdots & \vdots \end{pmatrix}$$

---

A NORMAL matrix commutes with its hermitian conjugate

$$[N^\dagger, N] = 0$$

Every normal matrix is diagonalizable

Example: hermitian matrix, unitary matrix

→) ~~any~~ two matrices that $\boxed{\text{commute}}$ ~~are~~ can be simultaneously diagonalized by the same (similarity) ~~similarity~~ matrix $S$

→) or if they are simultaneously diagonalized ⇒ they commute

$$SAS^{-1} = D \Rightarrow \underline{A = S^{-1}DS} \qquad SBS^{-1} = E \Rightarrow \underline{B = S^{-1}ES}$$

$$[A,B] = AB - BA = S^{-1}DSS^{-1}ES - S^{-1}ESS^{-1}DS = S^{-1}DES - S^{-1}EDS = S^{-1}\underbrace{[D,E]}_{\text{diagonal always commute}}S = 0$$

→) operators that ∘) commute are <u>COMPATIBLE</u> observables

and <u>share</u> eigen[vectors / functions

∘) don't commute are <u>INCOMPATIBLE</u> observables

don't share $\psi$'s

↳ like $x$ and $p$

→) The <u>hermitian conjugate</u> (or <u>adjoint</u>) of an operator $\hat{Q}$ is the operator $\hat{Q}$ such that

operators

$$\begin{cases} \langle \alpha | \hat{Q}\beta \rangle = \langle \hat{Q}^{+}\alpha | \beta \rangle \\ \langle \alpha | \hat{Q}^{+}\beta \rangle = \langle Q\alpha | \beta \rangle \end{cases}$$

<u>but</u>

The operator is <u>hermitian</u> if $\overbrace{Q^{+} = Q}^{\text{finite dim}}$

that is

$$\boxed{\langle \alpha | Q\beta \rangle = \langle Q\alpha | \beta \rangle}$$

<u>orthonormal</u> <u>basis</u> $\langle \alpha |$ – row $|\beta\rangle$ – column

$$\underline{\langle \alpha | \hat{Q} | \beta \rangle} = a^{+} Q\, b = (Q^{+}a)^{+}\, b = \underline{\langle \hat{Q}^{+}\alpha | \beta \rangle}$$

# Generalized Statistical Interpretation

We saw that

$$\underset{\text{hermitian}}{H}\,\psi_n = \underset{\text{eigenvalues}}{E_n}\,\underset{\text{eigenfunctions}}{\psi_n}$$

$$\langle \psi_m | \psi_n \rangle = \delta_{nm} \implies \Psi(x,t) = \sum c_n \psi_n(x)\, e^{-iE_n t/\hbar}$$

$$\boxed{\langle H \rangle = \sum |c_n|^2 E_n} \quad \begin{cases} |c_1|^2 \text{ prob. for } E_1 \\ |c_2|^2 \text{ prob. for } E_2 \\ \vdots \end{cases}$$

$$\boxed{\sum |c_n|^2 = 1}$$

Let's extend this to any observable

If we measure an Observable $Q(x,p)$ on a particle in state $\Psi(x,t)$, we get one eigenvalue of the hermitian operator $\hat{Q}(x, \frac{\hbar}{i}\frac{d}{dx})$

a) spectrum of $\hat{Q}$ is discrete

prob. of getting eigenvalue $q_n$ associated with eigenfunction $f_n(x)$ is

$$\boxed{|c_n|^2} \quad \text{where} \quad c_n = \langle f_n | \Psi \rangle$$

c) spectrum is continuous

prob. is in the range $dz$ for getting $q(z)$ associated with $f_z(x)$

$$\boxed{|c(z)|^2\, dz} \quad \text{where} \quad c(z) = \langle f_z | \Psi \rangle$$

$$\Psi(x,t) = \sum_n c_n(t)\, f_n(x)$$

$\rightarrow)$ $\sum_n |c_n|^2 = 1$

$$1 = \langle \Psi | \Psi \rangle = \left\langle \sum c_{n'}^* f_{n'}^* \,\Big|\, \sum c_n f_n \right\rangle$$

$$= \sum_{n'} \sum_n c_{n'}^* c_n \underbrace{\langle f_{n'} | f_n \rangle}_{\delta_{n'n}}$$

$$= \boxed{\sum_n |c_n|^2} = 1$$

$\rightarrow)$ $\langle Q \rangle = \sum_n q_n |c_n|^2$

$$\langle Q \rangle = \langle \Psi | Q | \Psi \rangle = \left\langle \sum_{n'} c_{n'}^* f_{n'} \,\Big|\, \underbrace{Q \sum c_n f_n}_{q_n f_n} \right\rangle$$

$$= \sum_{n'} \sum_n c_{n'}^* c_n\, q_n \underbrace{\langle f_{n'} | f_n \rangle}_{\delta_{n'n}}$$

$$= \boxed{\sum_n |c_n|^2 q_n}$$

**NOTE**: Upon $\boxed{\text{measurement}}$, the wave function **COLLAPSES** to the corresponding eigenstate

Example: operator $\hat{A}$ has two normalized eigenstates $\phi_1$ and $\phi_2$ with eigenvalues $a_1$ and $a_2$.
If observable A is measured and we get $a_1$
the state of the system (which could have been a superposition of $\phi_1$ and $\phi_2$)
immediately collapses and becomes $\boxed{\phi_1}$

Example 3.8

$$H = \begin{pmatrix} h & g \\ g & h \end{pmatrix}$$ basis is $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$

$$E_+ = h + g \qquad |s_+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

$$E_- = h - g \qquad |s_-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

If the system starts ~~at~~ out in state $\begin{pmatrix}1\\0\end{pmatrix}$, what is its state at time $t$ ?

$$|s(0)\rangle = \begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}\left(|s_+\rangle + |s_-\rangle\right)$$

$$|s(t)\rangle = \frac{1}{\sqrt{2}}\left(|s_+\rangle e^{-iE_+t/\hbar} + |s_-\rangle e^{-iE_-t/\hbar}\right)$$

$$= \frac{1}{2}\begin{pmatrix}1\\1\end{pmatrix} e^{-iE_+t/\hbar} + \frac{1}{2}\begin{pmatrix}1\\-1\end{pmatrix} e^{-iE_-t/\hbar} = e^{-iht/\hbar}\begin{pmatrix} \dfrac{e^{-igt/h} + e^{+igt/h}}{2} \\ \dfrac{e^{-igt/h} - e^{+igt/h}}{2} \end{pmatrix}$$

$$= e^{-iht/\hbar}\begin{pmatrix}\cos(gt/\hbar) \\ -i\sin(gt/\hbar)\end{pmatrix}$$

at $t=0 \implies |s(0)\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ (phase)

at $\frac{gt}{\hbar} = \frac{\pi}{2} \implies |s\left(\frac{\pi\hbar}{2g}\right)\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ phase

at $\frac{gt}{\hbar} = \pi \longrightarrow \begin{pmatrix}1\\0\end{pmatrix}$ phase

# Dirac Notation

$$\left.\begin{array}{l} |\alpha\rangle \\ \\ |\mathcal{S}(t)\rangle \end{array}\right\} \text{basis is not specified}$$

## VECTOR with respect to a BASIS

Once you write $|\alpha\rangle$ as $\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$ $\rightarrow$ the basis $|e_1\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix}$, $|e_2\rangle = \begin{pmatrix} 0 \\ 1 \\ \vdots \end{pmatrix}$, etc

is specified

$\Psi(x,t) = \langle x | \mathcal{S}(t) \rangle$ $\rightarrow$ basis of position is specified

$\phi(p,t) = \langle p | \mathcal{S}(t) \rangle$ $\rightarrow$ basis of momentum is specified

## OPERATOR with respect to a BASIS

$$\langle e_m | \hat{Q} | e_n \rangle \equiv Q_{mn}$$

Example : in the basis $|e_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|e_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \quad \text{where} \quad \begin{array}{l} m_{11} = \langle e_1 | M | e_1 \rangle \\ m_{12} = \langle e_1 | M | e_2 \rangle \\ m_{21} = \langle e_2 | M | e_1 \rangle \\ m_{22} = \langle e_2 | M | e_2 \rangle \end{array}$$

Operator transforms one vector into another: $|\beta\rangle = \hat{Q}|\alpha\rangle$

$\rightarrow$ with respect to a basis, the equation becomes

$$\left.\begin{array}{l} |\alpha\rangle = \sum_n a_n |e_n\rangle, \quad a_n = \langle e_n | \alpha \rangle \\ |\beta\rangle = \sum_n b_n |e_n\rangle, \quad b_n = \langle e_n | \beta \rangle \end{array}\right\} \Rightarrow \sum_n b_n |e_n\rangle = \sum_n a_n Q |e_n\rangle \xrightarrow{\langle e_m |} \sum_n b_n \langle e_m | e_n \rangle = \sum_n a_n \langle e_m | Q | e_n \rangle$$

$$b_m = \sum_n Q_{mn} a_n$$

$$\begin{cases} |\alpha\rangle \to \text{ket} \to \text{vector space} \\ \quad \text{(column vector)} \\ \langle\beta| \to \text{bra} \to \text{dual space} \\ \quad \text{(row vector)} \end{cases}$$

↳ collection of all bras

- Suppose $|\alpha\rangle$ is a normalized vector

  $\hat{P} \equiv |\alpha\rangle\langle\alpha|$ is the <u>projector</u> operator

  it picks out the portion of any vector that lies along $|\alpha\rangle$

$$\hat{P}|\beta\rangle = |\alpha\rangle\langle\alpha|\beta\rangle = \langle\alpha|\beta\rangle\,|\alpha\rangle$$

- $\hat{P}$ is idempotent $\boxed{\hat{P}^2 = \hat{P}}$

(Prob 3.21)

$$\hat{P}^2|\beta\rangle = P\,(P|\beta\rangle) = P\left(\langle\alpha|\beta\rangle\,|\alpha\rangle\right) = \langle\alpha|\beta\rangle\,\underbrace{\langle\alpha|\alpha\rangle}_{1}\,|\alpha\rangle$$

$$= \langle\alpha|\beta\rangle\,|\alpha\rangle = \hat{P}|\beta\rangle$$

↳ $\hat{P}^2 = \hat{P}$

- If $\{|e_n\rangle\}$ is a discrete <u>orthonormal</u> basis, that is, $\langle e_m|e_n\rangle = \delta_{mn}$

then $\boxed{\sum_n |e_n\rangle\langle e_n| = \mathbb{1}}$ → identity operator

because if this operator acts on any vector $|\alpha\rangle$ we recover $|\alpha\rangle$

$$\sum_n |e_n\rangle\underbrace{\langle e_n|\alpha\rangle}_{c_n} = \sum c_n|e_n\rangle = |\alpha\rangle$$

Schwartz inequality (Problem A 5)

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$$

Let

$$|\gamma\rangle = |\beta\rangle - \frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}|\alpha\rangle$$

since

$$\langle\gamma|\gamma\rangle \geq 0 \Rightarrow \left(\langle\beta| - \frac{\langle\alpha|\beta\rangle^*}{\langle\alpha|\alpha\rangle}\langle\alpha|\right)\left(|\beta\rangle - \frac{\langle\alpha|\beta\rangle|\alpha\rangle}{\langle\alpha|\alpha\rangle}\right)$$

$$= \langle\beta|\beta\rangle - \frac{\langle\alpha|\beta\rangle\langle\beta|\alpha\rangle}{\langle\alpha|\alpha\rangle} - \cancel{\frac{\langle\alpha|\beta\rangle^*\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}} + \cancel{\frac{\langle\alpha|\beta\rangle\langle\alpha|\beta\rangle^*\langle\alpha|\alpha\rangle}{\langle\alpha|\alpha\rangle\langle\alpha|\alpha\rangle}} \geq 0$$

$$\hookrightarrow \langle\beta|\beta\rangle \geq \frac{\langle\alpha|\beta\rangle(\langle\alpha|\beta\rangle)^*}{\langle\alpha|\alpha\rangle}$$

$$\hookrightarrow \boxed{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2}$$

# Uncertainty Principle

uncertainty
dispersion
standard deviation of observable $A$ : $\sigma_A$ (or uncertainty) / variance $\sigma_A^2$

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

$$\sigma_A^2 = \langle (A - \langle A\rangle)^2\rangle = \langle \Psi | (A - \langle A\rangle)^2 | \Psi\rangle =$$

$$= \langle (A - \langle A\rangle)\Psi | (A - \langle A\rangle)\Psi\rangle = \langle f | f\rangle$$

$$\begin{cases} |f\rangle = (A - \langle A\rangle)|\Psi\rangle \\ |g\rangle = (B - \langle B\rangle)|\Psi\rangle \end{cases}$$

$$\sigma_B^2 = \langle (B - \langle B\rangle)^2\rangle = \langle g | g\rangle$$

(Schwartz inequality)

$$\rightarrow \sigma_A^2 \sigma_B^2 = \langle f|f\rangle\langle g|g\rangle \geqslant |\langle f|g\rangle|^2$$

$$|z|^2 = [Re(z)]^2 + [Im(z)]^2 \geqslant [Im(z)]^2 = \left[\frac{z - z^*}{2i}\right]^2$$

$$\langle f|f\rangle\langle g|g\rangle \geqslant \left[\frac{\langle f|g\rangle - \langle f|g\rangle^*}{2i}\right]^2 \qquad \langle f|g\rangle^* = \langle g|f\rangle$$

$$\rightarrow \langle f|g\rangle = \langle (A - \langle A\rangle)\Psi | (B - \langle B\rangle)\Psi\rangle = \langle \Psi | (A - \langle A\rangle)(B - \langle B\rangle) | \Psi\rangle =$$

$$= \langle \Psi | AB - A\langle B\rangle - \langle A\rangle B + \langle A\rangle\langle B\rangle | \Psi\rangle = \langle AB\rangle - \langle A\rangle\langle B\rangle$$

$$\rightarrow \langle g|f\rangle = \langle BA\rangle - \langle A\rangle\langle B\rangle$$

$$\langle f|g\rangle - \langle f|g\rangle^* = \langle f|g\rangle - \langle g|f\rangle = \langle AB\rangle - \langle BA\rangle = \langle [A,B]\rangle$$

$$\boxed{\sigma_A^2 \sigma_B^2 \geqslant \left(\frac{\langle [A,B]\rangle}{2i}\right)^2} \leftarrow$$ (generalized) uncertainty principle

$$\sigma_A^2 \sigma_B^2 = \left( \frac{\langle [A,B] \rangle}{2i} \right)^2$$

$$[x, p] = i\hbar$$

$$\sigma_x^2 \sigma_p^2 \geq \left( \frac{i\hbar}{2i} \right)^2 = \frac{\hbar^2}{4}$$

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

Heisenberg uncertainty principle

uncertainty principle for every pair of $\left\{ \begin{array}{l} \text{observables whose operators don't commute} \\ \text{incompatible observables} \end{array} \right.$

HW - Prob. 3.13

↓

use test function

b) $[x^n, p] = i\hbar n x^{n-1}$

$$[x^n, p] g = x^n \frac{\hbar}{i} \cancel{\frac{\partial g}{\partial x}} - \frac{\hbar}{i} n x^{n-1} g - \frac{\hbar}{i} \cancel{x^n \frac{\partial g}{\partial x}} = -\frac{\hbar}{i} n x^{n-1} g$$

$$\Rightarrow \boxed{[x^n, p] = i\hbar n x^{n-1}}$$

# Continuous Spectra

If the spectrum of a hermitian operator is continuous,
the eigenfunctions are not normalizable

Ex. 3.2 $\underbrace{\text{eigenfunctions}}_{f_p(x)}$ and $\underbrace{\text{eigenvalues}}_{p}$ of $\hat{p}$

$$\frac{\hbar}{i}\frac{d}{dx}f_p(x) = p\, f_p(x)$$

$$\Rightarrow f_p(x) = A e^{ipx/\hbar} \longrightarrow \text{NOT square-integrable}$$

$$\boxed{\delta(p-p') = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{iu(p-p')}\, du}$$

→) restrict to / assume / p - real

$$\int_{-\infty}^{\infty} f_{p'}^{*}(x)\, f_p(x)\,dx = |A|^2 \int_{-\infty}^{\infty} e^{i(p-p')x/\hbar}\, dx \overset{u = x/\hbar}{=} |A|^2 \int_{-\infty}^{\infty} e^{i(p-p')u}\, \hbar\, du$$

$$= |A|^2\, 2\pi\hbar\, \delta(p-p') \qquad \text{if} \quad \boxed{A = \frac{1}{\sqrt{2\pi\hbar}}}$$

$$\Rightarrow \int_{-\infty}^{\infty} f_{p'}^{*}(x)\, f_p(x)\, dx = \boxed{\langle f_{p'} | f_p \rangle = \delta(p-p')}$$

→) "orthonormal" — non-normalizable

ORTHONORMAL

→) complete $\boxed{\text{Axiom}}$

$$f(x) = \int_{-\infty}^{\infty} c(p)\, f_p(x)\, dp$$

to find $c(p)$

$$\boxed{c(p) = \langle f_p | f \rangle}$$

$$\langle f_{p'} | f \rangle = \int dx \int dp\, c(p)\, \frac{e^{-ip'x/\hbar}}{\sqrt{2\pi\hbar}}\, \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} = \int dp\, c(p)\, \delta(p-p') = \boxed{c(p')}$$

NOTE

$$f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$ ← eigenfunction of the momentum operator

$$f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \left[ \cos\left(\frac{px}{\hbar}\right) + i \sin\left(\frac{px}{\hbar}\right) \right]$$

↳ to find the wavelength: $\frac{p\lambda}{\hbar} = 2\pi$

$$\boxed{\lambda = \frac{2\pi\hbar}{p}}$$ ⇒ The $\lambda$ of the eigenfunctions of $\hat{p}$ is the de Broglie's $\lambda$.

Momentum vs. Position space

up to now, most of our studies were in position space

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x\, \psi(x)\, dx$$

eigenfunctions of $\hat{p}$: $f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$

$$c(p) = \langle f_p | \psi \rangle$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar}\, \Psi(x,t)\, dx$$

$$\boxed{\phi(p,t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{-ipx/\hbar}\, \Psi(x,t)\, dx}$$ ← $\phi(p,t)$ is the Fourier transform of $\Psi(x,t)$

momentum space wave function

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar}\, \phi(p,t)\, dp}$$ ← $\Psi(x,t)$ is the inverse Fourier transform of $\phi(p,t)$

position space wave function

Ex 34 A particle of mass $m$ is bound in the delta function well

$V(x) = -\alpha\delta(x)$. What is the probability that a measurement of its momentum would yield a value greater than $p_0 = \frac{m\alpha}{\hbar}$?

$$\Psi(x,t) = \sqrt{\frac{m\alpha}{\hbar}}\; e^{-m\alpha|x|/\hbar^2}\; e^{-iEt/\hbar}$$

we need $\phi(p,t)$

$$\phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\,\Psi(x,t)\,dx = \frac{\sqrt{m\alpha}}{\hbar\sqrt{2\pi\hbar}}\, e^{-iEt/\hbar}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\, e^{-m\alpha|x|/\hbar^2}\,dx$$

$$= \frac{\sqrt{m\alpha}}{\hbar\sqrt{2\pi\hbar}}\, e^{-iEt/\hbar}\left[\underbrace{\int_{-\infty}^{0} e^{x\left(-\frac{ip}{\hbar}+\frac{m\alpha}{\hbar^2}\right)}dx}_{\frac{e^{x(\dots)}\big|_{\infty}^{0}}{-\frac{ip}{\hbar}+\frac{m\alpha}{\hbar^2}}} + \underbrace{\int_{0}^{\infty} e^{x\left(-\frac{ip}{\hbar}-\frac{m\alpha}{\hbar^2}\right)}dx}_{\frac{e^{-x(\dots)}\big|_{0}^{\infty}}{-\frac{ip}{\hbar}-\frac{m\alpha}{\hbar^2}} = \frac{1}{\frac{ip}{\hbar}+\frac{m\alpha}{\hbar^2}}}\right]$$

$$= \frac{\sqrt{m\alpha}}{\hbar\sqrt{2\pi\hbar}}\, e^{-iEt/\hbar}\left[\frac{+\cancel{ip/\hbar}+m\alpha/\hbar^2-\cancel{ip/\hbar}+m\alpha/\hbar^2}{\left(p^2/\hbar^2+m^2\alpha^2/\hbar^4\right)}\right]$$

$$= \frac{\sqrt{m\alpha}}{\hbar\sqrt{2\pi\hbar}}\, e^{-iEt/\hbar}\,\frac{2m\alpha}{\left(p^2+m^2\alpha^2/\hbar^2\right)} = \sqrt{\frac{2}{\pi}}\, e^{-iEt/\hbar}\,\frac{\sqrt{(m\alpha/\hbar)^3}}{p^2+(m\alpha/\hbar)^2} = \boxed{\sqrt{\frac{2}{\pi}}\,\frac{p_0^{3/2}\,e^{-iEt/\hbar}}{p^2+p_0^2}}$$

probability → measurement greater than $p_0$

$$\int_{p_0}^{\infty}|\phi(p,t)|^2\,dp = \frac{2}{\pi}\,p_0^3\int_{p_0}^{\infty}\frac{1}{(p^2+p_0^2)}\,dp = \boxed{0.0908}$$

## Prob. 3.10

Is the ground state of the infinite square well an eigenfunction of momentum?

$$\psi_1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$$

$$\hat{p}\,\psi_1 = \frac{\hbar}{i}\sqrt{\frac{2}{a}}\,\frac{\pi}{a}\cos\left(\frac{\pi x}{a}\right) = \frac{\hbar}{i}\frac{\pi}{a}\,\mathrm{cotg}\left(\frac{\pi x}{a}\right)\boxed{\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)} = \underbrace{\frac{\hbar}{i}\frac{\pi}{a}\,\mathrm{cotg}\left(\frac{\pi x}{a}\right)}_{\text{NOT a const}}\psi_1$$

↳ $\psi_1$ is NOT an eigenfunction of $\hat{p}$

## Prob. 3.11

Find $\phi(p,t)$ for a particle in the ground state of the harmonic oscillator

$$\psi_0(x,t) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}\, e^{-i\omega t/2}$$

$$\phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\,\psi_0(x,t)\,dx = \frac{1}{(\pi m\omega\hbar)^{1/4}}\, e^{-p^2/2m\omega\hbar}\, e^{-i\omega t/2}$$

(complete square ...)

What is the prob. that a measurement of $p$ on a particle in this state would yield a value outside the classical range (for the same energy)?

maximum $p$ classically } all $E$ is kinetic

$$E = \frac{\hbar\omega}{2} = \frac{p^2}{2m} \Rightarrow p = \pm\sqrt{m\hbar\omega}$$

$$\int_{-\infty}^{-\sqrt{m\hbar\omega}} |\phi(p,t)|^2\,dp + \int_{\sqrt{m\hbar\omega}}^{\infty} |\phi(p,t)|^2\,dp = \boxed{0.16}$$

(use mathematica)

Prob. 3.12

$$\langle x \rangle = \int \phi^*(p,t) \left(-\frac{\hbar}{i}\frac{\partial}{\partial p}\right) \phi(p,t)\, dp$$

$$\langle x \rangle = \int \Psi^* \, x \, \Psi \, dx =$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{ipx/\hbar} \phi(p,t)\, dp$$

$$= \frac{1}{2\pi\hbar} \int dp' \int dp \int dx \; e^{-ip'x/\hbar} \phi^*(p',t) \underbrace{x \, e^{ipx/\hbar} \phi(p,t)}$$

$$\frac{\hbar}{i}\frac{\partial}{\partial p} e^{ipx/\hbar}$$

$$= \frac{1}{2\pi\hbar} \int dp' \int dp \int dx \; e^{-ip'x/\hbar} \phi^*(p',t) \frac{\hbar}{i} \left(\frac{\partial}{\partial p} e^{ipx/\hbar}\right) \phi(p,t)$$

$$= \frac{1}{2\pi\hbar} \int dp' \int dx \; e^{-ip'x/\hbar} \phi^*(p',t) \frac{\hbar}{i} \left[ \cancel{e^{ipx/\hbar} \phi(p,t)\Big|_{-\infty}^{\infty}} - \int e^{ipx/\hbar} \frac{\partial}{\partial p}\phi(p,t)\, dp \right]$$

$$= \underbrace{\frac{1}{2\pi\hbar} \int dp' \int dp \; \phi^*(p',t) \int dx \; e^{i(p-p')x/\hbar}}_{\delta(p-p')} \left[ \left(-\frac{\hbar}{i}\frac{\partial}{\partial p}\right) \phi(p,t) \right]$$

$$= \int dp \; \phi^*(p,t) \left(-\frac{\hbar}{i}\frac{\partial}{\partial p}\right) \phi(p,t)$$

$$Q(\hat{x}, \hat{p}) \longrightarrow \begin{cases} Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right) \\ Q\left(-\frac{\hbar}{i}\frac{\partial}{\partial p}, p\right) \end{cases}$$

# QM in 3D

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

$$H = \frac{p^2}{2m} + V = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + V(x,y,z)$$

$$\left.\begin{aligned} p_x &= \frac{\hbar}{i}\frac{\partial}{\partial x} \\ y & \qquad\quad y \\ z & \qquad\quad z \end{aligned}\right\} \quad \boxed{\vec{p} = \frac{\hbar}{i}\vec{\nabla}}$$

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi}$$

$$\underline{\text{Laplacian}} \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

~~dens.~~ prob. dens. $|\Psi(x,y,z,t)|^2$

prob. to find particle in infinitesimal volume in time $\underline{t}$

$$|\Psi(x,y,z,t)|^2 \, dx\, dy\, dz = |\Psi(\vec{r},t)|^2 \, d^3\vec{r}$$

$$\int |\Psi(\vec{r},t)|^2 \, d^3\vec{r} = 1$$

if potential is indep. of time

$V(x,y,z,\cancel{t})$

stationary states

$\hookrightarrow \Psi_n(\vec{r},t) = \psi_n(\vec{r})\, e^{-iE_n t/\hbar}$

time-indep. Schröd. eq.

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi}$$

$$\Psi(\vec{r},t) = \sum c_n \psi_n(\vec{r})\, e^{-iE_n t/\hbar}$$

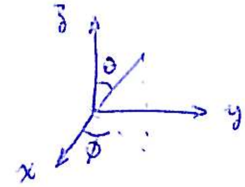
$\longrightarrow \quad [x, p_x] = \hbar i \qquad [x, p_y] = 0$

# Summary - overview

$\longrightarrow$ $V(r)$ : potential depends only on the distance from the origin (classical mech. $\longrightarrow$ central forces)

$\Big\}$ Coulomb $\boxed{\text{const}/r}$ gravitational $\boxed{\text{const}/r}$

<u>spherical coordinates</u>: $x = r \sin\theta \cos\phi$
$y = r \sin\theta \sin\phi$
$z = r\cos\theta$




<u>time-indep.</u> Schröd. eq.

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi \Rightarrow \quad (\text{Eq. } 4.14)$$

$\downarrow$

strategy to solve it

$\longrightarrow$ separation of variables: $\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$

$\downarrow$

every step has a constant associated with it

<u>before</u>

- position vs. time $\Rightarrow$ $\boxed{E}$ was the const ($\boxed{\text{energy}}$ is conserved)

each conserved quantity has a quantum number associated with it

E (quantized) $\longrightarrow$ n $\rightarrow$ $\boxed{\text{principal quantum number}}$

<u>now</u>

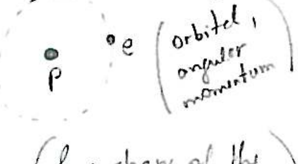
- $r$ vs. angles $\Rightarrow$ $\boxed{l(l+1)}$ is the const

$l$ associated with cons. of total $\boxed{\text{angular momentum}}$
azimuthal quantum number

- $\Theta$ vs $\phi$ $\Rightarrow$ $\boxed{m^2}$ is the const.

m associated with cons. of $\boxed{\text{angular momentum in } z}$
($m \rightarrow$ orientation of the orbital) magnetic quantum number

hydrogen atom




($l \rightarrow$ shape of the orbital)

→) 3 equations to solve

◦) $\Phi(\phi) \to m \to$ easy $\to \Phi(\phi) = e^{im\phi}$

put m into next eq which now deps on $\ell$

◦) $\Theta(\theta) \to \ell \to P_\ell^m(\cos\theta)$ } associated Legendre function

$Y_\ell^m(\theta,\phi) = \Theta(\theta)\,\Phi(\phi)$

$Y_\ell^m(\theta,\phi) = (\text{Norm})\, e^{im\phi} P_\ell^m(\cos\theta)$

SPHERICAL HARMONICS

◦) $R(r) \to n$ (E: energy) $\to$ solution depends on the potential $V(r)$

◦) infinite spherical well

◦) hydrogen atom / Coulomb $\frac{\text{const}}{r}$

→) Hydrogen atom

$$\boxed{E_n = \frac{E_1}{n^2}} \qquad n = 1, 2, 3 \ldots$$

$E_1 = -13.6\ \text{eV}$ (ground state energy)

$$E_1 = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]$$

mass, charge, permittivity of space

$E_1 = -13.6\ \text{eV}$ (binding energy)

$E_2 = -3.4\ \text{eV}$

↳ easier to ionize the atom

associated Laguerre polynomial

$$\boxed{\psi_{n\ell m} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}}\; e^{-r/na}\left(\frac{2r}{na}\right)^\ell \left[L_{n-\ell-1}^{2\ell+1}(2r/na)\right] Y_\ell^m(\theta,\phi)}$$

→ orthogonal since $Y_\ell^m$ are orthogonal

$$\boxed{a \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2}} = 0.529 \times 10^{-10}\ \text{m}$$

→ most probable position of the electron in the ground state

↳ Bohr radius

(spherical harmonics)

→) algebraic method for $Y_\ell^m(\theta, \phi)$

idea is to look at angular momentum $\vec{L} = \vec{r} \times \vec{p}$

•) $L_x, L_y, L_z$ → DO NOT commute
⇓
CAN NOT know all 3 directions

don't share same eigenfunctions

•) $L_x, L_y, L_z$ commute with square of the total angular momentum

$$L^2 \equiv L_x^2 + L_y^2 + L_z^2$$

$L^2$ and $L_i$ share the same eigenfunctions

spherical harmonics $Y_\ell^m$ are eigenfunctions of $L_z$ and $L^2$

$$\boxed{L^2 Y_\ell^m = \hbar^2 \ell(\ell+1) Y_\ell^m} \quad \text{and} \quad \boxed{L_z Y_\ell^m = \hbar m Y_\ell^m}$$

use ladder operators

$$L_\pm \equiv L_x \pm i L_y$$

→) $H, L^2, L_z$ commute, are compatible observables, have the same eigenfunctions

$$H\psi = E\psi \qquad L^2\psi = \hbar^2 \ell(\ell+1)\psi \qquad L_z\psi = \hbar m \psi$$

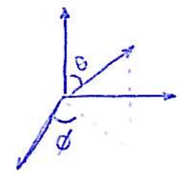
HW. 4.2, 4.3, 4.13(a), 4.18, 4.19

## Spherical coordinates

$z = r\cos\theta$

$x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$




$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi} \leftarrow \text{time indep. Schröd. eq.}$$

$\psi(r,\theta,\phi)$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\overset{\text{partial}}{\frac{\partial}{\partial r}}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\overset{\text{partial}}{\frac{\partial}{\partial\theta}}\left(\sin\theta\frac{\partial}{\partial\theta}\psi\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right] + V\psi = E\psi$$

◦) $V(r) \leftarrow$ only $r$

◦) look for solutions that are separable

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$$

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{r^2}\overset{\text{ordinary}}{\frac{d}{dr}}\left(r^2\frac{dR}{dr}\right) + \frac{R}{r^2\sin\theta}\overset{\text{partial}}{\frac{\partial}{\partial\theta}}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] + V(r)RY = ERY$$

$$\times\frac{1}{RY}\times\left(-\frac{2mr^2}{\hbar^2}\right)$$

$$\underbrace{\left\{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left[V(r) - E\right]\right\}}_{\boxed{l(l+1)}} + \underbrace{\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2}\right\}}_{\boxed{-l(l+1)}} = 0$$

radial equation — const

angular equation — const

## Angular Equation

$\times \left( Y \sin^2\theta \right)$

$$\hookrightarrow \quad \sin\theta \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = -\ell(\ell+1)\sin^2\theta \, Y$$

separation of variables

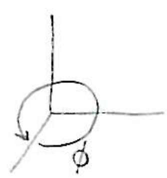
$$Y(\theta,\phi) = \Theta(\theta)\,\Phi(\phi)$$

$\times \dfrac{1}{\Theta\Phi}$

$$\hookrightarrow \quad \underbrace{\frac{1}{\Theta}\left[\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right)\right] + \ell(\ell+1)\sin^2\theta}_{m^2} + \underbrace{\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}}_{-m^2} = 0$$

•) $\dfrac{d^2\Phi}{d\phi^2} = -m^2\,\Phi \Rightarrow \boxed{\Phi(\phi) = e^{im\phi}}$ //     $m$ ⊕ and ⊖

const absorbed in $\Theta$




after $2\pi$ back to the same point

$$\hookrightarrow \quad \Phi(\phi + 2\pi) = \Phi(\phi)$$

$$\hookrightarrow \quad e^{im2\pi} = 1 \quad \Rightarrow \quad \underline{\overline{m = 0, \pm 1, \pm 2, \dots}}$$

c) The $\theta$ equation

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + \left[\ell(\ell+1)\sin^2\theta - m^2\right]\Theta = 0$$

$$\boxed{\Theta(\theta) = A\, P_\ell^m(\cos\theta)}$$

associated Legendre function

$$P_\ell^m(x) \equiv (1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|} \underbrace{P_\ell(x)}_{\text{Legendre polynomial}}$$

$$P_\ell(x) \equiv \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell$$

$\Rightarrow$ $\ell \geq 0$ because there is no factorial of $-\ell$

Exs. $P_0(x) = 1$

$P_1(x) = \frac{1}{2}\frac{d}{dx}(x^2-1) = x$

$\vdots$

$|m| < \ell$ (if $|m| > \ell \Rightarrow P_\ell^m = 0$ because $P_\ell$ is a polynomial of degree $\ell$)

therefore:

$$\boxed{\Theta(\theta) = A\, P_\ell^m(\cos\theta)}$$

with $\boxed{\ell \geq 0}$ integer (azimuthal quantum number) and $\boxed{|m| < \ell}$ (magnetic quantum number)

$\Rightarrow$ $m = \underbrace{-\ell, -\ell+1, \ldots, -1, 0, +1, \ldots \ell-1, \ell}_{(2\ell+1)\text{ values}}$

Normalization

$$\int |\psi|^2 \, d^3\vec{r} = \iiint |\psi|^2 \, r^2 \sin\theta \, dr \, d\theta \, d\phi$$

$$= \underbrace{\int_0^\infty |R|^2 r^2 \, dr}_{1} \; \underbrace{\int_0^{2\pi} d\phi \int_0^\pi \sin\theta \, d\theta \, |Y|^2}_{1} = 1$$

it is convenient to normalize radial and angular parts separately

Normalized angular wave function $\rightarrow$ SPHERICAL HARMONICS

$$\boxed{Y_\ell^m(\theta,\phi) = \epsilon \sqrt{\frac{(2\ell+1)}{4\pi} \frac{(\ell-|m|)!}{(\ell+|m|)!}} \; e^{im\phi} \, P_\ell^m(\cos\theta)}$$

$$\begin{cases} \epsilon = (-1)^m & \text{for } m \geq 0 \\ \epsilon = 1 & \text{for } m \leq 0 \end{cases}$$

they are orthogonal

$$\int_0^{2\pi} d\phi \int_0^\pi \sin\theta \, d\theta \, \left(Y_\ell^m\right)^* \left(Y_{\ell'}^{m'}\right) = \delta_{\ell\ell'} \, \delta_{mm'}$$

Prob. 4.3 ([illegible])

$$Y_0^0 = (-1)^0 \sqrt{\frac{1}{4\pi}}\; e^0\; P_0^0(\cos\theta) = \boxed{\left(\frac{1}{4\pi}\right)^{1/2}}$$

$$Y_2^1 = (-1)^1 \sqrt{\frac{5}{4\pi}\;\frac{1}{3!}}\; e^{i\phi}\; P_2^1(\cos\theta)$$

$$P_2^1(x) = \sqrt{1-x^2}\;\frac{d}{dx}\;\underbrace{\frac{1}{4 \cdot 2!}\;\frac{d^2}{dx^2}\;(x^2-1)^2}$$

$$\frac{1}{8}\,\frac{d}{dx}\left[2\,(x^2-1)\,(2x)\right] = \frac{1}{4}\left[(2x)^2 + 2(x^2-1)\right] = \frac{3x^2-1}{2}$$

$$P_2^1(x) = \sqrt{1-x^2}\;\; 3x$$

$$Y_2^1 = -\sqrt{\frac{5}{24\pi}}\; e^{i\phi}\; 3\cos\theta\,\sin\theta \;=\; \boxed{-\sqrt{\frac{15}{8\pi}}\;\sin\theta\,\cos\theta\; e^{i\phi}}$$

Hw. [illegible] AND 4.2

## Angular Momentum

$l, m \rightarrow$ related to angular momentum

$\vec{L} = \vec{r} \times \vec{p}$

$$\begin{tikzcd} x \arrow[r, bend left] & y \arrow[r, bend left] & z \arrow[ll, bend left] \end{tikzcd}$$

$$\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = \hat{i}\,\underbrace{(y p_z - z p_y)}_{L_x} + \hat{j}\,\underbrace{(z p_x - x p_z)}_{L_y} + \hat{k}\,\underbrace{(x p_y - y p_x)}_{L_z}$$

$L_x, L_y, L_z \rightarrow$ incompatible, they cannot be determined at the same time
do not share the same eigenvectors

$$[L_x, L_y] = \left[(y p_z - z p_y), (z p_x - x p_z)\right] = y p_x \underbrace{[p_z, z]}_{-\hbar i} + p_y x \underbrace{[z, p_z]}_{\hbar i} =$$

$$= \hbar i\,(x p_y - y p_x) = \boxed{\hbar i\, L_z}$$

$\boxed{[L_y, L_z] = i\hbar L_x}$ $\qquad$ $\boxed{[L_z, L_x] = i\hbar L_y}$

$$\sigma_{L_x}^2 \sigma_{L_y}^2 \geq \underbrace{\left(\frac{\langle [L_x, L_y] \rangle}{2i}\right)^2}_{\frac{\langle i\hbar L_z \rangle}{2i}} \qquad \sigma_{L_x}^2 \sigma_{L_y}^2 \geq \frac{\hbar^2 \langle L_z \rangle^2}{4} \Rightarrow \boxed{\sigma_{L_x} \sigma_{L_y} \geq \frac{\hbar}{2} |\langle L_z \rangle|}$$

$$\boxed{\begin{tikzcd} L_x \arrow[r, bend left, "i\hbar L_z"] & L_y \arrow[r, bend left, "i\hbar L_x"] & L_z \arrow[ll, bend left, "i\hbar L_y"] \end{tikzcd}}$$

for the commutators

Square of the total angular momentum

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$\left[L^2, \begin{matrix} L_x \\ L_y \\ L_z \end{matrix}\right] = 0 \quad \longleftrightarrow \quad [L^2, \vec{L}] = 0$$

$$[L^2, L_x] = [L_y^2, L_x] + [L_z^2, L_x]$$

$[AB, C] = A[B,C] + [A,C]B$

$$\downarrow$$

$$= L_y \underbrace{[L_y, L_x]}_{-i\hbar L_z} + \underbrace{[L_y, L_x]}_{-i\hbar L_z} L_y + L_z \underbrace{[L_z, L_x]}_{i\hbar L_y} + \underbrace{[L_z, L_x]}_{i\hbar L_y} L_z = \boxed{0}$$

$L^2$ is compatible with each component $L_x, L_y, L_z$

→) Let us pick $L_z$ and find the eigenfunctions shared by $L^2$ and $L_z$

$$\boxed{L^2 f = \lambda f} \quad \text{and} \quad \boxed{L_z f = \mu f}$$

→) to find $\lambda, \mu$, we introduce the ladder operators

$$\boxed{L_\pm \equiv L_x \pm i L_y}$$

$$\boxed{[L^2, L_\pm] = 0}$$

$$[L_z, L_\pm] = \underbrace{[L_z, L_x]}_{i\hbar L_y} \pm i \underbrace{[L_z, L_y]}_{-i\hbar L_x} = \pm\hbar(L_x \pm i L_y) = \boxed{\pm \hbar L_\pm}$$

Therefore, if $f$ is an eigenfunction of $L^2, L_z$

then $(L_\pm f)$ is also their eigenfunction, because

$$L^2 (L_\pm f) \overset{[L^2, L_\pm]=0}{=} L_\pm (L^2 f) = \boxed{\lambda (L_\pm f)}$$

$$L_z (L_\pm f) = L_\pm \underbrace{L_z f}_{\mu f} \pm \hbar L_\pm f = \boxed{(\mu \pm \hbar)(L_\pm f)}$$

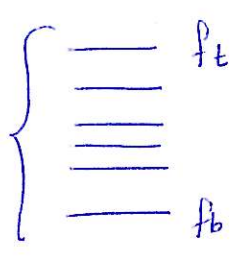
$$\Downarrow$$

$L_+$ : raising operator

$L_-$ : lowering operator

→) For each value $\lambda$, there is a ladder of eigenstates of $L_z$ with eigenvalues separated by $\hbar$

they are all degenerate in $L^2$, i.e., they all have the same eigenvalue $\lambda$




the lowest and highest eigenvalues of $L_z$ are limited by $\lambda$

$$\begin{cases} L_z f_t = \mu_t f_t \\ L_+ f_t = 0 \end{cases}$$ because $\mu$ cannot be $> \lambda$

$$\begin{cases} L_z f_b = \mu_b f_b \\ L_- f_b = 0 \end{cases}$$

∘) Let us write

$$L_z f_t = \hbar l f_t \qquad L_z f_b = \hbar \bar{l} f_b$$

and see how $\hbar l$ and $\hbar \bar{l}$ relate to $\lambda$

$$L_{\pm}L_{\mp} = (L_x \pm iL_y)(L_x \mp iL_y) = L_x^2 \mp i\overbrace{(L_xL_y - L_yL_x)}^{i\hbar L_z} + L_y^2$$

$$= L_x^2 + L_y^2 + L_z^2 - L_z^2 \pm \hbar L_z$$

$$= L^2 - L_z^2 \pm \hbar L_z$$

$$\boxed{L^2 = L_{\pm}L_{\mp} + L_z^2 \mp \hbar L_z}$$

$$L^2 f_t = (\cancel{L_-L_+} + L_z^2 + \hbar L_z) f_t = (\hbar^2 \ell^2 + \hbar^2 \ell) f_t = \boxed{\hbar^2 \ell(\ell+1) f_t}$$

$$L^2 f_b = (\cancel{L_+L_-} + L_z^2 - \hbar L_z) f_b = (\hbar^2 \bar{\ell}^2 - \hbar^2 \bar{\ell}) f_b = \boxed{\hbar^2 \bar{\ell}(\bar{\ell}-1) f_b}$$

since from $f_b$ to $f_t$, they all have the same eigenvalue $\lambda$ $\left\{ \begin{array}{l} L^2 f_t = \lambda f_t \\ \vdots \\ L^2 f_b = \lambda f_b \end{array} \right.$

$$\Rightarrow \ell(\ell+1) = \bar{\ell}(\bar{\ell}-1) \Rightarrow \begin{cases} \bar{\ell} = \cancel{\ell+1} & \text{which makes no sense} \\ \boxed{\bar{\ell} = -\ell} \end{cases}$$

$$L_z f_b = \hbar \bar{\ell} f_b = (-\hbar \ell) f_b$$

Raising

$$L_z(L_+ f_b) = L_+ L_z f_b + \hbar L_+ f_b = (-\hbar \ell + \hbar)(L_+ f_b)$$

$$\vdots$$

$$L_z f_t = (\hbar \ell) f_t$$

$$\Rightarrow \boxed{L_z f = \hbar m f} \quad \text{where} \quad m = \underbrace{-\ell, -\ell+1, -\ell+2, \ldots, 0, 1, \ldots \ell-1, \ell}_{(2\ell+1)}$$

$$\boxed{L^2 f_\ell^m = \hbar^2 \ell(\ell+1) f_\ell^m} \qquad \boxed{L_z f_\ell^m = \hbar m f_\ell^m}$$

$$\boxed{f_\ell^m = Y_\ell^m}$$

- By the algebraic method we found the eigenvalues of $L^2$ and $L_z$

- We now ~~construct~~ find the eigenfunctions
and show that they are the spherical harmonics

$$f_l^m = Y_l^m$$

- $L^2$ and $L_z$ are hermitian
$\hookrightarrow$ $Y_l^m$ are orthogonal (for $\neq$ eigenvalues)

$$\vec{L} = \vec{r} \times \vec{p} = \frac{\hbar}{i}\, \vec{r} \times \vec{\nabla}$$

(extra material) $\rightarrow$ $\left\{ \begin{array}{l} \vec{\nabla} = \hat{r} \dfrac{\partial}{\partial r} + \hat{\theta} \dfrac{1}{r} \dfrac{\partial}{\partial \theta} + \hat{\phi} \dfrac{1}{r\sin\theta} \dfrac{\partial}{\partial \phi} \\ \vec{r} = r\,\hat{r} \end{array} \right.$  $\hat{r}, \hat{\theta}, \hat{\phi}$ } unit vectors

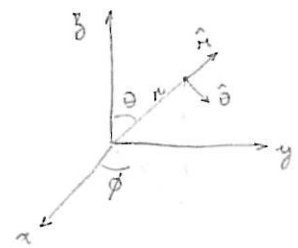
$$\vec{L} = \frac{\hbar}{i} \left[ r \cancel{(\hat{r} \times \hat{r})} \frac{\partial}{\partial r} + (\hat{r} \times \hat{\theta}) \frac{\partial}{\partial \theta} + (\hat{r} \times \hat{\phi}) \frac{1}{\sin\theta} \frac{\partial}{\partial \phi} \right]$$

$$\hat{r} \times \hat{\theta} = \begin{vmatrix} \hat{r} & \hat{\theta} & \hat{\phi} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{vmatrix} = \hat{\phi} \qquad \hat{r} \times \hat{\phi} = \begin{vmatrix} \hat{r} & \hat{\theta} & \hat{\phi} \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{vmatrix} = -\hat{\theta}$$

$$\boxed{\vec{L} = \frac{\hbar}{i} \left[ \hat{\phi} \frac{\partial}{\partial \theta} - \hat{\theta} \frac{1}{\sin\theta} \frac{\partial}{\partial \phi} \right]}$$

since (extra material) $\rightarrow$ $\left\{ \begin{array}{l} \hat{\theta} = \cos\theta \cos\phi\, \hat{\imath} + \cos\theta \sin\phi\, \hat{\jmath} - \sin\theta\, \hat{k} \\ \hat{\phi} = -\sin\phi\, \hat{\imath} + \cos\phi\, \hat{\jmath} \end{array} \right.$

$$x = r \sin\theta \cos\phi$$
$$y = r \sin\theta \sin\phi$$
$$z = r \cos\theta$$




$$\boxed{\vec{r} = r\,\hat{r} = r\left[\sin\theta\cos\phi\,\hat{\imath} + \sin\theta\sin\phi\,\hat{\jmath} + \cos\theta\,\hat{k}\right]}$$

• $\hat{r} = \dfrac{\frac{\partial \vec{r}}{\partial r}}{\left|\frac{\partial \vec{r}}{\partial r}\right|} = \boxed{\sin\theta\cos\phi\,\hat{\imath} + \sin\theta\sin\phi\,\hat{\jmath} + \cos\theta\,\hat{k}}$

• $\hat{\theta} = \dfrac{\frac{\partial \vec{r}}{\partial \theta}}{\left|\frac{\partial \vec{r}}{\partial \theta}\right|}$

$$\frac{\partial \vec{r}}{\partial \theta} = r\left[\cos\theta\cos\phi\,\hat{\imath} + \cos\theta\sin\phi\,\hat{\jmath} - \sin\theta\,\hat{k}\right]$$

$$\left|\frac{\partial \vec{r}}{\partial \theta}\right| = \sqrt{r^2\left(\cos^2\theta\cos^2\phi + \cos^2\theta\sin^2\phi + \sin^2\theta\right)} = r$$

$$\Rightarrow \boxed{\hat{\theta} = \cos\theta\cos\phi\,\hat{\imath} + \cos\theta\sin\phi\,\hat{\jmath} - \sin\theta\,\hat{k}}$$

• $\hat{\phi} = \dfrac{\frac{\partial \vec{r}}{\partial \phi}}{\left|\frac{\partial \vec{r}}{\partial \phi}\right|}$

$$\frac{\partial r}{\partial \phi} = r\left[-\sin\theta\sin\phi\,\hat{\imath} + \sin\theta\cos\phi\,\hat{\jmath}\right]$$

$$\left|\frac{\partial r}{\partial \phi}\right| = \sqrt{r^2\left(\sin^2\theta\sin^2\phi + \sin^2\theta\cos^2\phi\right)} = r\sin\theta$$

$$\Rightarrow \boxed{\hat{\phi} = -\sin\phi\,\hat{\imath} + \cos\phi\,\hat{\jmath}}$$

$$\vec{L} = \overbrace{\frac{\hbar}{i}\left(-\sin\phi\frac{\partial}{\partial\theta} - \underbrace{\frac{1}{\sin\theta}\cos\theta}_{\cot g\theta}\cos\phi\frac{\partial}{\partial\phi}\right)}^{L_x}\hat{i}$$

$$+\overbrace{\frac{\hbar}{i}\left(\cos\phi\frac{\partial}{\partial\theta} - \underbrace{\frac{1}{\sin\theta}\cos\theta}_{\cot g\theta}\sin\phi\frac{\partial}{\partial\phi}\right)}^{L_y}\hat{j}$$

$$+\underbrace{\frac{\hbar}{i}\frac{\cancel{\sin\theta}}{\cancel{\sin\theta}}\frac{\partial}{\partial\phi}}_{L_z}\hat{k}$$

$$\boxed{L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}}$$

$$L_\pm = L_x \pm i L_y$$

$$L_\pm = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_+L_- = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + i\frac{\partial}{\partial\phi}\right)$$

$$L^2 = L_+L_- + L_z^2 - \hbar L_z$$

$$L^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \underbrace{\cot^2\theta\frac{\partial^2}{\partial\phi^2} + \cancel{i\frac{\partial}{\partial\phi}} + \frac{\partial^2}{\partial\phi^2}}_{\frac{\cos^2\theta+\sin^2\theta}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}} + \cancel{\frac{1}{i}\frac{\partial}{\partial\phi}}\right)$$

$$= \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)$$

$$\boxed{L^2 = -\hbar^2 \left[ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \right]}$$

we saw that the eigenvalues of $L^2$ were $\hbar^2 \ell(\ell+1)$:

$$L^2 f_\ell^m = \hbar^2 \ell(\ell+1) f_\ell^m$$

$\hookrightarrow$ but this is Eq (4.18) in the book $\rightarrow$ the angular equation leading the spherical harmonics $Y_\ell^m$

$\Rightarrow \boxed{f_\ell^m = Y_\ell^m}$

Notice that, as we showed before, $f_\ell^m$ is an eigenfunction of $L_z$

$$\boxed{L_z f_\ell^m = \hbar m f_\ell^m}$$

$$\hookrightarrow \frac{\hbar}{i}\frac{\partial}{\partial\phi} f_\ell^m = \hbar m f_\ell^m$$

Therefore: spherical harmonics are eigenfunctions of $L^2$ and $L_z$

$H, L^2, L_z \rightarrow$ commute, share the same eigenfunctions

$$H\Psi = E\Psi \qquad L^2\Psi = \hbar^2 \ell(\ell+1)\Psi \qquad L_z\Psi = \hbar m \Psi$$

<u>Obs</u> $m = -\ell, -\ell+1, \dots 0, \dots, \ell-1, \ell$

when studying $L_+, L_-$, we saw that maximum $\ell$ is obtained starting from $-\ell$ after $N$ steps

$$-\ell + N = \ell \Rightarrow \boxed{\ell = N/2} \Rightarrow \ell \text{ is integer or half-integer}$$

this is different from what we obtained with the separation of variables

(more comments later ...)

## Radial Equation

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left[V(r) - E\right]R = l(l+1)\,R$$

change variables: $u(r) \equiv r\,R(r)$

$R = \frac{u}{r}$ $\qquad \frac{dR}{dr} = \frac{1}{r}\frac{du}{dr} - \frac{u}{r^2} = \boxed{\frac{r\,(du/dr) - u}{r^2}}$

$$\frac{d}{dr}\left[r^2 \frac{dR}{dr}\right] = \frac{d}{dr}\left[r\,\frac{du}{dr} - u\right]$$

$$= \frac{du}{dr} + r\frac{d^2u}{dr^2} - \frac{du}{dr} = \boxed{r\,\frac{d^2u}{dr^2}}$$

the equation becomes

$$r\frac{d^2u}{dr^2} - \frac{2mr^2}{\hbar^2}V\frac{u}{r} - l(l+1)\frac{u}{r} = -\frac{2mr^2}{\hbar^2}E\frac{u}{r}$$

$(\times)\ -\frac{\hbar^2}{2mr}$

$$\hookrightarrow\ -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \underbrace{\left[V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]}_{V_{eff}\ \text{(effective potential)}} u = E\,u$$

Normalization condition: $\int_0^\infty |R|^2 r^2\,dr = \boxed{\int_0^\infty |u|^2\,dr = 1}$

$\boxed{\text{Students go through Example 4.1}} \leftarrow$ HW

# Hydrogen Atom

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$$

Defining

$$K \equiv \frac{\sqrt{-2mE}}{\hbar}$$ $E < 0$ for bound states

$\div$ Eq. (4.53) by $E$

$$\hookrightarrow \frac{1}{K^2}\frac{d^2u}{dr^2} = \left[1 - \frac{me^2}{2\pi\epsilon_0\hbar^2 K}\frac{1}{Kr} + \frac{l(l+1)}{(Kr)^2}\right]u$$

Introducing

$$\rho \equiv Kr \qquad \rho_0 \equiv \frac{me^2}{2\pi\epsilon_0\hbar^2 K}$$

$$\boxed{\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]u}$$

Asymptotic solutions

$$\rho \to \infty \Rightarrow \frac{d^2u}{d\rho^2} = u$$

$$u(\rho) = Ae^{-\rho} + \underbrace{Be^{\rho}}_{\text{blows up for } \rho\to\infty}$$

$\hookrightarrow B = 0$

$$\boxed{u(\rho) \sim Ae^{-\rho}}$$

$$\rho \to 0 \Rightarrow \frac{d^2u}{d\rho^2} = \frac{l(l+1)}{\rho^2}u$$

$$u(\rho) = C\rho^{l+1} + \underbrace{D\rho^{-l}}_{\text{blows up for } \rho\to 0}$$

$\hookrightarrow D = 0$

$$\boxed{u(\rho) \sim C\rho^{l+1}}$$

This is done so that now we can write $\boxed{u(\rho) = \rho^{l+1}e^{-\rho}v(\rho)}$

and hope that $v(\rho)$ will be easier to find than $u(\rho)$

$$\frac{du}{d\rho} = l+1\, \rho^{l} e^{-\rho} v - \rho^{l+1} e^{-\rho} v + \rho^{l+1} e^{-\rho} \frac{dv}{d\rho} = \rho^{l} e^{-\rho} \left[ (l+1-\rho) v + \rho \frac{dv}{d\rho} \right]$$

$$\frac{d^2u}{d\rho^2} = l \rho^{l-1} e^{-\rho} [\quad] - \rho^{l} e^{-\rho} [\quad] + \rho^{l} e^{-\rho} \left[ - v + (l+1-\rho) \frac{dv}{d\rho} + \frac{dv}{d\rho} + \rho \frac{d^2v}{d\rho^2} \right]$$

$$= \rho^{l} e^{-\rho} \left[ \frac{l(l+1-\rho) v}{\rho} + \frac{l \rho\, dv/d\rho}{\rho} - (l+1-\rho) v - \rho \frac{dv}{d\rho} - v + (l+1-\rho) \frac{dv}{d\rho} + \frac{dv}{d\rho} + \rho \frac{d^2v}{d\rho^2} \right]$$

$$= \rho^{l} e^{-\rho} \left\{ \left[ -2l - 2 + \rho + \frac{l(l+1)}{\rho} \right] v + (2l + 2 - 2\rho) \frac{dv}{d\rho} + \rho \frac{d^2v}{d\rho^2} \right\}$$

Putting all together in the radial equation

$$\rho^{l} e^{-\rho} \left\{ \rho \frac{d^2v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + \left[ -2l - 2 + \cancel{\rho} + \frac{l(l+1)}{\rho} - \rho \left( \cancel{1} - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2} \right) \right] v \right\} = 0$$

$$\Rightarrow \quad \boxed{\rho \frac{d^2v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + [\rho_0 - 2(l+1)] v = 0}$$

Assume the solution $v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$ (power series in $\rho$)

we need to find the coefficients

$$\begin{cases} \dfrac{dv}{d\rho} = \sum_{j=0}^{\infty} j c_j \rho^{j-1} = \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^j \\ \dfrac{d^2v}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^{j-1} \end{cases}$$

our goal is to have all terms in the radial eq with the same power: $\rho^j$

can rewrite as $\sum_{j=1}^{\infty} j c_j \rho^j$ and it makes no difference if we include $j=0$ $\rightarrow \sum_{j=0}^{\infty} j c_j \rho^j$

in the radial eq. for $v$:

$$\sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^{j} + 2(l+1) \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^j - 2 \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^{j+1} + [\rho_0 - 2(l+1)] \sum_{j=0}^{\infty} c_j \rho^j = 0$$

Equating the coefficients

$$j(j+1)\,c_{j+1} + 2(l+1)(j+1)\,c_{j+1} - 2j\,c_j + [\rho_0 - 2(l+1)]\,c_j = 0$$

$$c_{j+1} = \left\{ \frac{2(j+l+1)-\rho_0}{(j+1)(j+2l+2)} \right\} c_j \quad \leftarrow \text{ recursion formula for } c_j$$

(start with $c_0$ → found later with normalization)

For large $j$

$$c_{j+1} \cong \frac{2j}{j(j+1)}\, c_j = \frac{2}{j+1}\, c_j$$

(Obs: could drop 1 in $j+1$; we are keeping it for cleaner expressions)

$$\Rightarrow c_1 = \frac{2}{1} c_0$$

$$c_2 = \frac{2 c_1}{2} = \frac{2^2}{2.1} c_1$$

$$c_3 = \frac{2}{3} c_2 = \frac{2^3}{3.2.1} c_0 \Rightarrow \boxed{c_j = \frac{2^j}{j!} c_0} \Rightarrow v(\rho) = c_0 \sum_{j=0}^{\infty} \frac{2^j}{j!} \rho^j$$

$\to e^{2\rho}$

$$\Rightarrow u(\rho) = \rho^{l+1} e^{-\rho} v(\rho) = \boxed{c_0 \rho^{l+1} e^{\rho}}$$

→ but it blows up for $\rho \to \infty$

therefore, the series must terminate

$$c_{j_{max}+1} = 0 \Rightarrow \boxed{2(j_{max} + l + 1) - \rho_0 = 0}$$

numerator in the recursion formula

Defining:

$$\boxed{n \equiv j_{max} + l + 1} \Rightarrow \boxed{\rho_0 = 2n}$$

principal quantum number

$\rho_0 = 2n \quad , \quad \rho_0 = \frac{me^2}{2\pi\epsilon_0 \hbar^2 K} \quad , \quad K^2 = -\frac{2mE}{\hbar^2}$

$$\Rightarrow \frac{2mE}{\hbar^2} = -\left(\frac{me^2}{2\pi\epsilon_0\hbar^2}\right)^2 \frac{1}{4n^2}$$

$$\boxed{E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n_2}}$$ $n = 1, 2, 3, \ldots$

Bohr formula (obtained in 1913 by mixing classical phys. while (Schröd. eq. in 1924)

$$\boxed{a \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}\,m} \leftarrow \text{Bohr radius} \Rightarrow \begin{cases} \rho_0 = me^2/2\pi\epsilon_0\hbar^2 K \\ \rho_0 = 2/aK = 2n \\ \boxed{K = \frac{1}{an}} \end{cases}$$

$$\boxed{\rho = \frac{r}{an}}$$

$\boxed{n=1} \Rightarrow E_1 = -13.6\,eV$ ground state

$\boxed{n=2} \Rightarrow E_2 = \frac{-13.6\,eV}{4} = -3.4\,eV$

→) Spatial wave functions for hydrogen are labeled by 3 quantum numbers $(n, l, m)$

$$\Psi_{nlm}(r, \theta, \phi) = R_{nl}(r)\, Y_l^m(\theta, \phi)$$

$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho) \quad , \quad \rho = Kr \quad , \quad R(r) = \frac{u(r)}{r}$

$$R_{nl}(r) = \frac{1}{r}\rho^{l+1} e^{-\rho} v(\rho)$$

polynomial of degree $j_{max}$ $\Big\}$ coefficients determined by recursion formula

Ground state: $\boxed{n=1}$

$$n = j_{max} + \ell + 1 \qquad \begin{cases} j_{max}, \ell \geq 0 \\ n \geq 1 \end{cases}$$

$n = 1 \Rightarrow j_{max} = \ell = 0$

$$\boxed{\ell = 0} \Rightarrow \boxed{m = 0}$$

$$\psi_{100}(r, \theta, \phi) = R_{10}(r)\, Y_0^0(\theta, \phi)$$

•) $j_{max} = 0 \Rightarrow v(\rho) = c_0 \longrightarrow R_{10}(r) = \frac{c_0}{r} \rho e^{-\rho}$

$$\rho = Kr = \frac{r}{an} \xRightarrow{(n=1)} \boxed{R_{10}(r) = \frac{c_0}{a} e^{-r/a}}$$

Normalizing

$$\int_0^\infty |R_{10}|^2 r^2 \, dr = \frac{|c_0|^2}{a^2} \int_0^\infty e^{-2r/a} r^2 \, dr = |c_0|^2 \frac{a}{4} = 1$$

$$\boxed{c_0 = 2/\sqrt{a}}$$

•) $Y_0^0 = 1/\sqrt{4\pi}$

therefore $$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

$E_1 = -13.6 \text{ eV}$

First excited state(s) $\boxed{n=2}$

$$n = j_{max} + l + 1 \implies \begin{cases} j_{max} = 1, & l = 0 \\ j_{max} = 0, & l = 1 \end{cases}$$

$n \to 2$

$$c_{j+1} = \left\{ \frac{2(j+l+1) - \rho_0}{(j+1)(j+2l+2)} \right\} c_j \qquad \rho_0 = 2n$$

$\boxed{l=0} \implies \boxed{m=0}$

$\boxed{l=1} \implies \boxed{m=-1,0,+1}$

four different states with the same energy

o) $j_{max} = 1$, $l = 0$

$j_{max} \to j = 0, 1$

$$c_1 = \frac{2(0+0+1-2)}{(0+1)(0+0+2)} c_0 \implies \boxed{c_1 = -c_0}$$

$$c_2 = \frac{2(1+0+1-2)}{(1+1)(1+0+2)} c_1 \implies \boxed{c_2 = 0}$$

so

$$v(\rho) = c_0 - c_0 \rho = c_0 \left(1 - \frac{r}{2a}\right) \qquad \rho = \frac{r}{2a}$$

$2 \leftarrow n$

$$R_{20}(r) = c_0 \left(1 - \frac{r}{2a}\right) \frac{1}{r} \left(\frac{r}{2a}\right)^1 e^{-r/2a}$$

$$\boxed{R_{20}(r) = \frac{c_0}{2a}\left(1 - \frac{r}{2a}\right) e^{-r/2a}}$$

$\to$ then normalize to find $c_0$

o) $j_{max} = 0$, $l = 1$ $\to v(\rho) = c_0$, $\rho = r/2a$

$$R_{21}(r) = \frac{c_0}{r} \left(\frac{r}{2a}\right)^{1+1} e^{-r/2a}$$

$$\boxed{R_{21}(r) = \frac{c_0}{4a^2} r e^{-r/2a}}$$

$\to$ normalize to find $c_0$

HW

Example 4.1

Prob. 4.11, 4.12, 4.13

Prob. 4.21

For arbitrary n

$$\ell = 0, 1, 2, \dots n-1$$

For each $\ell$

$$m = \underbrace{-\ell, -\ell+1, \dots 0, 1, \dots \ell-1, \ell}_{(2\ell+1)\text{ values}}$$

$\Rightarrow$ The total degeneracy of the energy level $E_n$

$$d(n) = \sum_{\ell=0}^{n-1} (2\ell+1) = 1+3+5+\dots+(2n-1) = \frac{(\text{initial} + \text{final})\left(\begin{smallmatrix}\text{number}\\ \text{of terms}\end{smallmatrix}\right)}{2}$$

(arithmetic series)

$$\boxed{d(n) = n^2}$$

$\rightarrow$ Polynomial $\boxed{v(\rho) = L_{n-\ell-1}^{2\ell+1}(2\rho)}$

where $L_{q-p}^{p}(x) \equiv (-1)^p \left(\frac{d}{dx}\right)^p L_q(x)$ and $L_q(x) \equiv e^x \left(\frac{d}{dx}\right)^q (e^{-x} x^q)$

(associated Laguerre polynomial) (Laguerre polynomial)

$\Rightarrow$ Normalized hydrogen wave functions

$$\boxed{\psi_{n\ell m} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}}\; e^{-r/na} \left(\frac{2r}{na}\right)^\ell \left[L_{n-\ell-1}^{2\ell+1}(2r/na)\right] Y_\ell^m(\theta,\phi)}$$

$\Rightarrow$ Wave functions are orthogonal

$$\int \psi_{n\ell m}^* \psi_{n'\ell'm'} r^2 \sin\theta \, dr \, d\theta \, d\phi = \delta_{nn'} \delta_{\ell\ell'} \delta_{mm'}$$

# SPIN

In classical mechanics

rigid object has

→ orbital angular momentum

$\vec{L} = \vec{r} \times \vec{p}$

(Earth around sun)

→ spin angular momentum

$\vec{S} = I\vec{\omega}$

(Earth daily rotation)

(can be decomposed into orbital angular momenta of constituent parts)

By analogy

In quantum mechanics

→ orbital angular momentum (extrinsic angular momentum)

Ex. $e^-$ around the nucleus in H atom

(spherical harmonics)

→ $\boxed{\text{spin}}$ – nothing to do with motion in space

not $\cancel{f(\theta,\phi,r)}$

$e^-$ is structureless point particle

= INTRINSIC angular momentum $\vec{S}$

Algebraic theory of spin follows that of orbital angular momentum

(formulas derived from rotational invariance in 3D)

$$[S_x, S_y] = i\hbar S_z \qquad [S_y, S_z] = i\hbar S_x \qquad [S_z, S_x] = i\hbar S_y$$

$$\left\{ \begin{aligned} S^2 |sm\rangle &= \hbar^2 s(s+1) |sm\rangle \\ S_z |sm\rangle &= \hbar m |sm\rangle \end{aligned} \right\}$$

Ket notation, because eigenstates of spin are NOT functions

[For $\vec{L}$, we can use $|\ell m\rangle$ (Ket) or $Y_\ell^m(\theta,\phi)$ (function)]

As in Prob. 4.18

$$L_\pm f_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)}\, f_\ell^{m\pm 1}$$

$\left\{ \begin{array}{l} (L_\pm)^\dagger = L_\mp \\ \text{because } L_x, L_y \text{ are hermitian} \end{array} \right.$

$L_\pm f_\ell^m = A_\ell^m f_\ell^{m\pm 1}$

$$\langle f_\ell^m | L_\mp L_\pm | f_\ell^m \rangle = \langle f_\ell^m | L^2 - L_z^2 \mp \hbar L_z | f_\ell^m \rangle = \langle f_\ell^m | \hbar^2 \ell(\ell+1) - \hbar^2 m^2 \mp \hbar^2 m | f_\ell^m \rangle$$

$$\langle L_\pm f_\ell^m | L_\pm f_\ell^m \rangle = |A_\ell^m|^2 = \hbar^2 \ell(\ell+1) - \hbar^2 m(m\pm 1)$$

$$\boxed{A_\ell^m = \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)}}$$

$$\boxed{S_\pm |s\, m\rangle = \hbar\sqrt{s(s+1) - m(m\pm 1)}\; |s\,(m\pm 1)\rangle}$$

Comment : ◦) for orbital angular momentum $\ell$ is a nonnegative integer so that Eq. (4.28) with $\ell!$ makes sense

However, from the algebraic method we saw that $m$ goes from $-\ell$ to $\ell$ in $N$ integer steps $\Rightarrow -\ell + N = \ell$

$\Rightarrow \underbrace{\ell = N/2}$

which says that $\ell$ may be an $\boxed{\text{integer}}$ or a ~~half-integer~~

contradicts separation of variables

◦) for spin angular momentum then $s$ can indeed be integer or half-integer

$\left\{ \begin{array}{l} \pi \text{ meson: } s=0 \\ e^-: s = 1/2 \\ \text{photon: } s=0 \\ \text{graviton: } s=2 \end{array} \right.$

$\boxed{s = 0, 1/2, 1, 3/2, \ldots}$ $\boxed{m = -s, -s+1, \ldots\, s-1, s}$

Every elementary particle has a specific and fixed spin (while $\ell$ can change)

# SPIN 1/2

↳ particles that make ordinary matter
protons, neutrons, electrons
quarks, leptons ($e^-$, neutrinos, muons)

$s = 1/2 \Rightarrow m = -1/2$ or $+1/2 \Rightarrow$ there are only <u>two</u> eigenstates of $S_z$

$$\begin{cases} \boxed{\text{spin up}} \; |\uparrow\rangle \quad \left|\frac{1}{2}\;\frac{1}{2}\right\rangle \longrightarrow \chi_+^{(z)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \boxed{\text{spin down}} \; |\downarrow\rangle \quad \left|\frac{1}{2}\;-\frac{1}{2}\right\rangle \longrightarrow \chi_-^{(z)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{cases}$$

∘) Using these two states as basis vectors, we can write any general state of a spin-1/2 particle as a <u>two-element</u> $\underbrace{\text{column matrix}}_{\text{vector}}$ (<u>spinor</u>)

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_- \qquad \Big\{ \text{general state}$$

notation $\chi_\pm$ or $\chi_\pm^z$ to remember that these are eigenstates of $S_z$

∘) spin operators : <u>2x2 matrices</u>

$$\begin{cases} S^2\chi_+ = \hbar^2 s(s+1)\chi_+ = \frac{3}{4}\hbar^2\chi_+ \\ S^2\chi_- = \frac{3}{4}\hbar^2\chi_- \end{cases}$$

[assuming $\chi_\pm$ are eigenstates of $S^2$ besides $S_z$ (analogy with $L$)]

$$S^2 = \begin{pmatrix} c & d \\ e & f \end{pmatrix}$$

$$S^2\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} c \\ e \end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix} 1 \\ 0 \end{pmatrix} \Longrightarrow \begin{cases} c = 3/4\,\hbar^2 \\ e = 0 \end{cases}$$

$$S^2\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} d \\ f \end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix} 0 \\ 1 \end{pmatrix} \Longrightarrow \begin{cases} d = 0 \\ f = 3/4\,\hbar^2 \end{cases}$$

$$\boxed{S^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}$$

$$\left\{ \begin{aligned} S_z \chi_+ &= \begin{pmatrix} c & d \\ e & f \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ S_z \chi_- &= \begin{pmatrix} c & d \\ e & f \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned} \right\} \quad \boxed{S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

$$S_\pm |s\, m\rangle = \hbar \sqrt{s(s+1) - m(m\pm1)}\; |s\ (m\pm1)\rangle$$

$$\left\{ \begin{aligned} & S_+ \chi_+ = 0 \qquad\qquad S_- \chi_- = 0 \\ & S_+ \chi_- = \hbar \sqrt{1/2\,(3/2) - (-1/2)(-1/2 + 2/2)}\; \chi_+ = \hbar \chi_+ \\ & S_- \chi_+ = \hbar \sqrt{1/2\,(3/2) - (1/2)(1/2 - 2/2)}\; \chi_- = \hbar \chi_- \end{aligned} \right.$$

$S_+$

$$\left\{ \begin{aligned} & \begin{pmatrix} c & d \\ e & f \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow \begin{cases} c = 0 \\ e = 0 \end{cases} \\ & \begin{pmatrix} c & d \\ e & f \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow \begin{cases} d = \hbar \\ f = 0 \end{cases} \end{aligned} \right.$$

$S_-$

$$\left\{ \begin{aligned} & \begin{pmatrix} C & D \\ E & F \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow \begin{cases} D = 0 \\ F = 0 \end{cases} \\ & \begin{pmatrix} C & D \\ E & F \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow \begin{cases} C = 0 \\ E = \hbar \end{cases} \end{aligned} \right.$$

$$\boxed{S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}} \qquad \boxed{S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}}$$

Since $S_\pm = S_x \pm i S_y \Rightarrow S_x = (S_+ + S_-)/2$ and $S_y = (S_+ - S_-)/(2i)$

$$\boxed{S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}} \qquad \boxed{S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}$$

◦) We can write $\vec{S} = \frac{\hbar}{2} \vec{\sigma}$

where

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are PAULI MATRICES

◦) Note: $S_x$, $S_y$, $S_z$, $S^2$ are hermitian (they represent observables)

but $S_+$ and $S_-$ are NOT

◦) The eigenspinors of $S_z$ are $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

eigenvalue $+\hbar/2$ eigenvalue $-\hbar/2$

so if we measure $S_z$

on a particle in a general state $\chi = \begin{pmatrix} a \\ b \end{pmatrix}$

we get $+\hbar/2$ with probability $\boxed{|a|^2}$

and $-\hbar/2$ with probability $\boxed{|b|^2}$

where $|a|^2 + |b|^2 = 1$

because (spinor is NORMALIZED)

◦) What happens if we measure $S_x$ ?

First

We need to write the general state $\chi$ in the basis vectors consisting of the eigenvectors of $S_x$

(eigenspinors)

Eigenvalues and eigenvectors of $S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

characteristic equation

$$\begin{vmatrix} -\lambda & \hbar/2 \\ \hbar/2 & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda^2 = \left(\frac{\hbar}{2}\right)^2 \Rightarrow \boxed{\lambda = \pm \frac{\hbar}{2}}$$

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \pm \frac{\hbar}{2}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \Rightarrow \begin{pmatrix} \beta \\ \alpha \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \Rightarrow \boxed{\beta = \pm \alpha}$$

after normalizing

$$\chi_+^{(x)} = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \qquad \chi_-^{(x)} = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$$

eigenvalue $+\hbar/2$ eigenvalue $-\hbar/2$

Therefore the general state

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = \boxed{\left(\frac{a+b}{\sqrt{2}}\right)\chi_+^{(x)} + \left(\frac{a-b}{\sqrt{2}}\right)\chi_-^{(x)}}$$

If you measure $S_x \Rightarrow \begin{cases} \frac{|a+b|^2}{2} \text{ is the prob. of getting } +\hbar/2 \\ \frac{|a-b|^2}{2} \quad \text{"} \quad -\hbar/2 \end{cases}$

Example 4.2 $\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 1+i \\ 2 \end{pmatrix}$ What are the probs. for $+\hbar/2$ and $-\hbar/2$ if you measure $S_z$ and $S_x$? Compute $\langle S_x \rangle$.

$$S_z \begin{cases} +\hbar/2 \Rightarrow |1+i|^2/6 = \boxed{1/3} \\ -\hbar/2 \Rightarrow 4/6 = \boxed{2/3} \end{cases}$$

$$S_x \begin{cases} +\hbar/2 \Rightarrow |3+i|^2/(6.2) = \boxed{5/6} \\ -\hbar/2 \Rightarrow |-1+i|^2/(6.2) = \boxed{1/6} \end{cases} \Rightarrow \langle S_x \rangle = \frac{5}{6}\frac{\hbar}{2} - \frac{1}{6}\frac{\hbar}{2} = \boxed{\hbar/3}$$

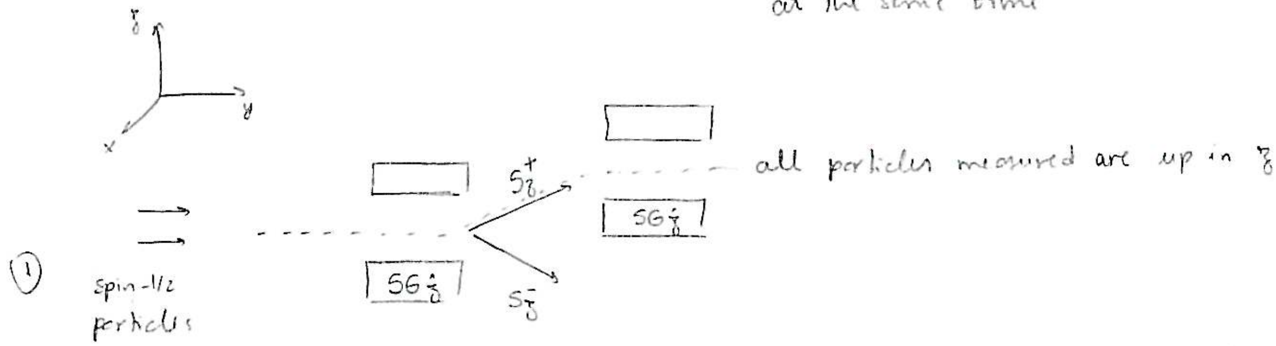
# Stern-Gerlach experiment

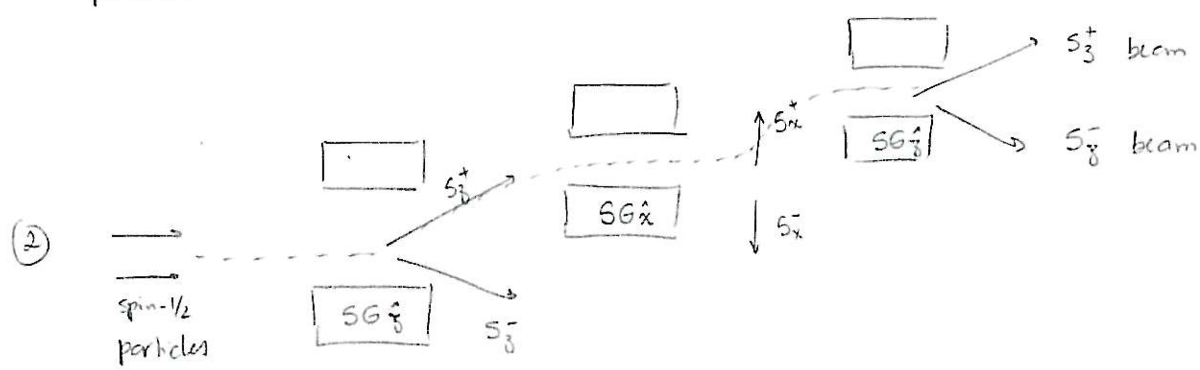
www.youtube.com/watch?v=waK4eKNXB4A

Modern Quantum Mechanics by J. J. Sakurai

$S_x, S_y, S_z$ do not commute $\Rightarrow$ cannot know $S_x$ and $S_z$ precisely at the same time

uncertainty principle




Measurement disturbs the system

HW 4.26, 4.27, 4.28, 4.29

4.34, 4.38, 4.49, ~~[illegible]~~

## Addition of Angular Momenta

Suppose we have two spin-1/2 particles. Example: $e + p$ in the ground state of H $\Downarrow$ $(\ell=0)$

What is the TOTAL angular momentum of the atom?

$$\vec{S} = \underbrace{\vec{S}^{(1)}}_{\substack{\text{acts only}\\ \text{on spin 1}\\ \chi_1}} + \underbrace{\vec{S}^{(2)}}_{\substack{\text{acts only}\\ \text{on spin 2}\\ \chi_2}}$$

•) There are four possibilities:

$$\begin{aligned} S_z \chi_1 \chi_2 &= \left(S_z^{(1)} + S_z^{(2)}\right)\chi_1\chi_2 \\ &= \left(S_z^{(1)}\chi_1\right)\chi_2 + \chi_1\left(S_z^{(1)}\chi_2\right) \\ &= \hbar m_1 \chi_1\chi_2 + \hbar m_2 \chi_1\chi_2 \\ &= \boxed{\hbar(m_1+m_2)\chi_1\chi_2} \end{aligned}$$

| | |
|---|---|
| $\uparrow\uparrow$ | $m=1$ |
| $\uparrow\downarrow$ | $m=0$ |
| $\downarrow\uparrow$ | $m=0$ |
| $\downarrow\downarrow$ | $m=-1$ |

$\uparrow\downarrow$, $\downarrow\uparrow$ ? $\longrightarrow$ eigenstates of $S_z$ but not of $S^2$

it appears that $\boxed{s=1}$, but there is an extra $m=0$

•) Apply $S_- = S_-^{(1)} + S_-^{(2)}$ to state $\uparrow\uparrow$

$$S_-(\uparrow\uparrow) = \left(S_-^{(1)}\uparrow\right)\uparrow + \uparrow\left(S_-^{(2)}\uparrow\right) = \hbar\left(\downarrow\uparrow + \uparrow\downarrow\right) \Longrightarrow \boxed{m=0}$$

so the three states with $\boxed{s=1}$ are

$$|s\,m\rangle = \left\{\begin{array}{l} |1\,1\rangle = \uparrow\uparrow \\ |1\,0\rangle = \frac{1}{\sqrt{2}}\left(\uparrow\downarrow + \downarrow\uparrow\right) \\ |1\,{-1}\rangle = \downarrow\downarrow \end{array}\right\} \; s=1 \;\; \text{(triplet)}$$

But we can also have a state orthogonal to the triplet where

$S=0$ (singlet)

$$|s\,m\rangle = |0\,0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$$

Therefore, the combination of two spin-1/2 particles can carry a total spin of 1 or 0

To confirm: prove that the triplet states are eigenvectors of $S^2$ with eigenvalue $2\hbar^2$ $\longleftarrow$ $S^2\,|\text{triplet}\rangle \underset{(s=1)}{=} \hbar^2\,1(1+1)\,|\text{triplet}\rangle$

and the singlet is an eigenvector of $S^2$ with eigenvalue 0 $\longleftarrow$ $S^2\,|\text{singlet}\rangle \underset{(s=0)}{=} 0$

$$S^2 = (\vec{S}^{(1)} + \vec{S}^{(2)}) \cdot (\vec{S}^{(1)} + \vec{S}^{(2)}) = (S^{(1)})^2 + 2\,\vec{S}^{(1)} \cdot \vec{S}^{(2)} + (S^{(2)})^2$$

$$\left.\begin{array}{l} \circ)\ (S^{(1)})^2 \uparrow = \hbar^2 \frac{1}{2}\left(\frac{3}{2}\right)\uparrow = \frac{3}{4}\hbar^2 \uparrow \\ \circ)\ (S^{(1)})^2 \downarrow = \hbar^2 \frac{1}{2}\left(\frac{3}{2}\right)\downarrow = \frac{3}{4}\hbar^2 \uparrow \end{array}\right\} \text{same for } (S^{(2)})^2$$

$\circ)$ $\vec{S}^{(1)} \cdot \vec{S}^{(2)} = S_x^{(1)} S_x^{(2)} + S_y^{(1)} S_y^{(2)} + S_z^{(1)} S_z^{(1)}$

$$\left\{\begin{array}{l} S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Rightarrow S_x\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix},\ S_x\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \Rightarrow S_y\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar i}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix},\ S_y\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar i}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Rightarrow S_z\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix},\ S_z\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{array}\right.$$

$\circ)$ $\vec{S}^{(1)} \cdot \vec{S}^{(2)}(\uparrow\downarrow) = \hbar^2/4\,(\downarrow\uparrow) + \hbar^2/4\,(\downarrow\uparrow) - \hbar^2/4\,(\uparrow\downarrow) = \hbar^2/4\,(2\downarrow\uparrow - \uparrow\downarrow)$

$\circ)$ $\vec{S}^{(1)} \cdot \vec{S}^{(2)}(\downarrow\uparrow) = \hbar^2/4\,(2\uparrow\downarrow - \downarrow\uparrow)$

$\circ)$ $\vec{S}^{(1)} \cdot \vec{S}^{(2)} \, |10\rangle = \vec{S}^{(1)} \cdot \vec{S}^{(2)} \, \frac{1}{\sqrt{2}} \left( \uparrow\downarrow + \downarrow\uparrow \right) =$

$$= \frac{\hbar^2}{4} \frac{1}{\sqrt{2}} \left( 2\downarrow\uparrow - \uparrow\downarrow + 2\uparrow\downarrow - \downarrow\uparrow \right) = \frac{\hbar^2}{4} |10\rangle$$

$\circ)$ $\vec{S}^{(1)} \cdot \vec{S}^{(2)} \, |00\rangle = \vec{S}^{(1)} \cdot \vec{S}^{(2)} \, \frac{1}{\sqrt{2}} \left( \uparrow\downarrow - \downarrow\uparrow \right) =$

$$= \frac{\hbar^2}{4} \frac{1}{\sqrt{2}} \left( 2\downarrow\uparrow - \uparrow\downarrow - 2\uparrow\downarrow + \downarrow\uparrow \right) = -\frac{3\hbar^2}{4} |00\rangle$$

$$\Rightarrow \quad S^2 |10\rangle = \left( \underbrace{\frac{3}{4}\hbar^2}_{(S^{(1)})^2} + \underbrace{\frac{3}{4}\hbar^2}_{(S^{(2)})^2} + 2 \underbrace{\frac{\hbar^2}{4}}_{\vec{S}^{(1)} \cdot \vec{S}^{(2)}} \right) |10\rangle$$

$$\boxed{S^2 |10\rangle = 2\hbar^2 |10\rangle}$$

$$\Rightarrow \quad S^2 |00\rangle = \left( \frac{3}{4}\hbar^2 + \frac{3}{4}\hbar^2 + 2 \left( -\frac{3}{4}\hbar^2 \right) \right)$$

$$\boxed{S^2 |00\rangle = 0}$$