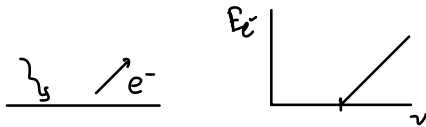


lec 1.

Early 20th Century: light can act like particle (photons).

$$E = h\nu \quad h = 6.63 \times 10^{-27} \text{ energy sec}$$

photo-electric effect:



de Broglie:

particles can act like wave: $\lambda = h/p$.

Davisson & Germer experiment:

Observed interference of electron diffraction.

Rules of QM:

complex function



1) Particle described by $\psi(\vec{x}, t)$, a wave function or **state** of the particle.

2) Probability of finding particle in d^3x about $\vec{x}$ is proportional to

$$dP(\vec{x}, t) = C |\psi(\vec{x}, t)|^2 d^3x \quad C \text{ constant}$$

where

$$1 = \int dP = C \cdot \int |\psi(\vec{x}, t)|^2 d^3x$$

3) Measurement of quantity A only yields set of allowed values $\{a\}$ called eigenvalues, associated with each a is a state ψ_a , called **eigenstate**.

In state ψ_a , measure A , get $A=a$ with certainty.

But if $\psi = \sum_a C_a \psi_a$. Measure A , then get $A=a$ with probability

$$P_a = |C_a|^2 / \sum_b |C_b|^2.$$

If you measure value a at time t_0 , state immediately after is ψ_a .

4) State $\psi(\vec{x}, t)$ satisfies Schrödinger Eq:

(*)

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

$$\hbar = h/2\pi.$$

m = mass of particle.

∇^2 = Laplacian.

V = potential Energy classical particle would have

Comments:

- 1) (*) is linear: If ψ_1, ψ_2 are solutions, so is $c_1\psi_1 + c_2\psi_2$, $c_1, c_2 \in \mathbb{C}$.
- 2) (*) is 1st order in time. So only need to specify $\psi(\vec{x}, t_0)$.

Example: free particle in 1D ($V=0$):

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi$$

Try:

$$\psi = X(x) T(t).$$

Substitute and divide by ψ . Set each side to const $\hbar\omega$: Get

$$\psi(x, t) = e^{i(kx - \omega t)} \quad \omega = \frac{\hbar k^2}{2m}.$$

$$E = \hbar\omega = \frac{(\hbar k)^2}{2m} = \frac{p^2}{2m}.$$

But ψ not square integrable.

General solution:

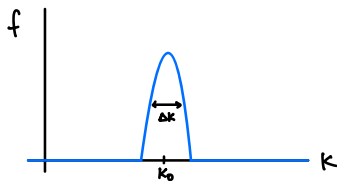
$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{i[kx - \omega(k)t]} dk. \quad g(k) \text{ arbitrary complex funct.}$$

Set $t=0$. $\psi(x, 0)$ is square integrable if $g(k)$ is. Just standard Fourier transf.

For any potential $V(x, t)$ at $t=0$:

$$\text{Write } g(k) = f(k) e^{i\alpha(k)} \quad f \text{ real.}$$

Assume f is sharply peaked:



And assume $\alpha(k)$ doesn't vary rapidly over $[k_0 - \frac{\Delta k}{2}, k_0 + \frac{\Delta k}{2}]$.

Then

$$\alpha(k) \approx \alpha(k_0) + \alpha'(k_0)(k - k_0).$$

Set

$$x_0 := -\alpha'(k_0).$$

Then $k = (K - K_0) + K_0$ gives

$$\psi(x, 0) = \frac{e^{i[k_0 x + \alpha(k_0)]}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k) e^{i(k - k_0)(x - x_0)} dk.$$

If $x - x_0$ oscillates when $k - k_0$ varies by Δk , integral is small. Need roughly $\Delta x \Delta k \approx 1$. (Heisenberg uncertainty).

Starting with

$$\psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int g(k) e^{ikx} dk$$

Since $p = \hbar k$. Probability of measuring $p = \hbar k$ should be proportional to $|g(k)|^2 dk$.

Replace k with p :

$$\psi(x, 0) = \int g\left(\frac{p}{\hbar}\right) e^{ipx/\hbar} \frac{dp}{\sqrt{2\pi\hbar}}.$$

Define

$$\bar{\psi}(p) = \frac{g(p/\hbar)}{\sqrt{\hbar}}.$$

Then

$$\psi(x, 0) = \int \bar{\psi}(p) e^{ipx/\hbar} \frac{dp}{\sqrt{2\pi\hbar}}$$

Parseval's relation:

$$\begin{aligned} \int |\psi(x, 0)|^2 dx &= \int |g(k)|^2 dk \\ &= \int |g\left(\frac{p}{\hbar}\right)|^2 \frac{dp}{\hbar} \\ &= \int |\bar{\psi}(p)|^2 dp. \end{aligned}$$

If $\psi(x)$ normalized, so is $\bar{\psi}(p)$.

Prob of finding particle between x and $x+dx$ is $|\psi(x, 0)|^2 dx$.

with momentum between p and $p+dp$ is $dP(p) = |\bar{\psi}(p)|^2 dp$.

Time evolution of a free particle. ($V=0$ necessary).

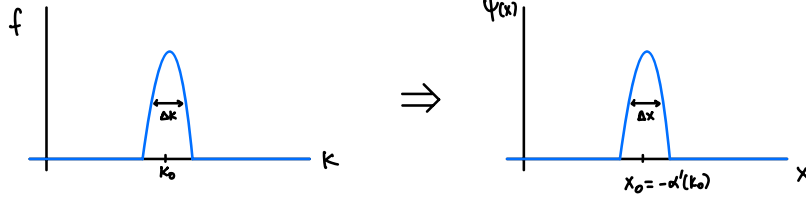
$$\psi(\hat{x}, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{i[kx - \omega(k)t]} dk. \quad \omega(k) = \frac{\hbar k^2}{2m}.$$

$$e^{i(kx - \omega t)} = e^{ik(x - v_p t)}$$

$$v_p = \frac{\hbar k}{2m} = \frac{p}{2m}.$$

Note v_p differs from classical answer by $1/2$. This v_p is phase velocity.

Consider wave packet $g(k) = f(k) e^{i\alpha}$



lec 2.

General Solution to free particle:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int g(k) e^{i[kx - \omega(k)t]} dk \quad \omega(k) = \frac{\hbar k^2}{2m}$$

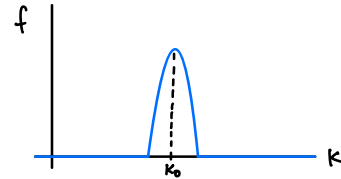
phase velocity of 1 mode:

$$e^{i[kx - \omega(k)t]} = e^{ik(x - v_p t)}$$

$$v_p = \frac{\hbar k}{2m} = \frac{p}{2m} = \frac{1}{2} v_{\text{classical}}$$

But we should look at group velocity of $\psi(x,t)$.

If $g(k) = f(k) e^{i\alpha(k)}$ w/ f peak around k_0



Expand

$$\alpha(k) - \omega(k)t \approx \alpha(k_0) - \omega(k_0)t + \underbrace{(\alpha'(k_0) - \omega'(k_0)t)}_{:= -X_0(t)}(k - k_0)$$

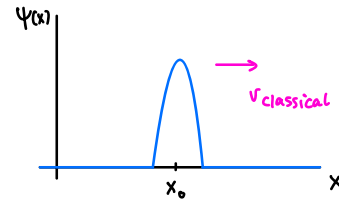
Then

$$\psi(x,t) = \frac{e^{i[k_0 x + \alpha(k_0) - \omega(k_0)t]}}{\sqrt{2\pi}} \int f(k) e^{i(k - k_0)(x - X_0(t))} dk$$

Max of ψ at $X_0(t)$.

Moves with velocity

$$v_0 = \frac{dX_0}{dt} = \frac{d\omega}{dk} = \frac{\hbar k}{m} = \frac{p}{m} = v_{\text{classical}}$$



For general time independent potential $V(\vec{x})$:

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

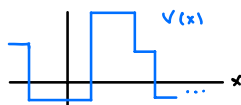
Try $\psi(x,t) = T(t) \varphi(x)$. Each side $\equiv E$.

$$T(t) = e^{-iEt/\hbar}$$

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

Eigenvalue Equation.

For piecewise constant potentials,



$$\psi(x,t) = e^{-iEt/\hbar} e^{ikx}$$

where if $V=V_0$,

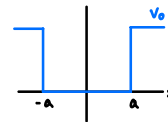
$$\frac{\hbar^2 k^2}{2m} = E - V_0. \quad (\text{RHS can be } + \text{ or } -).$$

Boundary Conditions:

- 1) When V jumps, ψ and $\frac{\partial \psi}{\partial x}$ must be continuous.
- 2) At $x = \pm \infty$, ψ can't grow exponentially. ψ can oscillate.
- 3) If $V_0 = \infty$, then $\psi = 0$.

Results:

- ① square well: For $E < V_0$, only certain E allowed.
For $E > V_0$, all E are allowed.



- ② $E < V_0$, particles can tunnel through the barrier.



..... End of Review

I. Mathematical Foundations of QM:

States: Vectors in a vector space V , denoted by $|\alpha\rangle$ (kets)

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle \in V$$

$$c \cdot |\alpha\rangle \in V \quad \forall c \in \mathbb{C}.$$

Basis: a countable set of linearly independent $|\alpha_i\rangle$ s.t. any

$$|\alpha\rangle = \sum_i c_i |\alpha_i\rangle \quad c_i \in \mathbb{C}$$

Dimension: # of basis vectors.

Inner Product: $\langle \alpha | \beta \rangle \in \mathbb{C}$ s.t.

$$1) \langle \alpha | \beta_1 + c_2 \beta_2 \rangle = c_1 \langle \alpha | \beta_1 \rangle + c_2 \langle \alpha | \beta_2 \rangle.$$

$$2) \langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle^*$$

$$3) \langle \alpha | \alpha \rangle \geq 0. \quad \langle \alpha | \alpha \rangle = 0 \Leftrightarrow |\alpha\rangle = 0.$$

Norm of $|\alpha\rangle$ is $|\alpha| = \langle\alpha|\alpha\rangle^{1/2}$.

Orthogonal: $\langle\alpha|\beta\rangle = 0$.

Note from (2): If $|\alpha\rangle = c|\gamma\rangle$, then $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^* = \langle\beta|c\alpha\rangle^* = (c\langle\beta|\alpha\rangle)^* = c^*\langle\alpha|\beta\rangle$.

$\langle\alpha| = c^*\langle\gamma|$. Inner product is anti-linear in 1st factor.

The dual of V is the space of linear maps: $V \rightarrow \mathbb{C}$.

Given the inner product, every vector is associated with a dual vector

$$|\alpha\rangle \leftrightarrow \langle\alpha| \quad c|\alpha\rangle \leftrightarrow c^*\langle\alpha|$$

(bra :)

where

$$(\langle\alpha|)(|\beta\rangle) = \langle\alpha|\beta\rangle.$$

If $\dim V = \infty$:

Defⁿ: A sequence of vectors $|\alpha_1\rangle, |\alpha_2\rangle, \dots$ is a Cauchy sequence if $\forall \varepsilon > 0, \exists N > 0$ s.t. $|\alpha_i - \alpha_j| < \varepsilon \quad \forall i, j > N$.

Defⁿ: A vector space w/ inner product is a Hilbert space if every Cauchy sequence converges: i.e., $\exists |\alpha\rangle$ s.t. $\lim_{j \rightarrow \infty} |\alpha_j - \alpha| = 0$.

Example 1:

Let $V = \{ \text{sequences of } \mathbb{C} \text{ \#s } (a_1, a_2, \dots) \text{ with } a_i = 0 \text{ for all but finitely many } i \}$.

inner product

$$\langle(x_n)|y_n\rangle = \sum_{n=1}^{\infty} x_n^* y_n.$$

Not a Hilbert space!

Let $|\alpha_j\rangle = (1, \frac{1}{2}, \frac{1}{3}, \dots, \frac{1}{j}, 0, 0, \dots)$. Cauchy.

But conv. to $\alpha = (1, \frac{1}{2}, \frac{1}{3}, \dots, \frac{1}{n}, \dots) \notin V$.

Example 2:

$$V = \{ \text{cts } \mathbb{C}\text{-valued functions on } \mathbb{R}^3 \text{ s.t. } \int |f|^2 < \infty \}.$$

$$\langle f|g \rangle = \int f^*(x) g(x) d^3x.$$

Not Hilbert space. Because can approach discontinuous functions with cts functions arbitrarily.

Example 3:

$$V = \{ \infty \text{ seqs } (x_n) \text{ s.t. } x_n \in \mathbb{C}, \sum |x_n|^2 < \infty \} := \ell^2(\mathbb{C}).$$

$$\langle (x_n) | (y_n) \rangle = \sum x_n^* y_n.$$

is a Hilbert space.

Example 4. $V = \{ \text{square integrable } \mathbb{C}\text{-functions on } \mathbb{R}^3 \} / \sim := L^2(\mathbb{R}^3).$

$$\langle f|g \rangle = \int f^*(x) g(x) d^3x.$$

$\uparrow$
 $f \sim g$ iff $|f-g| \neq 0$
for a measure 0 set.

is a Hilbert space.

lec 3.

Linear Operator

a map $A: V \rightarrow V$ s.t. $A(c_1|\alpha_1\rangle + c_2|\alpha_2\rangle) = c_1 A|\alpha_1\rangle + c_2 A|\alpha_2\rangle$.

$$(A+B)|\alpha\rangle = A|\alpha\rangle + B|\alpha\rangle.$$

$$(cA)|\alpha\rangle = c \cdot A|\alpha\rangle.$$

$$[A, B] = AB - BA$$

$$\{A, B\} = AB + BA$$

Examples:

$$\textcircled{1} I|\alpha\rangle = |\alpha\rangle$$

$$\textcircled{2} |\alpha\rangle\langle\beta| \text{ is an operator : } |\gamma\rangle \rightarrow \langle\beta|\gamma\rangle|\alpha\rangle.$$

Adjoint: A also maps dual space to itself

$$\langle\alpha|A : |\beta\rangle \rightarrow \langle\alpha|A|\beta\rangle.$$

But dual of $A|\alpha\rangle$ is not $\langle\alpha|A$. Define **adjoint** of A , denoted $A^\dagger$, s.t. $\langle\alpha|A^\dagger$ is the dual of $A|\alpha\rangle$.

$$\langle\alpha|A^\dagger|\beta\rangle = \langle\beta|A|\alpha\rangle^*$$

$$\text{Example: } A = iI, \quad \langle\alpha|A^\dagger|\beta\rangle = \langle\beta|A|\alpha\rangle^* = -i\langle\alpha|\beta\rangle \Rightarrow A^\dagger = -iI.$$

Properties of adjoint:

$$\textcircled{1} (cA)^\dagger = c^* A^\dagger.$$

$$\textcircled{2} (A^\dagger)^\dagger = A.$$

$$\textcircled{3} (AB)^\dagger = B^\dagger A^\dagger.$$

$$\text{pf: If } |\gamma\rangle = B|\alpha\rangle, \text{ then } \langle\alpha|(AB)^\dagger|\beta\rangle = \langle\beta|AB|\alpha\rangle^* = \langle\beta|A|\gamma\rangle^*$$

$$= \langle\gamma|A^\dagger|\beta\rangle$$

$$\stackrel{|\gamma\rangle = B|\alpha\rangle}{\langle\gamma| = \langle\alpha|B^\dagger}} = \langle\alpha|B^\dagger A^\dagger|\beta\rangle$$

□

An operator is **Hermitian** if $A = A^\dagger$.

An operator is **unitary** if $AA^\dagger = I = A^\dagger A$.

Unitary operator preserve norm:

$$|A\alpha|^2 = \langle A\alpha | A\alpha \rangle = \langle \alpha | A^\dagger A | \alpha \rangle = \langle \alpha | \alpha \rangle = |\alpha|^2.$$

In terms of orthonormal basis $|u_i\rangle$, i.e., $\langle u_i | u_j \rangle = \delta_{ij}$.

kets $\rightarrow$ column vectors bras $\rightarrow$ row vectors operators $\rightarrow$ matrices.

$$|\psi\rangle = \sum_j c_j |u_j\rangle$$

$$\langle \varphi | = \sum_i b_i \langle u_i |$$

$$\langle \varphi | \psi \rangle = \sum_{ij} b_i c_j \delta_{ij} = \sum_i b_i c_i.$$

For operator A , matrix element of A is

$$A_{ij} = \langle u_i | A | u_j \rangle.$$

We can reconstruct operator:

$$A = \sum_{ij} A_{ij} |u_i\rangle \langle u_j|$$

$$A|\psi\rangle = \sum_{ijk} A_{ij} c_k |u_i\rangle \underbrace{\langle u_j | u_k \rangle}_{\delta_{jk}} = \sum_{ij} A_{ij} c_j |u_i\rangle.$$

$$\text{Identity} = \sum_i |u_i\rangle \langle u_i|.$$

Adjoints:

$$A_{ij}^\dagger = \langle u_i | A^\dagger | u_j \rangle = \langle u_j | A | u_i \rangle^* = A_{ji}^*.$$

eigenvalue
 $\downarrow$

Defⁿ: An **eigenvector** is a **nonzero** vector s.t. $A|\psi\rangle = \lambda|\psi\rangle$.

If $|\psi\rangle$ is e.vector, so is $c|\psi\rangle$. If there is only 1 e.vector for λ , we say λ is **nondegenerate**. If $|\psi\rangle, |\varphi\rangle$ both e.vectors with e.values λ , so is $c_1|\psi\rangle + c_2|\varphi\rangle$.

Set of e.vectors w/ same e.value form a vector space.

Finding e.vectors

1) Solve a differential Equation;

2) If an operator A leaves N -dim subspace invariant, then use linear algebra:

• Let $|u_i\rangle$ $i=1, \dots, N$ be an O.N. basis of subspace.

- $A|\psi\rangle = \lambda|\psi\rangle \Rightarrow \langle u_i | A|\psi\rangle = \lambda \langle u_i | \psi\rangle$

- insert $I = \sum_j |u_j\rangle \langle u_j|$ into Eq above:

$$\sum_j \langle u_i | A | u_j \rangle \langle u_j | \psi \rangle = \lambda \langle u_i | \psi \rangle$$

$$\sum_j A_{ij} c_j = \lambda c_i$$

$$\sum_j (A_{ij} - \lambda \delta_{ij}) c_j = 0 \quad \text{requires} \quad \det(A_{ij} - \lambda \delta_{ij}) = 0.$$

(always have N complex solutions for λ).

Eigenvalues of Hermitian operators:

① E. values are real.

pf: If $A|\psi\rangle = \lambda|\psi\rangle$, then $\langle\psi|A|\psi\rangle = \lambda\langle\psi|\psi\rangle$. Thus $\langle\psi|A|\psi\rangle^* = \lambda^* \langle\psi|\psi\rangle$

$$\text{So } (\lambda - \lambda^*) \langle\psi|\psi\rangle = 0 \Rightarrow \lambda = \lambda^*. \quad \square \quad \langle\psi|A|\psi\rangle = \langle\psi|A^\dagger|\psi\rangle \quad (A^\dagger = A).$$

② E. vectors associated with different e. values are orthogonal.

pf: $A|\psi\rangle = \lambda|\psi\rangle$, $A|\varphi\rangle = \mu|\varphi\rangle$. $\langle\varphi|A|\psi\rangle = \lambda\langle\varphi|\psi\rangle$, $\langle\psi|A|\varphi\rangle^* = \mu\langle\varphi|\psi\rangle$

But $\langle\psi|A|\varphi\rangle^* = \langle\varphi|A|\psi\rangle$ for $A = A^\dagger$. Thus $(\lambda - \mu)\langle\varphi|\psi\rangle = 0$. $\lambda \neq \mu$

so $\langle\varphi|\psi\rangle = 0$. $\square$

If λ is degenerate, can pick ON basis for subspace of eigenvectors with e. val λ .

So e. vectors of Hermitian op. form O.N. set.

If $\dim = \infty$, Some Hermitian operator have no E. vectors. e.g. position operator in $L^2(\mathbb{R})$.

If $\dim < \infty$, E. vectors of Hermitian operator form an ON. basis.

pf: Suppose not. let W be the subspace of vectors which are perpendicular to all

e. vectors. Then $\forall |w\rangle \in W$, $A|w\rangle \in W$ because A is Hermitian:

$$\langle\psi|A|w\rangle = \langle w|A|\psi\rangle^* = \lambda\langle w|\psi\rangle^* = 0.$$

By (*), always exists 1. e. vector in W . Contradiction. $\square$

Commuting Operators:

Let A, B both Hermitian and $[A, B] = 0$,

If $A|\psi\rangle = a|\psi\rangle$ & set $|\chi\rangle = B|\psi\rangle$. Then since $[A, B] = 0$,

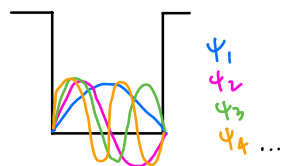
$$A|\chi\rangle = AB|\psi\rangle = BA|\psi\rangle = aB|\psi\rangle = a|\chi\rangle.$$

So $|\chi\rangle$ is an e.vector of A w/ same e.value.

- If a is nondegenerate eigenvalue, then $|\chi\rangle = b|\psi\rangle$. Then $B|\psi\rangle = b|\psi\rangle$. So $|\psi\rangle$ is e.state of B as well.
- If a is degenerate, $A|\psi_i\rangle = a|\psi_i\rangle$ $i=1, \dots, g$. Then $B|\psi_i\rangle$ is a linear comb of $|\psi_i\rangle$ for $AB=BA$. Find e.states of B on this g -dim subspace. Get ON set of e.vectors of B in eigenspace of A w/ e.value a . Thus we get an O.N. set of e.vectors of both B & A .

Conclusion: If A, B Hermitian, $[A, B] = 0$, $\exists$ an O.N. set of simultaneous eigenstates. (In finite dim, they can be a basis).

For square well, e.states of H form a basis.



If $\{A, B, C, \dots\}$ Hermitian, commute & simultaneous e.values all non-deg.

This is called complete set of commuting variables. States labeled by these e.values,

Position & Momentum Operators:

$$X\psi(x) = x\psi(x). \quad \langle\phi|X|\psi\rangle = \int \phi^*(x) \cdot x \cdot \psi(x) dx$$

If ψ is square integrable, $x\psi$ may not be square integrable! e.g. $\psi(x) = \frac{1}{x}$.

Lec 4.

Position & Momentum Operator

$|\psi(x)|^2$ Prob. of finding particle at x .

Average position:

$$\langle \psi | X | \psi \rangle = \int x |\psi(x)|^2 dx.$$

This is Hermitian:

$$\langle \psi | X^\dagger | \varphi \rangle = \langle \varphi | X | \psi \rangle^* = \left(\int \varphi^*(x) x \psi(x) dx \right)^* = \int \psi^*(x) x \varphi(x) dx = \langle \psi | X | \varphi \rangle.$$
$$X^\dagger = X.$$

Define $f(X)$ by

$$f(X) \psi(x) = f(x) \psi(x).$$

Recall Prob. of finding momentum p is $|\bar{\psi}(p)|^2$ where

$$\bar{\psi}(p) = \int \frac{dx}{(2\pi\hbar)^{1/2}} \psi(x) e^{-ipx/\hbar}.$$

Average momentum $\int p |\bar{\psi}(p)|^2 dp = \langle \psi | P | \psi \rangle$ where P multiplies $\bar{\psi}(p)$ by p .

Let

$$\begin{aligned} f(x) &= \int \frac{dp}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \left(\frac{\hbar}{i} \frac{\partial}{\partial x} e^{-ipx/\hbar} \bar{\psi}(p) \right) \\ &= \frac{\hbar}{i} \frac{\partial}{\partial x} \int \frac{dp}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \bar{\psi}(p) \\ &= -i\hbar \frac{\partial}{\partial x} \psi(x). \end{aligned}$$

Thus in the position space,

$$P = -i\hbar \frac{\partial}{\partial x}.$$

Note that P is not defined on the entire $L^2(\mathbb{R})$. At least the input needs to be differentiable. And the derivative must be in $L^2(\mathbb{R})$.

P is Hermitian:

$$\begin{aligned} \langle \psi | P^\dagger | \varphi \rangle &= \langle \varphi | P | \psi \rangle^* = \left(\int dx \varphi^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x) \right)^* \\ &= - \left(\int dx \frac{\hbar}{i} \frac{d}{dx} \varphi^*(x) \psi(x) \right)^* \\ &= \int dx \psi^*(x) \frac{\hbar}{i} \frac{d}{dx} \varphi(x) \\ &= \langle \psi | P | \varphi \rangle. \end{aligned}$$

$$P = P^\dagger.$$

Example like $x^L e^{-x^2} \sin x$ is L^2 but does not vanish at ∞ , but derivative not in L^2 .

integrate by part

We can throw away boundary term because we only consider functions in the domain of P : Continuous function whose derivative is square integrable. So $\varphi^*(x) \psi(x) |_{-\infty}^{\infty} = 0$.

In 3D: X_j multiplies by x_j , $P_j = -\frac{\hbar}{i} \frac{\partial}{\partial x_j}$.

For any state ψ ,

$$[X_j, P_k] \psi = x_j \frac{\hbar}{i} \frac{\partial}{\partial x_k} \psi - \frac{\hbar}{i} \frac{\partial}{\partial x_k} (x_j \psi) = i\hbar \delta_{jk} \psi.$$

So

$$[X_j, P_k] = i\hbar \delta_{jk}$$

$$[X_j, X_k] = 0$$

$$[P_j, P_k] = 0.$$

Eigenstates:

Want $X|x'\rangle = x'|x'\rangle$ where x' is a real number.

So $x \psi_{x'}(x) = x' \psi_{x'}(x)$ So $\psi_{x'}(x) = 0$ when $x \neq x'$. Thus $\psi_{x'}(x) = \delta(x-x')$.

allow δ -function normalized states:

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

Now view $\psi(x)$ has coefficients of expansion of $|\psi\rangle$ in $|x\rangle$:

$$|\psi\rangle = \int dx \psi(x) |x\rangle.$$

$|x\rangle$ are complete:

$$\int dx |x\rangle \langle x| = I.$$

$$\int dx \langle \phi|x \rangle \langle x|\psi \rangle = \langle \phi|\psi \rangle.$$

More rigorously, define the **spectrum** of an operator A to be all $\lambda \in \mathbb{C}$ s.t.

$(A - \lambda I)$ not invertible.

Momentum Operator:

$$P|p'\rangle = p'|p'\rangle$$

$$\frac{\hbar}{i} \frac{d}{dx} \psi_{p'}(x) = p' \psi_{p'}(x)$$

$$\psi_{p'}(x) \propto e^{ip'x/\hbar}.$$

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

$$\psi_{p'}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ip'x/\hbar} = \langle x|p' \rangle.$$

So

$$\begin{aligned}\langle p' | \psi \rangle &= \langle p' | \int dx |x\rangle \langle x | \psi \rangle = \int dx \langle p' | x \rangle \langle x | \psi \rangle \\ &= \int dx \frac{e^{-ip'x/\hbar}}{\sqrt{2\pi\hbar}} \psi(x) \\ &= \bar{\psi}(p).\end{aligned}$$

Momentum eigenspace are complete:

$$\int dp |p\rangle \langle p| = \mathbb{I}.$$

$|\psi\rangle$ abstract state, position & momentum representations are just expansions of $|\psi\rangle$ in $|x\rangle$ or $|p\rangle$.

Translation Operator

$$T(a) |x'\rangle = |x'+a\rangle \quad \text{on basis } \{|x'\rangle\}, \text{ so defined on entire Hilbert space.}$$

Claim: $T(a)$ unitary.

$$\text{pf. } T(a) |x'\rangle = |x'+a\rangle \Rightarrow \langle x'+a| = \langle x'| T^\dagger(a).$$

$$\langle x' | T^\dagger(a) T(a) |x\rangle = \langle x'+a | x+a \rangle = \delta(x-x') = \langle x' | x \rangle.$$

$$\text{So } T^\dagger(a) T(a) = \mathbb{I}.$$

□

$$\text{Also: } T(a) T(b) = T(a+b), \quad T(0) = \mathbb{I}.$$

So ordinary translations form a group since $\exists$ a product & identity & inverse.

In QM, they are represented by unitary operators.

What is $T(a) |p\rangle$?

$$\begin{aligned}T(a) |p\rangle &= \int dx T(a) |x\rangle \langle x | p \rangle = \int dx |x+a\rangle e^{ipx/\hbar} / (2\pi\hbar)^{1/2} & x' = x+a \\ &= \int dx' |x'\rangle e^{ip(x'-a)/\hbar} / (2\pi\hbar)^{1/2} \\ &= e^{-ipa/\hbar} \int dx' |x'\rangle \langle x' | p \rangle \\ &= e^{-ipa/\hbar} |p\rangle.\end{aligned}$$

$\Rightarrow |p\rangle$ is an eigenstate of $T(a)$ with eigenvalue $e^{-ipa/\hbar}$. Thus

$$T(a) = e^{-iPa/\hbar}$$

If $a = \epsilon$ (small), expand:

$$T(\epsilon) = I - \frac{i}{\hbar} P \epsilon + \dots \quad (*)$$

Momentum is the **generator** of translations.

In general, if $A^\dagger = A$, e^{iA} is unitary. Since $(e^{iA})^\dagger = e^{-iA^\dagger} = e^{-iA}$. So
 $(e^{iA})^\dagger (e^{iA}) = e^{-iA} e^{iA} = I$.

Note: $\frac{i}{\hbar} P = \frac{\partial}{\partial x}$.

Why minus sign in (*)?

$$x' := x + a$$

$$T(a) \int dx \psi(x) |x\rangle = \int dx \psi(x) |x+a\rangle \stackrel{\downarrow}{=} \int dx' \psi(x'-a) |x'\rangle$$

Lec 5.

Mean Value & Root Mean Square Approximation.

Given a Hermitian operator A with $A|u_n\rangle = a_n|u_n\rangle$. Let $|\psi\rangle = \sum c_n|u_n\rangle$ be a normalized state. Probability of measuring a_n is $|c_n|^2$. Average:

$$\langle A \rangle = \sum a_n |c_n|^2$$

for

$$\langle \psi | A | \psi \rangle = \sum_{m,n} a_n c_m^* c_n \overset{\delta_{mn}}{\langle u_m | u_n \rangle} = \sum_n a_n |c_n|^2.$$

Similarly, if $A|V_r\rangle = r|V_r\rangle$ for continuous r , and

$$|\psi\rangle = \int dr c(r) |V_r\rangle.$$

Then

$$\begin{aligned} \langle \psi | A | \psi \rangle &= \left(\int dr c^*(r) \langle V_r | \right) A \left(\int ds c(s) |V_s\rangle \right) \\ &= \left(\int dr c^*(r) \langle V_r | \right) \left(\int ds s \cdot c(s) |V_s\rangle \right) \\ &= \iint dr ds c^*(r) c(s) \cdot s \delta(r-s) \\ &= \int dr r |c(r)|^2 = \langle A \rangle. \end{aligned}$$

Fluctuations: For any Hermitian A , Consider $A - \langle A \rangle I$. Clearly

$$\langle A - \langle A \rangle I \rangle = 0.$$

But

$$\langle (A - \langle A \rangle I)^2 \rangle \neq 0.$$

Define the **root mean square** (RMS) deviation to be

$$\Delta A = \langle (A - \langle A \rangle I)^2 \rangle^{1/2}.$$

Expanding:

$$(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2.$$

Example: For **Gaussian** $|\psi(x)|^2 = \frac{1}{(2\pi)^{1/2}\sigma} e^{-x^2/2\sigma}$, we have

$$\langle x \rangle = 0, \langle x^2 \rangle = \sigma^2 \Rightarrow \Delta x = \sigma.$$

Proof of uncertainty principle:

Let A, B be 2 Hermitian operators. Let $\bar{A} = A - \langle A \rangle I$ and $\bar{B} = B - \langle B \rangle I$, then

$$(\Delta A)^2 (\Delta B)^2 = \langle \bar{A}^2 \rangle \langle \bar{B}^2 \rangle.$$

In state $|\psi\rangle$,

$$(\Delta A)^2 (\Delta B)^2 = \langle \bar{A}^2 \rangle \langle \bar{B}^2 \rangle.$$

$$= \langle \psi | \bar{A}^2 | \psi \rangle \langle \psi | \bar{B}^2 | \psi \rangle$$

$$= \| \bar{A} | \psi \rangle \|^2 \cdot \| \bar{B} | \psi \rangle \|^2$$

$$\bar{A}^\dagger = \bar{A}, \bar{B}^\dagger = \bar{B}$$

$$\geq |\langle \psi | \bar{A} \bar{B} | \psi \rangle|^2$$

by Schwarz inequality

$$= |\langle \psi | \frac{1}{2} (\bar{A} \bar{B} + \bar{B} \bar{A}) | \psi \rangle + \langle \psi | \frac{1}{2} (\bar{A} \bar{B} - \bar{B} \bar{A}) | \psi \rangle|^2$$

If $C^\dagger = -C$, $\langle \psi | C | \psi \rangle = -\langle \psi | C^\dagger | \psi \rangle = -\langle \psi | C | \psi \rangle^*$
 $\Rightarrow \langle \psi | C | \psi \rangle$ purely imaginary.

$$= |\langle \psi | \frac{1}{2} (\bar{A} \bar{B} + \bar{B} \bar{A}) | \psi \rangle|^2 + |\langle \psi | \frac{1}{2} (\bar{A} \bar{B} - \bar{B} \bar{A}) | \psi \rangle|^2$$

Dropping the 1st term and write, for 2nd term, we have by def of $\bar{A}, \bar{B}$:

$$[\bar{A}, \bar{B}] = [A, B].$$

Thus

$$(\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} |\langle \psi | [A, B] | \psi \rangle|^2$$

$$(\Delta A)(\Delta B) \geq \frac{1}{2} |\langle [A, B] \rangle|.$$

Uncertainty Principle

Example: $A = X, B = P, \Delta X \Delta P \geq \frac{\hbar}{2}$.

In 3D: $\Delta X_i \Delta P_j = \frac{\hbar}{2} \delta_{ij}$.

Can you saturate inequality (so that it's equality)?

For equality to hold:

a) $\bar{A} | \psi \rangle = \lambda \bar{B} | \psi \rangle$ for some $\lambda \in \mathbb{C}$ (so Schwarz ineqn is equality).

b) $\langle \psi | \bar{A} \bar{B} + \bar{B} \bar{A} | \psi \rangle = 0$ (so 1st term we throw doesn't contribute).

$$a) \Rightarrow (\Delta A)^2 = \langle \psi | \bar{A}^2 | \psi \rangle = \| \bar{A} | \psi \rangle \|^2 = |\lambda|^2 \| \bar{B} | \psi \rangle \|^2 = |\lambda|^2 (\Delta B)^2.$$

$$\text{So } \Delta A = |\lambda| \cdot (\Delta B)$$

$\| \bar{B} | \psi \rangle \|^2$ which is non zero for $|\psi\rangle \neq 0$. If $|\psi\rangle = 0$, ineqn is trivially saturated.

$$b) \Rightarrow \langle \psi | \bar{A} \bar{B} | \psi \rangle + \langle \psi | \bar{B} \bar{A} | \psi \rangle = 0 \Rightarrow (\lambda^* + \lambda) \langle \psi | \bar{B}^2 | \psi \rangle = 0 \Rightarrow \lambda^* + \lambda = 0$$

$$= \lambda^* \langle \psi | \bar{B}^2 | \psi \rangle \quad \text{by a)}$$

$$\Rightarrow \lambda \text{ purely imaginary.}$$

Therefore, a) with imag. $\lambda \Rightarrow$ b).

Let $A=P$, $B=X$. $\Delta X \Delta P = \frac{\hbar}{2} = |\lambda| (\Delta X)^2$ by above.

So by above, for saturated state

$$\lambda = \frac{i\hbar}{2(\Delta X)^2}$$

Assuming $\langle P \rangle = \langle X \rangle = 0$, then by a):

$$\frac{\hbar}{i} \frac{d}{dx} \psi = \lambda x \psi.$$

So

$$\psi(x) = N e^{i\lambda x^2/2\hbar} = N e^{-x^2/4(\Delta X)^2}.$$

Thus if a state is saturated, it is a Gaussian. Note that:

$$|\psi(x)|^2 = N^2 e^{-x^2/2(\Delta X)^2}.$$

So standard dev. is indeed ΔX .

Claim: Gaussians do not always minimize uncertainty.

$$\psi(x) = \int \bar{\psi}(p) e^{ipx/\hbar} \frac{dp}{(2\pi\hbar)^{1/2}}.$$

$\bar{\psi}(p)$ also a Gaussian. Under time evolution, pick up a phase $e^{-iP^2/2m\hbar}$, does not change ΔP , but increases ΔX .

II. Quantum Dynamics.

Classical Hamiltonian:

$$H = \frac{\vec{P}^2}{2m} + V(x).$$

In QM: $P = \frac{\hbar}{i} \nabla$. So quantum Hamiltonian:

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(X)$$

Schrodinger's Eq:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle. \quad (*)$$

H is Hermitian since P^2 & X are.

$$\Rightarrow \frac{d}{dt} \langle \psi(t) | \psi(t) \rangle = -\frac{1}{i\hbar} \langle \psi(t) | H | \psi(t) \rangle + \frac{1}{i\hbar} \langle \psi(t) | H | \psi(t) \rangle = 0.$$

So norm is preserved.

Write

time evolution operator

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle.$$

Since norm preserved, $U(t)$ is unitary. Easy to see

$$U(t) = e^{-iHt/\hbar} \quad \text{clearly solves } (*)$$

c.f. $T(a) = e^{-iPa/\hbar}$.

Hamiltonian generates time translation.

In terms of energy eigenstates: $H|\alpha\rangle = E_\alpha|\alpha\rangle$, $\langle\beta|\alpha\rangle = \delta_{\beta\alpha}$.

$$\langle\beta|H|\alpha\rangle = e^{-iE_\alpha t/\hbar} \delta_{\beta\alpha}.$$

$$U(t) = \sum_\alpha e^{-iE_\alpha t/\hbar} |\alpha\rangle\langle\alpha|.$$

For any $|\psi(0)\rangle$, Expand

$$|\psi(0)\rangle = \sum_\alpha c_\alpha |\alpha\rangle,$$

$$|\psi(t)\rangle = \sum_\alpha c_\alpha e^{-iE_\alpha t/\hbar} |\alpha\rangle.$$

In position basis:

$$K(x, t; x') \equiv \langle x|U(t)|x'\rangle. \quad K \text{ called propagator.}$$

Now

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

So:

$$\psi(x, t) = \int dx' K(x, t; x') \psi(x', 0).$$

K satisfies (*) in (x, t) for fixed x' :

$$\begin{aligned} K(x, t; x') &= \langle x|U(t)|x'\rangle \\ &= \langle x|U(t) \sum_\alpha |\alpha\rangle\langle\alpha||x'\rangle \\ &= \sum_\alpha \langle x|\alpha\rangle e^{-iE_\alpha t/\hbar} \langle\alpha|x'\rangle \\ &= \sum_\alpha \underbrace{\psi_\alpha(x) e^{-iE_\alpha t/\hbar}}_{\text{Solves Schrödinger Eq}} \psi_\alpha^*(x') \end{aligned}$$

$\{|\alpha\rangle\}$ energy eigenbasis

$$\psi_\alpha(x) = \langle x|\alpha\rangle.$$

For free particle:

$$K(x, t; x') = \left(\frac{m}{2\pi i \hbar t}\right)^{1/2} e^{im(x-x')^2/2\hbar t}.$$

Obtain by using $\int dp |p\rangle\langle p|$ rather than $\sum_\alpha |\alpha\rangle\langle\alpha|$.

lec 6.

$$U = e^{-iHt/\hbar}$$

Time dependence of expectation values: In energy eigenstates:

$$|\psi(0)\rangle = |\alpha\rangle \quad H|\alpha\rangle = E_\alpha |\alpha\rangle.$$

For any observable A:

$$\begin{aligned}\langle\psi(t)|A|\psi(t)\rangle &= \langle\alpha| e^{iE_\alpha t/\hbar} A e^{-iE_\alpha t/\hbar} |\alpha\rangle \\ &= \langle\alpha| A |\alpha\rangle \\ &= \langle\psi(0)|A|\psi(0)\rangle.\end{aligned}$$

But in general

$$\begin{aligned}|\psi(0)\rangle &= \sum_\alpha c_\alpha |\alpha\rangle \\ \langle\psi(t)|A|\psi(t)\rangle &= \sum_{\alpha\beta} c_\alpha^* c_\beta \langle\alpha|A|\beta\rangle e^{i(E_\alpha - E_\beta)t/\hbar}\end{aligned}$$

will evolve in time.

Note: Time evolution of matrix element

$$\langle\psi|A|\varphi\rangle = \langle\psi|U^\dagger A U|\varphi\rangle = \langle\psi|U^\dagger A U|\varphi\rangle.$$

Heisenberg Rep:

$$A^H(t) = U^\dagger(t) A U(t).$$

Operators now satisfy equation

$$\frac{dA^H}{dt} = \frac{dU^\dagger}{dt} A U + U^\dagger A \frac{dU}{dt}$$

But

$$\frac{dU}{dt} = -\frac{i}{\hbar} H U \quad \frac{dU^\dagger}{dt} = \frac{i}{\hbar} U^\dagger H.$$

$$\Rightarrow \frac{dA^H}{dt} = -\frac{i}{\hbar} \left[U^\dagger H \underbrace{U U^\dagger}_I A U - U^\dagger A \underbrace{U U^\dagger}_I H U \right]$$

$$= -\frac{i}{\hbar} [H A^H - A^H H]$$

$$= \frac{i}{\hbar} [A^H, H]$$

Note $U^\dagger H U = H$
for $U = e^{-iHt/\hbar}$

$$\frac{dA^H}{dt} = \frac{1}{i\hbar} [A^H, H]$$

Heisenberg Eq. of Motion

Comments:

1) In classical mechanics, if A is a function of x, p , then

$$\frac{dA}{dt} = [A, H]_{\text{Poisson Brackets}}$$

2) $\frac{dH}{dt} = 0$.

3) Expectation values in Schrödinger and Heisenberg rep. agree.

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

HW1: $[X, F(p)] = i\hbar F'(p)$ $[P, G(x)] = -i\hbar G'(x)$.

So

$$H = U^\dagger H U$$

$$\frac{dx^H}{dt} = \frac{1}{i\hbar} [U^\dagger x U, H] \stackrel{\downarrow}{=} \frac{U^\dagger}{i\hbar} [x, H] U = U^\dagger \frac{p}{m} U = \frac{p^H}{m}$$

$$\frac{dp^H}{dt} = \frac{1}{i\hbar} [U^\dagger p U, H] = \frac{U^\dagger}{i\hbar} [p, H] U = -U^\dagger V'(x) U = -V'(x^H)$$

So this is the classical Eq of motion.

Define $|\varphi(t)\rangle =$ eigenstate of the time dependent operator $A^H(t)$ at time t . (Although in Heisenberg picture states do not evolve).

If $A(0)|\varphi(0)\rangle = \lambda|\varphi(0)\rangle$ and $A^H(t) = U^\dagger(t) A U(t)$. Then $|\varphi(t)\rangle = U^\dagger(t) |\varphi(0)\rangle$

pf. $A^H(t) |\varphi(t)\rangle = (U^\dagger A U) U^\dagger |\varphi(0)\rangle = U^\dagger A |\varphi(0)\rangle = \lambda |\varphi(t)\rangle$ □

In general, if $|\varphi_i\rangle$ are e. states of A at time $t=0$.

$$|\psi\rangle = \sum_i c_i |\varphi_i\rangle. \quad c_i = \langle \varphi_i | \psi \rangle$$

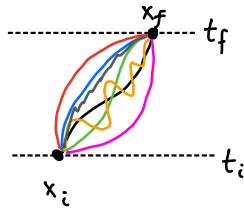
In Schrödinger Pic: $c_i(t) = \langle \varphi_i | U(t) | \psi \rangle$

In Heisenberg Pic: $c_i(t) = \langle \varphi_i | U(t) | \psi \rangle$
↑
 $|\varphi_i(t)\rangle = U^\dagger(t) |\varphi_i(0)\rangle$

Now let $|x, t\rangle$ be a Heisenberg L. state of position. Then $\langle x_f, t_f | x_i, t_i \rangle$ is **transition amplitude** to go from x_i at $t=t_i$ to x_f at $t=t_f$. We can evolve any state by

$$\begin{aligned}\Psi(x_f, t_f) &= \langle x_f, t_f | \Psi \rangle = \langle x_f, t_f | \int dx_i | x_i, t_i \rangle \langle x_i, t_i | \Psi \rangle \\ &= \int dx_i \langle x_f, t_f | x_i, t_i \rangle \langle x_i, t_i | \Psi \rangle \\ &= \int dx_i \langle x_f, t_f | x_i, t_i \rangle \Psi(x_i, t_i).\end{aligned}$$

Feynman's Path Integral.



Consider all paths $x(t)$ from x_i to x_f for each path, compute

$$S[x(t)] = \int_{t_i}^{t_f} dt \left[\frac{1}{2} m \dot{x}^2 - V(x) \right]$$

View $e^{iS[x(t)]/\hbar}$ as contribution to total amplitude:

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}[x(t)] e^{iS[x(t)]/\hbar}.$$

↑
integrate over all paths
 $x(t)$ s.t. $x(t_i) = x_i, x(t_f) = x_f$.

Classical limit: $\Delta x, \Delta p \rightarrow 0$ since measure infinitely accurate, so $\Delta x \Delta p \geq \frac{\hbar}{2} > 0$ implies $\hbar \rightarrow 0$. If $\delta S = 0$, nearby path contributes constructively. If $\delta S \neq 0$, nearby path contributes destructively.

$\mathcal{D}[x(t)]$:

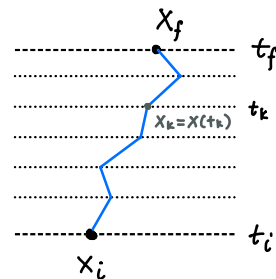
Divide $t_f - t_i$ into N segments. Assume path is straight line on each segment. path $x(t)$ specified by $x_k = x(t_k)$. Just integrate

over $(N-1)$ x_k 's :

Normalization factor

$$\int \mathcal{D}[x(t)] = \lim_{N \rightarrow \infty} C^N(\Delta t) \int dx_{N-1} dx_{N-2} \cdots dx_2$$

Assume $C^N(\Delta t)$ independent of $V(x)$.



For free particle, (x_{j-1}, t_{j-1}) to (x_j, t_j) :

$$S = \int_{t_{j-1}}^{t_j} dt \frac{1}{2} m \dot{x}^2 = \frac{m}{2\Delta t} (x_j - x_{j-1})^2$$

$$\langle x_j, t_j | x_{j-1}, t_{j-1} \rangle = C(\Delta t) \exp \left[\frac{im(x_j - x_{j-1})^2}{2\hbar \Delta t} \right]$$

Demand

$$\lim_{\Delta t \rightarrow 0} \langle x_j, t_j | x_{j-1}, t_{j-1} \rangle = \delta(x_j - x_{j-1}).$$

This fixes

$$C(\Delta t) = \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{1/2}.$$

Check:

$$\lim_{\Delta t \rightarrow 0} \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{1/2} \int dx_j e^{im(x_j - x_{j-1})^2 / 2\hbar \Delta t} = 1.$$

Let

$$\xi = (x_j - x_{j-1}) / \sqrt{\Delta t}$$

The above limit now becomes

$$\left(\frac{m}{2\pi i \hbar} \right)^{1/2} \int d\xi e^{i\xi^2} \dots = 1.$$

Path integral composition:

$$\langle x_f, t_f | x_i, t_i \rangle = \int dx_o \langle x_f, t_f | x_o, t_o \rangle \langle x_o, t_o | x_i, t_i \rangle.$$

Lec 7.

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}[X(t)] e^{iS[X(t)]/\hbar}$$

Claim: This satisfies Schrödinger's Equation.

Focus on the last step: divide path into n steps

$$\langle x_n, t_n | x_1, t_1 \rangle = \int dx_{n-1} c(\Delta t) \exp\left[\frac{im}{2\hbar} \frac{(x_n - x_{n-1})^2}{\Delta t} - \frac{iV\Delta t}{\hbar}\right] \cdot \langle x_{n-1}, t_{n-1} | x_1, t_1 \rangle$$

Let $\xi = x_{n-1} - x_n$, $x = x_n$, $t = t_{n-1}$. Then above reads:

$$\langle x, t + \Delta t | x_1, t_1 \rangle = \left(\frac{m}{2\pi i \hbar \Delta t}\right)^{1/2} \int d\xi \exp\left[\frac{im\xi^2}{2\hbar \Delta t} - \frac{iV\Delta t}{\hbar}\right] \langle x + \xi, t | x_1, t_1 \rangle.$$

Expand in $\Delta t + \xi$:

$$\text{LHS} = \langle x, t | x_1, t_1 \rangle + \Delta t \frac{\partial}{\partial t} \langle x, t | x_1, t_1 \rangle$$

$$\text{RHS} = \left(\frac{m}{2\pi i \hbar \Delta t}\right)^{1/2} \int d\xi \exp\left[\frac{im\xi^2}{2\hbar \Delta t}\right] \left(1 - \frac{iV\Delta t}{\hbar} + \dots\right) \left(\langle x, t | x_1, t_1 \rangle + \mathcal{O}(\xi) + \frac{\xi^2}{2} \frac{\partial^2}{\partial x^2} \langle x, t | x_1, t_1 \rangle\right).$$

this term is $\int_{-\infty}^{\infty} d\xi \exp\left(\frac{im\xi^2}{2\hbar \Delta t}\right) (\dots)(\xi) = 0$.

this term mult. by 1. when integrated is just $\langle x, t | x_1, t_1 \rangle$

$$\text{for: } \left(\frac{m}{2\pi i \hbar \Delta t}\right)^{1/2} \int d\xi \exp\left[\frac{im\xi^2}{2\hbar \Delta t}\right] = 1$$

Take $\frac{d}{dm}$ of $\int d\xi e^{im\xi^2/2\hbar \Delta t} = \left(\frac{2\pi i \hbar \Delta t}{m}\right)^{1/2}$ to get

$$\int d\xi \xi^2 e^{im\xi^2/2\hbar \Delta t} = \sqrt{2\pi} \left(\frac{i\hbar \Delta t}{m}\right)^{3/2}$$

gives

$$\Delta t \frac{\partial}{\partial t} \langle x, t | x_1, t_1 \rangle = \left(\frac{m}{2\pi i \hbar \Delta t}\right)^{1/2} \sqrt{2\pi} \left(\frac{i\hbar \Delta t}{m}\right)^{3/2} \frac{1}{2} \frac{\partial^2}{\partial x^2} \langle x, t | x_1, t_1 \rangle - \frac{i}{\hbar} V \Delta t \langle x, t | x_1, t_1 \rangle$$

throw away $\mathcal{O}(\Delta t^2)$

Divide by Δt and multiply by $i\hbar$:

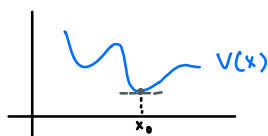
$$i\hbar \frac{\partial}{\partial t} \langle x, t | x_1, t_1 \rangle = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \langle x, t | x_1, t_1 \rangle + V \langle x, t | x_1, t_1 \rangle$$

As $\Delta t \rightarrow 0$, $\langle x, t | x_1, t_1 \rangle = \langle x_n, t_{n-1} | x_1, t_1 \rangle \rightarrow \langle x_n, t_n | x_1, t_1 \rangle$. So probability amplitude satisfies the Schrödinger Equation.

Harmonic Oscillator.

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 X^2.$$

General Potential:



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

Approximate all potential at a lowest pt by harmonic oscillator potential.

Define :

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

annihilation (lowering) operator

$$a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2} \left(x - i\frac{p}{m\omega}\right)$$

creation (raising) operator

We have

$$[a, a^\dagger] = \frac{i}{2\hbar} (-i[X, p] + i[p, X]) = 1. \quad \Rightarrow [a, a^\dagger] = 1.$$

and

$$aa^\dagger = \frac{m\omega}{2\hbar} \left(x^2 + \frac{p^2}{m^2\omega^2}\right) + \frac{i}{2\hbar} [X, p] = \frac{H}{\hbar\omega} - \frac{1}{2}.$$

Denote

$$N := aa^\dagger$$

number operator

So

$$H = \hbar\omega \left(N + \frac{1}{2}\right).$$

Let $|n\rangle$ be eigenstates of the number operator, $N|n\rangle = n|n\rangle$. They are eigenstates of H as well:

$$H|n\rangle = E_n|n\rangle \quad E_n = \left(n + \frac{1}{2}\right)\hbar\omega.$$

Note:

$$[AB, C] = A[B, C] + [A, C]B$$

$$[N, a] = [a^\dagger a, a] = a^\dagger [a, a] + [a^\dagger, a]a = -a.$$

In general:

$$[A, B]^\dagger = -[A^\dagger, B^\dagger].$$

So

$$[N, a^\dagger] = a^\dagger.$$

Therefore,

$$\begin{aligned} Na^\dagger|n\rangle &= ([N, a^\dagger] + a^\dagger N)|n\rangle \\ &= (n+1)a^\dagger|n\rangle. \end{aligned}$$

So $a^\dagger|n\rangle$ is e.state of N with e.value $n+1$. Similarly:

$$Na|n\rangle = ([N, a] + aN)|n\rangle = (n-1)a|n\rangle.$$

So $a|n\rangle$ is e.state of N with e.value $n-1$.

claim: Eigenvalues of N can't be negative.

pf: $n = \langle n | N | n \rangle = \langle n | a^\dagger a | n \rangle = \| a | n \rangle \|^2 \geq 0.$

□

So if n is not an integer, $a^p | n \rangle = (n-p) | n \rangle$ would be an eigenstate of N with negative e. val for $p > n$.

So n must be integers, and $\exists | 0 \rangle$ s.t. $a | 0 \rangle = 0.$

If $| 0 \rangle$ is unique, then all e. states are non-degenerate.

pf: Suppose $| n-1 \rangle$ not degenerate, but $| n \rangle$ is degenerate:

$$N | \varphi_n^i \rangle = n | \varphi_n^i \rangle \quad i=1, \dots, d.$$

Then $a | \varphi_n^i \rangle = c^i | n-1 \rangle$, $c^i \in \mathbb{C}$ for $| n-1 \rangle$ non-degenerate.

$$\Rightarrow a^\dagger a | \varphi_n^i \rangle = n | \varphi_n^i \rangle$$

$$\Leftrightarrow n | \varphi_n^i \rangle = c^i a^\dagger | n-1 \rangle$$

So $| \varphi_n^i \rangle \propto a^\dagger | n-1 \rangle$ which contradicts degeneracy.

□

Normalization:

$$a | n \rangle = c | n-1 \rangle. \quad c \in \mathbb{C}.$$

$$\text{Take norm: } \langle n | a^\dagger a | n \rangle = |c|^2 \quad \langle n | a^\dagger a | n \rangle = n.$$

Thus

$$a | n \rangle = \sqrt{n} | n-1 \rangle.$$

Similarly:

$$\begin{aligned} a^\dagger | n \rangle &= d | n+1 \rangle \Rightarrow \langle n | a a^\dagger | n \rangle = |d|^2. \\ &= \langle n | [a, a^\dagger] + a^\dagger a | n \rangle = n+1 \end{aligned}$$

So:

$$a^\dagger | n \rangle = \sqrt{n+1} | n+1 \rangle.$$

Thus

$$| 1 \rangle = a^\dagger | 0 \rangle \quad | 2 \rangle = \frac{a^\dagger}{\sqrt{2}} | 1 \rangle = \frac{(a^\dagger)^2}{\sqrt{2}} | 0 \rangle \quad | 3 \rangle = \frac{a^\dagger}{\sqrt{3}} | 2 \rangle = \frac{(a^\dagger)^3}{\sqrt{3!}} | 0 \rangle \dots$$

Therefore :

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle.$$

Note that $N^\dagger = (a^\dagger a)^\dagger = a^\dagger a = N$, so $\{|n\rangle\}_{n \in \mathbb{Z}_{\geq 0}}$ can be chosen to be O.N. Thus

$$\langle n' | a | n \rangle = \sqrt{n} \delta_{n', n-1}$$

$$\langle n' | a^\dagger | n \rangle = \sqrt{n+1} \delta_{n', n+1}.$$

Note:

$$X = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (a + a^\dagger)$$

$$P = i\left(\frac{m\hbar\omega}{2}\right)^{1/2} (a^\dagger - a).$$

lec 8.

Harmonic Oscillator:

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

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(X + \frac{iP}{m\omega}\right).$$

Ground state $a|0\rangle = 0$.

$$\left(X + \frac{iP}{m\omega}\right)|0\rangle = 0.$$

Define $x_0 = \sqrt{\frac{\hbar}{m\omega}}$. In position representation,

$$\left(x + x_0^2 \frac{d}{dx}\right)\psi_0(x) = 0.$$

Normalized Ground state:

$$\psi_0(x) = \frac{1}{\pi^{1/4} x_0} e^{-x^2/2x_0^2}.$$

Ground state is unique. By last time: ground state unique $\Rightarrow$ all excited states are nondegenerate. The excited states are: $|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$

$$\psi_1(x) = \langle x|a^\dagger|0\rangle = \frac{1}{\sqrt{2}x_0} \left(x - x_0^2 \frac{d}{dx}\right)\psi_0(x)$$

$\vdots$

$$\psi_n(x) = \left(\pi^{1/4} \sqrt{2^n n!} x_0^{n+1/2}\right)^{-1} \left(x - x_0^2 \frac{d}{dx}\right)^n e^{-x^2/2x_0^2}.$$

Also note:

$$X^2 = \frac{\hbar}{2m\omega} (a^2 + a^{\dagger 2} + a^\dagger a + a a^\dagger)$$

$$\langle 0|X^2|0\rangle = \frac{\hbar}{2m\omega} = \frac{x_0^2}{2} \quad \langle 0|P^2|0\rangle = \frac{\hbar m\omega}{2}.$$

$\uparrow$
only last term contributes.

$$\langle 0|\frac{P^2}{2m}|0\rangle = \frac{\hbar\omega}{4} = \langle 0|\frac{m\omega^2 X^2}{2}|0\rangle$$

So $\langle U \rangle_0 = \langle V \rangle_0$.

$$\langle 0|X|0\rangle = \langle 0|P|0\rangle = 0.$$

So for state $|0\rangle$:

$$(\Delta X)^2 = \langle X^2 \rangle = \frac{\hbar}{2m\omega}$$

$$(\Delta P)^2 = \langle P^2 \rangle = \frac{\hbar m\omega}{2}$$

$$(\Delta X)^2 (\Delta P)^2 = \frac{\hbar^2}{4}.$$

Uncertainty principle saturated.

In any excited state $|n\rangle$,

$$(\Delta X)^2 (\Delta P)^2 = (n + 1/2)^2 \hbar^2.$$

Time Evolution in Heisenberg Representation:

$$\frac{dP}{dt} = \frac{1}{i\hbar} [P, H]$$

For any $V(x)$, we saw $X(t)$ & $P(t)$ are same as classical eqns.

$$\frac{dP}{dt} = -m\omega^2 X \quad \frac{dX}{dt} = \frac{P}{m}.$$

Alternatively, one can use

$$\frac{da}{dt} = \frac{1}{i\hbar} [a, H] = -i\omega [a, N] = -i\omega a.$$

$$\Rightarrow a(t) = e^{-i\omega t} a(0).$$

Taking $+$:

$$\Rightarrow a^\dagger(t) = e^{i\omega t} a^\dagger(0).$$

$$\Rightarrow N = a^\dagger(0) a(0) \quad \text{time independent, for } [N, H] = 0.$$

Therefore:

$$X(t) = X(0) \cos(\omega t) + \frac{P(0)}{m\omega} \sin(\omega t).$$

$$P(t) = X(0) \sin(\omega t) + P(0) \cos(\omega t).$$

But $\langle X \rangle, \langle P \rangle$ don't always oscillate.

Coherent States:

nondegenerate for each λ , for a is just a differential operator.
 $\downarrow$
So $\forall \lambda \in \mathbb{C}$, $\exists!$ $|\lambda\rangle$ s.t.
 $a|\lambda\rangle = \lambda|\lambda\rangle.$

Defined by $a|\lambda\rangle = \lambda|\lambda\rangle$ where $\lambda \in \mathbb{C}$.

Expand in energy e. states:

$$|\lambda\rangle = \sum_{n=0}^{\infty} c_n |n\rangle. \quad c_n = \langle n|\lambda\rangle.$$

Since

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle,$$

$$\langle n| = \langle 0| \frac{a^n}{\sqrt{n!}}.$$

Hence

$$C_n = \langle n | \lambda \rangle = \frac{\lambda^n}{n!} \langle 0 | \lambda \rangle = \frac{\lambda^n}{n!} C_0.$$

So C_n 's determined by C_0 . Can determine C_0 by normalization:

$$1 = \langle \lambda | \lambda \rangle = \sum_{n=0}^{\infty} |C_n|^2 = |C_0|^2 \sum_{n=0}^{\infty} \frac{|\lambda|^{2n}}{n!} = |C_0|^2 e^{|\lambda|^2}.$$

Thus

$$C_0 = e^{-|\lambda|^2/2}.$$

$$C_n = \frac{\lambda^n}{n!} e^{-|\lambda|^2/2}.$$

So

$$|\lambda\rangle = e^{-|\lambda|^2/2} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} |n\rangle = e^{-|\lambda|^2/2} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} (a^\dagger)^n |0\rangle \\ = e^{-|\lambda|^2/2} e^{\lambda a^\dagger} |0\rangle.$$

Recall from HW1: If $[[A, B], B] = 0$ then $[A, f(B)] = [A, B] f'(B)$.

$$a e^{\lambda a^\dagger} |0\rangle = [a, e^{\lambda a^\dagger}] |0\rangle = \lambda e^{\lambda a^\dagger} |0\rangle.$$

Note: $|\lambda\rangle$ form an overcomplete basis, so not linearly independent.

Time dependence (Schrödinger Rep).

$$|\lambda(t)\rangle = e^{-iHt/\hbar} |\lambda\rangle_{t=0} = e^{-i\omega t/2} e^{-i\omega t N} |\lambda\rangle \\ = e^{-i\omega t/2} e^{-|\lambda|^2/2} \sum_n \frac{\lambda^n}{n!} e^{-i\omega t n} |n\rangle.$$

This just a coherent state with $\lambda \rightarrow \lambda e^{-i\omega t}$. So

$$|\lambda(t)\rangle = e^{-i\omega t/2} |\lambda e^{-i\omega t}\rangle.$$

Interpretation:

$$\langle X \rangle = \langle \lambda | X | \lambda \rangle = \frac{x_0}{\sqrt{2}} \langle \lambda | a + a^\dagger | \lambda \rangle \\ = \frac{x_0}{\sqrt{2}} (\lambda + \lambda^*) \\ = \sqrt{2} x_0 \operatorname{Re}(\lambda).$$

Similarly, $P = \frac{i\hbar}{\sqrt{2}x_0} (a^\dagger - a)$.

$$\langle P \rangle = \frac{i\hbar}{\sqrt{2}x_0} (\lambda^* - \lambda) = \frac{\sqrt{2}\hbar}{x_0} \operatorname{Im}(\lambda).$$

If we start with

$$\lambda = |\lambda| e^{i\gamma} \quad \text{at } t=0.$$

Thus

$$\langle \lambda(t) | X | \lambda(t) \rangle = |\lambda| \sqrt{2} x_0 \cos(\omega t - \gamma)$$

$$\langle \lambda(t) | P | \lambda(t) \rangle = -|\lambda| \left(\frac{\sqrt{2} \hbar}{x_0} \right) \sin(\omega t - \gamma).$$

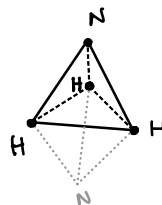
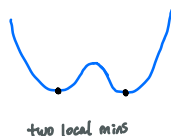
So $\langle X \rangle, \langle P \rangle$ just like classical particle.

Claim: These states saturate uncertainty principle $\forall t$.

pf: Next week's Hw :) $\square$

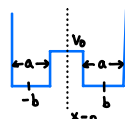
lec 9.

Double Well.

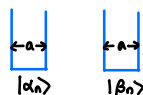


Ammonia molecule NH_3 has potential like this

Approximate the potential by



If $V_0 \rightarrow \infty$, we have 2 square wells



The energy eigenvalue is still the same as the single square well energy eigenvalue:

$$E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2$$

Eigenstates: $|\alpha_n\rangle, |\beta_n\rangle, |\alpha_n\rangle + |\beta_n\rangle$

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2.$$

Each is degenerate.

Clearly $\langle \alpha_n | \beta_m \rangle = 0$ because they have different support. Focus on 2 ground states.

In basis $|\alpha_1\rangle, |\beta_1\rangle$,

$$H_0 = \begin{pmatrix} E_1 & 0 \\ 0 & E_1 \end{pmatrix}.$$

For finite V_0 , add

$$W = -A \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

↑
a number

Total

$$H = H_0 + W = \begin{pmatrix} E_1 & -A \\ -A & E_1 \end{pmatrix}$$

Energy e.v.

$$E = E_1 \pm A.$$

degeneracy is broken. E. states

$$\frac{1}{\sqrt{2}} (|\alpha_1\rangle + |\beta_1\rangle) = |\chi_s\rangle.$$

for $E = E_1 - A$

$$\frac{1}{\sqrt{2}} (|\alpha_1\rangle - |\beta_1\rangle) = |\chi_a\rangle.$$

for $E = E_1 + A.$

Start with N below plane

$$|\psi(0)\rangle = |\alpha_1\rangle = \frac{1}{\sqrt{2}} (|\chi_s\rangle + |\chi_a\rangle).$$

So

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-iE_0 t/\hbar} [e^{iAt/\hbar} |\gamma_s\rangle + e^{-iAt/\hbar} |\gamma_a\rangle]$$

Write in terms of $|\alpha_1\rangle, |\beta_1\rangle$:

$$|\psi(t)\rangle = e^{-iE_0 t/\hbar} \left[\cos \frac{At}{\hbar} |\alpha_1\rangle + i \sin \frac{At}{\hbar} |\beta_1\rangle \right].$$

Prob of N to be above the plane is

$$\sin^2 \frac{At}{\hbar}$$

General Lessons.

Given 2 degenerate states & add perturbation:

- (1) Degeneracy is broken
- (2) Eigenstates will be symmetric & antisymmetric combinations.
- (3) Start with one, oscillate between them.

Parity (ref. Sec 4.2 of text)

In 1D define

$$\pi |x\rangle = |-x\rangle.$$

This is unitary:

$$\pi^\dagger \pi = \mathbb{I}.$$

But

$$\pi^2 = \mathbb{I}$$

So

$$\pi = \pi^\dagger.$$

From the prev. two lines, e. values of π are ± 1 .

Claim: $\pi X \pi = -X$. (*)

Pf. $\pi X \pi |x\rangle = \pi X |-x\rangle = -x \pi |-x\rangle = -x |x\rangle = -X |x\rangle.$

□

Note that (*) $\Rightarrow \pi X = -X \pi$, i.e., $\{\pi, X\} = 0$.

Wave functions: Given $\psi(x) = \langle x | \psi \rangle$. Parity inverted state has

$$\langle x | \pi | \psi \rangle = \langle -x | \psi \rangle = \psi(-x).$$

If $|\psi\rangle$ e. states of π ,

$$\pi |\psi\rangle = \pm |\psi\rangle \Rightarrow \psi(-x) = \pm \psi(x).$$

Now,

$$H = \frac{P^2}{2m} + V(x).$$

If V is even, the

$$[\pi, H] = 0.$$

$\exists$ simultaneous e. states.

Parity Selection Rule: If

$$\pi |\psi_i\rangle = \epsilon_i |\psi_i\rangle \quad \epsilon_i = \pm 1,$$

& A is odd under parity: $\pi A \pi = -A$. Then $\langle \psi_1 | A | \psi_2 \rangle = 0$ unless $|\psi_1\rangle, |\psi_2\rangle$ have opposite parity.

Pf: $\langle \psi_1 | A | \psi_2 \rangle = \langle \psi_1 | \pi (\pi A \pi) \pi | \psi_2 \rangle = -\epsilon_1 \epsilon_2 \langle \psi_1 | \psi_2 \rangle$. Clearly this vanishes unless $\epsilon_1 \epsilon_2 = -1$. $\square$

If A is even, then $\langle \psi_1 | A | \psi_2 \rangle = 0$ unless $|\psi_1\rangle, |\psi_2\rangle$ have same parity.

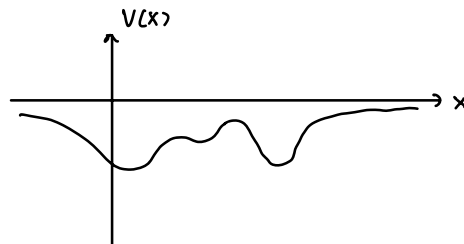
(i.e., $V < 0$)

General Properties of Attractive Potentials :

Energy Eigenstates ?

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

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



Claim: No degeneracy for bound states $E < 0$.

Pf: Suppose ψ & ϕ two Eigenstates with same energy E . Define Wronskian

$$W(x) = \psi\varphi' - \varphi\psi'$$

Then

$$\begin{aligned} W' &= \psi\varphi'' - \varphi\psi'' \\ &= \frac{2m}{\hbar^2} (V-E) (\psi\varphi - \varphi\psi) = 0. \end{aligned}$$

So W is constant. At $x \rightarrow \infty$, $\psi, \varphi \rightarrow 0$, so $W(\infty) = 0$. Thus $W = 0$ everywhere.

Thus $\psi\varphi' = \varphi\psi'$. So

$$\frac{\varphi'}{\varphi} = \frac{\psi'}{\psi} \Rightarrow \varphi, \psi \text{ proportional.}$$

Thus ψ, φ same eigenstate.

□

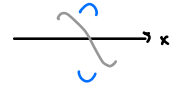
Case 1: Region with $V(x) - E > 0$.

ψ'' has same sign as ψ . So ψ is always curving away from x -axis.



Case 2: Region with $V(x) - E < 0$.

In general, ψ curve toward axis.

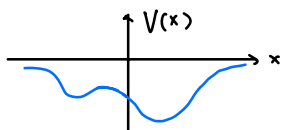


Match with ψ, ψ' continuous.

If $E < V_{\min}$, then always in case 1, so $\psi'' > 0$, not normalizable.

Lec 10.

Attractive Potential:



Eigenstates with $E < 0$:

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

For E close to $V_{\min}$, start with $\psi > 0$ at $x \rightarrow -\infty$. At large x , the solution is

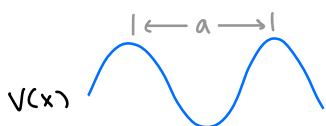
$$Ae^{kx} + Be^{-kx}.$$

As you increase E , A decreases for some E_0 , $A=0$ for 1st time. This is ground state. For $E = E_0 + \delta$, $A < 0$. Increase E , eventually, $A=0$, this gives the 1st excited state.

Summary : 1D attractive Potential: (i.e. $V < 0$, $V(\pm\infty) = 0$).

- (1) Always has at least one bound state (HWS).
- (2) Bound state energies are discrete, and lie in the range $V_{\min} < E < 0$.
- (3) Bound states are non-degenerate.
- (4) Ground state has no nodes (i.e. zero), 1st excited state has 1 node (if it exists).
- (5) If $V(-x) = V(x)$, then ground state is even, and parity of ψ_n alternates.

Periodic Potentials (Ref. Sec 4.3)



$$V(x \pm a) = V(x).$$

Recall the translation Operator

$$T(a) = e^{-iPa/\hbar}.$$

Periodicity means:

$$T^\dagger(a) V(x) T(a) = V(x).$$

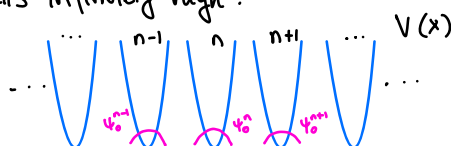
Since $T(a)^\dagger P^2 T(a) = P^2$, so $T(a)^\dagger H T(a) = H$. Thus

$$[T(a), H] = 0.$$

Can find simultaneous Eigenstate. First, suppose walls infinitely high:

Denote the ground state in the n^{th} well by $|n\rangle$.

Easy to see $\langle m | n \rangle = \delta_{mn}$.



We have $H|n\rangle = E_0|n\rangle$ where E_0 independent of n . State is infinitely degenerate.
But $T(a)|n\rangle = |n+1\rangle$.

Consider

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta} |n\rangle \quad \text{where } -\pi \leq \theta \leq \pi.$$

NOT Orthonormal for $\langle\theta|\theta'\rangle \neq 0$ if $\theta \neq \theta'$. Clearly $H|\theta\rangle = E_0|\theta\rangle$. Now

$$\begin{aligned} T(a)|\theta\rangle &= \sum_{n=-\infty}^{\infty} e^{in\theta} |n+1\rangle \\ &= \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta} |n\rangle \quad n \rightarrow n-1 \\ &= e^{-i\theta} |\theta\rangle. \end{aligned}$$

So $|\theta\rangle$ simult. eigenstate of $T(a)$ and H .

Now lower barrier to finite height. Let $\langle n|H|n\rangle = \tilde{E}_0$. Translation invariance $\Rightarrow \tilde{E}_0$ still independent of n . $|n\rangle$ defined as above. We expect

$$\langle n|H|n'\rangle \neq 0 \text{ only for } |n'-n| \leq 1$$

(i.e. when barrier high, tunnel from $|n'\rangle$ to $|n\rangle$ is possible only when the wells are adjacent. It's an "tight binding approximation"). Define

$$\langle n\pm 1|H|n\rangle = -\Delta \quad \text{indep of } n.$$

$$H|n\rangle = \tilde{E}_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle.$$

Set

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta} |n\rangle.$$

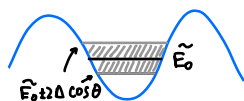
Then

$$H|\theta\rangle = \tilde{E}_0 \sum e^{in\theta} |n\rangle - \Delta \sum e^{in\theta} |n+1\rangle - \Delta \sum e^{in\theta} |n-1\rangle.$$

Shift $n \rightarrow n\pm 1$ in the last 2 terms, we get

$$\begin{aligned} H|\theta\rangle &= \tilde{E}_0 \sum e^{in\theta} |n\rangle - \Delta (e^{-i\theta} + e^{i\theta}) \sum e^{in\theta} |n\rangle \\ &= (\tilde{E}_0 - 2\Delta \cos\theta) |\theta\rangle. \end{aligned}$$

$|\theta\rangle$ is an energy eigenstate, θ continuous, so get continuous bands of energy eigenstates:



Degeneracy is lifted. Can include the next nearest neighbor coupling:

$$H|n\rangle = \tilde{E}_0 |n\rangle - \Delta(|n+1\rangle + |n-1\rangle) + \epsilon(|n+2\rangle + |n-2\rangle).$$

Then get eigenvalue of $|\theta\rangle$ to be

$$\tilde{E}_0 - 2\Delta \cos \theta + 2\epsilon \cos(2\theta) + \dots$$

What is $\psi_\theta(x)$?

$$\langle x|T(a)|\theta\rangle = e^{-i\theta} \langle x|\theta\rangle = e^{-i\theta} \psi_\theta(x).$$

On the other hand,

$$\begin{aligned} T(a)|x\rangle &= |x+a\rangle \\ \langle x+a| &= \langle x|T^\dagger(a) = \langle x|T(-a) \end{aligned}$$

Thus

$$e^{-i\theta} \psi_\theta(x) = \langle x|T(a)|\theta\rangle = \langle x-a|\theta\rangle = \psi_\theta(x-a).$$

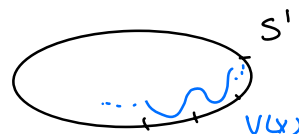
Solution is

$$\psi_\theta(x) = e^{ikx} \varphi_k(x) \leftarrow \text{periodic } \varphi_k(x+a) = \varphi_k(x)$$

where $k = \theta/a$. This is **Bloch's Theorem**.

Periodic Potential V on S^1 , $V(x) = V(x+a)$. Identify $V(x+Na) = V(x)$. That means we still have states $\{|n\rangle\}_n$, but now $1 \leq n \leq N$.

$$\begin{aligned} e^{ikx} &= e^{ik(x+Na)} \Rightarrow k = \frac{2\pi n}{Na} \\ &\Rightarrow \theta = \frac{2\pi n}{N}. \end{aligned}$$



Lec 11.

QM in 3D : Angular Momentum (Ref. Chapter 3).

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\mathbf{X})\psi = E\psi.$$

In few cases, try $\psi(x, y, z) = X(x)Y(y)Z(z)$.

Angular Momentum generates rotations : $e^{-i\mathbf{J}_k\varphi/\hbar}$ is rotation about k axis by amount φ .

$\mathbf{J}_k$ is a Hermitian operator, $e^{-i\mathbf{J}_k\varphi/\hbar}$ unitary.

Note, note starting with $\vec{J} = \vec{r} \times \vec{p}$.

Rotations : Orthogonal 3×3 matrices $SO(3)$.

e.g. Rotate about z -axis:

$$R_z(\varphi) = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

$$R_x(\varphi) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{bmatrix}$$

$$R_y(\varphi) = \begin{bmatrix} \cos\varphi & 0 & \sin\varphi \\ 0 & 1 & 0 \\ -\sin\varphi & 0 & \cos\varphi \end{bmatrix}$$

$R_x(\varphi)R_y(\tilde{\varphi}) \neq R_y(\tilde{\varphi})R_x(\varphi)$. For small rotations, $\varphi = \tilde{\varphi} = \varepsilon$, keeping terms $\mathcal{O}(\varepsilon^2)$,

$$R_x(\varepsilon) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 - \frac{\varepsilon^2}{2} & -\varepsilon \\ 0 & \varepsilon & 1 - \frac{\varepsilon^2}{2} \end{bmatrix}.$$

Claim: $R_x(\epsilon) R_y(\epsilon) R_x(-\epsilon) R_y(-\epsilon) = R_z(\epsilon^2)$ Keeping terms $O(\epsilon^2)$.

In QM, for every rotation R , we have a unitary operator $\mathcal{D}(R)$, s.t.

$$R_1 R_2 = R_3 \Rightarrow \mathcal{D}(R_1) \mathcal{D}(R_2) = \mathcal{D}(R_3)$$

$$\mathcal{D}(R^{-1}) \mathcal{D}(R) = \mathcal{D}(I) = I. \quad \Rightarrow \mathcal{D}(R^{-1}) = \mathcal{D}(R)^{-1} = \mathcal{D}^\dagger(R).$$

$(R_1 R_2) R_3 = R_1 (R_2 R_3)$ always true for operators.

Under rotation R of the system, $|\psi\rangle \rightarrow \mathcal{D}(R) |\psi\rangle$.

Rotation about axis $\hat{n}$ by φ given by

$$\mathcal{D}(R) = e^{-i \vec{J} \cdot \hat{n} \varphi / \hbar}.$$

Small rotation about x-axis:

$$\mathcal{D}(R_x(\epsilon)) = 1 - \frac{i J_x \epsilon}{\hbar} - \frac{J_x^2 \epsilon^2}{\hbar^2} \dots$$

$$\mathcal{D}(R_x(\epsilon)) \mathcal{D}(R_y(\epsilon)) \mathcal{D}(R_x(-\epsilon)) \mathcal{D}(R_y(-\epsilon))$$

$$\simeq \left(1 - \frac{i J_x \epsilon}{\hbar} - \frac{J_x^2 \epsilon^2}{\hbar^2}\right) \left(1 - \frac{i J_y \epsilon}{\hbar} - \frac{J_y^2 \epsilon^2}{\hbar^2}\right) \left(1 + \frac{i J_x \epsilon}{\hbar} - \frac{J_x^2 \epsilon^2}{\hbar^2}\right) \left(1 + \frac{i J_y \epsilon}{\hbar} - \frac{J_y^2 \epsilon^2}{\hbar^2}\right)$$

$O(\epsilon)$ term cancel, J_x^2 & J_y^2 cancel, 1st $-\frac{i J_x \epsilon}{\hbar}$ doesn't contribute

$$= 1 + \frac{J_y J_x \epsilon^2}{\hbar^2} - \frac{J_x J_y \epsilon^2}{\hbar^2}$$

$$= 1 - \frac{\epsilon^2}{\hbar^2} [J_x, J_y]$$

$$= \mathcal{D}(R_z(\epsilon^2)) \simeq 1 - \frac{i J_z \epsilon^2}{\hbar}.$$

$$\Rightarrow [J_x, J_y] = i \hbar J_z.$$

$$\left. \begin{aligned} [J_y, J_z] &= i \hbar J_x \\ [J_z, J_x] &= i \hbar J_y \end{aligned} \right\} \text{ Similarly.}$$

E. values of angular momentum:

$$J^2 \equiv J_x^2 + J_y^2 + J_z^2$$

Note

$$[J^2, J_x] = [J_y^2 + J_z^2, J_x] = J_y [J_y, J_x] + [J_y, J_x] J_y + J_z [J_z, J_x] + [J_z, J_x] J_z = 0.$$

Similarly

$$[J^2, J_y] = [J^2, J_z] = 0.$$

Look for simultaneous E. states of J^2 & J_z .

Assume

$$J^2 |a, b\rangle = a |a, b\rangle$$

$$J_z |a, b\rangle = b |a, b\rangle.$$

Define

$$J_{\pm} = J_x \pm iJ_y$$

Note

$$[J_+, J_-] = 2\hbar J_z.$$

$$[J_z, J_{\pm}] = \pm \hbar J_{\pm}.$$

$$[J^2, J_{\pm}] = 0.$$

So

$$\begin{aligned} J_z J_+ |a, b\rangle &= [J_z, J_+] |a, b\rangle + J_+ J_z |a, b\rangle \\ &= +\hbar J_+ |a, b\rangle + b J_+ |a, b\rangle \\ &= (b + \hbar) J_+ |a, b\rangle. \end{aligned}$$

So $J_+ |a, b\rangle$ e. state of J_z with e.v. $b + \hbar$

Similarly $J_- |a, b\rangle$ $b - \hbar$.

$$[J^2, J_{\pm}] = 0$$

$$\downarrow$$
$$J^2 J_{\pm} |a, b\rangle = a J_{\pm} |a, b\rangle.$$

Claim: $a \geq b^2$. (So cannot keep applying $J_{\pm} |a, b\rangle$ and not get 0 for fixed a).

$$\text{pf: } \langle a, b | J^2 - J_z^2 | a, b \rangle = \langle a, b | J_x^2 + J_y^2 | a, b \rangle = \|J_x |a, b\rangle\|^2 + \|J_y |a, b\rangle\|^2 \geq 0.$$

$$\text{But } \langle a, b | J^2 - J_z^2 | a, b \rangle = a - b^2.$$

□

So must be a state for each a s.t.

$$J_+ |a, b_{\max}\rangle = 0. \Rightarrow J_- J_+ |a, b_{\max}\rangle = 0.$$

$$\text{But } J_- J_+ = J_x^2 + J_y^2 - i(J_y J_x - J_x J_y) = J^2 - J_z^2 - \hbar J_z.$$

$$(\mathcal{J}^2 - \mathcal{J}_z^2 - \hbar \mathcal{J}_z) |a, b_{\max}\rangle = 0$$

$$a - b_{\max}^2 - b_{\max} \hbar = 0.$$

$$a = b_{\max}^2 + b_{\max} \hbar$$

Similarly, $\exists$ state st.

write in terms of $\mathcal{J}^2, \mathcal{J}_z$

↓

$$\mathcal{J}_- |a, b_{\min}\rangle = 0 \Rightarrow \mathcal{J}_+ \mathcal{J}_- |a, b_{\min}\rangle = 0.$$

$\Rightarrow$

$$a = b_{\min}^2 - b_{\min} \hbar$$

Equating two and solve for $b_{\max}$,

$$b_{\max} = -b_{\min}$$

(other solution $b_{\max} = b_{\min} - \hbar$, not physical).

Clearly $b_{\max} = b_{\min} + n\hbar$. Now set

$$j = b_{\max}/\hbar$$

$$b_{\max} - b_{\min} = n\hbar$$

$$(b_{\min} = -b_{\max}) \quad b_{\max} = \frac{n\hbar}{2}$$

$$\Rightarrow j = \frac{n}{2} \text{ (is integer or half integer)}$$

Then

$$a = j(j+1)\hbar^2$$

$$m = b/\hbar$$

$$b_{\min} \leq b \leq b_{\max}.$$

So

$$-j \leq m \leq j.$$

In these new labels: $|a, b\rangle \rightarrow |j, m\rangle$.

$$\mathcal{J}^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle$$

$$\mathcal{J}_z |j, m\rangle = m\hbar |j, m\rangle.$$

Comment:

1) j is integer or half integer.

Not all states arise in every problem.

2) Rotation about z axis. $e^{-i\mathcal{J}_z \varphi/\hbar}$

m integer states invariant under 2π rotations bosons.

" $\frac{1}{2}$ integer states change sign fermions.

3) For any direction $\hat{n}$, $[\mathcal{J}^2, \vec{\mathcal{J}} \cdot \hat{n}] = 0$, do the same.

lec 12.

Last time: $J^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle$

$$J_z |j, m\rangle = m\hbar |j, m\rangle.$$

The energy eigenstates are degenerate because $|j, m\rangle$ does not constrain radial dependence.

$|k, j, m\rangle$ and $|k', j', m'\rangle$ orthogonal, j, m are eigenvalues of Hermitian operator.
↑
label degeneracy

To get "standard" o.n. basis, pick o.n. basis for $M=j$:

$$|k_i, j, j\rangle \quad i=1, 2, \dots$$

Claim: $J_- |k_i, j, j\rangle$ are orthogonal for different k_i .

pf: Inner product of $J_- |k_2, j, j\rangle$ and $J_- |k_1, j, j\rangle$ and have

$$\begin{aligned} & \langle k_2, j, j | J_- J_- |k_1, j, j\rangle \\ &= \langle k_2, j, j | [J_+, J_-] |k_1, j, j\rangle - \langle k_2, j, j | J_- J_+ |k_1, j, j\rangle \quad [J_+, J_-] = 2\hbar J_z \\ &= 2j\hbar^2 \langle k_2, j, j | k_1, j, j\rangle \\ &= 2j\hbar^2 \delta_{k_1, k_2} \end{aligned}$$

by construction of $|k_i, j, j\rangle$.

□

Thus define

$$|k_i, j, j-1\rangle = \frac{1}{\hbar \sqrt{2j}} J_- |k_i, j, j\rangle.$$

In general, the norm of $J_- |k, j, m\rangle$ is: $\langle k, j, m | J_+ J_- |k, j, m\rangle$.

Use

$$J_+ J_- = J^2 - J_z^2 + \hbar J_z$$

to evaluate the inner product:

$$\langle k, j, m | J_+ J_- |k, j, m\rangle = [j(j+1) - m(m-1)]\hbar^2.$$

So given ON basis $|k, j, m\rangle$, define

$$|k, j, m-1\rangle = \frac{1}{\hbar [j(j+1) - m(m-1)]^{1/2}} J_- |k, j, m\rangle.$$

This implies

$$J_- |k, j, m\rangle = \hbar \sqrt{j(j+1) - m(m-1)} |k, j, m-1\rangle.$$

Similarly,

$$J_+ |k, j, m\rangle = \hbar \sqrt{j(j+1) - m(m+1)} |k, j, m+1\rangle.$$

Of course,

$$J_z |k, j, m\rangle = m\hbar |k, j, m\rangle.$$

Can also be written as

$$J_- |k, j, m\rangle = \hbar \sqrt{(j+m)(j-m+1)} |k, j, m-1\rangle$$

$$J_+ |k, j, m\rangle = \hbar \sqrt{(j-m)(j+m+1)} |k, j, m+1\rangle$$

Comparison of 1D HO and Angular Momentum Problem

1D QM ($\mathbb{R}$)	Angular Momentum (S^2 dependence)
$X, P \quad [X, P] = i\hbar$	$J_x, J_y, J_z \quad [J_x, J_y] = i\hbar J_z$
$a = \frac{1}{\sqrt{2\hbar}} (X + iP)$ $a^\dagger = \frac{1}{\sqrt{2\hbar}} (X - iP)$ $[a, a^\dagger] = 1$	$J_+ = J_x + iJ_y$ $J_- = J_x - iJ_y$ $[J_+, J_-] = 2\hbar J_z$
$N = a^\dagger a$ $[N, a] = -a \quad [N, a^\dagger] = a^\dagger$	$J^2 = J_x^2 + J_y^2 + J_z^2$ $[J_z, J_\pm] = \pm \hbar J_\pm$
Suppose $N n\rangle = n n\rangle$, then $a^\dagger n\rangle \propto n+1\rangle \quad a n\rangle \propto n-1\rangle$	Suppose $J^2 a, b\rangle = a a, b\rangle$, $J_z a, b\rangle = b a, b\rangle$, then $J_+ a, b\rangle \propto a, b+\hbar\rangle \quad J_- a, b\rangle \propto a, b-\hbar\rangle$
Must stop: $n = \langle n N n\rangle = \ a n\rangle\ ^2 \geq 0$ $\exists 0\rangle$ s.t. $a 0\rangle = 0 \Rightarrow n \in \mathbb{Z}$	Must stop: $a-b^2 = \langle a, b J^2 - J_z^2 a, b\rangle = \ J_x a, b\rangle\ ^2 + \ J_y a, b\rangle\ ^2 \geq 0$ $\exists J_+ a, b_{\max}\rangle = 0, J_- a, b_{\min}\rangle = 0 \Rightarrow$ $\begin{aligned} b_{\max} - b_{\min} &= n\hbar \\ J_- J_+ a, b_{\max}\rangle &= J_+ J_- a, b_{\min}\rangle = 0 \\ \Rightarrow b_{\max} &= -b_{\min} \\ \Rightarrow b_{\max} &= \frac{n\hbar}{2} = -b_{\min} \\ a &= b_{\max}(b_{\max} + \hbar) \end{aligned}$
$ n\rangle$ form O.N. basis of $L^2(\mathbb{R})$	$ j, m\rangle$ (for $j \in \mathbb{Z}$) are O.N. basis for $L^2(S^2)$

Orbital Angular Momentum.

In classical mechanics: $\vec{L} = \vec{r} \times \vec{p}$.

In QM, define: $\vec{L} = \vec{X} \times \vec{P}$. $\Rightarrow$ exerc. $[L_i, L_j] = i\hbar \epsilon_{ijk} L_k$.

Since $\vec{P} = \frac{\hbar}{i} \vec{\nabla}$:

We have:
$$L_z = \frac{\hbar}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

In polar coord:

$$x = r \sin \theta \cos \varphi$$

$$y = r \sin \theta \sin \varphi$$

$$z = r \cos \theta$$

We get

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \varphi}.$$

All L_x, L_y, L_z can be expressed in terms of $\partial/\partial \theta, \partial/\partial \varphi$. (Since radial momentum P_r never enters).

E. functions of L^2, L_z are spherical harmonics $Y_l^m(\theta, \varphi)$.

Convention: $j \rightarrow l$

$$L_z |l, m\rangle = m\hbar |l, m\rangle$$

$$\Rightarrow \frac{\hbar}{i} \frac{\partial}{\partial \varphi} Y_l^m(\theta, \varphi) = m\hbar Y_l^m(\theta, \varphi).$$

$$\Rightarrow Y_l^m(\theta, \varphi) = P_l^m(\theta) e^{im\varphi}.$$

To find P_l^m :

$$L_+ |l, l\rangle = 0 \quad L_+ = e^{i\varphi} \hbar \left(\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \varphi} \right).$$

$$\begin{aligned} \Rightarrow \left(\frac{\partial}{\partial \theta} - l \cot \theta \right) P_l^l(\theta) &= 0 \Rightarrow \frac{P_l'}{P_l} = l \cot \theta = \frac{l(\sin \theta)'}{\sin \theta} \\ &\Rightarrow P_l^l(\theta) \propto (\sin \theta)^l \end{aligned}$$

Normalize:

$$\int_{S^2} |Y_l^l(\theta, \varphi)|^2 \sin \theta d\theta d\varphi = 1 \Rightarrow Y_l^l(\theta, \varphi) = (-1)^l \sqrt{\frac{(2l+1)(2l)!}{4\pi}} \frac{1}{2^l l!} (\sin \theta)^l e^{il\varphi}.$$

Convention s.t. Y_l^0 is Legendre polynomial.

Similarly $L_- |l, -l\rangle = 0$.

$$L_- = e^{-i\varphi} \hbar \left(-\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \varphi} \right).$$

$$\Rightarrow Y_l^{-l} \propto (\sin \theta)^l e^{-il\varphi}.$$

In general:

$$Y_l^m(\theta, \varphi) = \frac{(-1)^l}{2^l l!} \left[\frac{(2l+1)}{4\pi} \frac{(l+m)!}{(l-m)!} \right] e^{im\varphi} \frac{1}{\sin^m \theta} \frac{d^{l-m}}{dx^{l-m}} (1-x^2)^l \Big|_{x=\cos \theta}.$$

lec 13,

Last time: $|l, m\rangle = Y_l^m(\theta, \varphi)$.

Try $l = \frac{1}{2}$. $L_+ |\frac{1}{2}, \frac{1}{2}\rangle = 0 \Rightarrow Y_{\frac{1}{2}}^{\frac{1}{2}}(\theta, \varphi) \propto (\sin\theta)^{\frac{1}{2}}$.

But this is a problem:

- $(\sin\theta)^{\frac{1}{2}}$ not in the domain of L^2

- Contradiction:

$$L_- |\frac{1}{2}, -\frac{1}{2}\rangle = 0 \Rightarrow Y_{\frac{1}{2}}^{-\frac{1}{2}}(\theta, \varphi) \propto (\sin\theta)^{\frac{1}{2}}$$

But $L_- |\frac{1}{2}, \frac{1}{2}\rangle$ not $\propto$ to $|\frac{1}{2}, -\frac{1}{2}\rangle$

$$\begin{aligned} \text{Pf: } L_- |\frac{1}{2}, \frac{1}{2}\rangle &\propto e^{-i\varphi} \left(-\frac{\partial}{\partial\theta} + i\cot\theta \frac{\partial}{\partial\varphi} \right) (\sin\theta)^{\frac{1}{2}} e^{i\varphi/2} \\ &= \left[-\frac{\cos\theta}{2(\sin\theta)^{\frac{1}{2}}} - \frac{1}{2} \frac{\cos\theta}{(\sin\theta)^{\frac{1}{2}}} \right] e^{-i\varphi/2} \\ &= -\frac{\cos\theta}{(\sin\theta)^{\frac{1}{2}}} e^{-i\varphi/2} \quad \text{not } \propto \text{ to } (\sin\theta)^{\frac{1}{2}}. \end{aligned}$$

□

This is the contradiction.

- Also, $|l, m\rangle$ where $l \in \mathbb{Z}$ form O.N. basis of $L^2(S^2)$.

- So conclude that there are no coordinate representations for $l = \frac{1}{2}, \frac{3}{2}, \dots$

We introduce them as a new type of angular momentum called **Spin** $\vec{S}$.

- Spin deg. of freedom observed by experiment.

Start with $j = \frac{1}{2}$:

Two S_z e. states $|+\rangle, |-\rangle$ with e.v. $\pm \frac{\hbar}{2}$.

Recall:

$$J_+ |j, m\rangle = \sqrt{(j-m)(j+m+1)} \hbar |j, m+1\rangle$$

$$J_- |j, m\rangle = \sqrt{(j+m)(j-m+1)} \hbar |j, m-1\rangle.$$

plug in $j = \frac{1}{2}$, $m = \pm \frac{1}{2}$:

$$S_+ |+\rangle = 0$$

$$S_+ |-\rangle = \hbar |+\rangle.$$

$$S_- |+\rangle = \hbar |-\rangle$$

$$S_- |-\rangle = 0$$

$$S_x |+\rangle = \frac{1}{2} (S_+ + S_-) |+\rangle = \frac{\hbar}{2} |-\rangle.$$

$$S_x |-\rangle = \frac{\hbar}{2} |+\rangle.$$

$$S_y |+\rangle = \frac{1}{2i} (S_+ - S_-) |+\rangle = \frac{i\hbar}{2} |-\rangle$$

$$S_y |-\rangle = -\frac{i\hbar}{2} |+\rangle.$$

Write $S_k = \frac{\hbar}{2} \sigma_k$, then

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

These are **Pauli matrices**.

Properties:

(1) $\sigma_k = \sigma_k^\dagger$.

(2) $\sigma_k^2 = I \Rightarrow \sigma_k^\dagger = \sigma_k^{-1} \Rightarrow \sigma_k$ unitary

(3) $\sigma_j \sigma_k + \sigma_k \sigma_j = 0$ if $j \neq k$.

(2) & (3) $\Rightarrow \{\sigma_j, \sigma_k\} = 2\delta_{jk} I$.

(4) $[\sigma_j, \sigma_k] = 2i\epsilon_{jkl} \sigma_l$.

(5) σ_k together with identity I form basis for all 2×2 matrices.

(6) e. values of σ_k are ± 1 . e. vectors of σ_x are $\frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle)$

σ_y are $\frac{1}{\sqrt{2}}(|+\rangle \pm i|-\rangle)$

Example: Spin Precession.

Spin $1/2$ particle with magnetic moment $\frac{e}{2mc}$.

External magnetic field has

$$H = \frac{e}{mc} \vec{S} \cdot \vec{B}$$

If $\vec{B}$ uniform,

$$H = \omega S_z \quad \omega = -\frac{eB}{mc}$$

Energy Eigenstates: $|+\rangle, |-\rangle$.

Start with Eigenstate of S_x with l. value $+\frac{\hbar}{2}$.

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$$

$$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle = \frac{1}{\sqrt{2}}(e^{-i\omega t/2}|+\rangle + e^{i\omega t/2}|-\rangle)$$

$$\langle \psi(t) | S_x | \psi(t) \rangle = \frac{1}{2} [\langle + | e^{i\omega t/2} + \langle - | e^{-i\omega t/2}] S_x [e^{-i\omega t/2} | + \rangle + e^{i\omega t/2} | - \rangle]$$

$$= \frac{\hbar}{4} (e^{-i\omega t} + e^{i\omega t}) = \frac{\hbar}{2} \cos(\omega t)$$

$$\langle \psi(t) | S_y | \psi(t) \rangle = \frac{\hbar}{2} \sin(\omega t)$$

Use formula on
previous
page. Only
 $\langle \pm | S_x | \mp \rangle$
non zero.

Claim: No "spreading of wavefn".

Pf: Time evolution is $e^{-iHt/\hbar} = e^{-i\omega t S_z/\hbar}$ is just a rotation. $\square$

For any vector $\vec{V}$,

$$\vec{V} \cdot \vec{\sigma} = V_x \sigma_x + V_y \sigma_y + V_z \sigma_z$$

$$(\vec{V} \cdot \vec{\sigma})^2 = V^i V^j \sigma_i \sigma_j$$

$$= \frac{1}{2} V^i V^j (\underbrace{\sigma_i \sigma_j + \sigma_j \sigma_i}_{2I \delta_{ij}})$$

$$= |\vec{V}|^2 \cdot I.$$

Rotation of Spin $1/2$ particle by ϕ in direction $\hat{n}$:

$$e^{-i\vec{S} \cdot \vec{n} \phi / \hbar} = e^{-i\vec{\sigma} \cdot \hat{n} \phi / 2}$$

$$= I - \frac{(\vec{\sigma} \cdot \hat{n})^2}{2!} \left(\frac{\phi}{2}\right)^2 + \frac{(\vec{\sigma} \cdot \hat{n})^4}{4!} \left(\frac{\phi}{2}\right)^4 + \dots$$

$$-i \left[(\vec{\sigma} \cdot \hat{n}) \frac{\phi}{2} - \frac{(\vec{\sigma} \cdot \hat{n})^3}{3!} \left(\frac{\phi}{2}\right)^3 + \dots \right]$$

$$= I \cos\left(\frac{\phi}{2}\right) - i(\vec{\sigma} \cdot \vec{n}) \sin\left(\frac{\phi}{2}\right).$$

By above,
 $(\vec{\sigma} \cdot \hat{n})^{2n} = I$

lec 14.

Pauli matrices only for spin $1/2$

↓

Recall: finite rotation of spin $1/2$ particle:

$$(\vec{\sigma} \cdot \hat{n})^2 = I$$

$$e^{-i\vec{\sigma} \cdot \hat{n} \phi / \hbar} = I \cos(\frac{\phi}{2}) - i(\vec{\sigma} \cdot \hat{n}) \sin(\frac{\phi}{2}).$$

General Case:

$$\langle j', m' | e^{-i\vec{J} \cdot \hat{n} \phi / \hbar} | j, m \rangle$$

Since $[J^2, J_i] = 0$, j unchanged by rotation. Set $j = j'$, vary m, m' , get a $(2j+1) \times (2j+1)$ matrix. For $j=1$, get 3×3 matrix using action $J_{\pm}$ on $|1, m\rangle$ and get

$$J_z = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

$$J_x = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad J_y = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}.$$

Note: $(\frac{J_i}{\hbar})^3 = \frac{J_i}{\hbar}$ for $i=x, y, z$. Therefore

$$\begin{aligned} e^{-i\vec{J} \cdot \hat{n} \phi / \hbar} &= I - \frac{i\vec{J} \cdot \hat{n}}{\hbar} \left(\phi - \frac{\phi^3}{3!} + \dots \right) - \left(\frac{\vec{J} \cdot \hat{n}}{\hbar} \right)^2 \left(\frac{\phi^2}{2} - \frac{\phi^4}{4!} + \dots \right) \\ &= I - i \sin \phi \left(\frac{\vec{J} \cdot \hat{n}}{\hbar} \right) + (\cos \phi - 1) \left(\frac{\vec{J} \cdot \hat{n}}{\hbar} \right)^2. \end{aligned}$$

Connection between finite rotations and $\mathcal{Y}_l^m(\theta, \phi)$:

Let l be integer, rotate in direction $\hat{n}$.

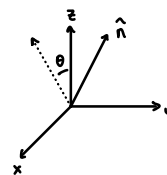
$$\mathcal{D}_{mm'}^{(l)} \equiv \langle l, m | e^{-i\vec{L} \cdot \hat{n} \phi / \hbar} | l, m' \rangle$$

To get $\hat{n}$ from $\hat{z}$, rotate by θ about $\hat{y}$ then rotate by ϕ about $\hat{z}$

$$|\hat{n}\rangle = e^{-iL_z \phi / \hbar} e^{-iL_y \theta / \hbar} |\hat{z}\rangle \equiv \mathcal{D} |\hat{z}\rangle$$

defined by LHS.

Position Eigenstates on $L^2(S^2)$.



Insert complete set of states:

$$|\hat{n}\rangle = \sum_{l', m'} \mathcal{D} |l', m'\rangle \langle l', m' | \hat{n}\rangle.$$

Contract with $\langle l, m |$:

$$\langle l, m | \hat{n}\rangle = \sum_{m'} \mathcal{D}_{mm'}^{(l)} \langle l, m' | \hat{n}\rangle.$$

But

$$\langle \hat{n} | l, m\rangle = Y_l^m(\theta, \varphi) \Rightarrow \langle l, m | \hat{n}\rangle = Y_l^{m*}(\theta, \varphi).$$

So

$$\langle l, m' | \hat{n}\rangle = Y_l^{m'*}(\theta=0, \varphi)$$

At $\theta=0$, $Y_l^m=0$ except when $m=0$: follows from

$$Y_l^m \propto \frac{1}{\sin^m \theta} \frac{d^{l-m}}{dx^{l-m}} (1-x^2)^l \Big|_{x=\cos \theta}.$$

$$Y_l^{0*} = \left(\frac{2l+1}{4\pi} \right)^{1/2}.$$

So

$$\mathcal{D}_{m0}^{(l)} = \left(\frac{4\pi}{2l+1} \right)^{1/2} Y_l^{m*}(\theta, \varphi).$$

Central Potential Problems.

Particle in 3D with $V(r)$ potential. $r^2 = X^i X_i$.

$$\left. \begin{array}{l} \text{HW 6} \Rightarrow [\vec{L}, r^2] = 0 \Rightarrow [\vec{L}, V(r)] = 0 \\ \quad \quad \quad \uparrow \\ \quad \quad \quad r = \sqrt{r^2}, \text{ Taylor Expand } V(\sqrt{r^2}) \\ \text{HW 6} \Rightarrow [\vec{L}, p^2] = 0 \end{array} \right\} \Rightarrow [\vec{L}, H] = 0.$$

$\exists$ simult. Eigenstates of H, L^2, L_z .

Want to relate L^2 to P^2 .

$$\vec{L} = \vec{X} \times \vec{P} \quad L_i = \sum_{j,k} \epsilon_{ijk} X^j P^k$$

Recall: $\epsilon_{ijk} \epsilon_{ilm} = \delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl}$.

Pf: RHS can only be $\pm 1, 0$, and antisymmetric in j, k and l, m .

□

Also,

$$\sum_{i,j,k} (\epsilon_{ijk})^2 = 6.$$

$$\Rightarrow L^2 = \sum_{j,k,l,m} (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}) X^j P^k X^l P^m$$

$$= \sum_{j,k}^{\text{sum over } j,m} X^j P^k \underbrace{X^j P^k}_{X^j P^k + [P^k, X^j]} - \underbrace{X^j P^k X^k P^j}_{P^k X^j + [X^j, P^k]}$$

$$= X^2 P^2 - i\hbar \vec{X} \cdot \vec{P} - \sum_{j,k} P^k X^j X^k P^j - i\hbar \vec{X} \cdot \vec{P}.$$

$$= - \sum_{j,k} \{X^k P^k + [P^k, X^k] \vec{X} \cdot \vec{P}\} = -(\vec{X} \cdot \vec{P})^2 + 3i\hbar (\vec{X} \cdot \vec{P})$$

$$= X^2 P^2 - (\vec{X} \cdot \vec{P})^2 + i\hbar (\vec{X} \cdot \vec{P}).$$

Since

$$X^2 = r^2 \quad \vec{X} \cdot \vec{P} = \frac{\hbar}{i} r \frac{\partial}{\partial r}$$

We get

$$P^2 = \frac{L^2}{r^2} - \frac{\hbar^2}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) - \frac{\hbar^2}{r} \frac{\partial}{\partial r}$$

$$= \frac{L^2}{r^2} - \hbar^2 \frac{\partial^2}{\partial r^2} - \frac{2\hbar^2}{r} \frac{\partial}{\partial r}$$

lec 15.

Central Potential Problem:

3D particle of mass μ , $V = V(r)$. SE:

$$\left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right] \psi = E \psi.$$

Last time expressed E as L . So above is

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{L^2}{2\mu r^2} + V(r) \right] \psi(r, \theta, \varphi) = E \psi(r, \theta, \varphi).$$

Try

$$\psi(r, \theta, \varphi) = R(r) Y_{\ell}^m(\theta, \varphi).$$

where

$$R(r) = u(r)/r.$$

Then SE:

$$-\frac{\hbar^2}{2\mu} (R'' + \frac{2}{r} R') + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} R + VR = ER$$

$$\Rightarrow -\frac{\hbar^2}{2\mu} u'' + V_{\text{eff}} u = E u \quad \text{where} \quad V_{\text{eff}} = V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}.$$

Boundary Conditions:

At $r \rightarrow \infty$, normalizability:

$$\int d^3x |\psi|^2 = \int d\Omega |Y_{\ell}^m(\theta, \varphi)|^2 \cdot \int r^2 \left(\frac{u}{r} \right)^2 dr < \infty \Rightarrow \int u^2 dr < \infty.$$

This requires $u \rightarrow 0$ faster than $\frac{1}{\sqrt{r}}$.

At $r \rightarrow 0$, we claim that $u(0) = 0$. Otherwise say $u(0) = C \neq 0$. Then $\psi \sim \frac{1}{r}$ as $r \rightarrow 0$, then $\nabla^2(\frac{1}{r}) \propto \delta(\vec{x})$, so SE will blow up at 0.

Asymptotic Solution:

$r \rightarrow \infty$ (assuming $V(r) \rightarrow 0$):

$$-\frac{\hbar^2}{2\mu} u'' = E u.$$

$r \rightarrow 0$ (assuming $r^2 V(r) \rightarrow 0$):

$$-\frac{\hbar^2}{2\mu} u'' + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} u = 0. \Rightarrow u(r) \sim r^{\ell+1}$$

for bound state $E < 0$,
solutions
 $\sim e^{-\kappa r}$.

throw away
solution
 $u \sim r^{-\ell}$
blows up.

Columb Problem:

$$V(r) = -\frac{Ze^2}{r}$$

let

$$\rho = Kr \quad K = \frac{\sqrt{2\mu|E|}}{\hbar} \quad \rho_0 = \frac{Ze^2 K}{|E|}$$

Then

$$\frac{V}{|E|} = \frac{-\rho_0}{Kr} = -\frac{\rho_0}{\rho}$$

Divide radial SE by $|E|$:

$$\left[\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{\rho_0}{\rho} - 1 \right] u(\rho) = 0. \quad (*)$$

Write

$$u(\rho) = \rho^{l+1} e^{-\rho} w(\rho) \quad (\text{have correct asym. behavior as } \rho \rightarrow \infty, 0)$$

Expand

$$w(\rho) = \sum_{k=0}^{\infty} a_k \rho^k$$

Plug in (*):

$$\sum_k a_k [k(k-1)\rho^{k-1} + 2(l+1)k\rho^{k-1} - 2k\rho^k + (\rho_0 - 2(l+1))\rho^k] = 0.$$

Shift index $k \rightarrow k+1$ in the 1st line and use $\sum_k C_k \rho^k = 0 \Rightarrow C_k = 0 \forall k$ gives:

$$a_{k+1} = \frac{2(k+l+1) - \rho_0}{(k+1)(k+2l+2)} a_k.$$

a_0 is fixed by normalizability, all other a_k determined.

But at large k :

$$\frac{a_{k+1}}{a_k} \sim \frac{2}{k} \Rightarrow w(\rho) = \sum_k a_k \rho^k \sim e^{2\rho} \quad \text{not normalizable.}$$

So power series $w(\rho) = \sum_k a_k \rho^k$ must terminate at some $k=N$.

Then

$$\begin{aligned} \rho_0 &= 2(N+l+1) & N &\equiv \text{Radial quantum number.} \\ &= \frac{Ze^2 K}{|E|} = \frac{Ze^2}{\hbar} \left(\frac{2\mu}{|E|} \right)^{1/2}. \end{aligned}$$

Solve for E :

$$E = \frac{-Z^2 e^4 \mu}{\hbar^2 p}$$

Set

$$n = N + l + 1 \Rightarrow E_n = -\frac{\mu Z^2 e^4}{2 \hbar^2 n^2} \quad n = 1, 2, 3, \dots$$

Degeneracy: $l = 0, 1, \dots, n-1$,

$$\sum_{l=0}^{n-1} (2l+1) = \frac{2(n-1)n}{2} + n = n^2.$$

Recall: fine structure constant:

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137} \Rightarrow E_n = -\frac{Z^2}{2} \frac{\alpha^2 \mu c^2}{n^2}$$

for e^- , $\mu c^2 = 5.1 \times 10^5 \text{ eV} \Rightarrow E_1 = -13.6 \text{ eV}$ (hydrogen $Z=1$).

Radial Wave Function:

$$R_{n,l}(r) = \frac{u_{n,l}(r)}{r} = \frac{r^{l+1} e^{-\rho} w(\rho)}{r} \quad \begin{matrix} \text{deg} = N \\ \swarrow \\ \text{associated} \\ \text{Laguerre polynomial.} \end{matrix}$$

$$\rho = Kr \quad K = \frac{\sqrt{2\mu|E|}}{\hbar} = \frac{\mu Z e^2}{\hbar^2 n}$$

Define $r_0 = \frac{\hbar^2}{\mu Z e^2}$. for $Z=1$, this is Bohr radius. $\sim 0.53 \times 10^{-8} \text{ cm}$.

$$R_{n,l}(r) = \frac{e^{-r/nr_0}}{r} \left(\frac{r}{nr_0} \right)^{l+1} w\left(\frac{r}{nr_0} \right)$$

e.g.

$$R_{1,0}(r) = 2r_0^{-3/2} e^{-r/r_0}$$

$$R_{2,0}(r) = 2r_0^{-3/2} \left(1 - \frac{r}{2r_0} \right) e^{-r/2r_0}$$

$$R_{2,1}(r) = (2r_0)^{-3/2} \frac{r}{\sqrt{3}r_0} e^{-r/2r_0}.$$

Comments:

(1) ∞ number of bound states: $E_n = \frac{E_1}{n^2}$.

(2) Spectroscopic Notation

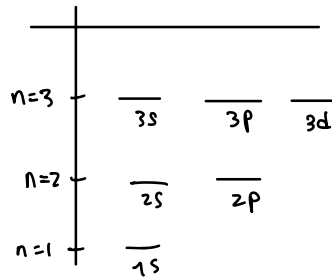
$$l=0 \leftrightarrow s$$

$$l=1 \leftrightarrow p$$

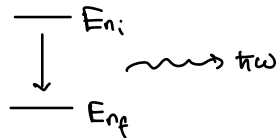
$$l=2 \leftrightarrow d$$

$$l=3 \leftrightarrow f$$

$$l=4 \leftrightarrow g$$



(3) Transitions:



$$h\omega = E_{n_i} - E_{n_f} = -\frac{Z^2 \alpha^2 \mu c^2}{2} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right).$$

Rydberg Formula (known long before QM).

Why does E_n depends only on n ?

Spherical Symmetry $\Rightarrow E$ indep. of L_z e.v. m .

V_{eff} depends on $l \Rightarrow$ Why doesn't E ?

Introduce

$$\vec{M} = \frac{1}{2\mu} (\vec{P} \times \vec{L} - \vec{L} \times \vec{P}) - \frac{Ze^2}{r} \vec{X}$$

Runge-Lenz Vector.

Properties (HW 8):

$$1) \vec{M}^\dagger = \vec{M}$$

$$2) [\vec{M}, H] = 0$$

$$3) [L_j, M_k] = i\hbar \epsilon_{jkl} M_l$$

$$4) [M_j, M_k] = \left(-\frac{2i\hbar}{\mu} H \right) \epsilon_{jkl} L_l.$$

$$5) M^2 = \frac{2H}{\mu} (L^2 + \hbar^2) + (Ze^2)^2.$$

Properties:

1) $\vec{M}^+ = \vec{M}$

$$2) [\vec{M}, H] = 0$$

$$3) [L_j, M_k] = i\hbar \epsilon_{jkl} M_l$$

$$4) [M_j, M_k] = \left(-\frac{29\hbar}{\mu} H\right) \varepsilon_{jkl} L_l$$

$$5) M^2 = \frac{2H}{\mu} (L^2 + \hbar^2) + (Ze^2)^2.$$

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Algebraic solution to Coulomb potential

$$\vec{M} = \frac{1}{2\mu} (\vec{P} \times \vec{L} - \vec{L} \times \vec{P}) - \frac{Ze^2}{r} \vec{X} \quad \text{Runge - Lens vector.}$$

Properties shown at top of page.

Focus on subspace with energy eigenvalue $E < 0$. Rescale

$$\vec{M}' = \left(-\frac{\mu}{2E}\right)^{1/2} \vec{M}.$$

$$\Rightarrow [M_f', M_k'] = i\hbar \epsilon_{fkl} L_l$$

Define

Define $\vec{I} := \frac{1}{2}(\vec{L} + \vec{M}')$, $\vec{K} := \frac{1}{2}(\vec{L} - \vec{M}')$

$$\Rightarrow [I_f, I_k] = \frac{1}{4} [L_f, L_k] + \frac{1}{4} [L_f, M_k'] + \underbrace{\frac{1}{4} [M_f', L_k] + \frac{1}{4} [M_f', M_k'] - \frac{1}{4} [L_k, M_f']}_{=0}$$

$$= \frac{1}{4} \hbar \varepsilon_{fkl} [L_l + M_l' + M_l' + L_l]$$

So

$$[I_f, I_k] = \frac{1}{2} \eta \hbar \epsilon_{f k l} (L_l + M_l') = \eta \hbar \epsilon_{f k l} I_l$$

$$\begin{aligned}
 [K_j, K_k] &= \frac{1}{4} [L_j, L_k] - \frac{1}{4} [L_j, M'_k] - \frac{1}{4} [M'_j, L_k] + \frac{1}{4} [M'_j, M'_k] \\
 &= \frac{1}{4} i\hbar \epsilon_{jkl} [L_l - M'_l - M'_l + L_l] \\
 &= \frac{1}{2} i\hbar \epsilon_{jkl} (L_l - M'_l)
 \end{aligned}$$

$$\Rightarrow [K_j, K_k] = i\hbar \epsilon_{jkl} K_l$$

$$\begin{aligned}
 [I_j, K_k] &= \frac{1}{4} [L_j, L_k] - \frac{1}{4} [L_j, M'_k] + \frac{1}{4} [M'_j, L_k] - \frac{1}{4} [M'_j, M'_k] \\
 &= \frac{1}{4} i\hbar \epsilon_{jkl} [L_l - M'_l + M'_l - L_l] = 0.
 \end{aligned}$$

$$[I_j, K_k] = 0$$

So we have 2 indep generators of rotations. Symmetry is $SO(3) \times SO(3) = SO(4)$.



In 3D: $\frac{3 \cdot 2}{2} = 3$ indep planes

In 4D: $\frac{4 \cdot 3}{2} = 6 = 3+3$.

Eigenvalues of $I^2 = j(j+1)\hbar^2$

Eigenvalues of $K^2 = k(k+1)\hbar^2$ $k, j = n/2$

$$I^2 - K^2 = \frac{1}{4} (L^2 + 2\vec{L} \cdot \vec{M}' + \vec{M}'^2 - L^2 + 2\vec{L} \cdot \vec{M}' - \vec{M}'^2)$$

$$\begin{aligned}
 [L_x, M'_x] &= 0 \Rightarrow L_x M'_x = M'_x L_x \quad \text{order doesn't matter} \\
 &\Rightarrow \vec{L} \cdot \vec{M}' = \vec{M}' \cdot \vec{L}
 \end{aligned}$$

$$= \vec{L} \cdot \vec{M}'$$

$$\vec{L} \cdot \vec{M}' = \frac{1}{2\mu} \underbrace{\vec{L} \cdot (\vec{P} \times \vec{L} - \vec{L} \times \vec{P})}_0 - \frac{Ze^2}{r} \underbrace{\vec{L} \cdot \vec{X}}_{=0 \text{ classically}}$$

$$QM: \vec{L} \cdot \vec{X} = \epsilon_{jkl} X^k \underbrace{P^l X^j}_{= X^j P^l, \text{ different components}} = \epsilon_{jkl} X^k X^j P^l = 0$$

$$\begin{aligned} \vec{L} \cdot (\vec{L} \times \vec{P}) &= \epsilon_{jkl} L^j L^k P^l \\ &= \frac{1}{2} \epsilon_{jkl} [L^j, L^k] P^l \\ &= \frac{1}{2} \hbar \epsilon_{jkl} \epsilon_{jkm} L^m P^l \quad [L_j, L_k] = \hbar \epsilon_{jkm} L_m \\ &= \frac{1}{2} \hbar 2 \delta_{lm} L^m P^l \\ &= \hbar \vec{L} \cdot \vec{P} = 0. \end{aligned}$$

$$\begin{aligned} \vec{L} \cdot (\vec{P} \times \vec{L}) &= \epsilon_{jkl} L^j P^k L^l \\ &= \frac{1}{2} \epsilon_{jkl} [L^j, P^k] L^l \\ &\quad \hbar \epsilon_{jkm} P^m \\ &= \hbar \vec{P} \cdot \vec{L} = 0 \end{aligned}$$

Conclusion: $\vec{L} \cdot \vec{M}' = 0 \Rightarrow L^2 = K^2 \Rightarrow \underbrace{L^2 + K^2}_{\frac{1}{2}(L^2 + M'^2)}$ has e.v. $2k(k+1)\hbar^2$.

Recall: $M^2 = \frac{2H}{\mu} (L^2 + \hbar^2) + (Ze^2)^2$

So $\frac{1}{2}(L^2 + M'^2) = \frac{1}{2}(L^2 - \frac{\mu}{2E} M^2)$ def of $\vec{M}'$

$$= - \frac{\mu(Ze^2)^2}{4E} - \frac{1}{2} \hbar^2 = 2k(k+1)\hbar^2$$

Note

$$2k(k+1) + \frac{1}{2} = \frac{1}{2}(4k^2 + 4k + 1) = \frac{1}{2}(2k+1)^2$$

Solve for E :

$$- \frac{\mu(Ze^2)^2}{4E} = \frac{1}{2}(2k+1)^2 \hbar^2 \Rightarrow E = - \frac{\mu(Ze^2)^2}{2\hbar^2(2k+1)^2}$$

Let $n=2k+1$
Get energy e.v.
for Coulomb potential

Degeneracy is supposed to be n^2 .

$$2k+1 = n \text{ from } K_z$$

$$2k+1 = n \text{ from } I_z$$

Total degeneracy is indeed n^2 .

Do we get same allowed range of L^2 ?

$$\vec{L} = \vec{I} + \vec{K}?$$

Addition of angular momentum

Example: 2 spin $\frac{1}{2}$ particles

Total of 4 states labelled by $|m_{1z}, m_{2z}\rangle$:

$$|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$$

Define total spin $\vec{S} = \vec{S}_1 + \vec{S}_2$. It satisfies

$$[S_x, S_y] = i\hbar S_z \text{ etc, since } [\vec{S}_1, \vec{S}_2] = 0.$$

Want eigenstates of $S^2 + S_z^2$:

$$\begin{aligned} \text{max } m: S_z |++\rangle &= (S_{1z} + S_{2z}) |++\rangle = \hbar |++\rangle \Rightarrow m=1 \text{ maximum} \\ &\Rightarrow s=1 \end{aligned}$$

$$|--\rangle \text{ has } s=1, m=-1.$$

$$|+-\rangle, |-+\rangle \text{ have } m=0.$$

Use

$$J_- |j, m\rangle = \sqrt{(j+m)(j-m+1)} \hbar |j, m-1\rangle$$

$$\begin{aligned} \Rightarrow J_- |1, 1\rangle &= \sqrt{2} \hbar |1, 0\rangle = J_-^{(1)} |++\rangle + J_-^{(2)} |++\rangle \\ &= \hbar (|-+\rangle + |+-\rangle) \end{aligned}$$

$$\Rightarrow |1, 0\rangle = \frac{1}{\sqrt{2}} (|-+\rangle + |+-\rangle)$$

Remaining state

$$|0,0\rangle = \frac{1}{\sqrt{2}} (|+-\rangle - |-+\rangle)$$

must be $\perp$ to others.

Lec 17.

Addition of Angular Momentum, General Case.

Given $\vec{J}_1, \vec{J}_2$. $[\vec{J}_1, \vec{J}_2] = 0$.

Set $\vec{J} = \vec{J}_1 + \vec{J}_2$. Find E. states of J^2, J_z .

$$[J^2, J_i^2] = 0 \quad i=1,2$$

New eigenstates $|j_1, j_2, j, m\rangle$ of J_1^2, J_2^2, J^2, J_z

Drop j_1, j_2 .

Write

Clebsch-Gordan Coefficient

↓

$$|j, m\rangle = \sum_{m_1, m_2} |m_1, m_2\rangle \langle m_1, m_2 | j, m\rangle$$

$|m_1, m_2\rangle$ E. states of J_{1z}, J_{2z} .

Note: $J_z = J_{1z} + J_{2z}$. So

$$0 = \langle m_1, m_2 | (J_z - J_{1z} - J_{2z}) | j, m\rangle$$

$$= (m - m_1 - m_2) \hbar \langle m_1, m_2 | j, m\rangle$$

for $\langle m_1, m_2 | J_{1z}$
 $= \langle m_1, m_2 | J_{1z}^+$
 $= m_1 \langle m_1, m_2 |$
 $m_1 \in \mathbb{R}$, similarly...

$$\Rightarrow m = m_1 + m_2.$$

Max m is $j_1 + j_2$.

Claim: $\min j = |j_1 - j_2|$

pf: Count states. There are $2j+1$ states for each j . Have a total of

$(2j_1+1)(2j_2+1)$ states. Define

$$f(n) = \sum_{j=0}^{n-1} (2j+1) = n(n-1) + n = n^2.$$

So

$$\sum_{j=j_{\min}}^{j_{\max}} (2j+1) = f(j_{\max}+1) - f(j_{\min}) = (j_1 + j_2 + 1)^2 - j_{\min}^2$$

This must equal $(2j_1+1)(2j_2+1)$.

$$\Rightarrow j_{\min}^2 = (j_1 + j_2 + 1)^2 - (2j_1+1)(2j_2+1) \Rightarrow j_{\min} = |j_1 - j_2|.$$

Intuitive Picture: Addition of Vectors:

Max length: $\vec{j}_1, \vec{j}_2 \rightarrow j_1 + j_2$

Min length: $\vec{j}_1, \vec{j}_2 \leftarrow j_1 - j_2$

But e.v. of J^2 is not $j^2 \hbar^2$
 but $j(j+1) \hbar^2$.

To find Clebsch-Gordan Coeff.

$$J_- |j, m\rangle = \sqrt{(j+m)(j-m+1)} \hbar |j, m-1\rangle$$

Start with $j = j_1 + j_2$ ^(*), $m = \max$.

$$|j, m=j\rangle = |m_1=j_1, m_2=j_2\rangle.$$

Act with $J_- = J_{1-} + J_{2-}$.

$$J_- |j, j\rangle = (J_{1-} + J_{2-}) |j_1, j_2\rangle$$

$$\sqrt{2j} \hbar |j, j-1\rangle = \sqrt{2j_1} \hbar |j_1-1, j_2\rangle + \sqrt{2j_2} \hbar |j_1, j_2-1\rangle$$

$$|j, j-1\rangle = \sqrt{\frac{j_1}{j}} |j_1-1, j_2\rangle + \sqrt{\frac{j_2}{j}} |j_1, j_2-1\rangle \quad (**)$$

(*) $\Rightarrow$ Correctly normalized.

Repeatedly applying J_- now $2j$ times.

Next, set $j = j_1 + j_2 - 1$.

Don't forget that j_1, j_2 are fixed, and we have restrictions $m_1 \leq j_1, m_2 \leq j_2$.
eg. $|j_1-2, j_2+1\rangle$ is not allowed although $m_1+m_2 = j_1+j_2-1$.

Highest m state must be linear combination of $|j_1-1, j_2\rangle, |j_1, j_2-1\rangle$ and $\perp$ to (**).

So

$$|j, m\rangle = |j_1+j_2-1, j_1+j_2-1\rangle = -\sqrt{\frac{j_2}{j_1+j_2}} |j_1-1, j_2\rangle + \sqrt{\frac{j_1}{j_1+j_2}} |j_1, j_2-1\rangle.$$

Example: $\vec{J} = \vec{L} + \vec{S}$ for Spin $1/2$.

In terms of ang. mom. E. states:

$$|l, m_l, m_s\rangle.$$

Fix l , find e. states of J^2, J_z .

$$j = l \pm \frac{1}{2}.$$

$$|j = l + \frac{1}{2}, m = l + \frac{1}{2}\rangle = |m_l = l, m_s = \frac{1}{2}\rangle$$

Apply J_- :

$$\sqrt{2l+1} |j = l + \frac{1}{2}, m_j = l - \frac{1}{2}\rangle = \sqrt{2l} |m_l = l-1, m_s = \frac{1}{2}\rangle + |m_l = l, m_s = -\frac{1}{2}\rangle$$

$$|l+\frac{1}{2}, l-\frac{1}{2}\rangle = \sqrt{\frac{2l}{2l+1}} |l-1, \frac{1}{2}\rangle + \sqrt{\frac{1}{2l+1}} |l, -\frac{1}{2}\rangle.$$

Apply J_- again:

$$\begin{aligned} \sqrt{2l \cdot 2} |l+\frac{1}{2}, l-\frac{3}{2}\rangle &= \sqrt{\frac{2l}{2l+1}} \left\{ \sqrt{(2l-1) \cdot 2} |l-2, \frac{1}{2}\rangle + |l-1, -\frac{1}{2}\rangle \right\} \\ &\quad + \sqrt{\frac{1}{2l+1}} \sqrt{2l} |l-1, -\frac{1}{2}\rangle. \end{aligned}$$

→ $J_1 + J_2$ to the 1st term above

→ $J_1 + J_2$ to the 2nd term above.

$$\Rightarrow |l+\frac{1}{2}, l-\frac{3}{2}\rangle = \sqrt{\frac{2l-1}{2l+1}} |l-2, \frac{1}{2}\rangle + \sqrt{\frac{2}{2l+1}} |l-1, -\frac{1}{2}\rangle.$$

Apply J_- n times:

$$|l+\frac{1}{2}, l+\frac{1}{2}-n\rangle = \sqrt{\frac{2l+1-n}{2l+1}} |l-n, \frac{1}{2}\rangle + \sqrt{\frac{n}{2l+1}} |l+1-n, -\frac{1}{2}\rangle.$$

let $m_j = l+\frac{1}{2}-n$:

$$|l+\frac{1}{2}, m_j\rangle = \sqrt{\frac{l+m_j+\frac{1}{2}}{2l+1}} |m_j-\frac{1}{2}, \frac{1}{2}\rangle + \sqrt{\frac{l-m_j+\frac{1}{2}}{2l+1}} |m_j+\frac{1}{2}, -\frac{1}{2}\rangle.$$

lec 18.

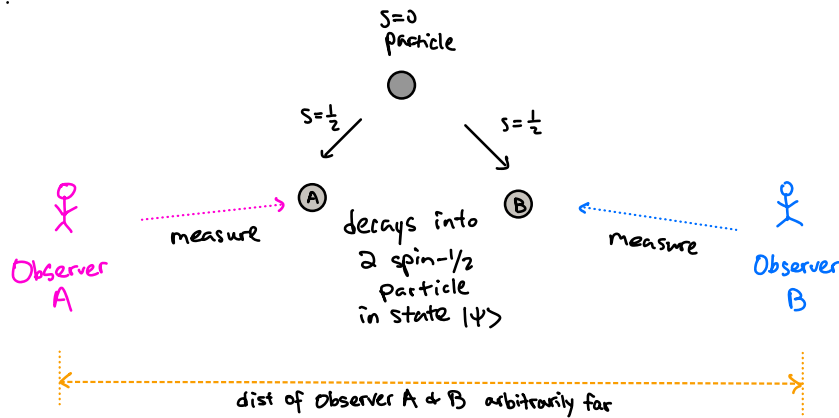
Quantum Entanglement & Bell's Inequality. (Ref. 3.10)

2 spin- $\frac{1}{2}$ particle in $S=0$ state:

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\hat{z}^+, \hat{z}^-\rangle - |\hat{z}^-, \hat{z}^+\rangle \right).$$

$m_1 \quad m_2 \qquad m_1 \quad m_2$

Imagine:



- If A measures $S_z = \frac{\hbar}{2}$ for $|\psi\rangle$, then $|\psi\rangle$ collapses to $|\hat{z}^+, \hat{z}^-\rangle$ immediately. Thus when B measure immediately after, he get $S_z = -\frac{\hbar}{2}$ with certainty.
- If A makes no measurement, B sees $\pm \frac{\hbar}{2}$ with equal probability.

Suppose A, B measures S_x , then $|\psi\rangle$ can also be written

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\hat{x}^+, \hat{x}^-\rangle - |\hat{x}^-, \hat{x}^+\rangle \right).$$

- Similar measurement story for S_x as above.
- Suppose A measure $S_z = \frac{\hbar}{2}$. Then $|\psi\rangle \rightarrow |\hat{z}^+, \hat{z}^-\rangle$. So for particle B, the state is $|\hat{z}^-\rangle = \frac{1}{\sqrt{2}} (|\hat{x}^+\rangle - |\hat{x}^-\rangle)$. If B measure S_x now, he will get $S_x = \pm \frac{\hbar}{2}$ with equal probability.
- Imagine A, B observers are so far away, and B measures particle B immediately after A does their measure. So no signal can reach B in the interval after A's measurement & before B's measurement. (Contradiction to SR ?)

Deterministic Model:

Every particle has definite S_z, S_x . 2nd particle always opposite:

1 st particle	2 nd particle
$(\hat{z}+, \hat{x}+)$	$(\hat{z}-, \hat{x}-)$
$(\hat{z}+, \hat{x}-)$	$(\hat{z}-, \hat{x}+)$
$(\hat{z}-, \hat{x}+)$	$(\hat{z}+, \hat{x}-)$
$(\hat{z}-, \hat{x}-)$	$(\hat{z}+, \hat{x}+)$

- Measure 1st particle, 2nd particle has definite result for same S_i .
- A measures $S_z = \pm \frac{\hbar}{2}$, then B measures $\pm \frac{\hbar}{2}$ for S_x .
- No measurement of 1st particle, then B measures $\pm \frac{\hbar}{2}$ for S_x .

Consider 3 directions $\hat{a}, \hat{b}, \hat{c}$ (not nesc. orthog.)

Only do 418 cases:

Population	particle 1	particle 2
N_1	$(\hat{a}+, \hat{b}+, \hat{c}-)$	$(\hat{a}-, \hat{b}-, \hat{c}+)$
N_2	$(\hat{a}+, \hat{b}-, \hat{c}+)$	$(\hat{a}-, \hat{b}+, \hat{c}-)$
N_3	$(\hat{a}+, \hat{b}-, \hat{c}-)$	$(\hat{a}-, \hat{b}+, \hat{c}+)$
N_4	$(\hat{a}-, \hat{b}-, \hat{c}+)$	$(\hat{a}+, \hat{b}+, \hat{c}-)$
... 4 more ...		

Let $P(\hat{a}+; \hat{b}+)$ be prob. that observer A measures $\vec{S}_1 \cdot \hat{a} = +\frac{\hbar}{2}$, and obs. B measures $\vec{S}_2 \cdot \hat{b} = +\frac{\hbar}{2}$.

In deterministic model, $N_{tot} = N_1 + \dots + N_8$,

$$P(\hat{a}+; \hat{b}+) = \frac{N_2 + N_3}{N_{tot}} \leq \frac{(N_1 + N_3)}{N_{tot}} + \frac{(N_2 + N_4)}{N_{tot}} = P(\hat{a}+; \hat{c}+) + P(\hat{c}+; \hat{b}+).$$

Compare with QM: let $\hat{a} = \hat{z}$.

$$\hat{b} = \sin\theta \hat{x} + \cos\theta \hat{z}$$

$\vec{S}_1 \cdot \hat{a}$ yields $+\frac{\hbar}{2}$ $P = \frac{1}{2}$

2nd particle in state $|\hat{z}-\rangle$:

$$\vec{\sigma} \cdot \hat{b} = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix}.$$

E. vector $\begin{bmatrix} \cos\theta/2 \\ \sin\theta/2 \end{bmatrix}$ e.v. $+1$ $\begin{bmatrix} \sin\theta/2 \\ -\cos\theta/2 \end{bmatrix}$ e.v. -1 .

Start with $|\hat{z}-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.

Prob to get $\vec{\sigma} \cdot \hat{b}$ be $+1$ is inner product² of $|\hat{z}-\rangle$ with $+1$ e.v. get

$$P(\hat{a}+; \hat{b}+) = \frac{1}{2} \sin^2 \frac{\theta_{ab}}{2}.$$

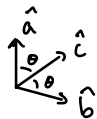
$$\theta \rightarrow \theta_{ab}.$$

(ineq above)

$$\text{Bell's Inequality} \Rightarrow \sin^2 \frac{\theta_{ab}}{2} \leq \sin^2 \frac{\theta_{ac}}{2} + \sin^2 \frac{\theta_{cb}}{2}$$

but this is wrong:

Suppose



all on the same plane.

θ small

$$\text{LHS} \approx \theta^2 \quad \text{RHS} \approx \frac{\theta^2}{4} + \frac{\theta^2}{4} = \frac{\theta^2}{2}. \quad \text{so LHS} \not\leq \text{RHS}.$$

Thus in QM, Bell's ineqn is violated. (Alain Aspect - experiment results confirm QM violate Bell's ineqn).

lec 19. (Topics, not on final)

24 hr take home final, starting noon Monday.

What is a measurement really?

Given 2 systems A, B with states $\mathcal{H}_A, \mathcal{H}_B$.

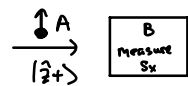
The combined system has states $\mathcal{H}_A \otimes \mathcal{H}_B$.

If $|a_i\rangle$ O.N. basis for $\mathcal{H}_A$, $|b_j\rangle$ O.N. basis for $\mathcal{H}_B$, a basis of $\mathcal{H}_A \otimes \mathcal{H}_B$ is

$$|a_i\rangle|b_j\rangle := |a_i\rangle \otimes |b_j\rangle.$$

If $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ is NOT of the form $|\psi_1\rangle_A |\psi_2\rangle_B$, the $|\psi\rangle$ is said to be **entangled**.

Suppose A = quantum system, B = measuring device.



$$|z+\rangle \underbrace{|0\rangle}_{\text{detector}} \longrightarrow |\hat{x}+\rangle|up\rangle + |\hat{x}-\rangle|down\rangle.$$

Not everything in QM can be assigned a probability. Probability can be assigned to situations that **decohere**. i.e. different contributions to $|\psi\rangle = \sum_{\alpha} c_{\alpha} |\psi_{\alpha}\rangle$ are orthogonal.

This holds due to interaction with environment. So really

$$|\psi\rangle = |\psi_1\rangle |a_1, \dots, a_N\rangle + |\psi_2\rangle |b_1, \dots, b_N\rangle + \dots$$

↑ environment
consisting of huge #N
of particles.

Even if $\langle a_i | b_i \rangle = 1 - \epsilon$, $|\epsilon| \leq 1$, we have each term

$$\begin{aligned} & (\langle a_1, \dots, a_N | \langle \psi_1 |) (|\psi_2\rangle |b_1, \dots, b_N\rangle) \\ &= \langle \psi_1 | \psi_2 \rangle \langle a_1, \dots, a_N | b_1, \dots, b_N \rangle \\ &\propto \prod_i \langle a_i | b_i \rangle = (1 - \epsilon)^N \simeq 0. \end{aligned}$$

So states contributing to $|\psi\rangle$ are orthogonal.

Mixed States (Density matrices).

Ensembles : large # of particles in different quantum state.
described by density matrices.

Suppose $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ entangled state as before,

$$|\psi\rangle = \sum_{ik} c_{ik} |a_i\rangle |b_k\rangle.$$

Operator that acts only on A: $\mathcal{O}_A$.

$$\begin{aligned}\langle \psi | \mathcal{O}_A | \psi \rangle &= \sum_{ijkl} \langle b_l | \langle a_j | c_{jl}^* \mathcal{O}_A c_{ik} | a_i \rangle | b_k \rangle \\ &= \sum_{j,k} c_{ik} c_{jk}^* \langle a_j | \mathcal{O}_A | a_i \rangle \quad \text{for } \langle b_l | b_k \rangle = \delta_{lk}.\end{aligned}$$

Define $\rho_{ij} = \sum_k c_{ik} c_{jk}^*$ density matrix

$$\rho = \sum_{ij} \rho_{ij} |a_i\rangle \langle a_j| \quad \text{density operator}$$

Clearly

$$\rho_{ij} = \langle a_i | \rho | a_j \rangle$$

Let

$$\mathcal{O}_{ji} = \langle a_j | \mathcal{O}_A | a_i \rangle$$

Then

$$\langle \psi | \mathcal{O}_A | \psi \rangle = \sum_{ij} \rho_{ij} \mathcal{O}_{ji} = \text{Tr}(\rho \mathcal{O}_A).$$

Properties of ρ :

1) ρ is Hermitian.

2) $\text{Tr} \rho = 1$: $\text{Tr} \rho = \sum \rho_{ii} = \sum c_{ik} c_{ik}^* = \langle \psi | \psi \rangle = 1$.

3) ρ is nonnegative : An operator O is nonnegative if $\langle \psi | O | \psi \rangle \geq 0$ for all $|\psi\rangle$.

pf: Obviously true if $|\psi\rangle = |a_i\rangle$. Since $\langle a_i | \rho | a_i \rangle = \rho_{ii} = \sum_k |c_{ik}|^2 \geq 0$. Any state $|\psi\rangle$ can be a basis state. $\square$

Conversely, any nonnegative Hermitian operator with $\text{Tr} = 1$ is a possible density matrix, i.e., mixed state for some system.

Given ρ , can diagonalize: Diagonal elements give probability that state is a corresponding eigenvectors $|v_i\rangle$, where

$$\rho = \begin{bmatrix} w_1 & & \\ & \ddots & \\ & & w_n \end{bmatrix} = \sum_i w_i |v_i\rangle\langle v_i|.$$

Lec 20.

Density Operator Continued.

If A is entangled with B, A described by density operator ρ .

i.e., any nonnegative, Hermitian operator with $\text{Tr } \rho = 1$

Diagonalize ρ :

$$\rho = \sum_i w_i |v_i\rangle\langle v_i|.$$

e.vectors of ρ , states of A.

If only 1 nonzero e.v. w , then $\rho = |v\rangle\langle v|$. This arises when the original state in $\mathcal{H}_A \otimes \mathcal{H}_B$ is a pure state: $|\psi\rangle = |v\rangle_A |\varphi\rangle_B$.

pf: If

$$\rho = |v\rangle\langle v|,$$

Then $\rho^2 = \rho$. So $\text{Tr } \rho^2 = 1$. Check that this is basis independent condition for ρ to describe pure state. In general,

$$\rho^2 = \begin{bmatrix} w_1^2 & & \\ & \ddots & \\ & & w_n^2 \end{bmatrix}$$

where $w_i > 0$ (ρ positive) and $\sum_i w_i = 1$ ($\text{Tr } \rho = 1$). So in general

$$\text{Tr } \rho^2 = \sum_i w_i^2 < 1.$$

Unless only 1 nonzero.

□

Interpretation of Wave Function.

Probability density

$$\tilde{\rho} = |\psi(\vec{x}, t)|^2.$$

Define

$$\vec{j} = \frac{\hbar}{m} \text{Im}(\psi^* \vec{\nabla} \psi).$$

One can show by Schrödinger Equation:

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

Thus $\vec{j}$ is probability flux (or current density).

Note:

$$\begin{aligned}\int d^3x \vec{j}(\vec{x}, t) &= \frac{1}{m} \int d^3x \frac{\hbar}{2i} (\psi^* \vec{\nabla} \psi - \underbrace{\psi \vec{\nabla} \psi^*}_{\text{integrate by parts}}) \\ &= \frac{\langle \vec{P} \rangle}{m} \quad (\text{using } \vec{P} = \frac{\hbar}{i} \vec{\nabla}).\end{aligned}$$

If write

$$\psi = \sqrt{\tilde{\rho}} e^{iS(\vec{x}, t)/\hbar}$$

Then

$$\vec{j} = \frac{\tilde{\rho}}{m} \vec{\nabla} S.$$

For free particle, $\psi \propto e^{i\vec{k} \cdot \vec{x}} \Rightarrow S = \hbar \vec{k} \cdot \vec{x}$ AND $\vec{\nabla} S = \hbar \vec{k} = \vec{P}$.

Charged Particle.

particle of charge e in (time indep) $\vec{E}$ & $\vec{B}$ field.

Potentials (classically):

$$\begin{aligned}\vec{E} &= -\vec{\nabla} \phi - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \\ \vec{B} &= \vec{\nabla} \times \vec{A}.\end{aligned}$$

Classical Hamiltonian:

$$H = \frac{1}{2m} \left(\vec{P} - \frac{e}{c} \vec{A} \right)^2 + e\phi$$

Use this in QM. Heisenberg Eq of Motion:

$$\frac{dX_i}{dt} = \frac{1}{i\hbar} [\vec{X}, H] = \frac{1}{m} \left(\vec{P} - \frac{e}{c} \vec{A} \right) \equiv \frac{1}{m} \vec{\pi}$$

$\vec{P}$ = usual canonical momentum = $\frac{\hbar}{i} \vec{\nabla}$.

$\vec{\pi}$ = Kinematic Momentum.

$$[\pi_i, \pi_j] = -\frac{e}{c} ([P_i, A_j] + [A_i, P_j]).$$

Use

$$[P, f(x)] = -i\hbar f'(x)$$

And get

$$\begin{aligned} [\pi_i, \pi_j] &= \frac{i\hbar e}{c} (\partial_i A_j - \partial_j A_i) \\ &= \frac{i\hbar e}{c} \epsilon_{ijk} B_k \end{aligned}$$

Write

$$H = \frac{\pi^2}{2m} + e\phi.$$

Use Heisenberg EOM above:

$$m \frac{d^2 \vec{X}}{dt^2} = \frac{d\vec{\pi}}{dt} = e \left[\vec{E} + \frac{1}{2c} \left(\frac{d\vec{X}}{dt} \times \vec{B} - \vec{B} \times \frac{d\vec{X}}{dt} \right) \right]$$

QM Lorentz force law.

Gauge transformations:

$$\tilde{A}_i = A_i + \partial_i \Lambda \quad \tilde{\phi} = \phi - \frac{1}{c} \frac{\partial \Lambda}{\partial t}.$$

What happens to ψ ?

Claim: If ψ satisfies

$$i\hbar \frac{\partial \psi}{\partial t} = \left[\frac{1}{2m} \left(\frac{\hbar}{i} \vec{\nabla} - \frac{e}{c} \vec{A} \right)^2 + e\phi \right] \psi,$$

then

$$\tilde{\psi} = e^{ie\Lambda/\hbar c} \psi$$

solves the SE above with $(A, \phi) \rightarrow (\tilde{A}, \tilde{\phi})$.

pf: Check:

$$\text{LHS} = i\hbar \frac{\partial \tilde{\psi}}{\partial t} = e^{ie\Lambda/\hbar c} \left[i\hbar \frac{\partial \psi}{\partial t} - \frac{e}{c} \frac{\partial \Lambda}{\partial t} \psi \right]$$

which cancels with
gauge transf. of ϕ on RHS.

First note:

$$\begin{aligned} & \left[\frac{\hbar}{i} \vec{\nabla} - \frac{e}{c} (\vec{A} + \vec{\nabla} \Lambda) \right] e^{ie\Lambda/\hbar c} \psi \\ &= e^{ie\Lambda/\hbar c} \left[\frac{\hbar}{i} \vec{\nabla} + \underbrace{\frac{e}{c} \vec{\nabla} \Lambda}_{\text{cancels with gauge transf. of } A} - \frac{e}{c} (\vec{A} + \vec{\nabla} \Lambda) \right] \psi = e^{ie\Lambda/\hbar c} \left[\frac{\hbar}{i} \vec{\nabla} - \frac{e}{c} \vec{A} \right] \psi. \end{aligned}$$

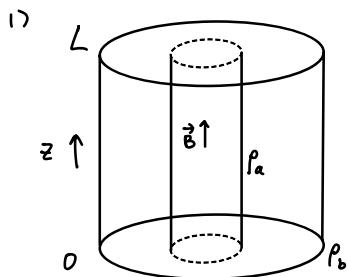
Now do this again but with

$$e^{ie\Delta/\hbar c} \psi \rightarrow \left(\frac{\hbar}{i} \vec{\nabla} - \frac{e}{c} \vec{A} \right) \psi$$

to verify $RHS = LHS$. □

$$\vec{\nabla} - \frac{ie}{\hbar c} \vec{A} \quad \text{called gauge covariant derivative.}$$

Examples where $\vec{A}$ & $\vec{\phi}$ have physical effects:



2 cylinders of radii ρ_a, ρ_b . Charged particle confined

$$\rho_a < \rho < \rho_b.$$

$\psi = 0$ at $\rho = \rho_a, \rho_b$. Also require $\psi = 0$ at $z = 0, z = L$.

Find energy e. values.

$$\nabla^2 = \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2}.$$

Suppose $\exists$ solenoid inside $\rho = \rho_a$, Can't set $A = 0$ in $\rho_a < \rho < \rho_b$:

$$\int \vec{B} \cdot d\vec{a} = \oint_C \vec{A} \cdot d\vec{s}.$$

If flux is $B_0 \pi \rho_a^2$, then

$$A_\phi = \frac{B_0 \rho_a^2}{2\rho}.$$

Can add any $\vec{\nabla} \Lambda$ to this.

E. States of
$$\frac{1}{2m} \left[\frac{\hbar}{i} \vec{\nabla} - \frac{e}{c} \vec{A} \right]^2 \psi = E \psi$$

will depend on B_0 .