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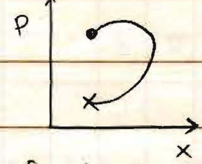
TOPIC

Quantum Mechanics

Classical Mechanics

- point particle (m)
- non-relativistic



→ state of system

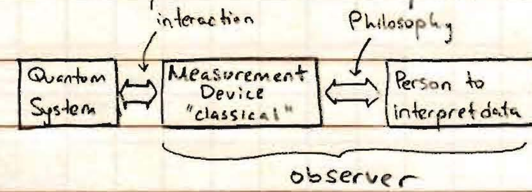
→ evolution - trajectory of phase space

→ eq of motion: $\dot{x} = \frac{\partial H}{\partial p}$; $\dot{p} = -\frac{\partial H}{\partial x}$

Quantum Mechanics

- point particles (m)
- non-relativistic

→ x and p are measured quantities



Schrödinger Wave Mechanics

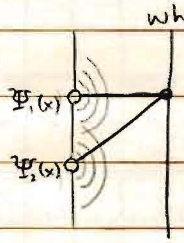
- state of the system - complex valued wave fct $\Psi(x,t)$
- equation of motion: $i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$ (Schrödinger equation)

Born's Statistical Interpretation

Probability of detecting a particle in $[x, x+dx]$ at time t:

$$dP = |\Psi(x,t)|^2 dx = \Psi^* \Psi dx$$

QM does not explain what e^- does in between



$$\Psi(x,t) = \Psi_1(x,T) + \Psi_2(x,T)$$

$|\Psi|^2$ ← interferance pattern

Experiment shows we need eq with wave like solutions

e^- → particle: $p = mv$

e^- → wave: $p = \hbar k = \hbar \frac{2\pi}{\lambda}$ (de Broglie)

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

$$i\hbar(-i\omega)\Psi = -\frac{\hbar^2}{2m}(ik)^2\Psi$$ ← different from wave equation

(Einstein) $E = \hbar\omega$

$$\hbar\omega \stackrel{?}{=} \frac{(\hbar k)^2}{2m}$$ (Dispersion Relation)

$$E = \frac{p^2}{2m}$$

GoldFibre

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SEPARATION OF VARIABLES I

Ex. Wave Eq.

$$\frac{\partial^2\Psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2\Psi}{\partial t^2} \qquad x \in [0, L] \quad t \in [0, \infty)$$

Boundary Conditions: $\Psi(0,t) = \Psi(L,t) = 0$

Initial Conditions: $\Psi(x,0) = 5\sin\left(\frac{2\pi}{L}x\right)$ $\qquad \left.\frac{d\Psi}{dt}\right|_{t=0} = 0$

Ansatz: $\Psi(x,t) = X(x) + T(t)$

$$\Psi(x,t) = X(x)T(t) \quad \leftarrow \text{pick this one}$$

$$X(x)\frac{\partial^2}{\partial t^2}T(t) = v^2 T(t)\frac{\partial^2}{\partial x^2}X(x)$$

$$\underbrace{\frac{1}{T}\ddot{T}}_{\text{depends only on } t} = \underbrace{v^2\frac{1}{X}X''}_{\text{depends only on } x} = -\omega^2 \quad \text{each side must be constant}$$

2 ODEs

$$\ddot{T}(t) + \omega^2 T(t) = 0 \rightarrow T(t) = A\cos(\omega t) + B\sin(\omega t)$$

$$X''(x) + \frac{\omega^2}{v^2}X(x) = 0 \xrightarrow{k^2 = \frac{\omega^2}{v^2}} X(x) = C\cos(kx) + D\sin(kx)$$

Boundary Conditions

$$\Psi(0,t) = 0 = X(0)T(t) \rightarrow X(0) = 0 \rightarrow C = 0$$

$$\Psi(L,t) = 0 \rightarrow X(L) = 0 \rightarrow X(L) = D\sin(kL) = 0$$

$\longrightarrow$ boundary cond "quantizes" k $\qquad k_n = \frac{n\pi}{L} \qquad n = \pm 1, \pm 2, \ldots$

and ω (pick positive root $kv = \omega$) $\qquad \omega_n = \frac{n\pi v}{L}$

$$\Psi(x,t) = D\sin\left(\frac{n\pi}{L}x\right)\left[A\cos\left(\frac{n\pi}{L}vt\right) + B\sin\left(\frac{n\pi}{L}vt\right)\right]$$

Initial Conditions

$$\Psi(x,0) = AD\sin\left(\frac{n\pi}{L}x\right) \overset{!}{=} 5\sin\left(\frac{2\pi}{L}x\right) \Longrightarrow AD = 5;\ n = 2$$

$$\frac{\partial\Psi}{\partial t}(x,0) = AB\sin\left(\frac{n\pi}{L}x\right)\left(\frac{n\pi v}{}\right. \qquad \Longrightarrow B = 0$$

$$\Psi(x,t) = 5\sin\left(\frac{2\pi}{L}x\right)\cos\left(\frac{2\pi}{L}vt\right)$$

$$\boxed{\Psi(x,t) = \frac{5}{2}\left[\sin\left(\frac{2\pi}{L}\{x+vt\}\right) + \sin\left(\frac{2\pi}{L}\{x-vt\}\right)\right]}$$

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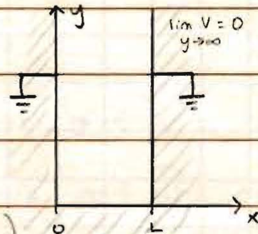
SEPARATION OF VARIABLES II

Ex. Laplace (2D)



$V(L,y)=0$
$V(0,y)=0$

$V(x,0)=V_0\sin\left(\frac{2\pi}{L}x\right)$

Asatz: $V = X(x)Y(y)$

$\nabla^2 V = Y\frac{\partial^2 X}{\partial x^2} + X\frac{\partial^2 Y}{\partial y^2} = 0$

$\underbrace{\frac{1}{X}X''}_{\text{only } x \text{ dependent}} = \underbrace{-\frac{1}{Y}Y''}_{\text{only } y \text{ dependent}} = -\alpha^2 \quad (\alpha \in \mathbb{C})$

2 ODEs

$X'' + \alpha^2 X = 0 \longrightarrow X(x) = A\cos(\alpha x) + B\sin(\alpha x)$

$Y'' - \alpha^2 Y = 0 \longrightarrow Y(y) = Ce^{\alpha y} + De^{-\alpha y}$

If α is purely real, then X oscillating, Y exp
If α is purely imaginary, then Y oscillating, X exp.

Boundary Conditions

① $X(0) = 0 \longrightarrow A$

② $X(L) = B\sin(\alpha L) = 0 \rightarrow$ pick $\alpha \in \mathbb{R} \rightarrow \alpha = \frac{n\pi}{L}$ $\quad$ n = integer

③ $y \to \infty \qquad \lim_{y\to\infty} Y(y) = 0 \longrightarrow C = 0$

④ $V(x,y) = \tilde{B}\sin\left(\frac{n\pi}{L}x\right)e^{-\frac{n\pi}{L}y}$

$V(x,0) = \tilde{B}\sin\left(\frac{n\pi}{L}x\right) \stackrel{!}{=} V_0\sin\left(\frac{2\pi}{L}x\right) \longrightarrow \tilde{B} = V_0,\ n = 2$

write as Fourier

$V_n(x,y) = \sin\left(\frac{n\pi}{L}x\right)e^{-\frac{n\pi}{L}y}$

$V(x,y) = \sum_{n=1}^{\infty} A_n V_n(x,y)$

$V(x,0) = \sum_{n=1}^{\infty} A_n V_n(x,0) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi}{L}x\right) \stackrel{!}{=} f(x)$

use Fourier's Trick

$\delta = \int_0^L \left(\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)\right)\left(\sqrt{\frac{2}{L}}\sin\left(\frac{m\pi}{L}x\right)\right)dx$

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LINEAR ALGEBRA I

Vector Spaces ($\mathbb{V}$)

- "objects" set of vectors $\mathbf{v} \in \mathbb{V}$

  scalars $a \in \mathbb{R}$ or $a \in \mathbb{C}$

  $\mathbf{v} + (-\mathbf{v}) = 0$

- "operations" addition $[\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u};\ \mathbf{u} + (\mathbf{v} + \mathbf{w}) = (\mathbf{u} + \mathbf{v}) + \mathbf{w};\ \mathbf{0} + \mathbf{u} = \mathbf{u}]$

  multiplication $[a(b\mathbf{v}) = (ab)\mathbf{v};\ a(\mathbf{u} + \mathbf{v}) = a\mathbf{u} + a\mathbf{v};\ (1)\mathbf{v} = \mathbf{v}]$

  $(a+b)\mathbf{v} = a\mathbf{v} + b\mathbf{v}$

Ex. ① $\mathbb{R}^2$ $\quad \mathbf{v} = \hat{i} + 2\hat{j}$

② $\mathbb{C}^2$ $\quad \mathbf{v} = i\hat{i} + (2i)\hat{j}$

③ Polynomial of degree 2

$\mathbf{v} = 1 + 2x + 3x^2$

Basis

can't throw a basis vector away and still span the space

For a $\mathbf{v} \in \mathbb{V}$, there is a linear comb. $\mathbf{v} = \sum_{i=1} a_i \mathbf{e}_i$

a set of linearly independent vectors that span $\mathbb{V}$. $\{\mathbf{e}_i\}_{i=1}^{N}$

Ex. $\mathbb{R}^2$

Basis $\hat{i}, \hat{j}$ $\quad \mathbf{v} = (1)\hat{i} + (2)\hat{j}$

Basis $\mathbf{e}_1 = \hat{i}$ $\quad \mathbf{v} = -\mathbf{e}_1 + 2\mathbf{e}_2$

$\mathbf{e}_2 = \hat{i} + \hat{j}$

We like to work with orthanormal basis vectors.

Ex. $\mathbb{R}^2$: $\hat{i}, \hat{j}$ $\qquad \mathbb{R}^2 \times \mathbb{R}^2 \rightarrow \mathbb{R}$

$\underbrace{\hat{i} \cdot \hat{i} = \hat{j} \cdot \hat{j} = 1}_{\text{length 1}} \qquad \underbrace{\hat{i} \cdot \hat{j} = 0}_{\text{orthogonal}}$

when are polynomials orthogonal?

$\mathbb{C}^2$: $\mathbf{v}\ (i)\hat{i} + (2i)\hat{j}$ $\qquad \mathbb{C}^2 \times \mathbb{C}^2 \rightarrow \mathbb{C}$

not a length

bad generalization $\rightarrow$ $\cancel{\mathbf{v} \cdot \mathbf{v} = (i)^2 + (2i)^2 = -5}$

instead, use complex conjugate

$\mathbf{v}^* \cdot \mathbf{v} = (-i)(i) + (-2i)(2i) = 5$

Introduce alternative notation: $\langle \mathbf{v} | \mathbf{v} \rangle = \mathbf{v}^* \cdot \mathbf{v} = \sum_{i=1}^{2} v_i^* v_i$

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LINEAR ALGEBRA II

Ex. $\mathbb{C}^2$ $\quad v = (i)\hat{\imath} + (2i)\hat{\jmath} \qquad w = \hat{\imath} + \hat{\jmath}$

$$\langle v|w\rangle = \begin{pmatrix} -i & -2i \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = -3i$$

$$\langle w|v\rangle = \begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} -i \\ -2i \end{pmatrix} = 3i$$

$$\langle w|v\rangle^* = \langle v|w\rangle$$

Inner Product $\langle \cdot | \cdot \rangle$

$\langle w|v\rangle^* = \langle v|w\rangle$

$\langle w|(a|v\rangle + b|u\rangle) = a\langle w|v\rangle + b\langle w|u\rangle$

$\langle v|v\rangle \geq 0$ (if it is 0, v is the zero vector)

Inner product spaces are vector spaces with an inner product.

Ex. Vector space of functions that are expressible as a Fourier sine series

$$f(x) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi}{L}x\right) \qquad a_n \in \mathbb{R},\ x \in [0, L]$$

Inner product

$$\langle f|g\rangle = \int_0^L f^*(x)\, g(x)\, dx$$

Basis Set

$|e_n\rangle \leftrightarrow e_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$

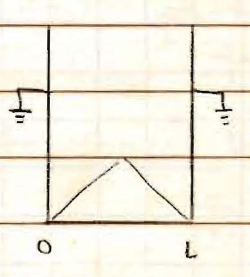
$$\langle e_m|e_n\rangle = \frac{2}{L}\int_0^L \sin\left(\frac{m\pi}{L}x\right)\sin\left(\frac{n\pi}{L}x\right) dx \overset{!}{=} \delta_{m,n} = \begin{cases} 0 & n \neq m \\ 1 & n = 1 \end{cases}$$

→ length is defined (norm) $\quad \|v\| = \sqrt{\langle v|v\rangle}$

→ orthogonality $\quad \langle v|w\rangle = 0 \longleftrightarrow$ v and w are orthogonal

$$|f\rangle = \sum_{n=1}^{\infty} a_n \sqrt{\frac{L}{2}}\, |e_n\rangle$$

$$f(x) = \sum_{n=1}^{\infty} a_n \sqrt{\frac{L}{2}}\, e_n(x)$$



$$a_n = \frac{8}{\pi n^2}\begin{cases} \frac{1}{4} & n = 1, 5, \dots \\ 0 & n = 2, 4, 6, \dots \\ -\frac{1}{4} & n = 3, 7, \dots \end{cases}$$

LINEAR ALGEBRA III

Dirac Notation

$| \ \rangle$ ket $\qquad$ $|\alpha\rangle$ kets are vectors in some vector space with complex scalars (label/name)

$\langle \ |$ bra

$\langle \ | \ \rangle$ braket = inner product

For a given basis $\{|e_i\rangle\}_{i=1}^{N}$, we can associate kets with complex column vectors

$$|\alpha\rangle = \sum_{i=1}^{N} \underbrace{a_i}_{a_i \in \mathbb{C}} |e_i\rangle \longleftrightarrow \alpha = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}$$

$\langle\alpha|$ bras are vectors in a different vector space (dual space)

Ex. $\langle e_m | e_n \rangle = \delta_{nm} = \begin{cases} 1 & m=n \\ 0 & m \neq n \end{cases}$

Ex. $|\alpha\rangle = \sum_{i=1}^{N} a_i |e_i\rangle \longrightarrow \langle\alpha| = \sum_{i=1}^{N} a_i^* \langle e_i|$

$$\langle\alpha|\alpha\rangle = \sum_{n=1}^{N}\sum_{m=1}^{N} (a_m^* \langle e_m|)(a_n|e_n\rangle) = \sum_{n=1}^{N}\sum_{m=1}^{N} a_m^* a_n \langle e_m|e_n\rangle$$
$$\stackrel{!}{=} \sum_{n=1}^{N} a_n^* a_n = \sum_{n=1}^{N} |a_n|^2 = (a_1^*, \dots, a_N^*)\begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}$$

This definition is consistent with our definition of inner products on $\mathbb{C}^N$.

① For every ket $|\alpha\rangle$ there exists a corresponding bra $\langle\alpha|$

② The associated coefficient vector in $\mathbb{C}^N$ is the complex conjugate transpose (conjugate row vector) $\langle\alpha| \longleftrightarrow (a_1^*, \dots, a_N^*)$

Operators $\hat{O}$

$\hat{\ }$ ← indicates an operator; O ← label/name

Operators map vectors to vectors in the same vector space

$$|\alpha\rangle, |\beta\rangle \in V \ ; \quad \hat{O}|\alpha\rangle = |\beta\rangle \ ; \quad \underbrace{\hat{I}}_{\text{identity operator}}|\alpha\rangle = |\alpha\rangle$$

Linear operators are finite dim (N) vector spaces

linear: $\hat{T}(a|\alpha\rangle + b|\beta\rangle) = a\hat{T}|\alpha\rangle + b\hat{T}|\beta\rangle$

For given basis we can associate $\hat{T}$ with $\mathbb{C}^{N\times N}$ matrix

$$\hat{T}|\alpha\rangle = |\beta\rangle \longleftrightarrow \begin{pmatrix} T_{11} & T_{12} & \cdots & T_{1N} \\ T_{21} & T_{22} & & \vdots \\ & & \ddots & \\ T_{N1} & \cdots & & T_{NN} \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$$

LINEAR ALGEBRA IV

One advantage of Dirac notation is that we specify the basis

basis $\{|e_i\rangle\}$ $\qquad a_m = \langle e_m|\alpha\rangle$

$$|\alpha\rangle = \sum_{n=1}^{N} a_n|e_n\rangle = \sum_{n=1}^{N} \overbrace{\langle e_n|\alpha\rangle}^{a_n}|e_n\rangle$$

$$|\beta\rangle = \sum_{n=1}^{N} b_m|e_m\rangle = \sum_{m=1}^{N} \langle e_m|\beta\rangle|e_m\rangle$$

Q: How do I get T_{mn}?

$$b_m = \langle e_m|\beta\rangle = \langle e_m|(\hat{T}|\alpha\rangle)$$
$$= \langle e_m|\left(\hat{T}\sum_n a_n|e_n\rangle\right)$$
$$= \sum_n \underbrace{\langle e_m|\hat{T}|e_n\rangle}_{T_{mn}} a_n$$

Ex. Identity

2D identity matrix: $\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \langle e_1|\hat{1}|e_1\rangle & \langle e_1|\hat{1}|e_2\rangle \\ \langle e_2|\hat{1}|e_1\rangle & \langle e_2|\hat{1}|e_2\rangle \end{pmatrix}$

2D identity operator: $\hat{1} = |e_1\rangle\langle e_1| + |e_2\rangle\langle e_2|$

in N dim: $\hat{1} = \sum_{n=1}^{N} |e_n\rangle\langle e_n|$

$$\hat{T} = \hat{1}\hat{T}\hat{1}$$
$$= \sum_{n=1}^{N}\sum_{m=1}^{N} |e_n\rangle\underbrace{\langle e_n|\hat{T}|e_m\rangle}_{\in\mathbb{C}}\langle e_m|$$
$$= \sum_{n=1}\sum_{m=1} \langle e_n|\hat{T}|e_m\rangle|e_n\rangle\langle e_m|$$

Preview / Motivation

	"Abstract"	For N-dim vector spaces, basis $\{|e_i\rangle\}$	∞-dim spaces in position representation
State of System	$|\psi\rangle$	$\begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}$	$\psi(x)$
Measurable Observables	$\hat{H}$ hermitian operators	$\mathbb{H}$ hermetian matrices	$\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ associated diff operator

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LINEAR ALGEBRA III

① Transpose Conjugate (hermetian conjugate)

$$A^{\dagger} = (A^{T})^{*} = (A^{*})^{T} \quad (\text{"A dagger"})$$

Ex. $\begin{pmatrix} i & 1 \\ 0 & 2i \end{pmatrix}^{\dagger} = \begin{pmatrix} -i & 0 \\ 1 & -2i \end{pmatrix}$ and $\begin{pmatrix} 1 \\ 2i \end{pmatrix}^{\dagger} = \begin{pmatrix} 1 & -2i \end{pmatrix}$

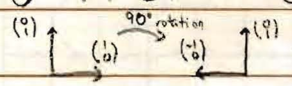
② Unitary Matrices

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

$$\delta_{mn} = (e_m^{*})^{T} e_n$$

$$UU^{\dagger} = UU^{-1} = \mathbb{1} = U^{\dagger}U \Leftrightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \vdots \\ 0 & \cdots & 1 \end{pmatrix} = \begin{pmatrix} \leftarrow e_1^{*} \rightarrow \\ \leftarrow e_2^{*} \rightarrow \\ \leftarrow e_n^{*} \rightarrow \end{pmatrix} \begin{pmatrix} e_1 & e_2 & \cdots & e_n \end{pmatrix}$$

Ex. $U = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \qquad U^{\dagger}U = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$



③ Hermetian Matrices

$$H^{\dagger} = H$$

Ex. general form of a 2×2 hermetian matrix?

$$\begin{pmatrix} z_1 & z_2 \\ z_3 & z_4 \end{pmatrix} = \begin{pmatrix} z_1^{*} & z_3^{*} \\ z_2^{*} & z_4^{*} \end{pmatrix} \qquad \{z_1, z_2, z_3, z_4\} \in \mathbb{C}$$

$\rightarrow z_1$ and z_4 are real, $z_2 = z_3^{*}$; $z_3 = z_2^{*}$ $\Longrightarrow$ $\begin{pmatrix} a & u+iv \\ u-iv & b \end{pmatrix}$ $a, b, u, v \in \mathbb{R}$

Eigenvalues and Eigenvectors

$$A v = \lambda v$$

λ ← eigenvalue, v ← eigenvectors

How to find λ and v?

Eval: $(A - \lambda\mathbb{1})v = 0$ • If $(A - \lambda\mathbb{1})$ were invertible, then $v = 0$ would be soln. We don't want that. Pick λ s t $(A - \mathbb{1}\lambda)$ is non-invertible.

eigenvalues: $\det(A - \lambda\mathbb{1}) = 0$

Ex. $H = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \longrightarrow \begin{vmatrix} -\lambda & -i \\ i & -\lambda \end{vmatrix} = \lambda^2 - (i)(-i) = \lambda^2 - 1 \stackrel{!}{=} 0 \Rightarrow \lambda_1 = 1, \lambda_2 = -1$

Evec: For a given λ_n solve $A v_n = \lambda_n v_n$ for v_n and normalize

$\rightarrow \lambda_1 = 1 \quad \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix} \qquad v_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$

$\rightarrow \lambda_2 = -1 \quad \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = -\begin{pmatrix} a \\ b \end{pmatrix} \qquad v_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$

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Linear Algebra III

Diagonalization

Assume we have N distinct eigenvalues $\lambda_1 \dots \lambda_N$

→ Form matrix $\mathbb{S} = [\mathbb{v}_1\ \mathbb{v}_2 \dots \mathbb{v}_N]$ $\mathbb{S}^{-1} \mathbb{A} \mathbb{S} = \mathbb{D}$

$\mathbb{D} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & & \vdots \\ 0 & \cdots & & \lambda_N \end{pmatrix}$ ← diagonal!

Why diagonalize? Algebra easy!

Ex. p^{th} power of $\hat{A}$: $\hat{A}^p |\alpha\rangle = ?$

- default $\{|e_n\rangle\}$ basis

$|\alpha\rangle = \sum_n \overbrace{\langle e_n|\alpha\rangle}^{a_n} |e_n\rangle \leftrightarrow \mathbb{a} = \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}$

$\hat{A} = \sum_m \sum_n \overbrace{\langle e_m|A|e_n\rangle}^{A_{mn}} |e_m\rangle\langle e_n| \leftrightarrow \mathbb{A}$

$\hat{A}^p|\alpha\rangle \leftrightarrow \mathbb{A}^p \mathbb{a} = ?$ (difficult)

Change of Basis!

- eigenvector $\{|v_n\rangle\}$ basis

$|\alpha\rangle = \sum_n \langle v_n|\alpha\rangle |v_n\rangle \longleftrightarrow \mathbb{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_n \end{pmatrix}$

$\hat{A} = \sum_n \lambda_n |v_n\rangle\langle v_n| \leftrightarrow \mathbb{D}$

$\hat{A}^p |\alpha\rangle \leftrightarrow \mathbb{D}^p \mathbb{b} = \begin{pmatrix} \lambda_1^p & & \\ & \ddots & \\ & & \lambda_N^p \end{pmatrix} \begin{pmatrix} b_1 \\ \vdots \\ b_N \end{pmatrix} = \begin{pmatrix} \lambda_1^p b_1 \\ \vdots \\ \lambda_N^p b_N \end{pmatrix}$ (easy)

→ not all matrices are diagonalizable

→ there are matrices $\mathbb{A}$ with eigenvectors that are <u>not</u> orthogonal

Hermetian Matrices

→ always diagonalizable

→ eigenvalues are real

$(\mathbb{H}\mathbb{v})^\dagger \mathbb{v} = \mathbb{v}^\dagger \mathbb{H}^\dagger \mathbb{v} = \mathbb{v}^\dagger \mathbb{H} \mathbb{v} = \lambda \mathbb{v}^\dagger \mathbb{v}$

$(\mathbb{H}\mathbb{v})^\dagger \mathbb{v} = (\lambda \mathbb{v})^\dagger \mathbb{v} = \lambda^* \mathbb{v}^\dagger \mathbb{v}$ $\lambda^* = \lambda$

→ eigenvectors are orthogonal $\xrightarrow{\text{normalize}}$ orthonormal $\mathbb{v}_n$

$\mathbb{H}$ is diagonalized by unitary matrix $\mathbb{U} = [\mathbb{v}_1, \dots, \mathbb{v}_N]$ $\mathbb{U}^\dagger \mathbb{H} \mathbb{U} = \mathbb{D}$

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LINEAR ALGEBRA III

Commutator

$[\mathbb{A}, \mathbb{B}] = \mathbb{A}\mathbb{B} - \mathbb{B}\mathbb{A}$

- If $\mathbb{A}$ and $\mathbb{B}$ commute, $[\mathbb{A}, \mathbb{B}] = 0$, then they diagonalized simultaneously

Ex. $\mathbb{A} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $\quad \lambda_1^A = 1 \quad \lambda_2^A = 1$ can pick any two orthogonal vetors as basi

$\mathbb{B} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\quad \lambda_1^B = 1 \quad \lambda_2^B = -1$

common basis: $v_1^{A\&B} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$ $\quad v_2^{A\&B} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$

in terms of Dirac Notation - use eigenvalues as label

$|\lambda_A, \lambda_B\rangle = |1, 1\rangle \leftrightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$

$|\lambda_A, \lambda_B\rangle = |1, -1\rangle \leftrightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$

PROBABILITY

A) Discrete Probabilities

- measure $N(j)$ events j
- total number of events $N = \sum_j N(j)$
- the probability of event j is $P = \frac{N(j)}{N}$
- the average of j is $\langle j \rangle = \sum_j j \frac{N(j)}{N}$
- average $f(j) = \sum_j f(j) \frac{N(j)}{N} \longrightarrow \langle j^2 \rangle = \sum_j j^2 \frac{N(j)}{N}$
- variance $\sigma^2 = \langle (j - \langle j \rangle)^2 \rangle$

$$\begin{aligned} &= \langle j^2 - 2j\langle j \rangle + \langle j \rangle^2 \rangle \\ &= \langle j^2 \rangle - 2\langle j \rangle \langle j \rangle + \langle j \rangle^2 \\ &= \langle j^2 \rangle - \langle j \rangle^2 \end{aligned}$$

- standard deviation $\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}$

B) Continuous Probabilities

Probability of x to be between a and b is

$$P = \int_a^b \rho(x)\, dx \quad \leftarrow \text{probability density}$$

Normalization forces particle to be somewhere:

$$1 = \int_{-\infty}^{+\infty} \rho(x)\, dx.$$

- average $\langle x \rangle = \int_{-\infty}^{+\infty} x \rho(x)\, dx$
- and $\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2 \rho(x)\, dx$

Ex. $\rho(x) = N x e^{-\alpha x}$ $\quad x \in [0, \infty]$

- Normalization: $1 = \int_0^\infty x e^{-\alpha x} dx = N\alpha^{-2}$

  $N = \alpha^2$

- Average: $\langle x \rangle = \int_0^\infty x \alpha^2 x e^{-\alpha x} dx = \alpha^2 \cdot \frac{2}{\alpha^3} = \frac{2}{\alpha}$

  $\langle x^2 \rangle = \int x^2 \alpha^2 x e^{-\alpha x} dx = \alpha^2 \frac{6}{\alpha^4} = \frac{6}{\alpha^2}$

$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{2}{\alpha^2}$

Need to know

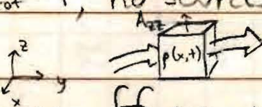
$$I_n = \int_0^\infty x^n e^{-\alpha x} dx$$

$$(-1)^n \frac{\partial^n}{\partial \alpha^n} e^{-\alpha x} = x^n e^{-\alpha x}$$

$$\begin{aligned} I_n &= (-1)^n \frac{d^n}{d\alpha^n} \int_0^\infty e^{-\alpha x} dx \\ &= (-1)^n [(-1)(-2)\dots(-n)]\, \alpha^{-1-n} \\ &= \frac{n!}{\alpha^{n+1}} \end{aligned}$$

PROBABILITIES

Continuity Equation

- Exists for conserved (continuous) quantities, including Probabilities
- We know that $P_{tot} = 1$, no sources or sinks of prob.
- For small volume  $\hat{j} \leftarrow$ flux/current and for small box:

$$\frac{d}{dt}\iiint \rho(x,t)\,dV + \oiint \hat{j}(x,t)\cdot dA = 0$$

$$\iiint \frac{\partial \rho}{\partial t}(x,t)\,dV + \iiint \nabla\cdot\hat{j}\,dV = 0$$

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla\cdot\hat{j} = 0}$$

continuity equation

Ex. Diffusion Equation

- assume $n(x,t)$ is the concentration of "stuff", where the total amount of stuff is conserved
- assume that flows down the concentration gradient

$$j = -D\frac{\partial n}{\partial x}$$

$$\boxed{\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2}}$$

DATE 2/12
TOPIC

QM Probability

Review

Ⓐ For a density $\rho(x,t)$ of a conserved quantity, the continuity eq. holds:

$$\frac{\partial \rho}{\partial x} = -\frac{\partial j}{\partial t}$$

flux

Ⓑ if $\rho(x,t)$ is a probability density:

- normalization $1 = \int_{-\infty}^{+\infty} \rho(x,t)\, dx$
- averages $\langle f \rangle = \int_{-\infty}^{+\infty} f(x)\, \rho(x,t)\, dx$

QM Postulates

① State of a QM system is given by $|\Psi\rangle \leftrightarrow \Psi(x,t)$

② Free evolution of system (no measurements) is given by Schö Eq.:

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

are these consistent?

classical potential pertaining to the physical system studied

③ Statistical interpretation: the probability density $\rho(x,t) = \Psi^*\Psi$ tells us the probability of finding the particle at position x. Then, the "expectation value" of a measurable quantity $f(x)$

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

Normalization

$$1 = \int_{-\infty}^{+\infty} \Psi^*(x,t)\Psi(x,t)\, dx$$

Since S.E. is linear if Ψ is a soln., then so is $\mathcal{N}\Psi$ can normalize any Ψ if:

① $\Psi \neq 0$

② the functions Ψ have to be square integrable

$$\int_{-\infty}^{+\infty} |\Psi|^2\, dx < \infty$$

(e.g smooth functions that fall of faster than $\frac{1}{\sqrt{x}}$ as $|x| \to \infty$)

DATE	2/12
TOPIC	

QM Probability

Probability Conservation

$$P_{tot} = \int \rho(x,t)\,dx = 1$$

$$\frac{dP_{tot}}{dt} = 0 \quad \text{check}$$

$$\Updownarrow \quad \text{that this}$$

$$\frac{\partial \rho}{\partial t} = -\frac{\partial j}{\partial x} \quad \text{holds}$$

$$\frac{dP_{tot}}{dt} = \int_{-\infty}^{+\infty} \frac{\partial \rho}{\partial t}\,dx = \int_{-\infty}^{+\infty} \left(\frac{\partial \Psi^*}{\partial t}\Psi + \Psi^* \frac{\partial \Psi}{\partial t}\right) dx$$

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

potential is real valued

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

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

check first that $\frac{dP_{tot}}{dt} = 0$:

integral by parts: $\displaystyle\int_{-\infty}^{+\infty} \frac{\partial^2 \Psi^*}{\partial x^2}\Psi\,dx = \underbrace{\frac{\partial \Psi^*}{\partial x}\Psi\Big|_{-\infty}^{+\infty}}_{0} - \int_{-\infty}^{+\infty} \frac{\partial \Psi^*}{\partial x}\frac{\partial \Psi}{\partial x}\,dx$

1. $\lim_{|x|\to\infty} \Psi \to 0$ (true b/c Ψ is normalizeable)
2. well behaved derivative as $|x| \to \infty$

$$\frac{dP_{tot}}{dt} = \frac{i\hbar}{2m}\int_{-\infty}^{+\infty} \left(\frac{\partial \Psi^*}{\partial x}\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi}{\partial x}\frac{\partial \Psi^*}{\partial x}\right) dx = 0$$

Summary: The SE and statistical interpretation are consistent for square integrable wave functions.

$$\frac{\partial \rho}{\partial t} = -\frac{i\hbar}{2m}\left(\frac{\partial^2 \Psi^*}{\partial x^2}\Psi - \Psi^* \frac{\partial^2 \Psi}{\partial x^2}\right)$$

$$\stackrel{!}{=} -\frac{\partial}{\partial x}\Big[\underbrace{\frac{i\hbar}{2m}\left(\frac{\partial \Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial \Psi}{\partial x}\right)}_{\text{flux } j}\Big]$$

$$\Psi(x,t) = \sqrt{\rho(x,t)}\, e^{i\phi(x,t)}$$

depends on $\phi(x,t)$ as well

We need SE b/c we can't express j in terms of ρ only.

SCHRÖDINGER WAVE MECHANICS

Schrödinger Wave Mechanics

Classical Mechanics Potential $V(x)$ $\longrightarrow$ If $V(x)$ is given and $\psi(x,0)$ [initial cond.] use SE to get $\Psi(x,t)$.

statistical integration

Observable $Q(x,p)$ $\longrightarrow$ Hermetian Operator $\hat{Q}: Q(\hat{x},\hat{p}) = Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)$

Prediction for Measurement Outcomes

e.g. expectation values

$$\underbrace{\langle \hat{Q} \rangle}_{\text{a number to be compared w/ experiment}} = \int_{-\infty}^{+\infty} \Psi^*(x,t)\, Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi(x,t)\, dx$$

Expectation values in Schrödinger wave mechanics (position representation)

$\Psi(x,t)$ state; $\rho(x,t) = |\Psi|^2$ (prob density)

$$\langle \hat{x} \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)\, x\, \Psi(x,t)\, dx$$

$$\int_{-\infty}^{+\infty} \frac{\partial \Psi^*}{\partial x}\Psi\, dx = \underbrace{\Psi^*\Psi\Big|_{-\infty}^{+\infty}}_{0} - \int_{-\infty}^{+\infty} \Psi^* \frac{\partial \Psi}{\partial x} dx$$

<u>Def</u>

$$\begin{aligned}
\langle \hat{p} \rangle &\stackrel{!}{=} m \frac{d}{dt}\langle x \rangle = m \int_{-\infty}^{+\infty} x \underbrace{\frac{\partial}{\partial t}\rho(x,t)}_{-\frac{\partial}{\partial x} j(x,t)} dx \\
&\stackrel{!}{=} -m \int_{-\infty}^{+\infty} x \frac{\partial j}{\partial x} dx \\
&\stackrel{!}{=} -m \left\{ \underbrace{x\, j(x,t)\Big|_{-\infty}^{+\infty}}_{0} - \int_{-\infty}^{+\infty} \underbrace{j(x,t)}_{\frac{i\hbar}{2m}\left(\frac{\partial \Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial \Psi}{\partial x}\right)} dx \right\} \\
&\stackrel{!}{=} \frac{i\hbar}{2} \int_{-\infty}^{+\infty} \left(\frac{\partial \Psi^*}{\partial x}\Psi - \Psi^* \frac{\partial \Psi}{\partial x} \right) dx \\
&\stackrel{!}{=} -i\hbar \int_{-\infty}^{+\infty} \Psi^* \left(\frac{\partial}{\partial x}\Psi \right) dx
\end{aligned}$$

<u>Example</u> Assume classically that the energy E is given by $H = \frac{p^2}{2m} + V(x)$

QM: Expectation Value

$$\langle \hat{H} \rangle = \int_{-\infty}^{+\infty} \underbrace{\Psi^*(x,t)\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t)}_{\text{LHS of SE}}\, dx$$

$\rightarrow$ should have RHS of SE be $E\Psi$

DATE 2/14

TOPIC

Schrödinger Wave Mechanics

Seperability of Variables

If V is time independant

$$\underbrace{V = V(x)}_{\hookrightarrow \text{ seporable}}$$

(doesn't depend on time)

Stationary SE

to wit: $\Psi(x,t) = \psi(x)\,\phi(t)$

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

$$\frac{1}{\psi}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi\right) = \frac{1}{\phi} i\hbar \frac{\partial \phi}{\partial t} \equiv E$$

$$\rightarrow \dot{\phi} = -i\frac{E}{\hbar} \Rightarrow \phi(t) = e^{-iEt/\hbar} \quad \rightarrow \quad \boxed{\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi_E(x) = E\psi_E(x)}$$

in Dirac notation $\hat{H}|\psi_E\rangle = E|\psi_E\rangle$

E is real because Ψ_E has to be normalizable

$$1 = \int \Psi^*(x,t)\Psi(x,t)\,dx$$

$$= \int \psi^*(x) e^{(\frac{i}{\hbar}E^* t)} \psi(x) e^{(-\frac{i}{\hbar}Et)}\,dx$$

$$= \underbrace{e^{\frac{1}{\hbar}(-\frac{E^*}{i}+\frac{E}{i})t}}_{e^{\frac{2t}{\hbar}\mathrm{Im}(E)}} \int \psi^*(x)\psi(x)\,dx$$

$e^{\frac{2t}{\hbar}\mathrm{Im}(E)} \longleftarrow$ has to be time independant $\Rightarrow \mathrm{Im}(E) = 0$

$$\langle \hat{H}\rangle = \langle \Psi_E|\hat{H}|\Psi_E\rangle = \int \Psi_E^* H \Psi_E\,dx$$

$$= \langle \psi|\hat{H}|\psi\rangle = \int \psi_E^* H \psi_E\,dx \qquad H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

$$= \langle \psi_E|E|\psi_E\rangle$$

$$= E\langle \psi_E|\psi_E\rangle = E$$

$$\langle \hat{H}^2\rangle = \langle \Psi_E|\hat{H}|\Psi_E\rangle$$

$$= \langle \Psi_E|\hat{H}\hat{H}|\Psi_E\rangle$$

$$= E^2$$

$$\sigma_E = \sqrt{\langle \hat{H}^2\rangle - \langle \hat{H}\rangle^2} = 0$$

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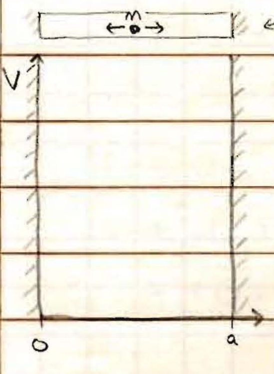
TOPIC	

Infinite Square Well

The ∞ $\square$ Well



$$V(x) = \begin{cases} 0 & x \in [0,a] \\ \infty & \text{otherwise} \end{cases}$$

SE is seperable. Ansatz: $\Psi(x,t) = \psi(x) e^{-\frac{i}{\hbar}E_n t}$

stationary SE $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = E\psi \quad x \in [0,a] \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$

($\psi = 0$ outside well)

$\psi'' + k^2\psi = 0 \longrightarrow \psi = A\sin(kx) + B\cos(kx)$

Match at boundary: $\psi(0) = 0 \longmapsto B = 0$; $\psi(a) = 0 \longmapsto k_n = \frac{n\pi}{a}$ $\quad n = 1, 2, 3, \ldots \longrightarrow E_n = \frac{\pi^2 n^2 \hbar^2}{2ma^2}$ (energy is quantized)

for each energy - energy eigenfunction: $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$

For a given initial condition: $\Psi(x,0) = f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$; $c_n = \langle \psi_n | f \rangle$

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

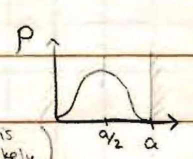
Ex. Initial conditions = energy eigenfunctions

$\Psi(x,0) = A\sin\left(\frac{\pi x}{a}\right) \xrightarrow{\text{normalize}} A = \sqrt{\frac{2}{a}}$

$\langle \hat{H} \rangle = \langle \Psi_1(x,t) | \hat{H} | \Psi_1(x,t) \rangle$

$= \int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) \hat{H} \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) \cancel{e^{\frac{i}{\hbar}E_1 t} e^{-\frac{i}{\hbar}E_1 t}} \, dx = E$

$\langle \hat{x} \rangle = \langle \Psi_1 | x | \Psi_1 \rangle = \langle \psi_1 | x | \psi_1 \rangle = \int_0^a \frac{2}{a}\sin^2\left(\frac{\pi x}{a}\right) x \, dx = \frac{a}{2}$



$\langle \hat{p} \rangle = \int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) dx = 0$ (avg momentum is 0 b/c equally likely to move in op dir)

Ex. Initial conditions = superpostions of energy eigenstates

$\Psi(x,0) = \underbrace{c_1\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)}_{\psi_1} + \underbrace{c_2\sqrt{\frac{2}{a}}\sin\left(\frac{4\pi x}{a}\right)}_{\psi_2} \qquad c_1 = \frac{1}{\sqrt{2}} \quad c_2 = \frac{1}{\sqrt{2}}e^{i\phi}$

orthonormal ψ

$\langle \Psi(x,0) | \Psi(x,0) \rangle = \sum_m \sum_n \int c_m^* \psi_m^*(x) c_n \psi_n(x) \, dx = \sum_n |c_n|^2 = 1$

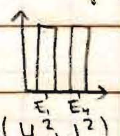
$|\Psi(x,0)\rangle = \sum_n \overset{\text{number}}{c_n} \underbrace{|\psi_n\rangle}_{\text{label}} = |\sum_n c_n \psi_n\rangle$

$\langle \Psi(x,0)| = \sum_n c_n^* \langle \psi_n | = \langle \sum_n c_n \psi_n |$

Most general equal weighted linear combination of ψ_1 and ψ_4

$\Psi(x,0) = \frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}e^{i\phi}\psi_4$ ← relative phase $\quad \Psi_4$

Histogram



$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2}}\psi_1(x)e^{-\frac{i}{\hbar}E_1 t} + \frac{e^{i\phi}}{\sqrt{2}}\psi_4(x)e^{-\frac{i}{\hbar}E_4 t}$ $\qquad \langle \hat{H} \rangle = \frac{\hbar^2\pi^2}{2ma^2}(4^2 + 1^2)$

scalar

$\langle \hat{H} \rangle = \langle \sum_m c_m \Psi_m | \hat{H} | \sum_n c_n \Psi_n \rangle = \sum_{m,n} c_m^* c_n \langle \Psi_m | E_n | \Psi_n \rangle = \sum_{n=1,4} |c_n|^2 E_n$

$\langle c_1\Psi_1 | x | c_4\Psi \rangle = -\frac{8\psi a}{15^2\pi^2} e^{-\frac{i}{\hbar}(E_4 - E_1)t + i\phi} \qquad \langle x \rangle = \frac{a}{2} - \frac{32a}{225\pi^2}\cos\left(\frac{E_4 - E_1}{\hbar}t + \phi\right)$

Harmonic Oscillator I

Review If $V = V(x)$

- Need to solve stationary SE $\longleftrightarrow$ eigenvalue problem

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi_n = E_n \Psi_n \longleftrightarrow \hat{H}|n\rangle = E_n|n\rangle$$

- If system state is $\Psi_n(x,t)$

$\rightarrow \rho(x,t) = |\Psi_n|^2 = \rho(x)$ time independant

$\rightarrow \langle\hat{O}\rangle$ expectation values when time independant

$$\langle\hat{H}\rangle = E_n \qquad \sigma_{\hat{H}} = 0$$

- If system state is a superposition

$$\Psi(x,t) = \sum_1 c_n \Psi_n \longleftrightarrow |\Psi\rangle = \sum_1 c_n|\Psi\rangle$$

$\rightarrow \rho(x,t), \langle x\rangle, \langle p\rangle$ depend on time; $\langle\hat{H}\rangle = \sum_1 |c_n|^2 E_n \qquad \sigma_{\hat{H}} \neq 0$

Measurements irreversibly project system onto an eigenstate of the measurement operator.

Ex (A) energy

$$\Psi_{before} = \sum c_n \Psi_n \xrightarrow[\text{means operator } \hat{H}]{\text{measurement yields } E_m} \Psi_{after} = \Psi_m$$

$\longrightarrow$ will remain in state Ψ_m forever

(B) position

$$\Psi_{before} = \sum_1 c_n \Psi_n \xrightarrow[\text{means operator } \hat{x}]{\text{measurement yields } x_0} \Psi_{after} = \delta(x - x_0)$$

$\longrightarrow$ since $\delta(x-x_0)$ is not a stationary solution it will delocalize with time.

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TOPIC	

Harmonic Oscillator 1

① Preliminaries

(1A) Hermetian matrices in inner products $\mathbb{H}^+ = \mathbb{H}$ and inner pr

consider vector $x = \mathbb{H}v$, $y = \mathbb{H}u$

Hermetian matrices can act to the left and right in an inner product

$$\langle x | u \rangle = (\mathbb{H}v)^+ u = v^+ \mathbb{H}^+ u = v^+ \mathbb{H} u$$

$$\langle v | y \rangle = v^+ \mathbb{H} u = v^+ \mathbb{H} u$$

$$\langle \mathbb{H}u | u \rangle = \langle u | \mathbb{H}^+ | u \rangle = \langle v | \mathbb{H} | u \rangle = \langle v | \mathbb{H} u \rangle$$

(1B) Hermetian operators act to the left and right in an inner pr

position $\hat{x}|f\rangle \longleftrightarrow x\, f(x)$

momentum $\hat{p}|f\rangle \longleftrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x} f(x)$

$$\langle \hat{x} f | g \rangle = \int (xf)^* g\, dx = \int f^* x\, g\, dx = \langle f | \hat{x} g \rangle$$

$$\langle \hat{p} f | g \rangle = \int_{-\infty}^{+\infty} \left(\frac{\hbar}{i}\frac{d}{dx} f\right)^* g\, dx = \int_{-\infty}^{+\infty} -\frac{\hbar}{i}(f^*)' g\, dx = \underbrace{-\frac{\hbar}{i} f^* g \Big|_{-\infty}^{+\infty}}_{0} + \int f^* \frac{\hbar}{i}\frac{d}{dx} g = \langle f | \hat{p} g \rangle$$

$$\boxed{\hat{x}^+ = \hat{x}} \qquad \boxed{\hat{p}^+ = \hat{p}}$$

Note on Dirac notation

$$\langle \hat{p} f | g \rangle = \langle f | \hat{p}^+ | g \rangle \overset{\hat{p}^+ = \hat{p}}{=} \langle f | \hat{p} | g \rangle = \langle f | \hat{p} g \rangle$$

(1C) Commutator $[\hat{x}, \hat{p}]$

position representation

$$[\hat{x}, \hat{p}]|f\rangle = (\hat{x}\hat{p} - \hat{p}\hat{x})|f\rangle \longrightarrow \left(x \frac{\hbar}{i}\frac{\partial}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x} x\right) f(x)$$

$$= -i\hbar\,(xf' - f - xf') = i\hbar f$$

$$= i\hbar |f\rangle$$

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

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

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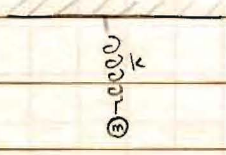
TOPIC

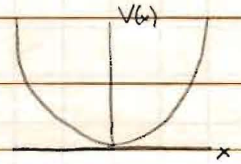
Harmonic Oscillator II

Problem Setup

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

$$\omega = \sqrt{\frac{k}{m}}$$





"boundary condition" $\lim_{|x|\to\infty} \psi(x) = 0$

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

SE: $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2x^2}{2}\right]\psi = E\psi$

$$\frac{1}{2m}\left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + (m\omega x)^2\right]\psi = E\psi$$

$$\underbrace{\frac{1}{2m}\left[\hat{p}^2 + (m\omega\hat{x})^2\right]}_{\hat{H}}|\psi\rangle = E|\psi\rangle$$

Solution Idea

try to factor $\hat{H}$

motivation from wave equation: $\left(\frac{\partial^2}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\right)\psi = \left(\frac{\partial}{\partial x} - \frac{1}{v}\frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial x} + \frac{1}{v}\frac{\partial}{\partial t}\right)\psi$

$L = x + vt$

$R = x - vt$

$= \frac{\partial}{\partial L}\frac{\partial}{\partial R}\psi = 0$

$\psi = \psi(L) \qquad \psi = \psi(R)$

$$\frac{1}{2m}(i\hat{p} + m\omega\hat{x})(-i\hat{p} + m\omega\hat{x})$$

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

$$= \frac{1}{2m}\left(\hat{p}^2 + (m\omega\hat{x})^2\right) + \frac{m\omega\hbar}{2m}$$

$$= \hat{H} + \frac{\hbar\omega}{2}$$

reverse order: $\frac{1}{2m}(-i\hat{p} + m\omega\hat{x})(i\hat{p} + m\omega\hat{x}) = \hat{H} - \frac{\hbar\omega}{2}$

Define a_+ and a_- Operators

$$\hat{a}_\pm = \frac{1}{\sqrt{2m\omega\hbar}}(\mp i\hat{p} + m\omega\hat{x})$$

$$= \frac{1}{\sqrt{2m\omega\hbar}}\left(\mp \hbar\frac{d}{dx} + m\omega\hat{x}\right)$$

$\hat{a}_-\hat{a}_+ = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} \longrightarrow \hat{H} = \hbar\omega(\hat{a}_-\hat{a}_+ - \frac{1}{2})$

$\hat{a}_+\hat{a}_- = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} \longrightarrow \hat{H} = \hbar\omega(\hat{a}_+\hat{a}_- + \frac{1}{2})$

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

$$[a_-, a_+] = 1$$

Harmonic Oscillator II

Properties of $\hat{a}_\pm$

- $[\hat{a}_-, \hat{a}_+] = 1$
- not hermetian

$$(\hat{a}_+)^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(-i\hat{p} + m\omega\hat{x})^\dagger$$
$$= \frac{1}{\sqrt{2m\hbar\omega}}(+i\hat{p}^\dagger + m\omega\hat{x}^\dagger)$$
$$= \hat{a}_-$$

- given a solution $\psi_n \leftrightarrow |n\rangle$, $\hat{H}|n\rangle = E_n|n\rangle$

  $\hat{a}_\pm$ will generate new solution

$$\hat{H}(\hat{a}_+|n\rangle) = \hbar\omega(\hat{a}_+\hat{a}_- + \tfrac{1}{2})(\hat{a}_+|n\rangle) = \hbar\omega\hat{a}_+\underbrace{(\hat{a}_-\hat{a}_+ + \tfrac{1}{2})}|n\rangle$$

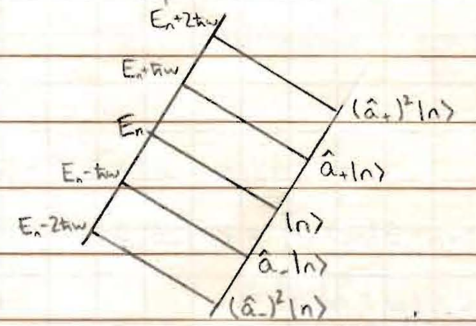
we get new eigenstates with energy

$$= \hat{a}_+[\hbar\omega(\hat{a}_+\hat{a}_- + \tfrac{1}{2}) + \hbar\omega]|n\rangle \qquad \hat{a}_+\hat{a}_- + [\hat{a}_-\hat{a}_+] = \hat{a}_+\hat{a}_- + 1$$
$$= \hat{a}_+(E_n + \hbar\omega)|n\rangle$$
$$= (E_n + \hbar\omega)(\hat{a}_+|n\rangle)$$

also,

$$\hat{H}(\hat{a}_-|n\rangle) = (E_n + \hbar\omega)(\hat{a}_-|n\rangle)$$

Ladder Operators



- There has to be a minimum state $|0\rangle$ such that $E_0 \geq V_{min} = 0$

  i.e. $\hat{a}_-|0\rangle = 0$ $\qquad |0\rangle \leftrightarrow \psi_0$

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

$$\psi_0 = Ne^{-\frac{m\omega}{2\hbar}x^2} \Leftarrow \frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar}x\,dx \rightarrow \ln\psi_0 = -\frac{m\omega}{2\hbar}x^2 + C_1$$

Normalization

Normalized Gaussian: $\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

want $1 = \int|\psi_0|^2dx = |N|^2\int e^{-\frac{m\omega}{\hbar}x^2}dx$

$\sigma^2 = \frac{\hbar}{2m\omega} \longrightarrow |N|^2 = \sqrt{\frac{m\omega}{\pi\hbar}}$

$$\boxed{\begin{aligned}\psi_0 &= \left(\frac{m\omega}{\hbar\omega}\right)^{1/4}e^{-\frac{m\omega}{2\hbar}x^2}\\ E_0 &= \frac{\hbar\omega}{2}\\ E_n &= \hbar\omega(n+\tfrac{1}{2})\end{aligned}}$$

$$\hat{H}|0\rangle = \hbar\omega(\hat{a}_+\hat{a}_- + \tfrac{1}{2})|0\rangle$$
$$= \frac{\hbar\omega}{2}|0\rangle$$

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HARMONIC OSCILLATOR III

Review: Harmonic Oscillator

$$\hat{H} = \frac{1}{2m}\left[-\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 + m^2\omega^2x^2\right]$$

$$= \hbar\omega\left[\hat{a}_+\hat{a}_- + \tfrac{1}{2}\right]$$

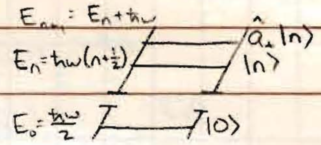
$$= \hbar\omega\left[\hat{a}_-\hat{a}_+ - \tfrac{1}{2}\right]$$

ground state $|0\rangle \longleftrightarrow \psi_0(x)$; $E_0 = \frac{\hbar\omega}{2}$; $\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$

raising operator

$$\hat{a}_+ = \frac{1}{\sqrt{2m\hbar\omega}}\left[-i\hat{p} + m\omega\hat{x}\right]$$

$$\hat{a}_+|n\rangle = A_{n+1}|n+1\rangle$$



here $\langle n|n\rangle = 1$, $\langle n+1|n+1\rangle = 1$, and A_{n+1} is not necessarily 1

Task: find A_{n+1} $\rightarrow$ then get $|n+1\rangle$ from $|n\rangle$: $|n+1\rangle = \frac{1}{A_{n+1}}\hat{a}_+|n\rangle$

$$|A_{n+1}|^2 = \langle \hat{a}_+n|\hat{a}_+n\rangle$$

$$= \langle n|(\hat{a}_+)^\dagger\hat{a}_+|n\rangle$$

$$= \langle n|\hat{a}_-\hat{a}_+|n\rangle$$

$$= \langle n|\hat{a}_-\hat{a}_+ - \tfrac{1}{2} + \tfrac{1}{2}|n\rangle$$

$$= \langle n|(n+\tfrac{1}{2}) + \tfrac{1}{2}|n\rangle$$

$$= (n+1)\langle n|n\rangle = n+1$$

So

$$\boxed{\begin{aligned}\hat{a}_+|n\rangle &= \sqrt{n+1}\,|n+1\rangle \\ \hat{a}_-|n\rangle &= \sqrt{n}\,|n-1\rangle\end{aligned}}$$

Check Orthogonality

① $\langle m|\hat{a}_+\hat{a}_-|n\rangle = \sqrt{n}\langle m|\hat{a}_+|n-1\rangle$

$$= \sqrt{n}\sqrt{n}\langle m|n\rangle$$

② $\langle m|\hat{a}_+\hat{a}_-|n\rangle = \left((\hat{a}_+\hat{a}_-)^\dagger|m\rangle\right)^\dagger|n\rangle$

$$= \left((\hat{a}_-)^\dagger(\hat{a}_+)^\dagger|m\rangle\right)^\dagger|n\rangle$$

$$\overset{①}{=} \left(\hat{a}_+\hat{a}_-|m\rangle\right)^\dagger|n\rangle$$

$$= \left(m|m\rangle\right)^\dagger|n\rangle$$

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

$0 = (m-n)\langle m|n\rangle$

if $m \neq n$ $\langle m|n\rangle = 0 \Rightarrow$ orthogonal

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HARMONIC OSCILLATOR III

Explicit Calculation of Wave Function

Define $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$ $\qquad \frac{d}{dx} = \sqrt{\frac{m\omega}{\hbar}} \frac{d}{d\xi}$

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2}$$

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

$$\begin{aligned}\psi_1 = \frac{\hat{a}_+}{\sqrt{0+1}}\psi_0 &= \frac{1}{\sqrt{0+1}}\frac{1}{\sqrt{2}}\left(-\frac{d}{d\xi} + \xi\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2} \\ &= \frac{1}{\sqrt{1}}\frac{1}{\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\underbrace{\left(-\left(-2\frac{\xi}{2}\right) + \xi\right)}_{2\xi} e^{-\xi^2/2}\end{aligned}$$

$$\begin{aligned}\psi_2 = \frac{\hat{a}_+}{\sqrt{1+1}}\psi_1 &= \frac{1}{\sqrt{2}}\frac{1}{2}\left(-\frac{d}{d\xi} + \xi\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(2\xi e^{-\xi^2/2}\right) \\ &= \frac{1}{2\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(-2 + 2\xi^2 + 2\xi^2\right) e^{-\xi^2/2}\end{aligned}$$

Hermite Polynomials

$H_n(\xi)$

$n=0$	1
$n=1$	2ξ
$n=2$	$4\xi^2$
$n=3$	$8\xi^2 - 12\xi$

Energy Eigenfunction of Harmonic Oscillator

$$\psi_n(\xi) = \frac{1}{\sqrt{n!}\sqrt{2^n}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n(\xi)\, e^{-\xi^2/2} \qquad \xi = \sqrt{\frac{m\omega}{\hbar}}\, x \quad n = 0, 1, 2, \ldots$$

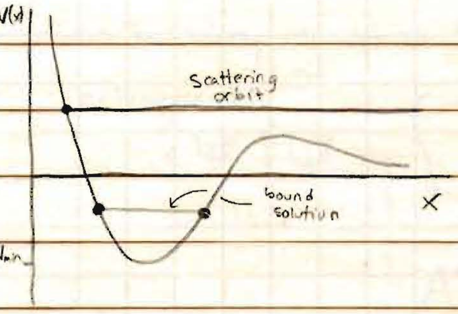
$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$ It is known that the ψ_n are a complete orthonormal basis for square integrable functions on $\mathbb{R}$.

Expectation Values

systems in state $|n\rangle \longrightarrow \langle \hat{x} \rangle = \langle n | \hat{x} | n \rangle \longrightarrow \hat{x} \propto (\hat{a}_+ + \hat{a}_-)$

FREE PARTICLE

Classical Mechanics

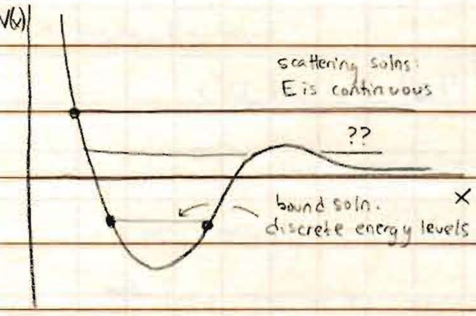


$E < V_{min}$ is not physical

$\frac{1}{2}mv^2 = E - V < 0$

$V \rightarrow$ imaginary (not physical)

Quantum Mechanics



$E < V_{min}$ not physical

$$-\frac{\hbar^2}{2m}\psi'' = (E-V)\psi$$

$$\psi'' = \underbrace{\frac{2m(E-V)}{\hbar^2}}_{\alpha}\psi \qquad \alpha > 0$$

$$\int \psi^* \psi'' \, dx = \alpha \int \psi^* \psi \, dx$$

$\psi = 0$ is only solution $\Longleftarrow$ $-\int (\psi')^* \psi' \, dx = \alpha \int |\psi|^2 dx$

Free Particle

$V(x) = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi \qquad \text{introduce } k = \pm\sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi'' + k^2\psi = 0 \longrightarrow \psi = Ae^{ikx} \qquad k \in \mathbb{R}$$

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

$$\Psi_E(x,t) = \psi(x)\, e^{-\frac{i}{\hbar}Et}$$

$$= Ae^{ikx - i\frac{k^2\hbar}{2m}t}$$

$$= Ae^{ik(x - \frac{k\hbar}{2m}t)}$$

travelling wave soln w/ V_{phase}:

$$V_p = \frac{\hbar k}{2m}$$

$k > 0$ right travelling
$k < 0$ left travelling

$$\Rightarrow V_p = \sqrt{\frac{E}{2m}}$$

compare to classical result ($E = \frac{1}{2}mv^2$)

$$V_{particle} = \sqrt{\frac{2E}{m}} \neq V_p$$

FREE PARTICLE

Properties

- no boundary condition $\leftrightarrow$ E, k are continuous
- orthogonality?

$$\langle \Psi_{E1} | \Psi_{E2} \rangle = \int_{-\infty}^{+\infty} \left(A_1^* e^{-ik_1 x + \frac{i}{\hbar} E_1 t} \right) \left(A_2 e^{-ik_2 x + \frac{i}{\hbar} E_2 t} \right) dx$$

$$= A_1^* A_2 e^{\frac{i}{\hbar}(E_1 - E_2)t} \underbrace{\int_{-\infty}^{+\infty} e^{-i(k_1 + k_2)x} \, dx}_{2\pi \delta(k_1 - k_2)}$$

if $k_1 \neq k_2$

the $\langle \Psi_E | \Psi_E \rangle = 0 \leftrightarrow$ orthogonal

- normalization

$$\langle \Psi_E | \Psi_E \rangle = |A|^2 \int_{-\infty}^{+\infty} dx = \infty$$

$\Rightarrow$ not normalizeable!!!

The energy eigenfunctions are not normalizable $\rightarrow$ are not a physical soln

$\rightarrow$ free particles cannot be in an energy eigenstate

$\rightarrow$ free particles do not have definite energy

Idea: Use energy eigenstates (traveling waves) as "basis fct" to construct a normalized solution through a continuous superposition

	bound soln	scattering soln
energy eigenstates	E_n, Ψ_n, n integer	$E_k, \Psi_k, \; k \in \mathbb{R}$
general solution	$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$	$\Psi(x,t) = \int \phi(k) \Psi_k(x,t) \, dk$

Math Interlude:
- Delta fct.
- Forier transf.
- Gaussian integral's

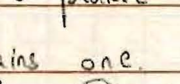
Dirac Delta Function

$$\int_{-\infty}^{\infty} f(x) \delta(x - x_0) \, dx = f(x_0)$$

- it is the continuous analog of the Kronecker $\delta_{mn} = \begin{cases} 1 & n = m \\ 0 & \text{otherwise} \end{cases}$

$$\int_a^b \delta(x) \, dx = \begin{cases} 1 & 0 \in (a,b) \\ 0 & \text{otherwise} \end{cases}$$

- roughly speaking $\delta(x) = \begin{cases} \infty & x = 0 \\ 0 & \text{otherwise} \end{cases}$ and $\int_{-\infty}^{+\infty} \delta(x) \, dx = 1$
- one can view δ as a limit of a peaked function as the peak width goe to zero and the area remains one. $\delta(x) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \eta\left(\frac{x}{\varepsilon}\right)$
- Ex: Gaussian $\delta = \lim_{\varepsilon \to 0} \frac{1}{\sqrt{2\pi}\, \varepsilon} e^{-\frac{1}{2}\left(\frac{x}{\varepsilon}\right)^2}$



FREE PARTICLE II

$E = \frac{\hbar^2 k^2}{2m}$ $\psi \propto e^{ikx}$ and want $\int_{-\infty}^{+\infty} \phi(k) e^{ikx - \frac{i}{\hbar}\frac{\hbar^2 k^2}{2m}t} dk$

Review: Fourier Transform

$f(x) \leftrightarrow F(k)$

$g(t) \leftrightarrow G(\omega)$

dimensions

x and k conjugate variables $[x] = \text{length}$

t and ω conjugate variables $[k] = \frac{1}{\text{length}}$

f and F are equivalent representation

Fourier transformations: $F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$

Inverse Fourier transformation: $f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{-ikx} dk$

→ conservation of norm $\int_{-\infty}^{+\infty} |f(x)|^2 dx = \int_{-\infty}^{+\infty} |F(k)|^2 dk$

$$F(k) \overset{!}{=} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(\bar{k}) e^{i\bar{k}x} d\bar{k} \right] e^{-ikx} dx$$

$$\overset{!}{=} \int_{-\infty}^{+\infty} F(\bar{k}) \underbrace{\left[\frac{1}{2\pi} \int e^{-i(k-\bar{k})x} dx \right]}_{\delta(k-\bar{k})} d\bar{k}$$

$$\delta(k-\bar{k}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left(\frac{1}{\sqrt{\pi}} e^{i\bar{k}x} \right) e^{-ikx} dx = \hat{F}\left[\frac{e^{ikx}}{\sqrt{2\pi}} \right]$$

2

Application

① orthogonality: e^{ikx}

$$\left\langle \frac{e^{ikx}}{\sqrt{\pi}} \middle| \frac{e^{i\bar{k}x}}{\sqrt{\pi}} \right\rangle = \int \frac{1}{2\pi} e^{-i(k-\bar{k})x} dx = \delta(k-\bar{k})$$

② solutions to free particle SE with initial $\psi_0(x)$

a) $\Psi(x,0) = \psi_0(x)$

FT of initial condition $\mathcal{F}[\psi_0(x)] = \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi_0(x) e^{-ikx} dx$

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

equivalent representation $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Phi(k,t) e^{ikx} dk$

$\xrightarrow[\text{to SE}]{\text{plug in}}$ $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Phi(k,t) e^{ikx} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} i\hbar \frac{\partial \Phi(k,t)}{\partial t} e^{ikx} dk$

$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\hbar^2 k^2}{2m} \Phi e^{ikx} dk$ = ———— " ————

$\frac{\hbar^2 k^2}{2m} \Phi = i\hbar \frac{\partial \Phi}{\partial t} \rightarrow \dot{\Phi} = -\frac{i}{\hbar} \frac{\hbar^2 k^2}{2m} \Phi \Rightarrow \Phi(k,t) = \Phi(k,0) e^{-i\frac{\hbar k^2}{2m}t}$

soln: $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)} dk$ with $\phi(k) = \int_{-\infty}^{\infty} \psi_0(x) e^{-ikx} dx$

FREE PARTICLE II

Example Gaussian

$$\psi_0(x) = \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2} \qquad \left(\text{Note: } \int_{-\infty}^{\infty} e^{-(Ax^2+Bx+C)}\,dx = \sqrt{\frac{\pi}{A}}\, e^{\frac{B^2}{4A}-C}\right.$$

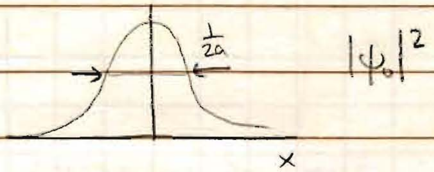
• Normalize: $$|\psi_0|^2 = \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-\frac{x^2}{2\sigma^2}} = \left(\frac{2a}{\pi}\right)^{1/2} e^{-2ax}$$

• FT of ψ_0: $$\phi(k) = \frac{1}{\sqrt{2\pi}} \int \left(\frac{2a}{\pi}\right)^{1/4} e^{-(ax^2+ikx)}\,dx$$
$$= \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\pi}{a}}\, e^{-\frac{k^2}{4a}}$$

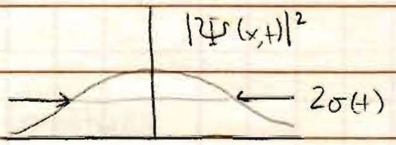
$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{2a}} e^{-\left(\frac{k^2}{4a} + i\frac{\hbar t}{2m} - ikx\right)}\,dk \qquad \left|\; A = \frac{1}{4a}\left(1+i\frac{2\hbar t a}{m}\right),\ B = -ix \right.$$
$$= \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{4\pi a}} \sqrt{\frac{\pi}{\frac{1}{4a}\left(1+i\frac{2\hbar t a}{m}\right)}}\ \exp\left(\frac{-x^2}{\frac{1}{a}\left(1+i\frac{2\hbar t a}{m}\right)}\right)$$

$$|\Psi|^2 = \Psi^*\Psi = \sqrt{\frac{4a}{2\pi}} \frac{1}{\sqrt{1+\frac{4\hbar^2 t^2 a^2}{m^2}}} \exp\left(-\frac{x^2}{1/a}\left(\frac{1}{1+i\frac{2\hbar t a}{m}} + \frac{1}{1-i\frac{2\hbar t a}{m}}\right)\right)$$
$$= \frac{1}{\sqrt{2\pi}} \frac{1}{\underbrace{\sqrt{\frac{1}{4a} + \frac{\hbar^2 t^2 a}{m^2}}}_{\sigma(t)}} \exp\left[-\frac{x^2}{\frac{4}{4a}} \underbrace{\frac{2}{\left(1+\frac{4\hbar^2 t^2 a^2}{m^2}\right)}}_{\sigma^2(t)}\right]$$
$$= \frac{1}{\sqrt{2\pi}\,\sigma(t)} e^{-\frac{x^2}{2\sigma(t)^2}}$$

$t = 0$

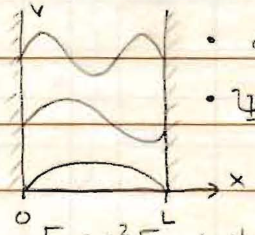


$t > 0$



bound states

energy eigenstates



- discrete values
- $\Psi(x,t) = \psi_n(x) e^{-\frac{i}{\hbar}E_n t}$

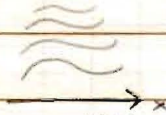
$$E_n = n^2 E_1 \; ; \; \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

general soln or superposition

$$\Psi(x,t) = \sum_n c_n \Psi_n(x,t)$$

$$c_n = \langle \Psi_n(x,0) | \Psi(x,0) \rangle$$
$$= \langle \psi_n(x) | \Psi(x,0) \rangle$$
$$= \int_{-\infty}^{+\infty} \psi_n^*(x) \Psi(x,0) \, dx$$

scattering states



- cont. energies
- $\Psi_k(x,t) = \frac{1}{\sqrt{2\pi}} e^{ikx - \frac{i}{\hbar}\frac{\hbar^2 k^2}{2m}t}$

not normalizable

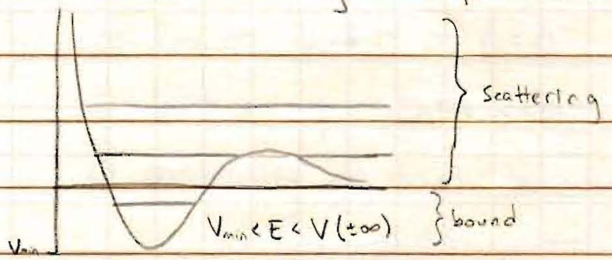
$$E_k = \frac{\hbar^2 k^2}{2m}$$

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

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

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

In QM, tunneling is possible:

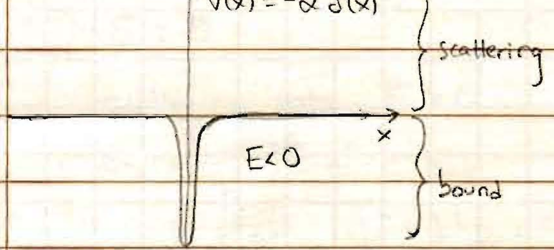


Boundary Conditions

(A) ψ is continuous

(B) $\frac{d\psi}{dx}$ is continuous, except where $|V(x)| = \infty$

Delta Function Well 1



$$\int_{-\infty}^{+\infty} V(x)\,dx = -\alpha$$

(A) Bound Solution

Is there a bound soln.?

- $x<0$: $-\frac{\hbar^2}{2m}\psi_-'' = -|E|\psi_-$

  $\kappa = \sqrt{\frac{2m|E|}{\hbar^2}}$ $\quad \psi'' - \kappa^2\psi = 0$

  $$\psi_-(x) = Ae^{\kappa x} + Be^{-\kappa x}$$

- $x>0$: $\psi_+(x) = Ce^{\kappa x} + De^{-\kappa x}$

  ① $x \to \infty$: $\psi_+ \to 0 \Rightarrow C = 0$

  ② $x \to -\infty$: $\psi_- \to 0 \Rightarrow B = 0$

  ③ continuity of ψ at boundary

  $$\psi_-(0) = \psi_+(0) \longrightarrow A = D$$

  $$\psi_-(x) = Ae^{\kappa x} \qquad \psi_+(x) = Ae^{-\kappa x}$$

  ④ $|V(0)| = \infty$

  - need a condition for discontinuity of ψ'
  - got it by integrating SE across boundary and taking $\varepsilon \to 0$ limit

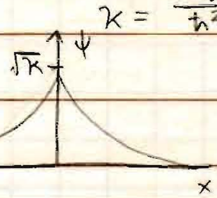
$$\lim_{\varepsilon\to 0}\Big[\underbrace{-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon}\frac{d^2\psi}{dx^2}dx}_{} + \underbrace{\int_{-\varepsilon}^{+\varepsilon}(-\alpha\delta(x))\psi(x)\,dx}_{-\alpha\psi(0)}\Big] = \underbrace{-|E|\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon}\psi(x)\,dx}_{0 \text{ b/c } \psi \text{ is cont.}}$$

$$-\frac{\hbar^2}{2m}\lim_{\varepsilon\to 0}\frac{d\psi}{dx}\Big|_{-\varepsilon}^{+\varepsilon} = -\frac{\hbar^2}{2m}\left(\psi_+'(0) - \psi_-'(0)\right)$$

$$\psi_+'(0) - \psi_-'(0) = -\frac{2m\alpha}{\hbar^2}\psi_\pm(0)$$

$$(-\kappa A) - (+\kappa A) = -\frac{2m\alpha}{\hbar^2}A$$

$$\kappa = \frac{m\alpha}{\hbar^2} \xrightarrow{\ \kappa^2 = \frac{2m|E|}{\hbar^2}\ } |E| = \frac{\hbar^2}{2m}\frac{m^2\alpha^2}{\hbar^4} = \frac{m\alpha^2}{2\hbar^2}$$



$$\Psi(x,t) = \begin{cases} \sqrt{\kappa}\, e^{\kappa x + \frac{i}{\hbar}|E|t} & x<0 \\ \sqrt{\kappa}\, e^{-\kappa x + \frac{i}{\hbar}|E|t} & x>0 \end{cases} \qquad E = -\frac{m\alpha^2}{2\hbar^2}$$

DELTA FUNCTION WELL I

(B) $E > 0$

<u>scattering soln</u> $E > 0$

- <u>$x < 0$</u>: $-\frac{\hbar^2}{2m}\psi_-'' = E\psi_-$

  $k = \sqrt{\frac{2mE}{\hbar^2}}$ $\quad \psi_-'' + k^2\psi_- = 0$

  $$\psi_- = Ae^{ikx} + Be^{-ikx}$$

- <u>$x > 0$</u>: $\psi_+ = Ce^{ikx} + De^{-ikx}$

  ① We know ψ is

  ② not normalizable $\quad [x \to \pm\infty]$

  ③ continuity of ψ

  $$\psi_-(0) = \psi_+(0)$$

  $$A + B = C + D$$

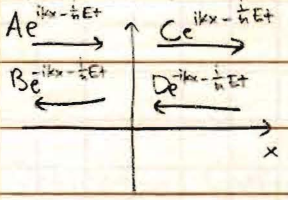
  ④ jump of ψ' at boundary

  $$\psi_+'(0) - \psi_-'(0) = -\frac{2m\alpha}{\hbar^2}\psi_-(0)$$

  $$ik(C-D) - ik(A-B) = -\frac{2m\alpha}{\hbar^2}(A+B) \quad \Big| \ \frac{-i}{k}$$

  $$C - D - A + B = 2i\beta(A+B) \quad \Big| \ \text{define } \beta = \frac{m\alpha}{\hbar^2 k}$$

Reflection and Transmission



$$A + B = C \to C - A = B$$

$$C - A + B = 2i\beta(A+B)$$

$$2B = 2i\beta(A+B) \longrightarrow \frac{B}{A} = \frac{i\beta}{1-i\beta}$$

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

Assume incoming wave from the left

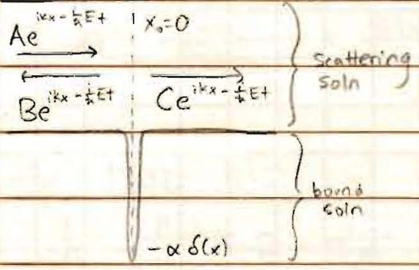
$$A \neq 0, \ D = 0$$

Reflection: B

Transmission: C

Delta Function Well II

Review



Boundary Conditions at x_0

① ψ is continuous

$$\lim_{\varepsilon\to 0}\left(\psi(x_0+\varepsilon)-\psi(x_0-\varepsilon)\right)=0$$

② a) $\frac{d\psi}{dx}$ continuous if $V(x)$ finite

b) if $|V(x_0)|=\infty$

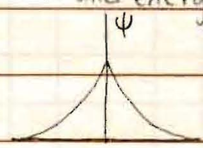
$$\Delta\frac{dx}{dt}=\lim_{\varepsilon\to 0}\left(\frac{d\psi}{dx}\bigg|_{x_0+\varepsilon}-\frac{d\psi}{dx}\bigg|_{x_0-\varepsilon}\right)=\frac{\hbar^2}{2m}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi(x)\,dx$$

bound states $\longleftrightarrow$ normalizable

③ $\psi(+\infty)=0$

④ $\psi(-\infty)=0$ $\Longrightarrow$ fixes coefficients and energies

⑤ $\int|\psi|^2dx=1$



scattering states $\longleftrightarrow$ not normalizable

reflection $\frac{B}{A}$

transmission $\frac{C}{A}$

Assumption: incoming particle from left $A\neq 0$, $D=0$

Reflection Coefficient

magnitude of probability flux density of reflected particle

$$R=\frac{-j_{\text{reflected}}}{j_{\text{incoming}}}$$

prob. flux density of incoming wave/particle

$$j=\frac{i\hbar}{2m}\left(\psi\frac{d\psi^*}{dx}-\psi^*\frac{d\psi}{dx}\right)=\frac{\hbar}{m}\,\mathrm{Im}\left(\frac{d\psi}{dx}\psi^*\right)$$

$$R=\frac{-\frac{\hbar}{m}\,\mathrm{Im}\left(\frac{d}{dx}(Be^{-ikx})B^*e^{ikx}\right)}{+\frac{\hbar}{m}\,\mathrm{Im}\left(\frac{d}{dx}(Ae^{-ikx})A^*e^{ikx}\right)}=\frac{-\mathrm{Im}(-ik|B|^2)}{\mathrm{Im}(ik|A|^2)}$$

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

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TOPIC	

Transmition Coefficient

$$T = \frac{j_{trans}}{j_{incoming}} = \frac{\frac{\hbar}{m}\,\mathrm{Im}\left(\frac{d}{dx}\left(Ce^{i\bar{k}x}\right)C^* e^{-i\bar{k}x}\right)}{\mathrm{Im}\left(ik|A|^2\right)} \rightarrow \boxed{T = \frac{|C|^2}{|A|^2}\frac{\bar{k}}{k}}$$

Probability conserv

$R + T = 1$

Ex Delta Well

$$\frac{B}{A} = \frac{i\beta}{1-i\beta} \Rightarrow R = \frac{\beta^2}{1+\beta^2}$$

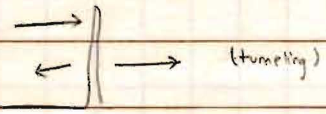
$$\frac{C}{A} = \frac{1}{1-i\beta} \Rightarrow T = \frac{1}{1+\beta^2}$$

$$k = \bar{k} = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\beta = \frac{m\alpha}{\hbar^2 k}$$

$\alpha^2 \propto \beta^2$ (sign independant)

$$R = \frac{\beta^2}{1+\beta^2}, \quad T = \frac{1}{1+\beta^2}$$



Ex. Step Potential