Quantum Mechanics I Review Guide

Vector Spaces

Vector Properties

i) Scalar Multiplication

$$|V\rangle \longrightarrow \alpha|V\rangle$$

ii) Vector Addition

$$|Z\rangle = \alpha|V\rangle + \beta|W\rangle$$

Also exist in vector space

iii) Null Vector

$$|V\rangle + |0\rangle = |V\rangle$$

iv) Opposite Vector

$$|V\rangle + |-V\rangle = |0\rangle$$

Linear Independence

A collection of vectors is linearly independent if

$$\sum_i \alpha_i |V_i\rangle = 0 \quad \text{iff} \quad a_i = 0 \ \forall i$$

A vector space is said to be n-dimensional if there are a maximum of n linearly independent vectors

A basis is a set of n linearly independent vectors in an n dimensional vector space

$$|V\rangle = \sum_{i=1}^{n} \alpha_i |V_i\rangle$$

unique coefficients

Arbitrary vector

Inner Product Spaces

Generalization of the dot product

$$A\cdot B = \sum_i A_i B_i$$

Properties

Linearity: $A\cdot(\alpha B + BC) = \alpha A\cdot B + BA\cdot C$

Symmetry: $A\cdot B = B\cdot A$

Non-zero: $A\cdot A \geq 0$ with equality if $A = 0$

For complex vector spaces

$$\langle W|V\rangle = \sum w_i^* v_i = [w_1^*, \dots w_n^*]\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$$

Properties

$\langle W|V\rangle = \langle V|W\rangle^*$

linear in ket

$\langle Z|(\alpha|V\rangle + B|W\rangle) = \alpha\langle Z|V\rangle + B\langle Z|W\rangle$

anti-linear in bra

$\langle(\alpha|V\rangle + B|W\rangle)|Z\rangle = \alpha^*\langle V|Z\rangle + B^*\langle W|Z\rangle$

$\langle V|V\rangle \geq 0$ with equality if $|V\rangle = 0$

Gram-Schmidt Process

Method to produce orthonormal basis

1. Normalize first vector
2. Find $|n'\rangle$ by subtracting the projection of existing O.N. vectors from $|n\rangle$
3. Normalize $|n'\rangle$ and add to set
4. Repeat 2 and 3

Schwartz Inequality

$$|\langle V|W\rangle|^2 \leq \langle V|V\rangle\langle W|W\rangle$$

Triangle Inequality

$$|V+W|^2 \leq |V| + |W|$$

$$|V| = \sqrt{\langle V|V\rangle}$$

Eigenvalue Problem

$$\Omega|\omega\rangle = \omega|\omega\rangle$$

Rescaling of the vector

eigenvalue

eigenvector

*Convention is to normalize eigenvectors

We find eigenvalues by solving for the zeros of the characteristic polynomial

$$|\Omega - \omega I| = 0$$

Solve eigenvectors after solving eigenvalue

$$\Omega|\omega\rangle = \omega|\omega\rangle$$

Every Hermetian operator has real eigenvalues and orthogonal eigenvectors

eigenvectors diagonalize Ω with eigenvalues on the diagonals

$$\langle \omega_i|\Omega|\omega_j\rangle = \omega_i \delta_{ij}$$

Degenerate eigenvectors yield a two dimensional eigenspace associated w/ eigenvalue

Select eigenvectors that obey conditions and are orthogonal

Eigenvalues of unitary operators are unimodular $(u_i = e^{i\theta_i})$

eigenvectors are orthogonal

If two Hermetian operators commute, we can find a common basis of eigenvectors

n operators to define a unique basis for n commuting operators

Operators

Operators act on vectors to produce other vectors

$$\Omega|V\rangle = |V'\rangle$$

Linear Operators

$$\Omega(\alpha|V\rangle + B|W\rangle) = \alpha\Omega|V\rangle + B\Omega|W\rangle$$

Fully specified by its action on basis vectors

We can represent linear operators as matricies

$$\langle i|j'\rangle = \langle i|\Omega|j\rangle = \Omega_{ij}$$

i^{th} component of the j^{th} basis vector after Ω acts on it

Identity Operator

$$I = \left[\sum_i |i\rangle\langle i|\right]$$

acts on $|V\rangle$ to yield $|V\rangle$

projection operator

Commutator

$$[\Omega, \Lambda] = \Omega\Lambda - \Lambda\Omega$$

Inverse Operators

Neutralize the action of the operator

$$\Omega|V\rangle = |W\rangle, \quad \Omega^{-1}|W\rangle = |V\rangle$$

$$\Omega\Omega^{-1} = I$$

$$(\Omega\Lambda)^{-1} = \Lambda^{-1}\Omega^{-1}$$

An operator that kills a non-zero vector cannot have an inverse (Determinant Vanishes)

Adjoint Operator

Analog of conjugated scalar

$$\langle\Omega V| = \langle V|\Omega^{\dagger}$$

$$\Omega^{\dagger}_{ij} = \Omega_{ji}^*$$

conjugate transpose

$$(\Omega\Lambda)^{\dagger} = \Lambda^{\dagger}\Omega^{\dagger}$$

Hermetian Operator

$$\Omega^{\dagger} = \Omega, \quad \Omega_{ij} = \Omega_{ji}^*$$

Analogs of real numbers

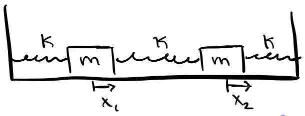
Unitary Operator

$$U^{\dagger}U = I, \quad U^{\dagger} = U^{-1}$$

Does not change inner products

Generalization of a rotation

Coupled Mass



Define $|x(t)\rangle = \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix}$ — from Newton's eq.

$$\frac{d^2 x(t)}{dt^2} = \Omega |x(t)\rangle \quad \text{where} \quad \Omega = \frac{k}{m}\begin{pmatrix} -2 & 1 \\ 1 & -2 \end{pmatrix}$$ time indep.

Normal Modes: Look for solutions of the form $|x(t)\rangle = f(t)|x\rangle$

$\ddot{f}(t) = f(t)\,\Omega|x\rangle$ ← plug into earlier eq.

$\Omega|x\rangle = \frac{\ddot{f}(t)}{f(t)}|x\rangle$ ← must be time independent

$\Omega|x\rangle = -\omega^2|x\rangle$

1) Initial state $|x\rangle$ must be an eigenstate of Ω

2) $f(t)$ is related to eigenvalue of Ω by $f(t) = f(0)\cos\omega t$

General Solution is a linear combination of eigensolutions

Lagrangian Mechanics

We define the Lagrangian to be $L = T - V$

Euler-Lagrange Equation

$$\frac{d}{dt}\left[\frac{\partial L}{\partial \dot{x}}\right] = \frac{\partial L}{\partial x}$$ ← generalize to all coordinates

Cyclic Coordinate

$$\frac{dp_i}{dt} = \frac{\partial L}{\partial q_i} = 0 \quad \text{if } q_i \text{ is cyclic}$$

↑ conservation of momentum coordinate

Hamiltonian Mechanics

1) Find the momenta p_i via the Lagrangian

$$p_i(q_i, \dot{q}_i) = \frac{\partial L}{\partial \dot{q}_i}$$

2) Construct the Hamiltonian

$\mathcal{H}(q,p) = T + V$ ← total energy in terms of q and p

3) Equations of Motion

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

Poisson Brackets

For a general variable $\omega(q,p)$ we can solve

$$\frac{d\omega}{dt} = \sum_{i=1}^{n}\left(\frac{\partial \omega}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \omega}{\partial p_i}\frac{\partial H}{\partial q_i}\right) = \{\omega, H\}$$

if $\{\omega, H\} = 0$, then ω is conserved!

Canonical Transformations

Coordinate transformations that preserve Hamilton Eq.'s form

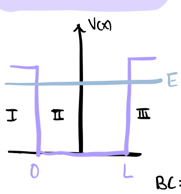
$$\{q_i'(q,p), p_j'(q,p)\} = \delta_{ij}$$

Ehrenfest's Theorem

time evolution of expected value

$$\frac{d\langle\Omega\rangle}{dt} = \frac{1}{i\hbar}\langle\psi|[\Omega, H]|\psi\rangle$$

Particle in a Box



Energy Eigenvalue Equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \to \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar}(E - V(x))\psi = 0$$

WLOG set to 1

III: $\psi_{III} = Ae^{-kx} + \cancel{Be^{kx}}$ $\quad k = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$

I: $\psi_I = \cancel{Ce^{-kx}} + De^{kx}$ ← ψ dies exponentially

II: $\psi_{II} = F\sin kx + G\cos kx$ $\quad k = \sqrt{\frac{2mE}{\hbar^2}}$ only specific E

BC: continuity and C^1 → 4 conditions, 3 parameters

Infinite Dimensions

We define the function $f(x)$ as follows

$$f(x) = \langle x|f\rangle$$

Inner product

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

Notice! $\int_0^L |x\rangle\langle x|\,dx = I$

Dirac Delta

$$\int_a^b \delta(x - x')\,dx' = 1$$ ← selects a point

therefore, $\int \delta(x-x')f(x')\,dx \simeq f(x)\int \delta(x-x')\,dx = f(x)$

$$\int \delta'(x-x')f(x)\,dx' = f'(x)$$

X operator

We define X to be the hermetian operator with $|x\rangle$ as a basis

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

K Operator

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

$$\langle x|K|f\rangle = -i\frac{df}{dx}$$

Postulates of Quantum Mechanics

Postulate I: The state

State of a particle is defined by a normalizable ket $|\psi\rangle$ defined in a hilbert space

Postulate II: Dynamical Variables

Independent variables x, p are represented by Hermetian operators X, P in hilbert space

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

$$\langle x|P|x'\rangle = -i\hbar\,\delta'(x - x')$$

For a general variable $\omega(x,p)$

$$\Omega(X, P) = \omega(x \to X, p \to P)$$

Postulate III: Results of Measurements

A variable corresponding to Ω is measured in $|\psi\rangle$ results in one of its eigenvalues with $P(\omega) = |\langle\omega|\psi\rangle|^2$ and the state collapses to the eigenstate $|\omega\rangle$

physical observables are only associated with hermetian

measuring commuting operators will not disturb eachother

Postulate IV: Dynamics

State vector obeys Schrodinger's Equation

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

$$H(X, P) = \mathcal{H}(x \to X, p \to P)$$

Free Particle

Energy Eigenvalue Equation

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_E}{\partial x^2}\right) = E\psi_E$$

$$\frac{\partial^2\psi_E}{\partial x^2} + \underbrace{\frac{2mE}{\hbar^2}}_{k^2}\psi_E = 0$$

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

$$2mE = k^2\hbar^2$$

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

$$p = \hbar k$$

$$p = \sqrt{2mE}$$

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

$$k = \sqrt{\frac{2mE}{\hbar}}, \quad p = \hbar k$$

$$= Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$$

→ ← opposing directions

two-fold degenerate states

need a commuting operator to properly label the states

Statistics in Quantum Mechanics

Expected Value

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

Variance/Uncertainity

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

Wavefunction $\psi_p(x)$

$\psi_p(x)$ is the eigenket of P in the x-basis

$$\psi_p(x) = \frac{1}{\sqrt{2\hbar\pi}}e^{ipx/\hbar}$$

Uncertainity Principle

Since X and P do not commute they cannot have a common eigenbasis. Therefore, you cannot have a state of definite X and P

Schrodinger Equation

$$i\hbar\frac{d|\psi\rangle}{dt} = H|\psi\rangle$$

We solve this like the coupled mass

Assume $|\psi(t)\rangle = |E\rangle f(t)$

and $H|E\rangle = E|E\rangle$ ← look for normal modes

$$i\hbar|E\rangle\dot{f} = f(t)E|E\rangle$$

$$i\hbar\frac{\dot{f}}{f} = E \longrightarrow f(t) = e^{-iEt/\hbar}$$

Normal Modes

$$|E(t)\rangle = |E\rangle e^{-iEt/\hbar}$$

General Solution

$$|\psi(t)\rangle = \sum_E c_E|E\rangle e^{-iEt/\hbar}$$

↑ time independent constants

$$c_E = \langle E|\psi(0)\rangle$$

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

$$U(t) = \sum_E |E\rangle\langle E|e^{-iEt/\hbar} \quad \text{s.t.} \quad |\psi(t)\rangle = U(t)|\psi(0)\rangle$$

↑ propagator

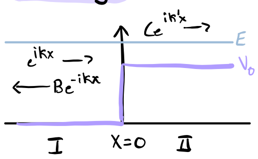
Imposing Boundary Conditions

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \quad \text{since } k = \frac{n\pi}{L} \quad n=1,\dots$$

$$\psi_n(x) = \sqrt{2/L}\,\sin\left[\frac{n\pi x}{L}\right]$$

There can be no degeneracy in $d=1$ if ψ vanishes at either or both infinities

Scattering



Transmission and Reflection

$$T = \frac{|C|^2 \frac{\hbar k'}{m}}{|1|^2 \frac{\hbar k}{m}} = |C|^2\left(\frac{k'}{k}\right)$$

$$R = \frac{|B|^2}{|1|^2}$$

Boundary Conditions

@ $x=0$ $\quad 1+B = C$

$ik(1-B) = ik'C$

$C = \frac{2k}{k+k'}$, $B = 1 - C = \frac{k-k'}{k+k'}$

Final T and R

$$R = \left(\frac{k-k'}{k+k'}\right)^2$$

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

$T+R = 1$ ✓

Harmonic Oscillator in X-basis

Hamiltonian: $H = \frac{P^2}{2m} + \frac{1}{2} m\omega^2 X^2$

$X \to x$, $P = -i\hbar \frac{d}{dx}$ ← X-basis representation

Schrodinger Eigenvalue Equation:

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

alternate representation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \tfrac{1}{2} m\omega^2 x^2\right)\psi = 0$$

Solution Steps:

1. Substitute $y = x/b$ — choose $b = \left(\frac{\hbar}{m\omega}\right)^{1/2}$ after analysis
2. Define $\varepsilon = E/\hbar\omega$

   Equation takes the form $\psi'' + (2\varepsilon - y^2)\psi = 0$

   negative due to physical restrictions

3. Consider the limit $y \to \infty$ — neglect $2\varepsilon\psi$ term

   $\psi'' - y^2\psi = 0 \longrightarrow \psi = Ay^m e^{-y^2/2}$

4. Consider the $y \to 0$ limit

   $\psi'' + 2\varepsilon\psi = 0 \longrightarrow \psi = A\cos(2\varepsilon)^{1/2} y + B\sin(2\varepsilon)^{1/2} y$

   Imposing $y^2 \approx 0$ condition

   $\psi(y) = u(y)e^{-y^2/2}$ where $u(y) \to A + cy$ $(y\to 0)$; $\to y^m$ $(y \to \infty)$

5. Notice that u obeys

   $$u'' + 2yu' + (2\varepsilon - 1)u = 0$$

   Express $u(y)$ as a power series

   $$u(y) = \sum_{n=0}^{\infty} C_n y^n$$

6. Plug powerseries into u differential equation

   $$\sum_{n=0}^{\infty} C_n\left[n(n-1)y^{n-2} - 2ny^n + (2\varepsilon - 1)y^n\right] = 0$$

   Exploit linear indep. of y^n

7. Solve recursive relation between C_{n+2} and C_n

   $$C_{n+2} = C_n \frac{(2n+1-2\varepsilon)}{(n+2)(n+1)}$$

Higher order solutions diverge

However, when $\varepsilon_n = \frac{2n+1}{2}$, $n = 0,1,2$ we can find solutions

parity: If n even: set $C_1 = 0$ ← kills odd terms; If n odd: set $C_0 = 0$ ← kills even terms

produces order n polynomial

Quantizes allowed Energies

$$\boxed{\varepsilon_n = n + 1/2 \longrightarrow E = (n + 1/2)\hbar\omega}$$

$$\boxed{\text{General Solution: } \psi_n = e^{-y^2/2} H_n(y)}$$

Take-aways

1. Zero-point energy $= \frac{\hbar\omega}{2}$ $(n=0)$
2. Levels are evenly spaces
3. $\psi_n(x)$ has n zeros and parity $(-1)^n$
4. Wave functions die exponentially past classical limits

We can use the above relations to define matricies

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

$$a = \begin{pmatrix} 0 & 1 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \quad a^\dagger = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 1 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 \\ \cdots & \cdots & \sqrt{3} & \cdots \end{pmatrix} \quad X = \sqrt{\frac{\hbar}{2m\omega}}\begin{pmatrix} 0 & 1 & 0 & \cdots \\ 1 & 0 & \sqrt{2} & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} \\ \vdots & & \sqrt{3} & \cdots \end{pmatrix} \quad P = i\sqrt{\frac{m\omega\hbar}{2}}\begin{pmatrix} 0 & -1 & 0 & \cdots \\ 1 & 0 & -\sqrt{2} & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} \\ \vdots & \vdots & \sqrt{3} & \cdots \end{pmatrix}$$

Dirac Harmonic Oscillator (H-basis)

Define the following operators

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

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

$[a, a^\dagger] = 1$

Notice

$$H = \hbar\omega\left(a^\dagger a + 1/2\right)$$

$$X = \sqrt{\hbar/2m\omega}\,(a + a^\dagger), \quad P = \sqrt{\frac{\hbar}{2m\omega}}\,(a^\dagger - a)$$

We can write the dimensionless Hamilton as follows

$$\hat{H} = \frac{H}{\hbar\omega} = a^\dagger a + 1/2$$

$$[a, \hat{H}] = a \quad \text{and} \quad [a^\dagger, \hat{H}] = -a^\dagger$$

Next, consider the eigenstate of $\hat{H}$

$\hat{H}|\varepsilon\rangle = \varepsilon|\varepsilon\rangle$ $\quad E = \hbar\omega\varepsilon$

$\hat{H}a|\varepsilon\rangle = a\hat{H}|\varepsilon\rangle - [a,\hat{H}]|\varepsilon\rangle$ ← commutator definition

$= a\varepsilon|\varepsilon\rangle - a|\varepsilon\rangle$

$= (\varepsilon - 1)a|\varepsilon\rangle$

$a|\varepsilon\rangle$ is eigenstate with energy $\varepsilon - 1$

Analogously, $\hat{H}a^\dagger|\varepsilon\rangle = (\varepsilon+1)a^\dagger|\varepsilon\rangle$

$a^\dagger|\varepsilon\rangle$ is an eigenstate with energy $\varepsilon + 1$

Ladder Operators

Lowering: $a|\varepsilon\rangle = C_-|\varepsilon - 1\rangle$

Raising: $a^\dagger|\varepsilon\rangle = C_+|\varepsilon + 1\rangle$

Since the ladder has a minimum, we label this state $|0\rangle$

$a|0\rangle = 0$ ← can't be further lowered

$a^\dagger a|0\rangle = 0$

$(\hat{H} - 1/2)|0\rangle = 0$

$\varepsilon_0 = 1/2$ so $E_0 = \frac{\hbar\omega}{2}$ — minimum energy state

Generalized, we recover the same result for other states

$$H|n\rangle = (n + 1/2)\hbar\omega|n\rangle$$

Solving for coefficients of the ladder operators

$$a|n\rangle = \sqrt{n}\,|n-1\rangle \quad \text{and} \quad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$a^\dagger a = n|n\rangle$$

Wavefunctions

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\left(\sqrt{\frac{m\omega}{2\hbar}}\,x - \sqrt{\frac{\hbar}{2m\omega}}\,\frac{d}{dx}\right)^n \psi_0(x)$$

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

Uncertainity Principle

Consider the shift operators

$\hat{X} = X - \langle X\rangle$ and $\hat{P} = P - \langle P\rangle$

$[\hat{X}, \hat{P}] = i\hbar$

Under these definitions

$(\Delta X)^2 = \langle \hat{X}^2\rangle$ and $(\Delta P)^2 = \langle \hat{P}^2\rangle$

$(\Delta X)^2(\Delta P)^2 = \langle\psi|\hat{X}^2|\psi\rangle\langle\psi|\hat{P}^2|\psi\rangle$

$= \langle\hat{X}\psi|\hat{X}\psi\rangle\langle\hat{P}\psi|\hat{P}\psi\rangle$

$\geq |\langle\hat{X}\psi|\hat{P}\psi\rangle|^2$ — Apply Schwarz

$= |\langle\psi|\hat{X}\hat{P}|\psi\rangle|^2$

$= \frac{1}{4}\left|\langle\psi|[\hat{X},\hat{P}] + [\hat{X},\hat{P}]_+|\psi\rangle\right|^2$

anti-commutator: $\hat{X}\hat{P} + \hat{P}\hat{X}$

$= \frac{1}{4}|\langle\psi|[\hat{X},\hat{P}]|\psi\rangle|^2 + \frac{1}{4}|\langle\psi|[\hat{X},\hat{P}]_+|\psi\rangle|^2$

$= \frac{1}{4}|\langle\psi|i\hbar|\psi\rangle|^2 + \frac{1}{4}|\langle\psi|[\hat{X},\hat{P}]_+|\psi\rangle|^2$

$= \frac{\hbar^2}{4} + \frac{1}{4}|\langle\psi|[\hat{X},\hat{P}]_+|\psi\rangle|^2$

$\geq \hbar^2/4$

$\therefore \Delta X \Delta P \geq \hbar/2$

Minimum Uncertainty Product

$\hat{X}|\psi\rangle = c\hat{P}|\psi\rangle$ — equality cond. for Schwarz

$\langle\psi|[\hat{X},\hat{P}]_+|\psi\rangle = 0$ — vanish 2nd term in $(\Delta X)^2(\Delta P)^2$

$\Rightarrow \hat{X}|\psi\rangle = i|c|\hat{P}|\psi\rangle$

in the X-basis

gaussian: $\psi(x) = A\exp\left[\frac{iP_0 x}{\hbar}\right]\exp\left[-\frac{(x-x_0)^2}{2\hbar|c|}\right]$

Uncertaintity Principle in Quantum HO

$$\langle H\rangle = \frac{\langle P\rangle^2}{2m} + \frac{1}{2} m\omega^2 \langle X\rangle^2$$

$$= \frac{(\Delta P)^2}{2m} + \frac{1}{2}m\omega^2(\Delta X)^2$$

Applying $\Delta P \geq \frac{\hbar}{2\Delta X}$

$$\geq \frac{\hbar^2}{8m(\Delta X)^2} + \frac{1}{2}m\omega^2(\Delta X)^2$$

Minimizing w.r.t ΔX we find

$$E_{min} = \frac{\hbar\omega}{2}$$

Multiple Particles

Two-Particle Schrödinger Equation — $\psi(x_1, x_2, t)$

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m_1}\frac{\partial^2\psi}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2\psi}{\partial x_2^2} + V\psi$$

Case 1: Non-interacting Particles $\quad V = V(x_1) + V(x_2)$

$H = H_1(X_1, P_1) + H_2(X_2, P_2)$ — Particles interact independently

$\psi(x_1, x_2, t) = \psi_1(x_1, t)\psi(x_2, t)$

← implies statistical independence

Case 2: Interacting Particles $\quad V = V(x_1 - x_2)$

$H = H_c(P_c) + H_r(X_r, P_r)$ — Solve via individual eigenvalue problem

$H\psi_E = E\psi_E$ where $E = E_c + E_r$

Many Identical Particles

Particles are indistinguishable given the lack of trajectories
requires label invariance

Normalized States

Symmetric : $|a,b;S\rangle = \frac{1}{\sqrt{2}}\left[|a,b\rangle + |b,a\rangle\right]$

Anti-symmetric : $|a,b;S\rangle = \frac{1}{\sqrt{2}}\left[|a,b\rangle - |b,a\rangle\right]$

Bosons always select symmetric states
Integer spin

Fermions always select anti-symmetric states
half-integer spin

} statistics

Wave functions

$|x_1,x_2;S/A\rangle = \frac{1}{\sqrt{2}}\left(|x_1,x_2\rangle \pm |x_2,x_1\rangle\right)$

$\psi(x_1,x_2;S/A) = \frac{1}{\sqrt{2}}\langle x_1,x_2;S/A|\psi;S/A\rangle$

$|\psi;S/A\rangle = \frac{1}{\sqrt{2}}\left(|n_1,n_2\rangle \pm |n_2,n_1\rangle\right)$

$\psi(x_1,x_2;S/A) = \frac{1}{\sqrt{2}}\left[\phi_{n_1}(x_1)\phi_{n_2}(x_2) \pm \phi_{n_2}(x_1)\phi_{n_1}(x_2)\right]$

$\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ ← particle in a box

ψ vanishes for fermions in the same state

Bosons have increased prob. to occupy same state

Translational Invariance

Active Transformation

We define a translation operator as $T(\varepsilon)|x\rangle = |x+\varepsilon\rangle$

$T(\varepsilon) = I - \frac{i\varepsilon}{\hbar}P$ ← generator of translations

Invariance now takes the form

$\langle\psi|H|\psi\rangle = \langle\psi_\varepsilon|H|\psi_\varepsilon\rangle$

$= \langle T(\varepsilon)\psi|H|T(\varepsilon)\psi\rangle$

$= \langle\psi|\left(I+\frac{i\varepsilon}{\hbar}P\right)H\left(I-\frac{i\varepsilon}{\hbar}P\right)|\psi\rangle$

$= \langle\psi|H|\psi\rangle + \frac{i\varepsilon}{\hbar}\langle\psi|[P,H]|\psi\rangle + \mathcal{O}(\varepsilon^2)$

when $\varepsilon \to 0$

$\langle\psi|[P,H]|\psi\rangle = 0$

Since $[H,P]=0$, they share an eigenbasis in which $\langle\dot{p}\rangle=0$ so the momentum eigenvalue stays constant in this state

Ehrenfest's Theorem: $\langle\dot{p}\rangle = 0$

Finite Transformations

$T(a) \longrightarrow e^{-a\frac{d}{dx}}$
X-basis

Since $[T(a),H]=0$ we can say $[T(a),U(t)]=0$

$T(a)U(t) = U(t)T(a)$

Passive Transformation

Alternatively, consider $T(\varepsilon)$ as

$T(\varepsilon)^\dagger X T(\varepsilon) = X + \varepsilon I$ $\quad T(\varepsilon) = I - \frac{i\varepsilon}{\hbar}P$

$T(\varepsilon)^\dagger P T(\varepsilon) = P$

Invariance takes the form: $T^\dagger(\varepsilon)HT(\varepsilon) = H$

$T^\dagger H T = H(T^\dagger X T, T^\dagger P T) = H(X+\varepsilon I, P) = H$

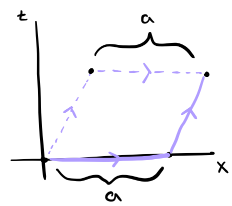
Analogous form to classical mechanics

Setting $T^\dagger(\varepsilon)HT(\varepsilon) - H = 0$ yields

$0 = -\frac{i\varepsilon}{\hbar}[H,P]$

Ehrenfest's Theorem: $\langle\dot{p}\rangle = 0$

Same point!



Experiments conducted in different locations yield the same result!

Time Translation Invariance

Consider infinitesimal time translations from t_1 and t_2

$|\psi(t_1+\varepsilon)\rangle = \left[I - \frac{i\varepsilon}{\hbar}H(t_1)\right]|\psi_0\rangle$

subtract equations

$|\psi(t_2+\varepsilon)\rangle = \left[I - \frac{i\varepsilon}{\hbar}H(t_2)\right]|\psi_0\rangle$

Assuming equivalence

$0 = \left(-\frac{i\varepsilon}{\hbar}\right)\left[H(t_2) - H(t_1)\right]|\psi_0\rangle$

$H(t_2) = H(t_1)$

∴ H is time-independent

Law of Conservation of Energy

Parity Invariance

$\Pi|x\rangle = |-x\rangle, \quad \Pi|p\rangle = |-p\rangle$

Notice $\Pi^2 = I$

i) $\pi = \pi^{-1}$

ii) Eigenvalues ± 1

iii) π hermitian and Unitary

Alternatively define $\pi^\dagger X\pi = -X,\ \pi^\dagger P\pi = -P$

$\Pi^\dagger H\Pi = H$ ← parity invariance

$[\pi, H] = 0$

Parity Invariance implies $\pi U(t) = U(t)\pi$

Rotations

2-Dimensions

Let $U(R(\phi_0,\hat{k}))$ or $U(R)$ represent our rotation operator

$U[R]|x,y\rangle = |x\cos\phi_0 - y\sin\phi_0,\ x\sin\phi_0 + y\cos\phi_0\rangle$

For infinitesimal rotations

$U[R(\varepsilon_z\hat{k})] = I - \frac{i\varepsilon_z L_z}{\hbar}$ ← generator of infinitesimal rotations

$L_z = XP_y - YP_x$

← Angular Momentum Operator

Finite Rotation

$U(R(\phi_0\hat{k})) = \exp\left(\frac{-i\phi_0 L_z}{\hbar}\right)$

In polar coordinates we can write

$L_z = i\hbar\frac{\partial}{\partial\phi}$ so that $U(R(\phi_0\hat{k})) = \exp\left(-\phi_0\frac{\partial}{\partial\phi}\right)$

↖ conserved with rotational invariance

$[L_z, H] = 0$

Angular Momentum in 2D

Solutions to the L_z eigenvalue problem

$L_z|\ell_z\rangle = \ell_z|\ell_z\rangle \longrightarrow \psi_{\ell_z}(\rho,\phi) = R(\rho)e^{i\ell_z\phi/\hbar} = R(\rho)\,\Phi_m(\phi)$

Angular portion of ψ when H is rotationally invariant

imposing hermicity + periodicity → $\ell_z = m\hbar \quad m = 0, \pm1, \pm2, \dots$
↖ magnetic quantum number

$\Phi_m(\phi) = (2\pi)^{-1/2}e^{-im\phi}$

State is specified by energy and angular momentum

If H is rotationally invariant

$\left[\frac{-\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) + V(\rho)\right]\psi_E(\rho,\phi) = E\psi_E(\rho,\phi)$ +

we have solution of the form

$\psi_{Em}(\rho,\phi) = R_{Em}(\rho)\,\Phi_m(\phi)$

⇓

$$\boxed{\left[\frac{-\hbar^2}{2\mu}\left(\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} - \frac{m^2}{\rho}\right) + V(\rho)\right]R_{Em}(\rho) = ER_{Em}(\rho)}$$

3-Dimensions

Angular Momentum Operators

$L_x = YP_z - ZP_y, \quad L_y = ZP_x - XP_z, \quad L_z = XP_y - YP_x$

$[L_i, L_j] = i\hbar\sum_{i=1}^{3}\varepsilon_{ijk}L_k$ ← Levi-Civita Symbol

Total Angular Momentum Operator

$L^2 = L_x^2 + L_y^2 + L_z^2 \qquad [L^2, L_i] = 0$

Rotation operator generalizes as

$U(R(\vec{\theta})) = e^{\frac{-i\theta\cdot L}{\hbar}}$

If a hamiltonian is invariant under arbitrary rotations

$[H, L_i] = 0 \longrightarrow [H, L^2] = 0$

Select a basis common to one L_i and H

Angular Momentum in 3D

Assume a common basis to L^2 and L_z

$L^2|\alpha,\beta\rangle = \alpha|\alpha,\beta\rangle \quad L_z|\alpha,\beta\rangle = \beta|\alpha,\beta\rangle$

Consider the raising and lowering operators

$L_\pm = L_x \pm iL_y$ s.t. $[L_z, L_\pm] = \pm\hbar L_\pm$

Raise and lower eigenvalue of L_z by $\hbar$ but leave L^2 intact

$[L^2, L_\pm] = 0$

We notice that

$L_+|\alpha,\beta\rangle = C_+(\alpha,\beta)|\alpha,\beta+\hbar\rangle$ and $L_-|\alpha,\beta\rangle = C_-(\alpha,\beta)|\alpha,\beta-\hbar\rangle$

Since $L^2 - L_z^2 = L_x^2 + L_y^2$ we see that $\alpha - \beta^2 \geq 0$

implying there exists states $|\alpha\,\beta_{max}\rangle$ and $|\alpha\,\beta_{min}\rangle$ s.t.

$L_+|\alpha\,\beta_{max}\rangle = 0, \quad L_-|\alpha\,\beta_{min}\rangle = 0$

$\Rightarrow \alpha = \beta_{max}(\beta_{max} + \hbar), \quad \alpha = \beta_{min}(\beta_{min} - \hbar)$

- $\beta_{max} = \beta_{min}$ w/ k steps between

$\beta_{max} = \frac{\hbar k}{2} \quad k = 0, 1, 2, \dots$

$\alpha = \hbar^2\left(\frac{k}{2}\right)\left(\frac{k}{2}+1\right)$

angular momentum of state

$$\boxed{\begin{aligned} L^2|\ell m\rangle &= \ell(\ell+1)\hbar^2|\ell,m\rangle \\ L_z|\ell m\rangle &= m\hbar|\ell,m\rangle \\ &\ell = 0, 1, \dots \\ &m = \ell, \ell-1, \dots, -\ell \end{aligned}}$$

Solving for constants

$J_\pm|jm\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}\,|j, m\pm1\rangle$

↖ generalized version of L

Any wavefunction can be expanded as

$\psi(r,\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} C_\ell^m(r)\,Y_\ell^m(\theta,\phi)$ ← spherical harmonic

For radially invariant problems

$\psi_{E,\ell,m}(r,\theta,\phi) = R_{E,\ell,m}(r)\,Y_\ell^m(\theta,\phi)$

Hydrogen Atom

Consider a single electron and an immobile proton

Schrodinger's Equation

$$\frac{d^2}{dr^2} + \frac{2m}{\hbar}\left[E + \frac{e^2}{r} - \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right] u_{E,\ell} = 0$$

coulomb's potential

$V = -e^2/r$

Corresponding wavefunctions

$$\psi_{E,\ell,m}(r,\theta,\phi) = R_{E,\ell}(r)\, Y_\ell^m(\theta,\phi) = \frac{u_{E,\ell}}{r} Y_\ell^m(\theta,\phi)$$

We can rewrite our differential equation w/ the following substitutions

$$\frac{d^2 v}{d\rho^2} - 2\frac{dv}{d\rho}\left[\frac{e^2\lambda}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right] v = 0$$

$\rho = \sqrt{\frac{2mW}{\hbar^2}}\, r \qquad u_{E,\ell} = e^{-\rho} v \qquad \lambda = \sqrt{\frac{2m}{\hbar^2 W}}$

$W = -E$

Next, express v as a power series

$$v = \rho^{\ell+1} \sum_{k=0}^{\infty} c_k \rho^k$$

behavior near $\rho = 0$

which produces the following recursive relation

$$\frac{c_{k+1}}{c_k} = \frac{-e^2\lambda + 2(k+\ell+1)}{(k+\ell+2)(k+\ell+1) - \ell(\ell+1)}$$

Requiring the power series to terminate at k

$$e^2\lambda = 2(k+\ell+1)$$

$$E = -W = \frac{-me^4}{2\hbar^2(k+\ell+1)^2} \qquad \begin{matrix} k = 0,1,2,\dots \\ \ell = 0,1,2,\dots \end{matrix}$$

$n = k+\ell+1 \longrightarrow$ principal quantum number

Allowed Energies

$$E_n = \frac{-me^4}{2\hbar^2 n^2} = \frac{-R_y}{n^2}$$

Rydberg

$n = 1,2,\dots$

degeneracy for each n is n^2

For a given n and ℓ we can solve for the wavefunctions

$$R_{n\ell} \sim e^{-r/na_0}\left(\frac{r}{na_0}\right)^{\ell} L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right)$$

associated Laguerre polynomial

bohr radius : $a_0 = \frac{\hbar^2}{me^2}$

most probable value of r in ground state