Free particle

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

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

$$k = \pm\frac{\sqrt{2mE}}{\hbar}$$

$$\psi_k(x) = A_k e^{ikx}$$

Orthonormality:

$$\begin{aligned}\int \psi_k^*(x)\psi_{k'}(x)dx = A_k A_{k'}\int e^{-ikx}e^{-ik'x}dx = A_k A_{k'}\int e^{-i(k-k')x}dx\\ = A_k A_{k'}\lim_{L\to\infty}\int_{-L}^{L} e^{-i(k-k')x}dx = A_k A_{k'}\lim_{L\to\infty}\frac{e^{-i(k-k')x}}{-i(k-k')}\Big|_{-L}^{L}\\ = A_k A_{k'}\lim_{L\to\infty}\frac{2sin(k-k')L}{k-k'} = A_k A_{k'}2\pi\delta(k-k')\end{aligned} \tag{1}$$

$$\lim_{L\to\infty}\frac{sin(Lx)}{\pi x} = \delta(x)$$

$$A_k A_{k'} = \frac{1}{\sqrt{2\pi}}$$

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

$$\int \psi_k^*(x)\psi_{k'}(x)dx = \delta(k-k')$$

Completeness:

$$f(x) = \int \phi(k)\psi_{k'}(x)dx = \frac{1}{\sqrt{2\pi}}\int \phi(k)e^{ikx}dx$$

$f(x) = \rightarrow FT \rightarrow \phi(k)$: momentum space wave function.

$$\phi(k) = \int \psi_k^*(x)f(x)dx = \frac{1}{\sqrt{2\pi}}\int f(x)e^{-kx}dx$$

General solution:

$$\Psi(x,t) = \int \phi(k)\psi_k(x)e^{\frac{-iEt}{\hbar}}dx = \frac{1}{\sqrt{2\pi}}\int \phi(k)e^{i(kx-\frac{E}{\hbar}t)}dx$$

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

Initial condition:

$$\Psi(x,0) = \int \phi(k)\psi_k(x)dx$$

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

Free particle=continuous, band particle=discrete, hence localization = quantization.

Velocity:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int \phi(k)e^{i(kx-\omega t)}dx; \omega = \omega(k) \textit{ dispersion relation}$$

Phase velocity: $v_{phase} = \frac{\omega}{k}$ can be larger than c. Group velocity $v_{group} = \frac{d\omega}{dk}$ is true velocity.

Eg: $E = \frac{\hbar^2k^2}{2m} = \hbar\omega$; $\omega = \frac{\hbar k^2}{2m}$; $v_{phase} = \frac{\hbar k}{2m}$; $v_{group} = \frac{\hbar k}{m}$; $v_{phase} = 2v_{group}$

Dirac δ function and δ function potential:

$$\delta(x) = 0, x \not\equiv 0 \tag{2}$$
$$= 0, x = 0 \tag{3}$$

$$\int_{-\infty}^{\infty} = 1$$

Properties of $\delta(x)$:

$$\int_{-\infty}^{\infty} \delta(ax)dx = \frac{1}{|a|}$$

$$\delta(ax) = \frac{\delta(x)}{|a|}$$

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

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

$$f(x) * \delta(x-a) = \int_{-\infty}^{\infty} f(\tau)\delta(\tau - (x-a))d\tau = f(x-a)$$

$$\delta(f(x)) = \Sigma_i \frac{\delta(x-x_i)}{|f'(x_i)|};\ x_i\ are\ zeros\ of\ f(x)$$

$$\delta(x) = \frac{dH(x)}{dx};\ Heaviside\ step\ fn$$

$$H(x) = 1, x > 0 \tag{4}$$
$$= 0.5, x = 0 \tag{5}$$
$$= 0, x < 0 \tag{6}$$

Dimension of $\delta(x)$ are $\frac{1}{[x]}$.

$$V(x) = -\alpha\delta(x),\ [\alpha] = [x][E]$$

Eg: Fermi pseudopotential $V_f(r) = \frac{2\pi\hbar^2}{m}b\ \delta(r)$, where b is bound scattering length.

Bound State, $E < 0, \not\equiv$

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

$$\psi(x) = Ae^{kx} + Be^{-kx}, k = \frac{\sqrt{-2mE}}{\hbar}$$

$$\begin{aligned}\psi(x) &= Ae^{kx}, x < 0 && (7)\\ &= Be^{-kx}, x > 0 && (8)\\ & && (9)\end{aligned}$$

Using continuity:

$$\psi(0^-) = \psi(0^+), A = B$$

$\frac{d\psi}{dx}$ is not continuous at ∞ potential.

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

Integrating from $-\epsilon$ to ϵ:

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

Taking the limit $\epsilon \to 0$:

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

$$\frac{d\psi}{dx}\Big|_{0^-}^{0^+} = -\frac{2m}{\hbar^2}\alpha A \not\equiv 0$$

$$-Ak - Ak = \frac{2m}{\hbar^2}\alpha A$$

$$k = \frac{m\alpha}{\hbar^2} = \frac{\sqrt{-2mE}}{\hbar}$$

$$E = \frac{-m\alpha^2}{2\hbar^2}$$

Normalization:

$$\int_{-\infty}^{\infty} |\psi|^2 dx = (A^2)(2)\int_0^{\infty} e^{-2kx} dx = (A^2)(2)\frac{1}{2k} = 1$$

$$A = \sqrt{k}$$

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

$$E = -\frac{m\alpha^2}{2\hbar^2}$$

Scattering state,$E > 0$:

$$x \neq 0, \frac{-\hbar^2}{2m}\frac{d^{\psi}(x)}{dx^2} = E\psi(x)$$

$$x < 0, \psi(x) = Ae^{ikx} + Be^{-ikx}$$

$$x > 0, \psi(x) = Ce^{ikx} + De^{-ikx}$$

where $k = \frac{\sqrt{2mE}}{\hbar}$.

Using continuity at 0^- and 0^+:

$$A + B = C + D$$

$$\frac{-\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{0^-}^{0^+} - \alpha\psi(0)$$

$$\frac{-\hbar^2}{2m}ik[(C - D) - (A - B)] = \alpha(A + B)$$

Consider $D = 0$, particle comes from the left:

$$A + B = C$$

$$(1 + 2\beta i)A + (-1 + 2\beta i)B = C, \beta = \frac{m\alpha}{k\hbar^2}$$

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

$$C(A) = \frac{1}{1-\beta i}A$$

Reflection coefficient:

$$R = \left|\frac{B}{A}\right|^2 = \frac{\beta^2}{1+\beta^2}$$

Transmission coefficient:

$$T = \left|\frac{C}{A}\right|^2 = \frac{1}{1+\beta^2}$$

Remarks:

- E inc, k inc, β dec, T inc, R dec
- α inc, β inc, T dec, R inc, $\alpha \to \infty$,$T \to 0$, $R \to 1$
- If $V \to -V$: no bound state, scattering state remains the same vs classical.

1D Finite Square Well

$$V(x) = \begin{cases} 0; & |x| \geq a \\ -V_0; & |x| < a \end{cases}$$

(1) Bound State $E < 0(E > -V_0)$ For $x < -a$:

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

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}$$

$$\psi(x) = Ae^{\kappa x} + Be^{-\kappa x}; B = 0$$

For $-a < x < a$:

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

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

$$\psi(x) = Ce^{kx} + De^{-kx}$$

For x>a:

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

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}$$

$$\psi(x) = Fe^{\kappa x} + Ge^{-\kappa x}; F = 0$$

$$\psi(x) = \begin{cases} Ae^{\kappa x}; & x < -a \\ Csinkx + Dcoskx; & -a < x < a \\ Ge^{-\kappa x}; & x > a \end{cases}$$

Continuity:

$$Ae^{-\kappa a} = -Csinka + Dcoska \tag{10}$$

$$A\kappa e^{-\kappa a} = -Cksinka + Dkcoska \tag{11}$$

$$Ge^{-\kappa a} = Csinka + Dcoska \tag{12}$$

$$-G\kappa e^{-\kappa a} = Cksinka - Dkcoska \tag{13}$$

$$10^2 + \frac{11}{k}^2 : A^2e^{-2\kappa a}(1 + \frac{\kappa^2}{k^2}) = C^2 + D^2$$
$$12^2 + \frac{12}{k}^2 : G^2e^{-2\kappa a}(1 + \frac{\kappa^2}{k^2}) = C^2 + D^2$$

For even wave function:

$$A = G$$

For odd wave function:

$$A = -G$$

$$10 - 12 : 0 = -2Csinka \Rightarrow C = 0$$

$$10, 12 \Rightarrow Ae^{-\kappa a} = Dcoska$$

$$11, 13 \Rightarrow Ake^{-\kappa a} = Dksinka$$

$$\kappa = ktanka$$

For odd, $D = 0$:

$$\kappa = -kcotka$$

Notice that:

$$k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2}$$

Let $ka = Z$, then:

$$Z^2 + k^2a^2 = \frac{2mV_0}{\hbar^2}a^2 = Z_0^2$$

$$ka = \sqrt{Z_0^2 - Z^2}$$

$$=> \sqrt{Z_0^2 - Z^2} = Ztanz$$

$$tanZ = \sqrt{\frac{Z_0}{Z}^2 - 1}$$

Wide($a \to \infty$), deep($V_0 \to \infty$):

$$Z_n \approx \frac{n\pi}{2}$$

where n=1,3,5... for even wave functions and n=2,4,6... for odd wave functions.

$$k_n = \frac{Z_n}{a} \approx \frac{n\pi}{2a}$$

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

which is same as inifinte square well.

Narrow($a \to 0$), shallow($V_0 \to 0$): If $Z_0 < \frac{\pi}{2}$, then one bound state.

Normalization of even wavefunction:

$$D^2 \int_0^a cos^2kxdx + A^2 \int_a^\infty e^{-2\kappa x}dx = \frac{1}{2}$$

$$D^2 \frac{1}{k}\frac{1}{2}(\frac{1}{2}sin2ka + ka) + A^2 \frac{1}{2k}e^{-2\kappa a} = \frac{1}{2}$$

$$Ae^{-\kappa a} = Dcoska$$

$$D^2 = \frac{\kappa k}{kcos^2ka + sinkacoska + \kappa ka} = \frac{\kappa}{1 + \kappa a}$$

$$D = \sqrt{\frac{\kappa}{1+\kappa a}}$$

$$A = \sqrt{\frac{\kappa}{1+\kappa a}} coska\ e^{\kappa a}$$

Normalization of odd wavefunction:

$$C^2 \int_0^a sin^2 kx dx + A^2 \int_a^\infty e^{-2\kappa x} dx = \frac{1}{2}$$

$$C^2 \frac{1}{k}\frac{1}{2}(-\frac{1}{2}sinka + ka) + A^2 \frac{1}{2\kappa} e^{-2\kappa a} = \frac{1}{2}$$

$$Ae^{-\kappa a} = -Csinka$$

$$C^2 = \frac{\kappa k}{ksin^2 ka - sinkacoska + \kappa ka} = \frac{\kappa}{1+\kappa a}$$

$$C = \sqrt{\frac{\kappa}{1+\kappa a}}$$

$$A = -\sqrt{\frac{\kappa}{1+\kappa a}} coska\ e^{\kappa a}$$

In summary:

For odd n:

$$\psi_n(x) = \begin{cases} Ae^{\kappa x}; & x < -a \\ Dcoskx; & -a < x < a \\ Ae^{-\kappa x}; & x > a \end{cases}$$

For even n:

$$\psi_n(x) = \begin{cases} Ae^{\kappa x}; & x < -a \\ Csinkx; & -a < x < a \\ -Ae^{-\kappa x}; & x > a \end{cases}$$

(2) Scattering State $E > 0$)

$$x < -a, \psi(x) = Ae^{ik_1 x} + Be^{-ik_1 x}, k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$-a < x < a, \psi(x) = Csink_2 x + Dcosk_2 x, k_2 = \frac{\sqrt{2m(E+V_0}}{\hbar}$$

$$x > a, \psi(x) = Fe^{ik_1 x} + Ge^{-ik_2 x}, G = 0$$

Consider G=0, particle comes from the left. Using continuity:

$$Ae^{-ik_1a} + Be^{ik_1a} = -Csink_2a + Dcosk_2a$$

$$ik_1(Ae^{-ik_1a} - Be^{ik_1a}) = k_2(Ccosk_2a + Dsink_2a)$$

$$Csink_2a + Dcosk_2a = Fe^{ik_1a}$$

$$k_2(Ccosk_2a - Dsink_2a) = ik_1Fe^{ik_1a}$$

$$F = \frac{e^{-2ik_1a}}{cos(2k_2a) - i\frac{k_1^2+k_2^2}{2k_1k_2}sin(2k_2a)}A$$

$$B = i\frac{sin(2k_2a)}{2k_2a}(k_2^2 - k_1^2)F$$

Reflection coefficient:

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

Transmission coefficient:

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

Remarks:

$$T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)}sin^2(\frac{2a\sqrt{2m(E+V_0}}{\hbar})$$

when

$$\frac{2a\sqrt{2m(E+V_0)}}{\hbar} = n\pi$$

or

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

the eigen energies. Then $T = 1$, the well becomes transparent.

Formalism: Algebra Mechanics and Vector-Matrix Representation

Hilbert Space: ∞ dimension linear space, could be discrete or continuous.

- Ket vector $|\psi >\to \psi(x)$
- Bra vector $< \psi| \to \int \psi^*(x)dx$
- Inner product $< \psi|\phi >\to \int \psi^* \phi dx$
- Normalization $< \psi|\psi >= 1$
- Orthogonality $< \psi|\phi >= 0$

Operator:

- Observable: $< A >=< \psi|A|\psi >$ Hermitian operator: $< A >$ of physical quantity must be real. $< A >^* =< A >$.

$$< \psi|A\psi >^* =< A\psi|\psi >=< \psi|A\psi >$$

[If $< A^T\psi|\phi >=< \psi|A\phi >$, then A^T is the Hermitian conjugate of A, $(A^T)^T = A$

$$=< A^T\psi|\psi >=> A^T = A$$

- All physical quantities are represented by Hermitian operators.
- Eigenstates and eigenvalues of Hermitian operators

$$A|\psi_n >= A_n|\psi_n >$$

- A_n are real:

$$< \psi_n|A|\psi_n >=< \psi_n|A_n|\psi_n >= A_n$$
$$< A\psi_n|\psi_n >= A_n^*$$

- Normalization : $< \psi_n|\psi_n >= 1$

- Orthogonality : $< \psi_n|\psi_m >= 0$

$$< \psi_n|\psi_n >= \delta_{nm}$$

Proof:

$$A|\psi_n >= A_n|\psi_n >; A|\psi_m >= A_m|\psi_m >$$

$$< \psi_n|A|\psi_m >=< \psi_n|A_m|\psi_m >= A_m < \psi_n|\psi_m >$$

$$< A\psi_n|\psi_m >= A_n^* < \psi_n|\psi_m >= A_n < \psi_n|\psi_m >$$

If $A_n \neq A_m$, then $< \psi_n|\psi_m >= 0$.
If $A_n = A_m$, then Gram-Schmidt orthogonalization.

- Completeness $|\psi >= \Sigma C_n|\psi_n >$, where $C_n < \psi_n|\psi >$.

$$|\psi >= \Sigma < \psi_n|\psi > |\psi_n >= \Sigma|\psi_n >< \psi_n|\psi >=> I = \Sigma|\psi_n >< \psi_n|$$

- Projection operator $\hat{P} = |\alpha >< \alpha|$, picks out the portion along $|\alpha >$.

- $< A >=< \psi|A|\psi >= (\Sigma_n C_n^* < \psi_n|)A(\Sigma_m C_m|\psi_m >) = \Sigma|C_n|^2 A_n$, where $|C_n|^2$ is the probability.

- Normalization:

$$1 =< \psi|\psi >= \Sigma_m C_m^* < \psi_m|\Sigma_n C_n|\psi_n >= \Sigma_{n,m} C_m^* C_n < \psi_m|\psi_n >= \Sigma|C_n|^2$$

Vector-Matrix Representation

- Heisenberg (1932 Nobel), Born (1954 Nobel), Jordan ($N\ a\ z\ i$).
  Given an operator and its eigenstates $|\psi_n>$.
- Vector:

$$|\psi >= \Sigma c_n|\psi_n > \to \begin{pmatrix} c_1 \\ . \\ . \\ . \\ c_n \end{pmatrix}$$

- Dual vector

$$< \psi| = \Sigma c_n^* < \psi_n| \to (c_1, ..., c_n^*)$$

- inner product:
  - $< \psi|\phi >= \Sigma c_n^* d_n$
  - $< \psi|\phi >^* =< \phi|\psi >$
  - Normalization: $< \psi|\psi >= 1 = \Sigma |c_n|^2$
  - Orthogonality: $< \psi|\phi >= 0 = \Sigma c_n^* d_n$
- Operator $A|\psi >= |\phi >$

$$|\psi >= \Sigma c_n|\psi_n >, |\phi >= \Sigma d_m|\psi_m >$$

$$A\Sigma_n c_n|\psi_n >= \Sigma_m d_m|\psi_m >$$

$$\Sigma_n < \psi_m|A|\psi_n > c_n = d_m$$

$$\Sigma_n A_{mn} c_n = d_{mn}$$

$$A_{mn} =< \psi_m|A|\psi_n >$$

-matrix element.

Rotation:

$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ A_{m1} & \dots & \dots & A_{mn} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_m \end{pmatrix}$$

- vector representation using different bases:

$$x : \Psi(x,t) =< x|\Psi(t) >; |\Psi(t) >= \int |x >< x|\psi(t) > dx$$

$$p : \Phi(p,t) =< p|\Psi(t) >; |\Psi(t) >= \int |p >< p|\psi(t) > dx$$

$$H : c_n(t) =< n|\Psi(t) >; |\Psi(t) >= \Sigma|n >< n|\Psi(t) >$$

$$\Psi(x,t) = \int < x|y > \Psi(y,t)dy = \int < x|p > \Phi(p,t)dp = \Sigma < x|n > c_n(t)$$

$$= \int \delta(x,y)\Psi(y,t)dy = \int \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px}\Phi(p,t)dp = \Sigma c_n(t)e^{-\frac{i}{\hbar}E_n t}\psi_n(x)$$

Time evolution of an operator

- Classical mechanics

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + [A, H](Poisson\ bracket)$$

- Quantum mechanics

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \frac{1}{i\hbar}[A, H](Commutator)$$

which is equivalent to Schroedinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi >= H|\psi >$$

Proof:

$$\frac{d < A >}{dt} = \frac{d}{dt} < \Psi|A|\Psi >$$

$$\frac{\partial}{\partial t} < \Psi|A|\Psi > + < \Psi|\frac{\partial A}{\partial t}|\Psi + < \Psi|A|(\frac{\partial}{\partial t}|\Psi >)$$

$$(i\hbar\frac{\partial}{\partial t}|\psi >= H|\psi > => \frac{\partial}{\partial t}|\psi >= \frac{1}{i\hbar}H|\psi > => \frac{\partial}{\partial t} < \psi| = -\frac{1}{i\hbar} < H\psi|)$$

$$= -\frac{1}{i\hbar} < H\Psi|A|\Psi > + < \frac{\partial A}{\partial t} + \frac{1}{i\hbar} < \psi|A|H\psi >$$

$$=< \frac{\partial A}{\partial t} + \frac{1}{i\hbar} < \Psi|AH - HA|\Psi >$$

$$=< \frac{\partial A}{\partial t} > + \frac{1}{i\hbar} < [A, H] >$$

- If $[A, H] = 0$, and A does not depend on t explicitly:

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} = 0$$

A is conserved.

- Schroedinger picture vs Heisenberg picture:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)>=H|\psi(t)>; |\psi(t)>=\hat{S}|\psi(0)>$$

$\hat{S}=e^{-\frac{i}{\hbar}Ht}$ - S matrix.

Procedure:

- Given H, solve $H|\psi_n>=E_n|\psi_n>$ to get E_n and $|\psi_n>$.
- General solution $|\psi(t)>=\Sigma c_n e^{-\frac{i}{\hbar}E_n t}|\psi_n>$.
  $|\psi(0)>=\Sigma c_n|\psi_n>=> c_n=<\psi_n|\psi(0)>$.
- Observable:

  $<H>=<\psi(t)|H|\psi(t)>=\Sigma_n c_n^* e^{\frac{i}{\hbar}E_n t}<\psi_n|\Sigma_m E_m c_m e^{-\frac{i}{\hbar}E_n t}|\psi_n>=\Sigma|c_n|^2 E_n$

Example: Two state system

Spin(up/down), bit(0/1), Schroedinger's cat (dead/alive), relationship(love/hate), exam(pass/fail).

$$\begin{pmatrix} E_1 & \\ & E_2 \end{pmatrix} => |\psi_1>=\begin{pmatrix}1\\0\end{pmatrix}=|\uparrow>, |\psi_2>=\begin{pmatrix}0\\1\end{pmatrix}=|\downarrow>$$

If:

$$|\psi(0)>=c_1|\uparrow>+c_2|\downarrow>=\begin{pmatrix}c_1\\c_2\end{pmatrix}$$

If $c_1=\frac{1}{2}, c_2=(?)\frac{\sqrt{3}}{2}$

$$|\psi(t)>=c_1 e^{-\frac{i}{\hbar}E_1 t}|\uparrow>+c_2 e^{-\frac{i}{\hbar}E_2 t}|\downarrow>=\begin{pmatrix}c_1 e^{-\frac{i}{\hbar}E_1 t}\\c_2 e^{-\frac{i}{\hbar}E_2 t}\end{pmatrix}$$

$$<H>=|c_1|^2 E_1+|c_2|^2 E_2$$

Uncertainty Principle (Heisenberg)

- If $[A, B] = 0$, then A,B can have the same eigen state.

$$A|\psi_n >= A_n|\psi_n >$$
$$BA|\psi_n >= A(B|\psi_n >)$$
$$B|\psi_n >= B_n|\psi_n >$$
$$BA_n|\psi_n >= A_n(B|\psi_n >)$$

- If $[A, B] \neq 0$, then $\sigma_A \sigma_B \geq \frac{1}{2}| < [A, B] > |$.

$\sigma_A^2 =< \Delta A|\Delta A >=< (A- < A >)^2 >=< A^2 - 2A < A > + < A >^2 >=< A^2 > - < A >^2$

Schwarz inequality:

$$< \alpha|\alpha >< \beta|\beta >\geq | < \alpha|\beta > |^2, (|\alpha|^2|\beta|^2 \geq |\alpha|^2|\beta|^2 cos^2\theta$$

$$\sigma_A^2\sigma_B^2 =< \Delta A|\Delta A >< \Delta B|\Delta B >\geq | < \Delta A|\Delta B > |^2$$

$$\Delta A\Delta B = \frac{1}{2}(\Delta A\Delta B - \Delta B\Delta A) + \frac{1}{2}(\Delta A\Delta B + \Delta B\Delta A) = \frac{1}{2}[\Delta A, \Delta B] + \Delta A, \Delta B$$

$[\Delta A, \Delta B]^\dagger = (\Delta A\Delta B - \Delta B\Delta A)^\dagger = (\Delta B)^\dagger(\Delta A)^\dagger - (\Delta A)^\dagger(\Delta B)^\dagger = \Delta B\Delta A - \Delta A\Delta B = -[\Delta$

...anti-Hermitian, imaginary.

$\Delta A, \Delta B^\dagger = (\Delta A\Delta B + \Delta B\Delta A)^\dagger = (\Delta B)^\dagger(\Delta A)^\dagger + (\Delta A)^\dagger(\Delta B)^\dagger = \Delta B\Delta A + \Delta A\Delta B = \Delta A, \Delta$

...Hermitian, real.

$$\sigma_A^2\sigma_B^2 \geq \frac{1}{4}| < [\Delta A, \Delta B] > |^2$$

$$[\Delta A, \Delta B] = \Delta A\Delta B - \Delta B\Delta A = (A- < A >)(B- < B >) - (B- < B >)(A- < A >)$$
$$= (AB- < A > B - A < B > + < A >< B >) - (BA- < B > A - B < A > +$$

$$\sigma_A^2\sigma_B^2 \geq \frac{1}{4}| < [A, B] > |^2, \sigma_A\sigma_B \geq \frac{1}{2}| < [A, B] > |$$

eg: $[x, p_x] = i\hbar$, $\sigma_x\sigma_{p_x} \geq \frac{1}{2}\hbar$.

Minimum uncertainty wave packet

$\Delta A = ia\Delta B$, a is real.
For position-momentum uncertainty relation:

$$(-i\hbar\frac{d}{d\chi} - <p>)\psi(\chi) = ia(\chi - <\chi>)\psi(\chi)$$

$$\frac{d}{d\chi}\psi + \frac{a}{\hbar}\chi\psi - \frac{i}{\hbar}(<p> - ia<\chi>)\psi = 0$$

$$\chi \to \infty, \frac{d\psi}{d\chi} + \frac{a}{\hbar}\chi\psi = 0$$

$$\psi(\chi) = c_1 e^{-\frac{a}{2\hbar}\chi^2}$$

Let $\psi(\chi) = \phi(\chi)e^{-\frac{a}{2\hbar}\chi^2}$:

$$\frac{d\phi}{d\chi}e^{-\frac{a}{2\hbar}\chi^2} + \phi(\chi)e^{-\frac{a}{2\hbar}\chi^2}(-\frac{a}{2\hbar}\chi) + \phi(\chi)e^{-\frac{a}{2\hbar}\chi^2}(\frac{a}{2\hbar}\chi) - \frac{i}{\hbar}(<p> - ia<\chi>)\phi(\chi)e^{-\frac{a}{2\hbar}\chi^2} = 0$$

$$\frac{d\phi}{d\chi} - \frac{i}{\hbar}(<p> - ia<\chi>)\phi(\chi)e^{-\frac{a}{2\hbar}\chi^2} = 0$$

$$\phi(\chi) = e^{\frac{i}{\hbar}(<p> - ia<\chi>)\chi}$$

$$\psi(\chi) = c_2 e^{-\frac{a}{2\hbar}\chi^2} e^{\frac{i}{\hbar}(<p> - ia<\chi>)\chi} = c_3 e^{-\frac{a}{2\hbar}(\chi - <\chi>)^2} e^{\frac{i}{\hbar}(<p>\chi}$$

...Gaussian in χ.

Energy-time uncertainty principle

$$\sigma_H \sigma_t \geq \frac{1}{2}\hbar$$

If A doesn't depend on t explicitly, $\frac{\partial A}{\partial t} = 0$, $\frac{dA}{dt} = \frac{1}{i\hbar}[A, H]$.

$$\sigma_A \sigma_H \geq \frac{1}{2}| <[A, H]> | = \frac{\hbar}{2}|\frac{d<A>}{dt}|$$

Define $\sigma_t = \frac{\sigma_A}{\frac{d<A>}{dt}}$, then $\sigma_H, \sigma_t \geq \frac{1}{2}\hbar$.

$\sigma_A = |\frac{d<A>}{dt}|\sigma_t =$ the amount of time it takes the expectation value of A to change by one standard deviation of σ_A.

3D Schroedinger Equation

$$[-\frac{\hbar^2}{2m}\nabla^2 + V(r)]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

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

Separation of variables $\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$:

$$\frac{1}{R}\frac{d}{dr}(r^2\frac{dR}{dr}) - \frac{2mr^2}{\hbar^2}[V(r)-E] + \frac{1}{Y}\frac{1}{sin\theta}\frac{\partial}{\partial\theta}(sin\theta\frac{\partial Y}{\partial\theta}) + \frac{1}{sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} = 0$$

$$l(l+1) - l(l+1) = 0$$

The angular equation let $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$:

$$\frac{1}{\Theta}[sin\theta\frac{d}{d\theta}(sin\theta\frac{d\Theta}{d\theta})] + l(l+1)sin^2\theta + \frac{1}{\Phi}\frac{d^2\Phi}{d^2\phi} = 0$$

...same as solving $\nabla^2\psi = 0$. Previous equation is same as:

$$m^2 - m^2 = 0$$

For Φ :

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2, \Phi(\phi) = e^{im\phi}$$

(-m is included by allowing m to run negative).
Symmetry:

$$\Phi(\phi) = \Phi(\phi + 2\pi)$$

$$=> e^{im\phi} = e^{im(\phi+2\pi)} => m = integer$$

For Θ:

$$sin\theta\frac{d}{d\theta}(sin\theta\frac{d\Theta}{d\theta}) + [l(l+1)sin^2\theta - m^2]\Theta = 0$$

$$\Theta(\theta) = AP_l^m(cos\theta)$$

$P_l^m(\chi)$: associated Legendre function/polynomial:

$$P_l^m(\chi) = (-1)^m(1-\chi^2)^{\frac{m}{2}}\frac{d^m}{d\chi^m}P_l(\chi), m > 0$$

Rodrigue's formula:

$$P_l(\chi) = \frac{1}{2^l l!}\frac{d^l}{d\chi^l}(\chi^2-1)^l$$

$$P_l^{-m}(\chi) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(\chi)$$

$$P_l^m(-\chi) = (-1)^{m+l} P_l^m(\chi)$$

$$P_0(\chi) = 1$$

$$P_1(\chi) = \chi$$

$$P_2(\chi) = \frac{1}{2}(3\chi^2 - 1)$$

$$P_3(\chi) = \frac{1}{2}(5\chi^3 - 3\chi)$$

If $|m| > l$, then $P_l^m = 0$, so $|m| \leq l$, m=-l,....,l (2l+1 values). $P_l^m(\chi)$ is always a polynomial in $cos\theta$ and $sin\theta$.

$$P_0^0 = 1$$

$$P_1^0 = cos\theta; P_1^1 = -sin\theta; P_1^{-1} = -\frac{1}{2}P_1^1$$

$$P_2^0 = \frac{1}{2}(3cos^2\theta - 1), P_2^1 = -3sin\theta cos\theta; P_2^2 = 3sin^2\theta$$

$$P_2^{-1} = -\frac{1}{6}P_2^1; P_2^{-2} = -\frac{1}{24}P_2^2$$

$$Y_l^m = (-1)^m \sqrt{\frac{(2l+1)(l-m!)}{4\pi(l+m!)}} P_l^m(cos\theta) e^{im\theta}$$

...spherical harmonics, solution of Laplace's equation. Vibration of a string: sin, cos. Vibration of a sphere: Y_l^m.

$$Y_l^{-m} = (-1)^m (Y_l^m)$$

$$\int_0^\pi d\theta \int_0^{2\pi} d\phi Y_l^m Y_{l'}^{m'} = \delta_{ll'}\delta_{mm'}$$

Normalization:

$$\int_0^\infty |R|^2 r^2 dr = 1; \int_0^{2\pi} d\phi \int_0^\pi d\theta(|Y|^2 sin\theta) = 1$$

Parity:

$$Y_l^m(\pi - \theta, \pi + \phi) = (-1)^l Y_l^m(\theta, \phi)$$

l=0:

$$Y_0^0 = \frac{1}{2}\sqrt{\frac{1}{\pi}}$$

l=1:

$$Y_1^{-1} = \frac{1}{2}\sqrt{\frac{3}{2\pi}} sin\theta e^{-i\phi}$$

$$Y_1^0 = \frac{1}{2}\sqrt{\frac{3}{\pi}} cos\theta$$

$$Y_1^{-1} = \frac{1}{2}\sqrt{\frac{3}{2\pi}} sin\theta e^{-i\phi}$$

l=2:

$$Y_2^{-2} = \frac{1}{4}\sqrt{\frac{15}{2\pi}} sin^2\theta e^{-2i\phi}$$

$$Y_2^{-1} = \frac{1}{2}\sqrt{\frac{15}{\pi}} sin\theta cos\theta e^{-i\phi}$$

$$Y_2^0 = \frac{1}{4}\sqrt{\frac{5}{\pi}} (3cos^2\theta - 1)$$

$$Y_2^1 = -\frac{1}{2}\sqrt{\frac{15}{\pi}} sin\theta cos\theta e^{i\phi}$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}} sin^2\theta e^{2i\phi}$$