Quantum Mechanics I

The unreasonable effectiveness of mathematics in the Natural World

Linear Vector Spaces

A. Vector Space Axioms

Consists of a collection of vectors

Vector Space Requirements

- Addition
- Scalar multiplication
- Zero vector

  $\vec{v}_1 + \vec{0} = \vec{v}_1$

  Non-trivial conditions
- Negative vector

  $\vec{v}_1 + (-\vec{v}_1) = \vec{0}$

Periodic functions satisfy vector space axioms

B. Linear Independence

$V_1 \dots V_n$ are linearly independent if $\alpha_1 v_1 + \alpha_2 v_2 + \dots + \alpha_n v_n = 0 \implies \alpha_i = 0$

C. Dimensionality

Maximum number of linearly independent vectors in a given vector space

Infinite dimensions have slightly different definitions and properties

Any set of n linearly independent vectors in an n-dimensional space form a basis

for arbitrary V in vector space

$$V = \sum_{i=1}^{n} \alpha_i \vec{v}_i$$

← basis vectors

↑ Vector components

Proof that each V has unique components

Suppose $V = \sum \alpha_i v_i$

$= \sum \alpha_i' v_i$

with respect to the basis selected

$\sum (\alpha_i - \alpha_i') v_i = 0$

only true if $(\alpha_i - \alpha_i') = 0$

$\therefore \alpha_i = \alpha_i'$

D. Vector Notation

Bra-ket notation

$$|v\rangle = \sum_{i=1}^{N} v_i \cdot |i\rangle$$

↑ basis

E. Inner Product

Dot Products

$\vec{A} = A_x \vec{i} + A_y \vec{j} + A_z \vec{k}$ or $\vec{A} = \sum_{i=1}^{3} \vec{e}_i A_i$

$\vec{B} = B_x \vec{i} + B_y \vec{j} + B_z \vec{k}$

$\vec{A} \cdot \vec{B} = A_x B_x + A_y B_y + A_z B_z$

Properties

- $\vec{A} \cdot \vec{B} = \vec{B} \cdot \vec{A}$
- $\vec{A} \cdot (\alpha \vec{B} + \beta \vec{C}) = \alpha \vec{A} \cdot \vec{B} + \beta \vec{A} \cdot \vec{C}$
- $\vec{A} \cdot \vec{A} \geq 0,\ 0$ iff $\vec{A} \neq \vec{0}$

  ← notion of length

Kronecker delta

$e_i \cdot e_j = \delta_{ij}$ ← orthonormal basis

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

Suppose

$$|v\rangle = \sum_{i=1}^{N} v_i |i\rangle \quad \text{and} \quad |w\rangle = \sum_{j=1}^{N} w_j |j\rangle$$

Inner product

$$\langle w|v\rangle = \sum_{i=1}^{N} w_i^* v_i$$ complex conjugate

$$\langle i|j\rangle = \delta_{ij}$$

Properties

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

$$\langle z|\alpha v + \beta w\rangle = \alpha\langle z|v\rangle + \beta\langle z|w\rangle$$ ← linear in the ket

$$\langle v|v\rangle = \sum |v_i|^2 \geq 0 \quad 0 \text{ iff } \vec{v} = 0$$

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

length of the vector

$$\langle \alpha v + \beta w|z\rangle = \alpha^*\langle v|z\rangle + \beta^*\langle w|z\rangle$$

Bras are associated with row vectors and kets are associated with column vectors

$$|v\rangle = \sum v_i |i\rangle$$

$$\langle v| = \sum \langle i| v^*$$

$$\langle v|w\rangle = (v_1^*, \ldots, v_N^*)\begin{pmatrix} w_1 \\ \vdots \\ w_N \end{pmatrix}$$

Inner product implies orthonormal basis

$\langle i|j\rangle = \delta_{ij}$

F. Vector Basis

A set of N linearly independent vectors in an N dimensional vector space

Any vector in the space can be represented by these vectors

$$|v\rangle = \sum_{i=1}^{N} \alpha |i\rangle$$ basis

Basis is not unique but the coefficients for a given basis are

G. Gram Schmidt Process

Convert N linearly independent vectors to N orthonormal vectors

$$\langle i|j\rangle = \begin{cases} 1 & i=j \\ 0 & i\neq j \end{cases}$$

Given $|I\rangle$ and $|II\rangle$ as two linearly independent vectors

1) $|1\rangle = \dfrac{|I\rangle}{|I|}$ ← rescale first vector

2) $|2'\rangle = |II\rangle - |1\rangle\langle 1|II\rangle$

$$|2\rangle = \frac{|2'\rangle}{|2'|}$$

H. Schwarz Inequality

$$|A\cdot B| \leq |A||B|$$ ← traditional dot product

$$|\langle v|w\rangle|^2 \leq \langle v|v\rangle\langle w|w\rangle$$

Proof:

Consider $|z\rangle = |v\rangle - \dfrac{|w\rangle\langle w|v\rangle}{\langle w|w\rangle}$ and apply $\langle z|z\rangle \geq 0$

$$\langle z|z\rangle = \left(\langle v| - \frac{\langle v|w\rangle\langle w|}{\langle w|w\rangle}\right)\left(|v\rangle - \frac{|w\rangle\langle w|v\rangle}{\langle w|w\rangle}\right) \geq 0$$

general rule

$\alpha|v\rangle + \beta|w\rangle \iff \langle v|\alpha^* + \langle w|\beta^*$

Turn every ket into a bra, bra into a ket, and swap the order of factors

$$\langle v|v\rangle + \frac{\langle v|w\rangle\langle w|w\rangle\langle w|v\rangle}{\langle w|w\rangle^2} - 2\frac{\langle v|w\rangle\langle w|v\rangle}{\langle w|w\rangle} \geq 0$$

$$\langle v|v\rangle\langle w|w\rangle \geq \langle v|w\rangle\langle w|v\rangle$$

$$|v|^2|w|^2 \geq |\langle v|w\rangle|^2$$

equality when $|v\rangle = \lambda|w\rangle$

I. Triangle Inequality

$$|v+w| \leq |v| + |w|$$

equality when $|v\rangle = \lambda|w\rangle$

$\lambda > 0$

Operators

A. Basic Definitions

$\Omega|v\rangle = |w\rangle$ ← feed in one vector and spit out another vector

general operators require every vector to be specified

Linear operators obey

$$\Omega(\alpha|v\rangle + \beta|w\rangle) = \alpha\Omega|v\rangle + \beta\Omega|w\rangle$$

$$\Omega|v\rangle = \Omega\left(\sum_{i=1}^{n}\alpha_i|i\rangle\right) = \sum\alpha_i\Omega|i\rangle$$

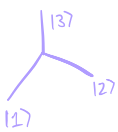
In linear operators if you know the fate of the basis, you know the action of the operator

Examples

$\Omega = I \rightarrow I|w\rangle = |w\rangle$

$\Omega = \alpha I \rightarrow \Omega|w\rangle = \alpha|w\rangle$

$R_x(\pi/2)$



$R_x|1\rangle = |1\rangle$

$R_x|2\rangle = |3\rangle$

$R_x|3\rangle = -|2\rangle$

B. Matrix Representation

Linear operator can be represented by a matrix

$$\Omega = \begin{pmatrix} \Omega|1\rangle & \cdots & \Omega|n\rangle \\ \vdots & \ddots & \vdots \\ \cdots & \cdots & \cdots \end{pmatrix}$$

$$\Omega|v\rangle = |v'\rangle$$

$$= \Omega\sum v_i|i\rangle$$

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

$$|v'\rangle = \sum v_i\Omega|i\rangle$$

$$\langle j|v'\rangle = \sum v_i\langle j|\Omega|i\rangle$$

$$v_j' = \sum_i \Omega_{ji}v_i$$

C. Multiple operators

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

$$\begin{pmatrix} V_1'' \\ \vdots \\ V_N'' \end{pmatrix} = \begin{pmatrix} \Lambda \end{pmatrix} \begin{pmatrix} \Omega \end{pmatrix} \begin{pmatrix} V_1 \\ \vdots \\ V_N \end{pmatrix}$$

$$\Lambda \Omega \neq \Omega \Lambda$$

$$[\Lambda, \Omega] = \Lambda \Omega - \Omega \Lambda \quad \leftarrow \text{commutator}$$

D. Inverse Operators

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

If $\Omega|V\rangle = 0$ and $|V\rangle \neq 0$ Ω does not have an inverse

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

E. Projection Operator / Outerproduct

$$|V\rangle = \sum v_i |i\rangle = \sum \underset{\substack{\uparrow \\ \text{coefficient} \\ v_i}}{\langle i|V\rangle} |i\rangle = \sum |i\rangle\langle i|V\rangle = \Big(\underbrace{\sum |i\rangle\langle i|}_{I}\Big)|V\rangle$$

$$I = \sum |i\rangle\langle i|$$

$$\begin{pmatrix} \ \end{pmatrix} \begin{pmatrix} \quad & \quad \end{pmatrix} = \begin{pmatrix} \quad & \quad \\ \quad & \quad \end{pmatrix}$$

Outerproduct returns an operator

$|i\rangle\langle i| = \mathbb{P}_i$ ← Projection operator

$$\mathbb{P}_i^2 = \mathbb{P}_i$$

$$\mathbb{P}_i \mathbb{P}_j = \delta_{ij} \mathbb{P}_i$$

Example: Find $(\Omega\Lambda)_{ij}$

$$\begin{aligned}(\Omega\Lambda)_{ij} &= (\Omega I \Lambda)_{ij} \\ &= \langle i|\Omega \left(\textstyle\sum |k\rangle\langle k|\right) \Lambda |j\rangle \\ &= \sum_k \Omega_{ik} \Lambda_{kj}\end{aligned}$$

F. Adjoint

$$\alpha|V\rangle = |\alpha V\rangle$$

$$\langle \alpha V| = \langle V|\alpha^*$$

Now consider $|\Omega V\rangle$

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

← adjoint

$$\begin{aligned}\langle i|\Omega^{+}|j\rangle &= \langle \Omega i|j\rangle \\ &= \langle j|\Omega i\rangle^* = \langle j|\Omega|i\rangle^* = \Omega_{ji}^* \end{aligned} \quad \longrightarrow \quad \boxed{\Omega^{+}_{ij} = \Omega_{ji}^*}$$

conjugate transpose

$$\boxed{(\Lambda\Omega)^{+} = \Omega^{+}\Lambda^{+}}$$

Consider $\langle \Omega(\Lambda V)|$

$$\begin{aligned} &= \langle \Lambda V|\Omega^{+} \\ &= \langle V|\Lambda^{+}\Omega^{+} \\ &= \langle V|(\Lambda\Omega)^{+} \end{aligned}$$

Finding the adjoint of an expression

- Convert every bra to a ket
- Convert every ket to a bra
- Convert every coefficient to its conjugate
- Convert every operator to its adjoint

G. Special Operators

Hermetian Operator

$\Omega = \Omega^{\dagger}$

$\Omega_{ij} = \Omega_{ji}^{*}$

Diagonals must be real

the product of two hermetian operators is not necessarily hermetian unless they commute

Unitary Operators

$U^{\dagger} U = I$

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

Viewed as rotational operators

Dot product is unaffected by unitary operator

If U_1 and U_2 are unitary, $U_1 U_2$ is as well

Rows and Columns of a unitary matricies are orthonormal

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

$|v'\rangle = \Omega |v\rangle = \Omega \sum v_j |j\rangle = \sum v_j \Omega |j\rangle$

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

Review

H. Eigenvalues

"developed by mathematicians having a good time"

For a given operator, $\Omega |v\rangle = |w\rangle$

Sometimes $\Omega |w\rangle = w |w\rangle$

Non-trivial operator

w is the eigenvalue

$|w\rangle$ is the eigenvector

Eigenvectors are directions, not vectors

Eigenvectors are always orthogonal

Hermetian operators have real and orthogonal eigenvalues/vectors

Solving for eigenvalues

Consider $\Omega = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = w \begin{pmatrix} u \\ v \end{pmatrix}$

$\underbrace{\begin{pmatrix} -w & 1 \\ 1 & -w \end{pmatrix}}_{\text{not invertible}} \underbrace{\begin{pmatrix} u \\ v \end{pmatrix}}_{\text{non-trivial}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow \det \begin{pmatrix} -w & 1 \\ 1 & -w \end{pmatrix} = 0$

since matricies that anhilate non-zero vectors are not invertible

$\therefore \det(\Omega) = 0$

Generally, for eigen values

$\Omega = \begin{pmatrix} \Omega_{11} & \cdots & \Omega_{n1} \\ \vdots & \ddots & \vdots \\ \Omega_{1n} & \cdots & \Omega_{nn} \end{pmatrix}$

solve $\det \underbrace{(\Omega - wI)}_{\text{Characteristic polynomial}} = 0$ for w

Now, for eigenvectors plug in eigenvalues and solve for each eigenvalue

$\underbrace{(\Omega - wI)}_{n \times n} \underbrace{(v)}_{n \times 1} = 0$ for v

Eigenvectors are typically normalized

Any observable is a real eigenvalue associated with a hermetian operator

Requires real diagonals since $\Omega_{ij} = \Omega_{ji}^*$

Proving eigenvalue/eigenvector properties of Hermetian operators

Consider Ω an arbitrary hermetian operator with eigenvectors w_i and w_j

$$\Omega|w_i\rangle = w_i|w_i\rangle \quad \text{and} \quad \Omega|w_j\rangle = w_j|w_j\rangle$$

1) $\langle w_j|\Omega|w_i\rangle = w_i\langle w_j|w_i\rangle$

$\langle w_i|\Omega|w_j\rangle = w_j\langle w_i|w_j\rangle \xrightarrow[\text{conjugate}]{\text{complex}} \langle w_j|\Omega|w_i\rangle = w_j^*\langle w_j|w_i\rangle$ 2)

Subtract 1) and 2)

$$0 = (w_i - w_j^*)\langle w_j|w_i\rangle$$

if $i=j$ $\langle w_i|w_i\rangle \neq 0$ so $w_i = w_i^*$ $\therefore$ w_i is real

if $i\neq j$ $(w_i - w_j)\langle w_j|w_i\rangle$ so $\langle w_j|w_i\rangle = 0$ $\therefore$ w_i and w_j are orthogonal

Assumes $w_i \neq w_j$

Degeneracy is when there is a repeated eigenvalue

The eigenvectors of a hermetian operator are an orthonormal basis

Consider

$$\Omega = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \longrightarrow w(w-2)^2 = 0$$

When $w=0$

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \longrightarrow \begin{matrix} u+w=0 \\ 2v=0 \\ w+u=0 \end{matrix} \longrightarrow \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}\cdot\underbrace{\frac{1}{\sqrt{2}}}_{\text{normalizing factor}}$$

when $w=2$

$$\begin{pmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \longrightarrow \begin{matrix} w-u=0 \\ 0=0 \\ u-w=0 \end{matrix} \longrightarrow \begin{pmatrix} 1 \\ x \\ 1 \end{pmatrix}\cdot\frac{1}{\sqrt{2+x^2}}, \quad \begin{pmatrix} 1 \\ y \\ 1 \end{pmatrix}\frac{1}{\sqrt{2+y^2}}$$

"two duds"

ensure it is orthogonal to previous eigenvectors

Any linear combination of n degenerate eigenvectors is also an eigenvector with the same eigenvalue

defines an n-dimensional space orthogonal to other eigenvectors with different eigenvalues

I. Unitary operators

$U|u\rangle = u|u\rangle$ where $u = e^{i\theta}$

Akin to complex numbers while hermetian operators are akin to real numbers

Consider $U|u_i\rangle = u_i|u_i\rangle$ and $U|u_j\rangle = u_j|u_j\rangle$

$$\langle u_j|U^\dagger = u_j^*\langle u_j|$$

$$\langle u_j|U^\dagger U|u_i\rangle = u_j^* u_i\langle u_j|u_i\rangle$$

if $j=i$ $\quad u_j^* u_i = 1;\ u_i = e^{i\theta}$

$j\neq i$ $\quad \langle u_j|u_i\rangle(u_j^* u_{i-1}) = 0$

so $\langle u_j|u_i\rangle = 0$

$U = e^{iH}$ ← via infinite series $= I + iH + (iH)^2 + \dots$

$U^\dagger = e^{-iH} = I - iH + (-iH)^2 + \dots$

Review

J. Commutators

If $[\Omega, \Lambda] = 0$ then they share a basis

Non-degeneracy

Suppose $\Omega|w\rangle = w|w\rangle$ $\qquad \Lambda|w\rangle = \lambda|w\rangle$

$\Lambda\Omega|w\rangle = w\,\Lambda|w\rangle$ $\qquad \Omega|w,\lambda\rangle = w|w,\lambda\rangle$

$\Omega(\Lambda|w\rangle) = w(\Lambda|w\rangle)$ $\qquad \Lambda|w,\lambda\rangle = \lambda|w,\lambda\rangle$

Suppose $w_1 = w_2 = w_0$

$\langle w_i|\Lambda|w_j\rangle = 0$ unless $w_i = w_j$ why?

$$0 = \langle w_i|[\Lambda,\Omega]|w_j\rangle = \langle w_i|\Lambda\Omega - \Omega\Lambda|w_j\rangle = (w_j - w_i)\langle w_i|\Lambda|w_j\rangle = 0$$

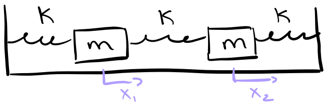
$$\Lambda \leftrightarrow \begin{array}{cc} w_1 = w_2 & w_3 \\ \left(\begin{array}{c|c} \lambda_1 \cdots \lambda_2 & O \\ \hline O & \end{array}\right) \end{array}$$

If two operators commute, they cannot impact the eigenvectors of eachother

two operators together can give you a non-degenerate basis

You need n commuting operators to single out a unique basis for n-degeneracies

Coupled Mass



Initial displacement $x_1(0)$ and $x_2(0)$ under the condition $\dot{x}_1(0) = 0 = \dot{x}_2(0)$

Applying Newton's Laws

$$m\ddot{x}_1 = -kx_1 + k(x_2 - x_1) = -2kx_1 + kx_2$$

$$m\ddot{x}_2 = -2kx_2 + kx_1$$

Pedestrian Approach

Add the equations

$$m(\ddot{x}_1 + \ddot{x}_2) = -k(x_1 + x_2)$$

$$x_+ = x_1 + x_2$$

$$m\ddot{x}_+ = -kx_+ \longrightarrow x_+(t) = x_+(0)\cos\sqrt{k/m}\,t$$

$$x_- = x_1 - x_2$$

$$m\ddot{x}_- = -3kx_- \longrightarrow x_-(t) = x_-(0)\cos\sqrt{3k/m}\,t$$

We can recover x_1 and x_2 by taking the sum/difference of x_+ and x_-

We refer to x_+ and x_- as normal coordinates

independent time evolutions

General Approach

Suppose we represent $x_1(t)$ and $x_2(t)$ via $|x(t)\rangle$

$$|x(t)\rangle = x_1(t)|1\rangle + x_2(t)|2\rangle$$

$$|1\rangle \rightarrow \begin{pmatrix}1\\0\end{pmatrix} \qquad |2\rangle \rightarrow \begin{pmatrix}0\\1\end{pmatrix}$$

$$|x(t)\rangle = \begin{pmatrix}x_1(t)\\x_2(t)\end{pmatrix}$$

Newton's Second Law

$$m|\ddot{x}\rangle = m\begin{pmatrix}\ddot{x}_1\\\ddot{x}_2\end{pmatrix} = k\begin{pmatrix}-2 & 1\\1 & -2\end{pmatrix}\begin{pmatrix}x_1\\x_2\end{pmatrix}$$

$$\frac{d^2}{dt^2}|x(t)\rangle = \Omega|x(t)\rangle$$

$$|\ddot{x}\rangle = \Omega|x\rangle$$

Ansatz: guess for the form of the solution and see if they exist

Impose $|x(t)\rangle = |x(0)\rangle f(t)$ ← Assumes some time dependence

$$\frac{d}{dt^2}\left(|x(0)\rangle f(t)\right) = \Omega|x(0)\rangle f(t)$$

$$\ddot{f}(t)\,|x(0)\rangle = f(t)\,\Omega|x(0)\rangle$$

$$\frac{\ddot{f}(t)}{f(t)}|x(0)\rangle = \Omega|x(0)\rangle$$

Demand $\frac{\ddot{f}(t)}{f(t)} = -w^2$

$$\Omega|X(0)\rangle = -w^2|X(0)\rangle$$ ← eigenvector of Ω

Now solve for eigenstates

$$\Omega|I\rangle = -w^2|I\rangle$$
$$\Omega|II\rangle = -w^2|II\rangle$$

Since $|\ddot{X}\rangle = \Omega|X\rangle$

form a basis

$$|\ddot{X}_I(t)\rangle = \Omega|X_I(t)\rangle$$
$$|\ddot{X}_{II}(t)\rangle = \Omega|X_{II}(t)\rangle$$

exploiting linearity

$$\frac{d^2}{dt^2}\left(\alpha|\ddot{X}_I(t)\rangle + \beta|\ddot{X}_{II}(t)\rangle\right) = \Omega\left[\alpha|X_I\rangle + B|X_{II}\rangle\right]$$

Finding a general solution

$$|X(t)\rangle = C_I|I\rangle\cos w_I t + C_{II}|II\rangle\cos w_{II} t$$

$$|X(0)\rangle = C_I|I\rangle + C_{II}|II\rangle$$

$$C_I = \langle I|X(0)\rangle$$
$$C_{II} = \langle II|X(0)\rangle$$

Therefore,

$$|X(t)\rangle = |I\rangle\langle I|X(0)\rangle\cos w_I t + |II\rangle\langle II|X(0)\rangle\cos w_{II} t$$
$$= \sum_{\alpha=I}^{II}\left(|\alpha\rangle\langle\alpha|\cos w_\alpha t\right)|X(0)\rangle$$
$$= U(t)|X(0)\rangle$$

↖ propagator : closed form solution for an arbitrary initial value state

Only works when time evolution is linear?

$$\begin{pmatrix} X_1(t) \\ X_2(t) \end{pmatrix} = \underbrace{\begin{pmatrix} \quad & \quad \\ \quad & \quad \end{pmatrix}}_{U}\begin{pmatrix} X_1(0) \\ X_2(0) \end{pmatrix}$$

Infinite Dimensions

We need infinite dimensions to accurately describe functions

A basis vector for every point in the domain

$$|f\rangle = \sum f(x_n)|n\rangle$$

$$\langle f|g\rangle = \sum_{n=1}^{N} f^*(x_n)\, g(x_n)$$ ← inner product blows up as $N \to \infty$

$\langle f|g\rangle = \int dx\ f^*(x)g(x)$ ← infinite dimension generalization

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

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

$$= \int dx\ \langle f|x\rangle\langle x|g\rangle$$

$$= \langle f|\underbrace{\left[\int |x\rangle\langle x|\,dx\right]}_{I}|g\rangle$$

$$I = \sum |n\rangle\langle n|$$

Consider

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

$$= \int \langle x|x'\rangle\langle x'|f\rangle\,dx$$

$$= \int \langle x|x'\rangle f(x')\,dx$$

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

kronecker delta

In infinite dimensions we need to redefine δ s.t. the above relation holds

$$\left.\begin{array}{ll} \delta(x,x') = 0 & x \neq x' \\ \delta(x,x') = \infty & x = x' \end{array}\right\}$$

heuristic actually a limit of functions

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

constant in the neighbourhood $x=x'$

dirac delta function

$$= f(x)\underbrace{\int \delta(x-x')\,dx}_{1}$$

Dirac delta is well defined in an integral

Gaussian definition of the dirac delta

$$\underbrace{\int e^{-x^2/\sigma^2}\,dx = \sqrt{\pi\sigma^2}}_{\text{Gaussian Function}} \longrightarrow \lim_{\sigma\to 0}\frac{1}{\sqrt{\pi\sigma^2}}\int e^{\frac{-(x-x')^2}{\sigma^2}} = 1 \longrightarrow \delta(x,x')$$

Require dirac delta for a functional dot product

Outerproduct only has meaning w/ a bra/ket?

Once again consider

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

$$\frac{df(x)}{dx} = \int \frac{d\delta}{dx}(x-x')\,f(x')\,dx'$$

Pay careful attention to $\frac{d\delta}{dx}$

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

pulls out derivative at $x'=x$

Summary

$$|f\rangle = \int |x\rangle \underbrace{\langle x|f\rangle}_{f(x)} dx$$

$$\langle g|f\rangle = \int g^* f \, dx$$

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

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

Operators in Infinite Dimensions

We define X s.t. $X|x\rangle = x|x\rangle$ where X is hermetian

basis vector

$$\langle x|X|f\rangle = \int \langle x|X|x'\rangle \langle x'|f\rangle \, dx'$$

gives us components

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

$$= x f(x)$$

Consider the eigenfunction of X

$$X|x_0\rangle = x_0 |x_0\rangle$$

$$= x|x_0\rangle \quad \leftarrow \text{defined action of } X$$

$$\langle x|x_0\rangle = \delta(x-x_0)$$

$$= x\,\delta(x-x_0)$$

$$= x_0\,\delta(x-x_0)$$

K operator

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

$$\langle x|K|f\rangle = \int \langle x|K|x'\rangle \langle x'|f\rangle \, dx'$$

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

$$= -i \frac{df}{dx}$$

K and X are the fundamental operators for any transformations of functions

Is K hermetian?

$$\langle x|K|x'\rangle \stackrel{?}{=} (\langle x'|K|x\rangle)^*$$

$$-i\,\delta'(x-x') \stackrel{?}{=} [-i\,\delta'(x'-x)]^*$$

$$= i\,\delta(x'-x)$$

Review

K is hermetian only if functions vanish at the boundary or are equivalent at the endpoints

periodic functions yield hermetian K

Eigenfunctions of K

$$[X,K]|f\rangle = XK|f\rangle - KX|f\rangle = x\left(-i\frac{df}{dx}\right) - \left(i\frac{d(xf)}{dx}\right) = +if$$

$$[X,K] = iI$$

$$K|k\rangle = k|k\rangle$$

$$\langle x|K|k\rangle = k\langle x|k\rangle$$

$$-i\frac{d\psi_k}{dx} = k\,\psi_k(x)$$

$$\psi_k(x) = Ae^{ikx}$$

High level Summary

$f(x)$ form a vector space

$|f\rangle$ is a ket

$f(x) = \langle x|f\rangle$ is a basis ket

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

$$= \int \langle f|x\rangle\langle x|g\rangle\,dx$$

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

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

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

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

$$X|x\rangle = x|x\rangle$$

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

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

$$X|f\rangle = xf$$

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

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

$$[X,K] = iI$$

Review of Mechanics

Newtonian mechanics is a local approach to motion

moment-by-moment

A. Lagrangian Mechanics

Lagrangian mechanics is a more general/global approach to motion

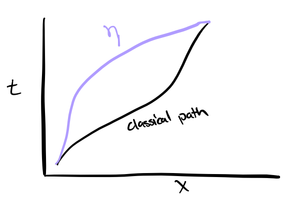
Motion follows the path of least action

$$S[x(t)] = \int_{t_1}^{t_2} \left[\tfrac{1}{2}m\dot{x}^2 - V(x)\right] dt$$

action

$$= \int_{t_1}^{t_2} \mathcal{L}(x,\dot{x},t)\,dt$$

Consider a perturbation from the classical path



$x_c + \underbrace{\delta x}_{\eta}$

$\dot{x}_c + \dot{\eta}$

$$\Rightarrow \delta S = \int \left(\underbrace{\frac{\partial \mathcal{L}}{\partial x}}\eta + \frac{d\mathcal{L}}{d\dot{x}}\dot{\eta}\right) dt$$

exploit arbitrary η to set 0

Path of Least Action

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}}\right) = \frac{\partial \mathcal{L}}{\partial x}$$ ← Euler Lagrange Equation

↑ momentum

We choose $\mathcal{L} = \frac{1}{2}m\dot{x}^2 - V(x)$ to replicate Newton's laws

$$\frac{\partial \mathcal{L}}{\partial \dot{x}} = m\dot{x} \qquad \frac{\partial \mathcal{L}}{\partial x} = -\frac{\partial V}{\partial x}$$

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}}\right) = m\ddot{x} = -\frac{\partial V}{\partial x}$$ ← One second order equation

Euler-Lagrange are invariant under coordinate changes

Conservation of a quantity is due to coordinates missing from the lagrange

B. Hamiltonian Mechanics

"Ghost of quantum mechanics resides in Hamiltonian mechanics"

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

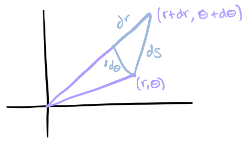
$T(p)$ not v

$$H = \sum_i p_i q_i - \mathcal{L}$$
$$= p\dot{x} - \frac{1}{2}m\dot{x}^2 + V$$
$$= p \cdot p/m - \frac{1}{2}m(p/m)^2 + V$$
$$= \frac{p^2}{2m} + V$$

$$\dot{q} = \frac{\partial H}{\partial p} \quad \text{and} \quad \dot{p} = -\frac{\partial H}{\partial q}$$ ← two first order equations

Only need initial position and momentum

Consider a particle moving in 2-Dimensions



$$(ds)^2 = (dr)^2 + (r d\theta)^2$$

$$\left(\frac{ds}{dt}\right)^2 = v^2 = r^2\left(\frac{d\theta}{dt}\right)^2 + \left(\frac{dr}{dt}\right)^2 = r^2\dot{\theta} + \dot{r}^2$$

$$\mathcal{L} = \frac{1}{2}m\left(\dot{r}^2 + r^2\dot{\theta}^2\right) - V(r,\theta)$$

$$P_r = \frac{\partial \mathcal{L}}{\partial \dot{r}} = m\dot{r} \qquad P_\theta = \frac{\partial \mathcal{L}}{\partial \dot{\theta}} = mr^2\dot{\theta}$$

generalized definition of momentum

Writing the Hamiltonian

must be written in velocities

$$H = \frac{m}{2}\left(\frac{P_r}{m}\right)^2 + \frac{m}{2}r^2\left(\frac{P_\theta}{mr^2}\right)^2 + V(r,\theta)$$

$$= \frac{P_r^2}{2m} + \frac{P_\theta^2}{2mr^2} + V(r,\theta)$$

Solving the Hamiltonian

$$\boxed{\begin{aligned} \dot{r} &= \frac{\partial H}{\partial P_r} = \frac{P_r}{m} \\ \dot{P}_r &= -\frac{\partial H}{\partial r} = -\frac{\partial V}{\partial r} - \frac{P_\theta^2}{mr^3} \end{aligned}} \qquad \boxed{\begin{aligned} \dot{\theta} &= \frac{\partial H}{\partial P_\theta} = \frac{P_\theta}{mr^2} \\ \dot{P}_\theta &= -\frac{\partial H}{\partial \theta} = -\frac{\partial V}{\partial \theta} \end{aligned}}$$

Summary of Hamiltonian Mechanics

1. Find the Lagrangian
2. Find the momentum analogs
3. Define the Hamiltonian
4. Solve for $\dot{p}$ and q for each variable

$$\dot{P}_i = -\frac{\partial H}{\partial q_i} \qquad \dot{q}_i = \frac{\partial H}{\partial P_i}$$

C. Poisson Bracket

Consider a general variable $\omega(q,p)$

$$\frac{\partial \omega}{\partial t} = \frac{\partial \omega}{\partial q}\dot{q} + \frac{\partial \omega}{\partial p}\dot{p}$$

$$= \frac{\partial \omega}{\partial q}\cdot\frac{\partial H}{\partial p} - \frac{\partial \omega}{\partial p}\cdot\frac{\partial H}{\partial q}$$ ← Apply Hamiltonian Definitions

$$= \{\omega, H\}$$ ← Poisson Bracket

$$\{\omega_1,\omega_2\} = \frac{\partial \omega_1}{\partial q}\cdot\frac{\partial \omega_2}{\partial p} - \frac{\partial \omega_1}{\partial p}\cdot\frac{\partial \omega_2}{\partial q}$$

$$\frac{dq}{dt} = \{q,H\} = \underbrace{\cancel{\frac{\partial q}{\partial q}}}_{1}\frac{\partial H}{\partial p} - \underbrace{\cancel{\frac{\partial q}{\partial p}}}_{0}\frac{\partial H}{\partial q} = \frac{\partial H}{\partial p}$$ ← Hamiltonian relationship

$$\{\omega,\lambda\Sigma\} = \{\omega,\lambda\}\Sigma + \lambda\{\omega,\Sigma\}$$ ← Akin to the commutator

$$\{\omega,\lambda\} = -\{\lambda,\omega\}$$

Quantities that are conserved poisson bracket to 0

D. Canonical Transformations

Hamiltonian mechanics exists in the phase space

Offers more transformations since we can work with q and p

However, Hamiltonian equations of motions will need to be rewritten in the new transformation

To preserve the form of hamiltonian equations across transformations, we require

$$\{q',p'\} = 1$$

↖ Canonical Transformation

We can compound infinitesimal canonic transformations to produce another canonical transformation

Process for generating Canonical Transformations

1. Take any $g(q,p)$

$$q' = q + \epsilon\frac{\partial g}{\partial p}$$

$$p' = p + \epsilon\frac{\partial g}{\partial q}$$ q-generating

$$\{q',p'\} = \{q,p\} + \underbrace{\epsilon\left\{\frac{\partial g}{\partial p},p\right\} - \epsilon\left\{q,\frac{\partial g}{\partial q}\right\}}_{} + O(\epsilon^2)$$

↖ drop quadratic infinitesimal terms

$$\epsilon\left(\left\{\frac{\partial g}{\partial p},p\right\} - \left\{q,\frac{\partial g}{\partial q}\right\}\right)$$

$$\frac{\partial^2 g}{\partial q\partial p} - \frac{\partial^2 g}{\partial p\partial q}$$

E. Conservation and Symmetry

$$H = \frac{P_1^2}{m} + \frac{P_2^2}{2m} + V(x_1,x_2)$$

↑ $V(x_1-x_2)$

$x_1 \to x_1 + c$

$x_2 \to x_2 + c$ $\qquad x = x_1 - x_2$

$H \to H$

$$\dot{P}_1 = -\frac{\partial H}{\partial x_1} = -\frac{\partial H}{\partial x}\cdot\frac{\partial x}{\partial x_1} = -\frac{\partial H}{\partial x}$$

$$\dot{P}_2 = -\frac{\partial H}{\partial x_2} = -\frac{\partial H}{\partial x}\cdot\frac{\partial x}{\partial x_2} = \frac{\partial H}{\partial x}$$

Consider a generic transformation

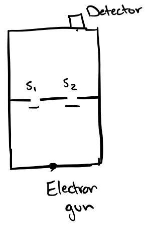
$q_i \to q_i + \delta q_i$

$p_i \to p_i + \delta p_i$

$$H(q_i, p_i) = H(q_i + \delta q_i, p_i + \delta p_i)$$

$$0 = \frac{\partial H}{\partial q_i}\delta q_i + \frac{\partial H_i}{\partial p_i}\delta p_i + \epsilon\left(\frac{\partial H}{\partial q_i}\cdot\frac{\partial g}{\partial p_i} - \frac{\partial H}{\partial p_i}\cdot\frac{\partial g}{\partial q_i}\right) = \epsilon\{H, g\} = 0$$

The Failure of Classical Mechanics



Let $I_1(x)$ represent the counts of electrons at point x with S_1 open

Let $I_2(x)$ represent the counts of electrons at point x with S_2 open

Let $I(x)$ represent the case where both slits are open

Under Newtonian Mechanics $I(x) = I_1(x) + I_2(x)$

motion only depends on local conditions

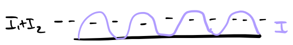
There exists x^* s.t. $I_1(x^*) \neq 0$ and $I_2(x^*) \neq 0$ but $I(x^*) = 0$

Opening of a second slit reduces electron count at a position

This phenomena cannot be explained via Newtonian mechanics

Not how quantum mechanics was discovered but the experiment was retroactively conducted to verify the essence of QM

Electron count result



This behavior is characteristic of waves, not particles

The calculated wavelength from the diffraction pattern

unexpected property $\lambda = \frac{2\pi\hbar}{p}$ $\approx 10^{-34}$ J·s $\qquad E = p^2/2m$

Only one detector is activated at a time

Electron is a particle but not a newtonian particle

Doesn't have a trajectory

For repeated trials we can define

$|\psi(x)|^2 dx = P(x)\,dx$ ← Conclusion from double slit experiment

wave associated w/ electron

We must reduce the intensity of light to see particle properties

unexpected property $p = \frac{2\pi\hbar}{\lambda}$

$E = pc$

Photons are relativistic particles w/ more complicated quantum mechanics

Energy and wavelength of electrons are not simply connected

Energy and wavelength of photons are directly connected

$E = \hbar\omega$

$p = \hbar k = \frac{2\pi\hbar}{\lambda}$

Electrons only have a definite location when you observe it

Laws of Classical Mechanics vs. Quantum Mechanics

Postulates	Classical Mechanics	Quantum Mechanics
I. State	(x,p)	$\lvert\psi\rangle \in$ Hilbert space ↖ ray (represents direction) $\lvert\psi\rangle = a\lvert\psi\rangle$ ← pick $\lvert\psi\rangle$ s.t. it is normalized
II. Observables dynamic variables ↗	$w(x,p)$	$\Omega(x,p)$ ← operaterize classical counterpart $X: \langle x\lvert X\rvert x'\rangle = x\,\delta(x-x')$ $P: \langle x\lvert P\rvert x\rangle = -i\hbar\,\delta'(x-x')$ $\quad \hbar = h/2\pi$ In a given basis $\lvert\psi\rangle \to \langle x\lvert\psi\rangle \to \psi(x)$ $\langle x\lvert X\rvert\psi\rangle = x\,\psi(x) = \int \langle x\lvert X\rvert x'\rangle \underbrace{\langle x'\lvert\psi\rangle}_{\psi(x')}\,dx'$ $\langle x\lvert P\rvert\psi\rangle = -i\hbar\frac{d\psi}{dx}$ Observables are operators in quantum theory
III. Measurement	Every observable has a definite value $w(x_0,p_0)$ Observable is real	Result of Ω measurement in the state $\lvert\psi\rangle$ is an eigenvalue of Ω Only eigenvalues are allowed $\Omega\lvert w_i\rangle = w_i\lvert w_i\rangle$ at state $\lvert\psi\rangle$ $P(w_i) = \lvert\langle w_i\lvert\psi\rangle\rvert^2$ $P(x) = \lvert\langle x\lvert\psi\rangle\rvert^2$ Right after measurement $\lvert\psi\rangle \to \lvert w_i\rangle$ ← Collapse of the state vector Usually $\lvert\psi\rangle$ is a superposition of $\lvert w_i\rangle$
IV. Time Evolution	$\dot{x} = \frac{\partial H}{\partial p}$ $\dot{p} = -\frac{\partial H}{\partial x}$ Hamiltonian Equations	$i\hbar\frac{\partial\lvert\psi\rangle}{\partial t} = H\lvert\psi\rangle$ Project both sides into x basis $i\hbar\frac{\partial\psi(x,t)}{\partial t} = \langle x\lvert H\rvert\psi\rangle$

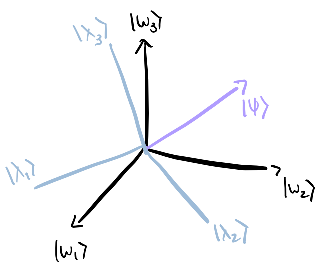
Consider the following example:

$$i\hbar\frac{d\lvert\psi\rangle}{dt} = H\lvert\psi\rangle \quad \text{where} \quad H = \frac{P^2}{2m} + \frac{1}{2}kx^2$$

In the x basis

$$i\hbar\frac{d\lvert\psi\rangle}{dt} = \frac{1}{2}\left(-\hbar^2\frac{\partial\psi}{\partial x^2}\right) + \frac{1}{2}kx^2\,\psi(x,t$$

3-dimensional Hilbert Space Example



$\Omega \in$ Mat (3x3)
$\Lambda \in$ Mat (3x3) ← given

$$\left.\begin{aligned} P(w_1) &= \lvert\langle w_1\lvert\psi\rangle\rvert^2 \\ P(w_2) &= \lvert\langle w_2\lvert\psi\rangle\rvert^2 \\ P(w_3) &= \lvert\langle w_3\lvert\psi\rangle\rvert^2 \end{aligned}\right\} \text{eigenvalues/vectors}$$

$$P(\lambda_1) = \lvert\langle\lambda_1\lvert\psi\rangle\rvert^2$$

$\vdots$

If we collapse $\lvert\psi\rangle$ to $\lvert w_2\rangle$ we find $P(\lambda_1) = \lvert\langle\lambda_1\lvert w_2\rangle\rvert^2$

If we return to w_2, the answer will be different

If two operators commute you can measure them in succession

You can use commuting operators to handle the problem of degeneracy

Can only test quantum theory with an ensemble

Statistics in Quantum Mechanics

$$\langle \Omega \rangle = \sum P(\omega_i)\, \omega_i$$ ← weighted average

expected value

$$= \sum |\langle \omega_i|\psi\rangle|^2 \omega_i$$

$$= \sum \langle\psi|\omega_i\rangle\langle\omega_i|\psi\rangle\, \omega_i$$

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

$$= \sum_i \langle\psi|\Omega\underbrace{|\omega_i\rangle\langle\omega_i|}_{\text{identity}}\psi\rangle$$

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

Uncertainity

$$(\Delta\Omega)^2 = \sum (\omega_i - \langle\Omega\rangle)^2 P(\omega_i)$$ ← Variance

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

Uncertainity refers to $\Delta\Omega$

$$X|x\rangle = x|x\rangle$$

$$\langle x'|X|x\rangle = x\langle x'|x\rangle$$

$$x'\,\delta(x-x') = x\,\delta(x'-x)$$

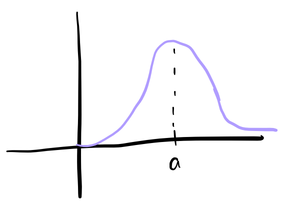
$$\langle\psi|X|\psi\rangle = \iint \langle\psi|x\rangle\langle x|X|x'\rangle\langle x'|\psi\rangle\, dx\, dx'$$

$$= \iint \psi^*(x)\; x\,\delta(x-x')\,\psi(x')\; dx\, dx'$$

$$= \int \psi^*(x)\,(x)\,\psi(x)\, dx$$

Gaussian Wave Function

$$\psi(x) = Ae^{-\frac{(x-a)^2}{2\Delta^2}}$$



Select A s.t. $|\psi(x)| = 1$

$$\int_{-\infty}^{\infty} e^{-\alpha x^2}\, dx = \sqrt{\pi/\alpha}$$

← fundamental equalities

$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} = \frac{1}{2\alpha}\sqrt{\pi/\alpha}$$

Normalizing $\psi(x)$

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

$$A = \frac{1}{(\pi\Delta^2)^{1/4}}$$

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

Expected Value of X

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

Uncertainity of X

$$(\Delta X)^2 = \langle (X - \langle X \rangle)^2 \rangle = \frac{1}{\sqrt{\pi\Delta^2}} \int e^{-(x-a)^2/\Delta^2} (x-a)^2\, dx = \frac{\Delta^2}{2}$$

$$\Delta X = \frac{\Delta}{\sqrt{2}}$$

Expected Value of P

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

gaussian is real

$$= \frac{1}{2} \int \left(-i\hbar \frac{d(\psi)^2}{dx}\right) dx = \frac{-i\hbar}{2} \psi^2 \Big|_{-\infty}^{\infty} = 0$$

$\langle P \rangle$ for any real ψ that vanishes at infinity

Uncertainity for P

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

$$= \int \psi^* \left(-\hbar^2 \frac{d^2}{dx^2}\right) \psi$$

$$(\Delta P)^2 = \langle \psi | P^2 | \psi \rangle = \langle \psi | P P | \psi \rangle = \langle P\psi | P\psi \rangle = \int \left| i\hbar \frac{d\psi}{dx} \right|^2 dx = \hbar^2 \int \left(\frac{d\psi}{dx}\right)^2 dx = \frac{\hbar^2}{\sqrt{\pi\Delta^2}} \int \frac{(x-a)^2}{\Delta^2} e^{-(x-a)^2/\Delta^2} dx$$

don't forget factor

$$\Delta P = \frac{\hbar}{\sqrt{2}\Delta}$$ ← inverse of uncertainity in position

Eigenvalues of P

$\langle P | p \rangle = p | p \rangle$

we want in terms of x-basis

$\langle x | P | p \rangle = \langle x | p | p \rangle = p \langle x | p \rangle$

$$\int dx \langle x | P | x' \rangle \langle x' | p \rangle = p\, \psi_p(x)$$

$$-i\hbar \frac{d}{dx} \psi_p(x) = p\, \psi_p(x)$$

State of definite momentum

$$\psi_p(x) = e^{ipx/\hbar} \rightarrow \psi_p^*(x) = e^{-ipx/\hbar}$$

$$|\psi_p(x)|^2 = \psi_p^*(x)\, \psi_p(x) = |A|^2$$ ← no x-dependence

Particle of definite position has indefinite momentum

$$\langle p|x\rangle = \int \langle p|x'\rangle\langle x'|x\rangle\, dx$$

$$= \int e^{-ipx'/\hbar}\, \delta(x'-x)\, dx = e^{-ipx/\hbar}$$

X and P do not share any eigenvectors

$$[X,P] = i\hbar$$

$$[X,P]\,|x_0,p_0\rangle = \text{something lmao}$$

Schrodinger Equation

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

$$= \left[\frac{p^2}{2m} + V(x)\right]|\psi(t)\rangle$$

$$|\psi(t)\rangle = |\psi(0)\rangle\, c(t)$$ ← look for solutions of this form

Normal mode

Schrodinger's Equation becomes

$$i\hbar\,|\psi(0)\rangle\, \dot{c}(t) = H\,|\psi(0)\rangle\, c(t)$$

$$i\hbar\,|\psi(0)\rangle \frac{\dot{c}(t)}{c(t)} = H\,|\psi(0)\rangle$$

Let $E = i\hbar \frac{\dot{c}}{c}$

implies

$\vdots$

$$c(t) = c(0)\, e^{-iEt/\hbar}$$

$$E\,|\psi(0)\rangle = H\,|\psi(0)\rangle$$

Propagator

via superposition

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

Consider

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

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

$$|\psi(t)\rangle = \sum_E |E\rangle\langle E|\psi(0)\rangle\, e^{-iEt/\hbar}$$ ← most general solution to schrodinger equation

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

propagator

$$\boxed{\begin{aligned} |\psi(t)\rangle &= U(t)\,|\psi(0)\rangle \\ U(t) &= \sum_E |E\rangle\langle E|\, e^{-iEt/\hbar} \end{aligned}}$$

$$U(t) = e^{-iHt/\hbar}\Big(\underbrace{\sum |E\rangle\langle E|}_{I}\Big) = e^{-iHt/\hbar}$$

Turn the operator into a matrix

$$\langle x|U(t)|x'\rangle = \sum_E \underbrace{\langle x|E\rangle}_{\psi_E(x)} \underbrace{\langle E|x'\rangle}_{\psi_E^*(x')} e^{-iEt/\hbar}$$

Schrodinger Equation for Eigenfunctions

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

$\langle x|H|E\rangle = E\langle x|E\rangle$ ← project into x basis

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

$$\frac{-\hbar^2}{2m}\frac{d^2\psi_E}{dx^2} + V(x)\psi_E(x) = E\,\psi_E(x)$$ ← time independent eigenvalue equation

General State

$$i\hbar\frac{\partial\psi}{\partial t}(x,t) = \left[\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\,\psi\right]$$ ← written in x-basis

time dependent equation

Solutions to time independent eigenvalue equation are the allowed energies of the system

Reconciling the Quantum and Classical Worlds

$\Delta p = \hbar/\Delta x$

if $\Delta x \sim 10^{-17}$ m
$\Delta p \sim 10^{-17}$ } functionally definite

Consider $|x_0, p_0\rangle$ where

$\langle x\rangle = x_0$

$\langle p\rangle = p_0$

$\dot{x}_0 = -\frac{\partial H}{\partial p}(x_0, p_0)$

Recall

$$\frac{d|\psi\rangle}{dt} = \frac{1}{i\hbar}H|\psi\rangle \quad \text{and} \quad \frac{d\langle\psi|}{dt} = -\frac{1}{i\hbar}\langle\psi|H$$

Consider an arbitrary operator Ω

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

$$= \frac{d\langle\psi|}{dt}\Omega|\psi\rangle + \langle\psi|\Omega\frac{d|\psi\rangle}{dt}$$

$$= \frac{1}{i\hbar}\left(-\langle\psi|H\Omega|\psi\rangle + \langle\psi|\Omega H\rangle\right)$$

$$= \frac{1}{i\hbar}\langle\psi|[\Omega,H]|\psi\rangle$$ ← Ehrenfest's Theorem

similar to poisson bracket

Now, lets reconsider $\langle x\rangle$

$$\frac{d\langle x\rangle}{dt} = \frac{dx_0}{dt} = \frac{1}{i\hbar}\langle\psi|[X,H]|\psi\rangle$$

V(x) commutes with X so we can ignore

$$= \frac{1}{i\hbar}\langle\psi|[X, P^2/2m]\psi\rangle$$

$$\dot{x}_0 = \bar{P}_0/m$$ ← classical result

Now consider momentum

$$\dot{P}_0 = \frac{d}{dt}\langle P\rangle = \frac{1}{i\hbar}\left\langle \psi \middle| \left[P, \frac{P^2}{2m} + V(x)\right] \middle| \psi \right\rangle$$

$$= \frac{1}{i\hbar}\langle \psi | [P, V(x)] | \psi\rangle$$

$$= \left\langle -\frac{dV(x)}{dx} \right\rangle = -\left\langle \frac{\partial H}{\partial x} \right\rangle$$

not classical Force

Classical and Quantum Mechanics allign when potential is relatively constant over the width of the wavefunction

Schrodinger's Equation

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

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

$X \to x$

$P \to -i\hbar \frac{d}{dx}$, $P^2 = -\hbar^2 \frac{d^2}{dx^2}$

Projecting into x-basis

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

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

limiting to time independent Hamiltonians

We look for solutions of the form

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

split position and time

Plug the above solution into schrodingers equation

$$E\,\psi_E(x,t)\,\cancel{e^{\frac{-iEt}{\hbar}}} = \cancel{e^{\frac{-iEt}{\hbar}}}\left[-\frac{\hbar^2}{2m}\frac{d^2\psi_E}{dx^2} + V(x)\,\psi_E(x) \right]$$

Eigenvalue equation

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

time independent Schrodinger Equation

Stationary State : $\psi_E(x)\, e^{-iEt/\hbar}$ doesn't depend on time

$$\langle \Omega \rangle = \int \psi_E^*(x)\,\cancel{e^{iEt/\hbar}}\ \Omega\ \psi_E(x)\,\cancel{e^{-iEt/\hbar}}\ dx$$

time dependence cancels

$$P(x,t) = |\psi_E(x)|^2$$

Also time independent

Probability will not change with time if the state is an eigenvector of the Hamiltonian

Free Particle

$V(x) = 0$

In classical mechanics the particle maintains its current dynamics

In quantum mechanics

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

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

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

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

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

$$p = \hbar k$$

$$\frac{\partial^2\psi_E}{\partial x^2} + k\,\psi_E = 0$$

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

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

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

opposing directions

two-fold degenerate states

need a commuting operator to properly label the states

$$U = \sum_{\alpha=1,2} |E\rangle\langle E|\, e^{-iEt/\hbar}$$

$$= \sum |E,\alpha\rangle\langle E,\alpha|\, e^{-iEt/\hbar}$$

$$= \sum_p |p\rangle\langle p|\, e^{-\frac{ip^2t}{2m\hbar}} \longrightarrow \int \frac{dp}{2\pi\hbar}\, |p\rangle\langle p|\, e^{\frac{-ip^2t}{2m\hbar}}$$

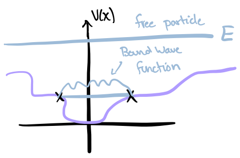
$$U(x,t,x',0) = \left(\sqrt{}\right) e^{\frac{i(x-x')^2 t m}{2\hbar}}$$

$$\psi(x,0) = \sqrt{}\; e^{\frac{-(x-a)^2}{2\Delta^2}} \cdot e^{ip_0 x}$$

$$\langle p\rangle = p_0$$

gaussian will get wider as it propogates with time

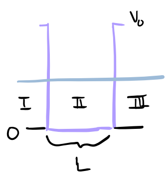
Particle w/ a Potential



$E < V(\infty)$ refers to bound states

$T = E - V(\infty)$ so no kinetic energy

Particle in a Box



In region III

$$\frac{\partial^2\psi_{III}}{\partial x^2} + \frac{2m}{\hbar^2}(E-V_0)\,\psi_{III} = 0$$

$$\frac{d^2\psi_{I}}{dx^2} = \frac{2m}{\hbar^2}(V_0-E)\,\psi_{III}$$

$$= k^2\psi \qquad \underbrace{k = \pm\sqrt{\frac{2m}{\hbar^2}(V_0-E)} \quad \text{or} \quad k = \pm\sqrt{\frac{2m}{\hbar^2}(E-V_0)}}_{?}$$

$$\psi_{III} = \cancel{Ce^{kx}} + De^{-kx}$$

can't blow up at infinity

As $V_0 \to \infty$, $k \to \infty$ and $\psi_{III} \to 0$

$$\psi_I = \psi_{III} \to 0$$

In region II

$$\frac{\partial^2\psi_{II}}{\partial x^2} + \frac{2m}{\hbar^2}E\,\psi_{II} = 0$$

$$\psi_{II} = Ae^{ikx} + Be^{-ikx} = A'\cos kx + B'\sin kx$$

ψ_{II} must vanish at the boundaries so ψ is continuous

$$\psi_{II}(0) = 0 \;, \quad \psi_{II}(L) = 0$$

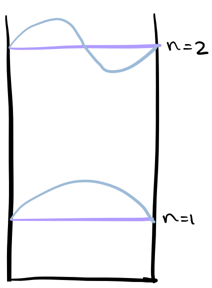
$$A' = 0 \qquad B'\sin kL = 0$$

set $kL = n\pi$ for $n = 1,2,3,\dots$

$$k = \frac{n\pi}{L}$$

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

$$\boxed{\psi_n = \sqrt{\frac{2}{L}}\,\sin\frac{n\pi x}{L}}$$



Energy is continuous when it is greater than the well height

Solutions in both directions

Energy is quantized within the well ← Bound States

Observations

1) Lowest Energy is not 0

Lowest energy is $E_1 = \frac{\hbar^2}{2mL^2}$, $E = 0$ violates uncertainty principle

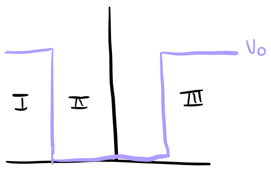
2) As you increase energy, there are more oscillations

3) Parity: Hamiltonian is invariant under operations

$$H(x) = H(-x) \to \psi(-x) = \pm\,\psi(x)$$

Consider a system with potential

$$\psi'' + \left(\frac{2m}{\hbar}(E - V(x))\right)\psi = 0$$



$$\text{I}: \psi_I'' = -\underbrace{\frac{2m}{\hbar^2}(E - V_0)}_{k_0^2}\psi_I$$

$$\text{II}: \psi_{II}'' = -\underbrace{\frac{2mE}{\hbar^2}}_{k}\psi_{II}$$

$$\text{III}: \psi_{III}'' = -\frac{2m}{\hbar^2}(E - V_0)\psi_{III}$$

$\longrightarrow$

set to 1 WLOG

$$\psi_I(x) = Ae^{ik_0x} + \cancel{Be^{-ik_0x}}$$

$$\psi_{II}(x) = Ce^{ikx} + De^{-ikx}$$

$$\psi_{III}(x) = \cancel{Fe^{ik_0x}} + Ge^{-ik_0x}$$

prevent wavefunction from blowing up

$\longrightarrow$

Boundary Conditions

- $\psi_I(L) = \psi_{II}(L)$
- $\psi_I'(L) = \psi_{II}'(L)$

$L \leftrightarrow R$

4 conditions

3 parameters w/ 4 conditions

Vary E to find special allowed solutions

Quantization of Energy!

Scattering

All energies obey

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

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

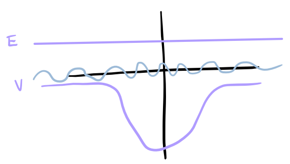
Simplest case when $V=0$

$$\frac{d^2\psi_E}{dx^2} + \underbrace{\frac{2m}{\hbar^2}E}_{k^2}\psi_E = 0$$

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

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

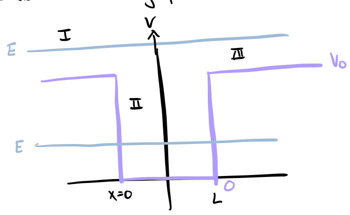
$$= Ae^{ipx/\hbar} + Be^{-ipx/\hbar} = \underbrace{A'\cos kx + B'\sin kx}_{\text{Only true for constant } V}$$



$k^2 \propto E - V$

maximized at bottom of well

Consider the following potential



(ψI) $Ae^{i\bar{k}x} + Be^{-i\bar{k}x}$ $\qquad \frac{\hbar^2\bar{k}^2}{2m} = E - V_0$

(ψII) $Ce^{ikx} + De^{-ikx}$ $\qquad \frac{\hbar^2k^2}{2m} = E$

(ψIII) $Fe^{i\bar{k}x} + Ge^{-i\bar{k}x}$

Boundary Conditions

$$\psi_I(x=0) = \psi_{II}(0)$$

$$\psi_I'(x=0) = \psi_{II}'(0)$$

$$A + B = C + D$$

$$i\bar{k}A - Bi\bar{k} = ik(C - D)$$

Repeat for II and III

4 conditions

5 parameters

W.LOG set A=1

We can write

$$\bar{k}^2 = \frac{2m(E - V_0)}{\hbar^2}$$

$$\bar{k} = \sqrt{\frac{-2m(V_0 - E)}{\hbar^2}}$$

$$\kappa = i\bar{k} = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

When $E < V_0$ — Blow up

$$\psi_I = e^{\kappa x} + \cancel{Be^{-\kappa x}}$$

$$\psi_{II} = C\cos kx + D\sin kx$$

$$\psi_{III} = \cancel{Fe^{\kappa x}} + Ge^{-\kappa x}$$

Blow up

Real exponentials in forbidden regions

$\longrightarrow$

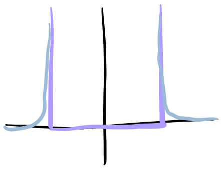
Overdetermined system

3 parameters

4 conditions

Only solvable in a specific situation

Consider a particle in a box $V_0 \to \infty$



exponential falls off but is non zero in classically forbidden regions

$\psi_I = e^{Kx} + \cancel{B e^{-Kx}}$ Blow up

$\psi_{II} = \cancel{C \cos kx} + D \sin kx$

$\psi_{III} = \cancel{F e^{Kx}} + G e^{-Kx}$

Blow up

$x = 0$

$C \cos kx \to 0$

$x = L$

$D \sin kL \to 0$

$kL = n\pi \quad n = 1, 2, \dots$

$\psi_n = A \sin \frac{n\pi x}{L}$

$n-1$ zeros in the wavefunction

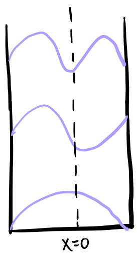
$n = 0 \to 0$ wavefunction

$n < 0 \to$ constant multiple

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

- All solutions are real and non-degenerate

Bound states have non-degeneracy in 1-Dimension

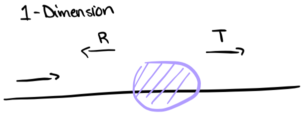


Symmetry of solutions

Parity Invariant

Doesn't distinguish left from right

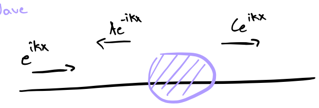
Scattering in 1-Dimension



T = prob of transmission
R = prob of reflection
$\Big\}\; T + R = 1$

R,T are function of input Energy

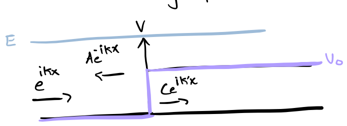
Plane Wave



$R = \frac{|A|^2}{1^2} \qquad T = \frac{|C|^2}{1^2}$

$T = \dfrac{|C|^2 \cancel{\frac{\hbar k}{m}}}{1 \cancel{\frac{\hbar k}{m}}}$ velocity term (current of particles)

Consider the following potential



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

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

Boundary Conditions

$x = 0 \quad 1 + A = C$

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

$C = \frac{2k}{k + k'} \qquad A = C - 1 = \frac{k - k'}{k + k'}$

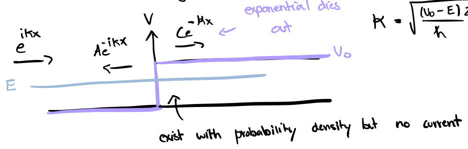
Resulting T and R

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

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

$T + R = 1$ ✓

Consider the following potential



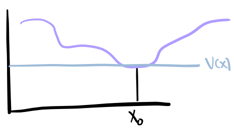
$$K = \sqrt{\frac{(V_0 - E)\,2m}{\hbar}}$$

Harmonic Oscillator

Classical System

$$\mathcal{H} = \frac{p^2}{2m} + \underbrace{\frac{1}{2}m\omega^2 x^2}_{\frac{1}{2}kx^2}$$

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



$$V(x) = \underbrace{\cancel{V(x_0)}}_{\text{Set to } 0} + \underbrace{\cancel{(x-x_0)V'}}_{\text{minimum}} + \frac{1}{2}(x-x_0)^2 V'' + \ldots$$

Any potential energy can be modeled as a harmonic oscillator around the minimum

Single Oscillator

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

Write schrödinger equation

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

Let $x = b \cdot y$ (Natural units)

$$\frac{1}{b^2} \cdot \frac{d^2\psi}{dy^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2 b^2 y^2\right)\psi = 0$$

$$\frac{d^2\psi}{dy^2} + \frac{2mb^2}{\hbar^2}E\psi - \frac{m^2\omega^2}{\hbar^2}b^4 y^2\psi = 0$$

Let $\frac{m^2\omega^2}{\hbar^2}b^4 = 1$ so that $b^2 = \frac{\hbar}{m\omega}$

$$\frac{d^2\psi}{dy^2} + \underbrace{\left(\frac{2E}{\hbar\omega}\right)}_{\epsilon}\psi - y^2\psi = 0$$

$$\epsilon = \frac{E}{\hbar\omega} \qquad y = \sqrt{\frac{m\omega}{\hbar}}\,x \quad \leftarrow \text{ resonable energies}$$

Putting it all together

$$\frac{d^2\psi}{dy^2} + 2\epsilon\psi - y^2\psi = 0$$

At small y

$$\psi \simeq A + By$$

At large y

$$\psi'' = y^2\psi$$

$$\psi = e^{-y^2/2} \leftarrow \text{ Asymptotically obeys differential equation}$$

We can write

$$\psi(y) = e^{-y^2/2}\, u(y)$$

Plug back into original differential equation

$$\psi'' + 2\epsilon\psi - y^2\psi = 0$$

$$\Rightarrow \quad u'' - 2u'y + (2\epsilon - 1)u = 0$$

$$u(y) = \sum_n^{\infty} c_n y^n \leftarrow \text{ power series expansion}$$

$$\Rightarrow \quad \sum_n n(n-1)\,y^{n-2}c_n - 2\sum_n n y\, c_n + (2\epsilon - 1)\sum y^n c_n = 0$$

$$\sum_{n=2}^{\infty} n(n-1)\,y^{n-2}c_n - 2\sum_{n=0}^{\infty} n y\, c_n + (2\epsilon - 1)\sum_{n=0} y^n c_n = 0$$

$n' = n - 2$

$$\sum_{n=0}^{\infty} (n+2)(n+1)\, y^n\, C_{n+2} - 2\sum n y^n C_n + \sum (2\epsilon-1)\, y^n C_n = 0$$

$$\sum_n y^n \underbrace{\left(C_{n+2}(n+1)(n+2) + (2\epsilon - 1 - 2n) C_n \right)}_{0} = 0$$

$$C_{n+2} = \frac{(2n+1-2\epsilon)C_n}{(n+1)(n+2)}$$ ← recursive definition of coefficients

C_1 and C_0 are arbitrary

u grows at e^{y^2} so $\psi(y)$ has funky behavior

If we restrict energy

$\epsilon = 2n^* + 1$ ← kills all even/odd terms after n^* in u

$E_n = \hbar\omega(n^* + 1/2)$

We set the other even/odd solution by setting C_0 or C_1 to 0

End with even/ odd series that ends at n^*

Wavefunctions are even or odd

For example select n^* s.t. $C_{n^*+2} = 0$

$$2n^* + 1 - 2\epsilon = 0$$

$$2\epsilon = 2n^* + 1$$

$$C_{n+2} = \frac{(2n+1-2\epsilon)C_n}{(n+1)(n+2)} = \frac{2(n-n^*)}{(n+1)(n+2)} C_n$$

↗ restricted coefficients

$n^* = 0$ $\quad C_0 e^{-1/2\, y^2} = C_0 e^{-\frac{m\omega}{2\hbar}x^2}$

Set odd to 0

$n^* = 1$ $\quad C_1 y e^{-y^2/2}$

Set even to 0

$n^* =$ $\quad C_0\left(e^{-1/2 y^2} + \frac{C_2}{C_0} y^2 e^{-1/2 y^2}\right)$ $\qquad \frac{C_2}{C_0} = \frac{2(n-n^*)}{(n+1)(n+2)} = \frac{4}{2} = 2$

⋮

General Solution

$\psi_n = e^{-y^2/2} H_n(y)$

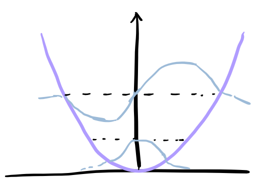
↖ Hermite Polynomial

Energy levels are evenly spaced $E_n = (n + 1/2)\hbar\omega$

linear in n

Use the language quanta of energy for the difference between each energy level

Each state is ground state + quanta



Classical peaks are inverse from the quantum system

For large quanta, the system peaks at the edges

correspondence principal

Systems with large quantum numbers behave classically

Dirac Harmonic Oscillator

Solve the problem in the energy basis (Basis independent approach)

Any relation between operators is independent of the provided basis

Define

$$a = \sqrt{\frac{m\omega}{2\hbar}}\, X + i\sqrt{\frac{1}{2m\omega\hbar}}\, P$$ ← Not Hermitian

Recall

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

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

$$P = \sqrt{\frac{\hbar m\omega}{2}}\, i\,(a^\dagger - a)$$

Consider

$$[a,a^\dagger] = \frac{-i}{2\hbar}[X,P] + \dots = 1$$

a is dimensionless

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

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

$$= \frac{\hbar\omega}{2}\left(a^\dagger a + aa^\dagger\right)$$

$\leftarrow$ $aa^\dagger = 1 + a^\dagger a$

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

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

$$\hat{H} = \frac{H}{\hbar\omega} = (a^\dagger a + 1/2)$$ $\leftarrow$ dimensionless hamiltonian

Consider

$$\epsilon = \frac{E}{\hbar\omega}$$

$$\hat{H}|\epsilon\rangle = \epsilon|\epsilon\rangle$$

$$\hat{H}a^\dagger|\epsilon\rangle = a^\dagger\hat{H}|\epsilon\rangle - [a^\dagger,\hat{H}]|\epsilon\rangle$$

$$[a^\dagger,\hat{H}] = [a^\dagger, a^\dagger a + 1/2] = [a^\dagger, a^\dagger a] = \cancel{[a^\dagger,a^\dagger]}a + a^\dagger[a^\dagger,a] = -a^\dagger$$

$$\hat{H}a^\dagger|\epsilon\rangle = (a^\dagger\hat{H} + a^\dagger)|\epsilon\rangle$$

$$= (a^\dagger\epsilon + a^\dagger)|\epsilon\rangle$$

$$\hat{H}a^\dagger|\epsilon\rangle = (\epsilon+1)\,a^\dagger|\epsilon\rangle$$ $\leftarrow$ eigenvector!

raising operator

$$a^\dagger|\epsilon\rangle = c_+|\epsilon+1\rangle$$

lowering operator

$$a|\epsilon\rangle = c_-|\epsilon-1\rangle$$

Any positive semidefinite operator cannot have a negative eigenstate

There must exist a state such that

$$a|0\rangle = 0$$

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

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

$$\epsilon_0 = 1/2$$

$$E_0 = \frac{\hbar\omega}{2}$$ $\leftarrow$ lowest energy

Let's solve for X and P operators in $\hat{H}$ basis

$$a^\dagger|\epsilon\rangle = c_+|\epsilon+1\rangle$$

$$\langle\epsilon|a = c_+^*\langle\epsilon+1|$$

$$\langle\epsilon|a\,a^\dagger|\epsilon\rangle = |c_+|^2\cdot\underbrace{\langle\epsilon+1|\epsilon+1\rangle}_{1}$$

$$\langle n|a^\dagger a + 1|n\rangle = |c_+|^2$$

level

$$n+1 = |c_+|^2$$

$$c_+ = \sqrt{n+1}\,e^{i\varphi}$$

$$= \sqrt{n+1}$$

Same logic: $c_- = \sqrt{n}$

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

With this in hand we can write the matrix representation of a and $a^\dagger$

$$a = \begin{array}{c} \\ n=0 \\ n=1 \\ n=2 \\ n=3 \\ n=4 \end{array} \begin{array}{c} \begin{array}{ccccc} n=0 & n=1 & n=2 & n=3 & n=4 \end{array} \\ \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} & 0 \\ 0 & 0 & 0 & 0 & \sqrt{4} \\ 0 & 0 & 0 & 0 & 0 \cdots \\ & & & & \vdots \end{pmatrix} \end{array} \qquad a^\dagger = \begin{array}{c} \\ n=0 \\ n=1 \\ n=2 \\ n=3 \\ n=4 \end{array} \begin{array}{c} \begin{array}{ccccc} n=0 & n=1 & n=2 & n=3 & n=4 \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 \cdots \\ & & & & \vdots \end{pmatrix} \end{array}$$

We can now solve for x and P

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

Consider the uncertainity of x

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

$$\langle x\rangle = \langle n|x|n\rangle \propto \langle n|(a+a^\dagger)|n\rangle = 0$$

only non zero for n+1 and n-1

$$\langle x^2\rangle = \langle n|x^2|n\rangle \propto \langle n|(a+a^\dagger)(a+a^\dagger)|n\rangle$$

only cross terms don't vanish

$$= \langle n|\, a^\dagger a + a a^\dagger\, |n\rangle$$

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

Solving for the wavefunctions

$$\psi_n(x) = \langle x|n\rangle$$

$$a|0\rangle = 0$$

$$\left(x + \frac{d}{dx}\right)|0\rangle = 0$$

rough combination of x and P

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

$$\frac{d\psi_0}{dx} = -x\,\psi_0$$

$$\psi_0(x) = e^{-x^2/2}$$

rough solution form

Normalize to find groundstate wavefunction

$$\sqrt{\frac{m\omega}{2\hbar}}\; e^{-\frac{m\omega}{2}x^2}$$

Apply raising operator

$$\langle x|a^\dagger|0\rangle = \langle x|1\rangle = \psi_1(x)$$

$$\langle x|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$$

Uncertainity Principle

Since X and P do not commute, we cannot have a definite position and momentum

Any bound waveform is the sum of definite wavelengths

decomposed via Fourier Analysis

Crude Intuition of Uncertainity Theorem

We know that

$$p = \hbar/\lambda$$

Consider the wave

$$p = \frac{\hbar}{\lambda} = \hbar/_{L/N} = \frac{N\hbar}{L}$$

$$\Delta p = \frac{\hbar}{L}(\Delta N) \approx \frac{\hbar}{L}$$ ← Δx

$$\Delta p \Delta x \simeq \hbar$$

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

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

Let $\bar{x} = x - \langle x\rangle$ and $\bar{p} = p - \langle p\rangle$

$$(\Delta x)^2(\Delta p)^2 = \langle\bar{x}^2\rangle\langle\bar{p}^2\rangle$$

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

↖ shifting by a coefficient doesn't change commutator

$$= \langle\psi|\bar{x}\bar{x}|\psi\rangle\langle\psi|\bar{p}\bar{p}|\psi\rangle$$

$$= \langle\bar{x}\psi|\bar{x}\psi\rangle\langle\bar{p}\psi|\bar{p}\psi\rangle$$

Applying Schwarz Inequality

$$(\Delta x)^2(\Delta p)^2 \geq |\langle\bar{x}\psi|\bar{p}\psi\rangle|^2$$

$$|\langle\varphi|\psi\rangle|^2 \leq \langle\varphi|\varphi\rangle\langle\psi|\psi\rangle$$

equality if $|\bar{p}\psi\rangle = c|\bar{x}\psi\rangle$

anti-commutator $xp+px$

$$(\Delta x)^2(\Delta p)^2 \geq |\langle\bar{x}\psi|\bar{p}\psi\rangle|^2 = |\langle\psi|xp|\psi\rangle|^2 = \left|\langle\psi|\frac{[x,p]+[x,p]_+}{2}|\psi\rangle\right|^2$$

$$(\Delta x)^2(\Delta p)^2 \geq \frac{1}{4}|\langle\psi|[x,p]+[x,p]_+|\psi\rangle|$$

$$[x,p] = i\hbar$$

$$(\Delta x)^2(\Delta p)^2 \geq \frac{\hbar^2}{4} + \frac{1}{4}|\langle\psi|[x,p]_+|\psi\rangle|$$

If the two vectors are parallel we find the lowest bound

$$(\Delta x)^2(\Delta p)^2 \geq \frac{\hbar^2}{4}$$

Consider $\bar{p}|\psi\rangle = c\bar{x}|\psi\rangle$

$$\langle\psi|\bar{p} = \langle\psi|\bar{x}\,c^*$$

$$0 = \langle\psi|xp+px|\psi\rangle = \langle\psi|x\,cx + xc^*x|\psi\rangle$$

$$= (c+c^*)\langle\psi|x^2|\psi\rangle$$

$$\bar{p}|\psi\rangle = i\,|c|\,\bar{x}|\psi\rangle \qquad c = i|c|$$

$$-i\hbar\frac{d\psi}{dx} = i|c|\,x\psi + \frac{p_0}{i}|\psi\rangle$$

$$\int\frac{d\psi}{\psi} = -\int\frac{|c|x}{\hbar}dx$$

$$\psi(x) = e^{\frac{-|c|(x-x_0)^2}{\hbar}}\,e^{\frac{ip_0x}{\hbar}}$$ ← minimum uncertainity wavefunction

Uncertainty Principle in the Quantum Harmonic Oscillator

$$\langle H\rangle = \frac{\langle p\rangle^2}{2m} + \frac{1}{2}m\omega^2\langle x\rangle^2$$

$$= \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2$$ applying $\langle x\rangle = \langle p\rangle = 0$

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

minimum energy is

$$\frac{\hbar\omega}{2}$$

Uncertainity Principle and the Hydrogen Atom

$$H = \frac{P_x^2 + P_y^2 + P_z^2}{2m} - \frac{e^2}{\sqrt{x^2+y^2+z^2}}$$

$$\langle H\rangle \simeq \frac{3(\Delta P)^2}{2m} - \frac{e^2}{\sqrt{3\Delta^2}}$$

$\Delta P_x = \Delta P_y = \Delta P_z$

$$= \frac{3}{2m}\frac{\hbar^2}{4\Delta^2} - \frac{e^2}{\sqrt{3}\Delta}$$

$$\langle H\rangle \simeq -\frac{me^4}{\hbar^2}\cdot c \leftarrow \text{order 1 number}$$

Actually $\frac{-me^4}{2\hbar^2}$

$$\Delta = \frac{\hbar}{me^2} \leftarrow \text{Bohr radius}$$

Uncertainity in Relativity

$$\Delta E\, \Delta t \geq \frac{\hbar}{2}$$

$\simeq \hbar$

no uncertainity in time

Consider a pure energy eigenstate

$$|\psi\rangle = |E\rangle e^{-iEt/\hbar}$$

All observations are independent of time

Δt is the time over which something significant happens

Consider the state

$$|\psi\rangle = |E_1\rangle e^{-iE_1t/\hbar} + |E_2\rangle e^{-E_2t/\hbar}$$

$$\Omega(t) = \langle\psi|\Omega|\psi\rangle$$

$$= \langle E_1|\Omega|E_1\rangle + \langle E_2|\Omega|E_2\rangle + \langle E_2|\Omega|E_1\rangle e^{-i(E_1-E_2)t/\hbar} + \langle E_1|\Omega|E_2\rangle e^{i(E_1-E_2)t/\hbar}$$

$$\simeq \text{const} + \cos\left(\frac{\Delta E}{\hbar}t\right)$$

period

$$\frac{\Delta E\, t}{\hbar} \simeq \pi$$

Multiple Particles

Recap of Single Particle

$|x\rangle \quad |\psi\rangle$

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

$P(x) = |\psi(x)|^2$

$P \to -i\hbar\frac{d}{dx} \qquad X \to x$

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

Two particle System

case 1: Particles are uncoupled

paste individual solutions together

Case 2: Potential is dependent on relative distance between particles

$$\mathcal{L} = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 - V(x_1 - x_2) \qquad \frac{1}{2}M\dot{x}_c + \frac{1}{2}\mu\dot{x}_r^2 - V(x_r)$$

$$\mathcal{H} = \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + V(x_1 - x_2) \xrightarrow{\text{Change of coordinates}} \frac{P_c^2}{2M} + \frac{P_r^2}{2\mu} + V(x_r)$$

Two particle Schrodinger Equation

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

Case 1: Non-interacting particles

$$V = V(x_1) + V(x_2)$$

$$\Rightarrow \quad H = H_1(X_1, P_1) + H_2(X_2, P_2)$$

$$i\hbar\frac{\partial\psi_1}{\partial t} = H_1\left(x_1, -i\hbar\frac{\partial}{\partial x_1}\right)\psi_1 \quad \text{and} \quad i\hbar\frac{\partial\psi_2}{\partial t} = H_2\left(x_2, -i\hbar\frac{\partial}{\partial x_2}\right)\psi_2$$

Final solution : $\psi = \psi_1 \psi_2 \leftarrow$ implies statistical independence

Case 2 : Interacting Particles

$V = V(x_1 - x_2)$

$\Rightarrow \quad H = H_c(P_c) + H_r(x_r, P_r)$

Each part evolves independently

Energy Eigenfunctions are the product of solutions to each part with energy equal to their sum

Solutions to $H \psi_E = E \psi_E$ are products of solutions to $H_c \psi_{E_c} = E_c \psi_{E_c}$ and $H_r \psi_{E_r} = E_r \psi_{E_r}$

with energy $E = E_c + E_r$

Direct Product Vectors

$|x_1, x_2\rangle = |x_1\rangle \otimes |x_2\rangle$ represents two particles in a 1D space

more to come later

Identical Particles

Identical particles can be distinguishable if they have distinct trajectories

Quantum particles do not have trajectories

All predictions must be the same if the particles are exchanged

Instead of $|a,b\rangle$ and $|b,a\rangle$ we say $\alpha|a,b\rangle + \beta|b,a\rangle$

$\alpha|b,a\rangle + \beta|a,b\rangle = \gamma(\alpha|ab\rangle + \beta|ba\rangle)$ $\leftarrow$ invariant

$\beta = \gamma\alpha$

$\alpha = \gamma\beta$

$\beta = \gamma^2 \beta$

$\gamma = \pm 1$

$|a,b\,;S\rangle = \frac{1}{\sqrt{2}}\left(|a,b\rangle + |b,a\rangle\right)$ $\leftarrow$ Symmetric (Bosons)

$|a,b\,;A\rangle = \frac{1}{\sqrt{2}}\left(|ab\rangle - |b,a\rangle\right)$ $\leftarrow$ Anti-Symmetric (Fermions)

no two fermions can have the same state

Postulate : Some particles are always bosonic or fermionic

Fermions have half integer spins

Bosons have integer angular momentum

Wavefunctions

$\psi(x_1,x_2) = \langle x_1,x_2|\psi\rangle$

$P(x_1,x_2) = |\langle x_1,x_2|\psi\rangle|^2$

$|\psi(S,A)\rangle = |n_1,n_2\,;S/A\rangle$

$= \dfrac{|n_1n_2\rangle \pm |n_2n_1\rangle}{\sqrt{2}}$

$|x_1,x_2\,;S/A\rangle = \dfrac{|x_1,x_2\rangle \pm |x_2,x_1\rangle}{\sqrt{2}}$

$\psi(x_1,x_2\,;S/A\rangle = \frac{1}{\sqrt{2}}\left(\langle x_1,x_2\,; S/A\,|n_1,n_2\,;S/A\rangle\right)$

$= \frac{1}{\sqrt{2}}\left[\dfrac{\langle x_1,x_2| \pm \langle x_2x_1|}{\sqrt{2}}\,\middle|\,\dfrac{|n_1n_2\rangle \pm |n_2n_1\rangle}{\sqrt{2}}\right.$

$= \frac{1}{2\sqrt{2}}\left(\langle x_1x_2|n_1n_2\rangle + \langle x_2x_1|n_2n_1\rangle \pm \langle x_1,x_2|n_2n_1\rangle \pm \langle x_2x_1|n_1n_2\rangle\right)$

$= \frac{1}{2\sqrt{2}}\left(\varphi_{n_1}(x_1)\varphi_{n_2}(x_2) + \varphi_{n_2}(x_2)\varphi_{n_1}(x_1) \pm \varphi_{n_2}(x_1)\varphi_{n_1}(x_2) \pm \varphi_{n_1}(x_2)\varphi_{n_2}(x_1)\right)$

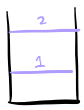
$= \frac{1}{\sqrt{2}}\left(\varphi_{n_1}(x_1)\varphi_{n_2}(x_2) + \varphi_{n_2}(x_1)\varphi_{n_1}(x_2)\right.$

$= \left\langle x_1,x_2\,\middle|\,\dfrac{|n_1,n_2\rangle \pm |n_2,n_1\rangle}{\sqrt{\ }}\right\rangle$

$\psi(x_1,x_2\,;S/A) = \langle x_1,x_2|n_1,n_2\,;S/A\rangle$

$$\int |\psi|^2 dx_1 dx_2 = \int \langle n_1 n_2 ; S/A | x_1, x_2 \rangle \langle x_1, x_2 | n_1, n_2 ; S/A \rangle \, dx_1 dx_2$$

2 Identical Particles in a box



$\varphi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$

$n_1 = 1$, $n_2 = 2$, both bosons

$$\psi(x_1, x_2) = \frac{\varphi_1(x_1)\varphi_2(x_2) + \varphi_2(x_1)\varphi_1(x_2)}{\sqrt{2}}$$

$n_1 = 1$, $n_2 = 2$, both Fermions

$$\psi(x_1, x_2) = \frac{\varphi_1(x_1)\varphi_2(x_2) - \varphi_2(x_1)\varphi_1(x_2)}{\sqrt{2}}$$

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_1(x_1) & \varphi_1(x_2) \\ \varphi_2(x_1) & \varphi_2(x_2) \end{vmatrix}$$ ← Determinant

Symmetries and Conservation Laws

Every conservation law is connected to the invariance of the Hamiltonian

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

If $\mathcal{H}(q + \delta q, p + \delta p) = \mathcal{H}(q, p)$

then $\frac{\partial \mathcal{H}}{\partial q} \delta q + \frac{\partial \mathcal{H}}{\partial p} \delta p = 0$

Consider $g(q, p)$ = generator

$$\delta q = \epsilon \frac{\partial g}{\partial p} \qquad \delta p = -\epsilon \frac{\partial g}{\partial q}$$

Now,

$$0 = \epsilon \frac{\partial \mathcal{H}}{\partial q} \frac{\partial g}{\partial p} - \epsilon \frac{\partial \mathcal{H}}{\partial p} \frac{\partial g}{\partial q}$$

$$= \epsilon \{\mathcal{H}, g\} = -\{g, \mathcal{H}\}$$

$$\frac{dg}{dt} = \{g, \mathcal{H}\}$$

Review

Translation Operator in Quantum Mechanics

$$T(a)|x\rangle = |x + a\rangle$$

$$\langle x | T(a) | \psi \rangle = \langle x | \psi_a \rangle = \psi_a(x)$$

$T^\dagger T = I$

↖ unitary operator

Unitary operators correspond to rotations in quantum mechanics

$$T^\dagger |x\rangle = |x - a\rangle$$

$$\langle x | T(a) | \psi \rangle$$

$$\langle T^\dagger (x) | \psi \rangle$$

$$\langle x - a | \psi \rangle = \psi(x - a)$$

T should be constructed as a function of $\underline{X}$ and $\underline{P}$

Consider $\langle x | T(\epsilon) | \psi \rangle = \psi(x - \epsilon)$

$= \psi(x) - \epsilon \frac{\partial \psi}{\partial x} + \dots$

taylor expansion ↗

$$= \left(I - \frac{i\epsilon}{\hbar} \underline{P}\right) \psi$$

$$T(\epsilon) = I - \frac{i\epsilon}{\hbar} \underline{P}$$

For a finite translation

$$T(a) = \lim_{N \to \infty} \left(I - i \frac{a}{N} \frac{P}{\hbar}\right)^N = e^{-i \frac{aP}{\hbar}} = e^{-a \frac{d}{dx}}$$

taylor expansion

$$e^{-a \frac{d}{dx}} \psi(x) = \psi(x - a)$$

We define invariance via expectation value

$$\langle \psi | H | \psi \rangle = \langle T\psi | H | T\psi \rangle \quad \forall \psi$$

$$\langle \psi | H - T^\dagger H T | \psi \rangle = 0$$

$$H = T^{\dagger} H T$$ ← translational invariance

$$\left(I + \frac{i\varepsilon}{\hbar} P\right) H \left(I - \frac{i\varepsilon P}{\hbar}\right) = 0$$

$$\cancel{H} + \frac{i\varepsilon}{\hbar}(PH - HP) = \cancel{H}$$

$$PH - HP = 0$$

$$[P,H] = 0$$

Via Ehrenfest's Theorem

$$\frac{d}{dt}\langle P \rangle = \frac{1}{i\hbar}[P,H] = 0$$

When two operators commute, we can find joint Eigenstates

Consider the Propagator

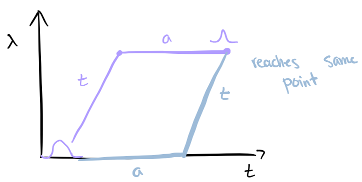
$$U(t) = e^{-iHt/\hbar}$$

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

$$PU(t) = U(t)P$$ ← since U is just an exponential of H

Implies

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



Active and Passive Transformations

$$\langle \psi | X | \psi \rangle = \langle X \rangle$$

$$\langle T(a)\psi | X | T(a)\psi \rangle = \langle X + a \rangle$$ ← operators are constant but states move

$$\langle \psi | T^{\dagger} X T | \psi \rangle = \langle X + a \rangle$$ ← States don't change, operators do

If this is true for every ψ

$$T^{\dagger} X T = X + a$$

↖ active transformation

Translationally invariant Hamiltonians only depend on coordinate differences

If the Hamiltonian changes with time

$$\frac{d}{dt}\langle H \rangle = \langle \psi | [H,H] | \psi \rangle + \langle \psi | \dot{H} | \psi \rangle$$

Ehrenfest's Theore ↗ Energy is conserved when H is independent of time

Parity

$$\Pi|x\rangle = |-x\rangle$$

$$\Pi^2 |x\rangle = |x\rangle \quad \text{for all } x$$

$$\Pi^2 = I$$

Π is also unitary

$$\Pi \Pi^{\dagger} = I$$

$$\Pi = \Pi^{\dagger}$$

$$\langle \Pi\psi | x | \Pi\psi \rangle = \int \psi(-x)\, x\, \psi(x)\, dx = -\langle \psi | x | \psi \rangle$$

$$= \langle \psi | \Pi^{\dagger} x \Pi | \psi \rangle$$

$$\Pi^{\dagger} x \Pi = -x$$

Parity Invariance

$$H(\Pi x \Pi, \Pi P \Pi) = H(x,p) = 0$$

$$H(-x,-p) = H(x,p)$$

$$\Pi H \Pi = H$$

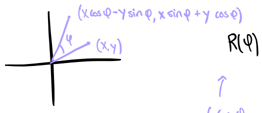
$$\Pi H = H \Pi$$

$$[\Pi, H] = 0$$

↖ For example, Harmonic Oscillator

Rotations

Rotation in 2D



$$R(\varphi)\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x\cos\varphi - y\sin\varphi \\ x\sin\varphi + y\cos\varphi \end{pmatrix}$$

$$R(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}$$

In QM we work with infinite dimensions

$$U(R(\varphi))|x,y\rangle = |x\cos\varphi - y\sin\varphi,\ x\sin\varphi + y\cos\varphi\rangle$$

Consider

$$\langle x,y|\psi\rangle = \psi(x,y)$$

$$\langle x,y|U(R)|\psi\rangle = \langle U^\dagger(R)\, xy|\psi\rangle$$

For an infinitesimal translation

$$U(R(\epsilon))|x,y\rangle = |x-\epsilon y,\ y+\epsilon x\rangle$$

$$\langle xy|U(R(\epsilon))|\psi\rangle = \langle x+\epsilon y,\ y-\epsilon x|\psi\rangle = \psi(x+\epsilon y,\ y-\epsilon x)$$

Now, let's apply the taylor expansion

$$\psi(x+\epsilon y,\ y-\epsilon x) = \psi(x,y) + \epsilon y\frac{\partial\psi}{\partial x} - \epsilon x\frac{\partial\psi}{\partial y}$$

$$= I - \frac{i}{\hbar}\epsilon L_z$$

$$L_z = XP_y - YP_x$$ ← Angular momentum analog

Rotational Invariance

$$\langle\psi|U^\dagger H U|\psi\rangle = \langle\psi|H|\psi\rangle \quad \forall\ |\psi\rangle$$

$$H(U^\dagger X U,\ U^\dagger Y U,\ U^\dagger P_x U,\ U^\dagger P_y U) = H(X,Y,P_x,P_y)$$

$$U^\dagger H U = H$$ → necessary condition for rotational invariance

$$U = I - \frac{i\epsilon}{\hbar}L_z$$

$$\left(I + \frac{i\epsilon}{\hbar}L_z\right)H\left(I - \frac{i\epsilon}{\hbar}L_z\right) = H$$

$$H + \frac{i\epsilon}{\hbar}\underbrace{[H, L_z]}_{0} = H$$

Exist simultaneous eigenstates for L_z and H

We see that the Hamiltonian takes the following form

$$U^\dagger H(X,Y,P_x,P_y)U = H(X\cos\varphi - Y\sin\varphi,\ X\sin\varphi + Y\cos\varphi,\ P_x\cos\varphi - P_y\sin\varphi,\ P_x\sin\varphi + P_y\cos\varphi)$$

Eigenstates of L_z operator

$$L_z = XP_y - YP_x$$

$$= x\left(-i\hbar\frac{\partial}{\partial y}\right) + y\left(i\hbar\frac{\partial}{\partial x}\right)$$

In polar coordinates, rotations only effect one coordinate

$$\psi(\rho,\phi) \to \psi(\rho,\phi)$$

$$= \left(I - \frac{i\epsilon}{\hbar}\left(-i\hbar\frac{\partial}{\partial\rho}\right)\right)\psi$$

$$L_z = -i\hbar\frac{\partial}{\partial\rho}$$

$$L_z|l_z\rangle = l_x|l_z\rangle$$

$$\langle\rho\varphi|l_z\rangle = \psi_{l_z}(\rho,\varphi)$$

$$-i\hbar\frac{\partial\psi_{l_z}}{\partial\varphi} = l_z\psi_{l_z}$$

$$\psi_{l_z}(\rho,\varphi) = R_l(\rho)\Phi_l(\varphi)$$

$$R_l(\rho)\left[-i\hbar\frac{d\Phi_l}{d\varphi}\right] = R_l(\rho)\, l_z\,\Phi_l(\varphi)$$

R is a spectator

$$\psi_\ell(\rho,\varphi) = R_\ell(\rho)\, e^{i/\hbar\, \ell_z \varphi}$$

Additional Requirement

$$e^{\frac{i}{\hbar}\ell_z(\varphi+2\pi)} = e^{i/\hbar\, \ell_z \varphi}$$

$$\frac{2\pi \ell_z}{\hbar} = 2\pi m \quad , m = 0,1,2,\ldots$$

$$\ell_z = m\hbar \qquad m = 0,1,2,\ldots$$

Schrodinger's Equation in 2D

$$\frac{-\hbar^2}{2\mu}\nabla^2\psi_E + V\psi_E = E\psi_E$$

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

if $V(\rho)$ then the problem is rotationally invariant

Eigenfunction: $e^{im\varphi} R_{mE}(\rho)$

Skipping some algebra

$$\frac{-\hbar^2}{2m}\left(\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{m^2}{\rho^2}\right)R_{mE}(\rho) + V(\rho)R_{mE} = E R_{mE}(\rho)$$

Rotations in 3-dimensions

$$\left.\begin{aligned} L_z &= xP_y - yP_x \\ L_x &= yP_z - zP_y \\ L_y &= zP_x - xP_z \end{aligned}\right\} \quad L^2 = L_x^2 + L_y^2 + L_z^2$$

$$[L^2, L_i] = 0$$

$$[L_x, L_y] = [yP_z - zP_y,\, zP_x - xP_z]$$

$$= [yP_z, zP_x] - [zP_y, xP_z]$$

$$= y\underbrace{[P_z, z]}_{-i\hbar}P_x - P_y[z, P_z]x$$

$$= -i\hbar\, yP_x + i\hbar\, P_y x$$

$$= i\hbar L_z$$

non-zero commutator shows that order of rotation does matter

Consider

$$L^2|\alpha,B\rangle = \alpha|\alpha,B\rangle$$

$$L_z|\alpha,B\rangle = B|\alpha,B\rangle$$

$$L_+ = L_x + iL_y$$

$$[L_z, L_+] = [L_z, L_x + iL_y]$$

$$= i\hbar L_y + i(-i\hbar L_x)$$

$$= \hbar(L_x + iL_y)$$

$$= \hbar L_+$$

$$L_z L_+|\alpha,B\rangle = (L_+L_z - [L_+,L_z])|\alpha,B\rangle$$

$$= L_+ B|\alpha,B\rangle + \hbar L_+|\alpha,B\rangle$$

$$= (B+\hbar)L_+|\alpha,B\rangle$$

eigenvalue of L_z is raised by B

$$L_\pm|\alpha,B\rangle = C_\pm|\alpha, B\pm\hbar\rangle$$

There must be a state you cannot raise

$L_+|\alpha,\beta^{max}\rangle = 0$

$L_-L_+|\alpha,\beta^{max}\rangle = 0$

$(L_x - iL_y)(L_x + iL_y)|\alpha,\beta^{max}\rangle = 0$

$(L_x^2 + L_y^2 + iL_xL_y)|\alpha,\beta^{max}\rangle = 0$

$\alpha = \beta^{max}(\beta^{max} + \hbar)$

$$\left\{\begin{array}{l} |\alpha,\beta^{max}\rangle \\ \vdots \\ |\alpha,\beta^{max}-\hbar\rangle \\ \vdots \\ |\alpha,-\beta^{max}\rangle \end{array}\right.$$

There is a state you cannot lower

$L_-|\alpha,\beta^{min}\rangle = 0$

$\alpha = \beta^{min}(\hbar - \beta^{min}$

$\beta^{min} = -\beta^{max}$

$$\beta^{max} - \beta^{min} = k\hbar$$

$$2\beta^{max} = k\hbar$$

$$\beta^{max} = \frac{k}{2}\hbar$$

Families of Solutions

$k=0$

$\alpha = 0$ $\quad |0,0\rangle$

$\beta = 0$

$k=1$

$\alpha = \frac{3}{4}\hbar^2$ $\quad |\tfrac{3}{4}\hbar^2|\hbar/2\rangle$ ← half integer eigenvalues

$\beta = \hbar/2 \, . . -\hbar/2$ $\quad |\tfrac{3}{4}\hbar^2|-\hbar/2\rangle$

$k=2$

$\alpha = 2\hbar^2$

$\beta = \hbar, 0, \hbar$

Only use integer solutions based on physical restrictions

$$J^2|\alpha,\beta\rangle = |\hbar^2(k/2)(k/2+1), m\hbar\rangle$$

$$= |\hbar^2(j)(j+1), m\hbar\rangle$$

$J = 0, \cancel{1/2}, 1, \cancel{3/2}, 2, \ldots$

ignore for L

$$\boxed{\begin{array}{l} L^2|l,m\rangle = l(l+1)\hbar^2|l,m\rangle \\ L_z|l,m\rangle = m\hbar|l,m\rangle \end{array}}$$

$l = 0,1,2,3, \ldots$

Solving for constants

$L_+|l,m\rangle = C_+|l,m+1\rangle$

$\langle l,m|L_- = (C_+)^*\langle l,m+1|$

$\langle l,m|L_-L_+|l,m\rangle = |C_+|^2$

$\langle l,m|(L_x - iL_y)(L_x + iL_y)|l,m\rangle = |C_+|^2$

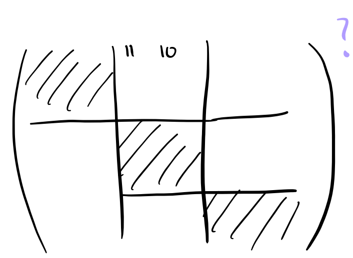
$\langle l,m|L_x^2 + L_y^2 + i[L_x,L_y]|l,m\rangle = |C_+|^2$

$\langle l,m|(L^2 - L_z^2 - \hbar L_z)|l,m\rangle = |C_+|^2$

$= \hbar^2 l(l+1) - m(m+1)\hbar^2$

$C_+ = \hbar\sqrt{l(l+1) - m(m+1)}$

$L_\pm|l,m\rangle = \hbar\sqrt{(l \mp m)(l \pm m+1)}\;|l,m\rangle$ →



Consider the state $|\ell\ell\rangle$

$$L_+ |\ell,\ell\rangle = 0$$

$$\langle r,\theta,\varphi | L_+ | \ell,\ell\rangle = 0$$

$$\left(\qquad \right) \psi_{\ell,\ell}(r,\theta,\phi) = 0$$

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

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

With rotational symmetry

$$\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right)\psi_\ell^\ell(\theta,\varphi) = 0$$

$$P_\ell^\ell(\theta)e^{i\ell\phi}$$

$$\left(\frac{\partial}{\partial\theta} - \ell\cot\theta\right)P_\ell^\ell(\theta) = 0$$

$$\frac{\partial P}{\partial\theta} = \ell\cot\theta\, P$$

$$P_\ell^\ell = A\sin^\ell\theta$$

$$\psi_\ell^\ell = Ne^{i\ell\varphi}\sin^\ell\theta$$

$$Y_\ell^{\ell-1} = (L_-)\psi_\ell^\ell$$

In three dimensions

$$\left.\begin{aligned}\psi_\ell^m(\theta,\varphi) = P_\ell^m(\theta)e^{im\phi} N_{\ell,m} \\ m = \ell, \dots \ell\end{aligned}\right\}$$ Spherical Harmonics

$$T(\theta,\varphi) = \sum \psi_\ell^m(\theta,\varphi)C_{\ell,m}$$

$$\psi_0^0(\theta,\varphi) = \frac{1}{\sqrt{4\pi}} = \int_{-1}^{1}\int_0^{2\pi}$$ ← integration over the surface of the sphere

Hydrogen Atom

Rydberg Formula for atomic transitions

$$E_{n_2 n_1} = R\left(1/n_2^2 - 1/n_1^2\right)$$

$$R = \frac{me^4}{2\hbar^2}$$

Schrodinger's Equation in spherical coordinates

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

$$H = \frac{P^2}{2m} + V = \frac{P^2}{2m} - \frac{e^2}{r}$$

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

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \underbrace{\frac{1}{r^2}\left(\frac{1}{\sin\phi}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\phi} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)}$$

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

Solution of the form:

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

Plugging it in:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial R}{\partial r}\cancel{Y}\right) - \frac{1}{r^2 \cancel{\hbar^2}}\, \ell(\ell+1)\cancel{\hbar^2}\, \cancel{Y_\ell^m} R + V(r)\cancel{Y}R = E\cancel{Y}R$$

$$\frac{\partial}{\partial r} \to \frac{d}{dr}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\ell(\ell+1)}{r^2}\cdot\frac{2m}{\hbar^2}R - \frac{2m}{\hbar^2}V R_{E,\ell} = E R_{E,\ell}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2m}{\hbar^2}\left(E + \frac{e^2}{r} - \frac{\ell(\ell+1)}{r^2}\right)R = 0$$

$R = \frac{u}{r}$, $u(0) = 0$

$r \to r$ for ease of notation

$$\boxed{\frac{d^2u}{dr^2} + \frac{2m}{\hbar^2}\left(E - V(r) - \frac{\ell(\ell+1)^2\hbar^2}{2mr^2}\right)u = 0}$$

As $r \to \infty$

$$\frac{d^2u}{dr^2} = -\frac{2mE}{\hbar^2}u$$

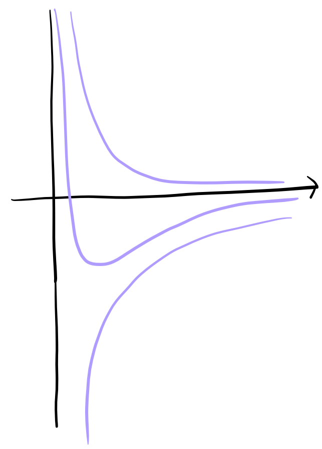
$E<0$ so solutions die exponentially

$E = -W$ where $W>0$

$$u'' = \frac{2mW}{\hbar^2} = k^2 u$$

$$k = \sqrt{\frac{2mW}{\hbar^2}}$$

$$\longrightarrow u = \cancel{Ae^{kr}} + Be^{-kr} \xrightarrow{r\to\infty} e^{-kr}$$



As $r \to 0$

$$u'' = \frac{\ell(\ell+1)}{r^2}u \longrightarrow u(r) = r^{\ell+1}$$

In natural units $r \to \rho\sqrt{\frac{\hbar^2}{2mW}}$

$$u(\rho) = e^{-\rho}v(\rho)$$

$kr \to \rho$, $u(\rho) = e^{-\rho}v(\rho)$

$$v'' - 2v' + \frac{\lambda e^2}{\rho}v - \frac{\ell(\ell+1)}{\rho^2}v = 0$$

$$\lambda = \sqrt{\frac{2m}{\hbar^2 W}}$$

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

↳ yields a two term recursion relation between c_k and c_{k+1}

$$v'' = \sum_{k=0}^{\infty} (\ell+k)(\ell+k-1)\rho^{\ell+k-2} c_k \qquad -\ell(\ell+1)\frac{v}{\rho^2} = -\ell(\ell+1)\sum_{k=0}^{\infty}\rho^{\ell+k-2} c_k$$

$$-2v' = \sum_{k=0}^{\infty} -2(\ell+k)\rho^{\ell+k-1} c_k \qquad \lambda e^2\frac{v}{\rho} = \lambda e^2\sum_{k=0}^{\infty}\rho^{\ell+k-1} c_k$$

Collecting like powers

$$\sum_{k=0}^{\infty} C_k \left[(\ell+k)(\ell+k-1) - \ell(\ell+1)\right] \rho^{\ell+k-2} + C_k \left[\lambda e^2 - 2\ell - 2k\right] \rho^{\ell+k-1} = 0$$

$$C_{k+1} \left[(\ell+k)(\ell+k+1) - \ell(\ell+1)\right] = C_k \left[\lambda e^2 - 2\ell - 2k\right]$$

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

$k \to \infty$ $\quad \dfrac{+2k}{k^2} = \dfrac{2}{k}$

?

Solutions only when $\lambda e^2 = 2(\ell + k^{max} + 1) = 2n$

$$\lambda = \sqrt{\frac{2m}{\hbar^2 W}} \qquad \lambda = \frac{2n}{e^2}, \quad \lambda^2 = \frac{4n^2}{e^4}$$

$$W = \frac{me^4}{2\hbar^2 n^2}$$

$$E = -\frac{me^4}{2\hbar^2 n^2} \qquad n = 1, 2, \ldots$$

recovers Rydberg constant

principal quantum number

Multiplicities of n

$n=1 \implies 1 = k^{max} + \ell + 1$ $\qquad$ 0^{th} order polynomial

$k^{max} = \ell = 0$

$$\psi_{1,0,0} = \rho^{\ell=0} C_0 \cdot e^{-\rho}$$

n, ℓ, m

falling exponential

$$\rho = r\sqrt{\frac{2mW}{\hbar^2}} = r\sqrt{\frac{2mW}{\hbar^2}} \cdot \sqrt{\frac{me^4}{2\hbar^2 n^2}} = r \cdot \frac{me^2}{\hbar^2 n} = \frac{r}{n a_0}$$

Bohr's Radius $\dfrac{\hbar^2}{me^2}$

$n=2 \implies 2 = k^{max} + \ell + 1$

$k^{max} + \ell = 1$

$k^{max} = 0, \ \ell = 1$ $\quad$ or $\quad$ $\ell = 0$ and $k^{max} = 1$

$m = \pm 1, 0$

Hidden symmetry

$n=2$ — $\ell=0$ $\quad$ — $m=1$ $\quad$ — $m=2$ $\quad$ — $m=3$ $\quad$ $\ell=1$

deg of degeneracy $= n^2$

$n=1$ —

Hydrogen atom potential has an additional symmetry

Wavefunctions

$k^{max} = 0, \ \ell = 1$

$$\psi_{2,1,m} = \rho^1 C_0 e^{-\rho} = \underbrace{\left(\frac{r}{a_0}\right) C_0 e^{-r/2a_0} Y_\ell^m}_{\text{normal units}}$$

$k^{max} = 1, \quad l = 0$

solve via recursion relation $= -1$

$$\varphi_{2,0,m} = \rho^0 (c_0 + c_1 \rho) e^{-\rho} = \underbrace{A\left(1 + \frac{c_1}{c_0}\frac{r}{2a_0}\right) e^{-r/2a_0}}_{\text{normal units}} Y_0^m$$

Define size of an atom via

$$\varphi_{n,n-1,m} = r^{n-1} e^{-r/2a_0} Y$$

$$P(r) = r^{2n} e^{-2r/na_0}$$

Find maximum

$$r^* = n^2 a_0$$

Important Numbers

$$\hbar c = 2000 \text{ e.V. A}$$

$$mc^2 = 0.5 \cdot 10^6 \text{ eV}$$

$$\alpha = \frac{e^2}{\hbar c} \simeq 1/137$$

Non-hydrogen Atoms

$|n, l, m\rangle$ is not degenerate for different l

$n=2$ $\uparrow\downarrow$ Li, Be $\uparrow\downarrow$ B, C $\uparrow\downarrow$ N, O $\uparrow\downarrow$ F, Ne

$n=1$ $\uparrow\downarrow$ H, He $l=0, m=0, s=\pm$