~~Quan~~ Quantum in 3 dimensions

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \Psi + V\Psi \quad , \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\int |\Psi|^2 d^3\vec{r} = 1 \quad , \quad \Psi_n(\vec{r},t) = \psi_n(\vec{r}) e^{-iE_n t/\hbar}$$

[time independent Schrodinger eq] $\rightarrow$ $\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi}$, general solution: $\Psi(\vec{r},t) = \sum c_n \psi_n(\vec{r}) e^{-iE_n t/\hbar}$

Spherical coordinates

$\rightarrow V(\vec{r}) \Rightarrow V(r)$ (central potential), Laplacian in spherical coordinates

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

In the schrodinger eq:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right) + \dots\right] + V\psi = E\psi \quad ,$$

look for seperable solutions $\psi(r,\theta,\phi) = R(r)\, Y(\theta,\phi)$

dividing out:

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

$\hookrightarrow$
$$\boxed{\begin{aligned} &\frac{1}{R}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r) - E) = l(l+1) \\ &\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial Y}{\partial \theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial \phi^2}\right] = -l(l+1) \end{aligned}}$$

each must be a constant that add's to 0, for the Y doesnt depend on r, so when changing it, r stays constant, thus if they are each are constants to add to 0.

The Angular Equation

$$\sin\theta \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial Y}{\partial \theta}\right) + \frac{\partial^2 Y}{\partial \phi^2} = -l(l+1)\sin^2\theta\, Y$$

, seperate again: $Y(\theta,\phi) = \Theta(\theta) \cdot \Phi(\phi)$

$\hookrightarrow$ [plugging in and dividing out] $\rightarrow$

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

$\leftarrow$ seperation constant

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2$$

(still both have to be a constant) $\leftarrow$ same reasons above

Φ equation:

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

its really $\pm m$, but if you let m run negative you just cover all the solutions
* constant factor will be absorbed into

↳ (we know) → $\Phi(\phi + 2\pi) = \Phi(\phi) \Rightarrow e^{im(\phi+2\pi)} = e^{im\phi} \rightarrow e^{2\pi i m} = 1$

↳ $\boxed{m = 0, \pm 1, \pm 2, \dots}$

Θ equation

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

↳ solution is: $\boxed{\Theta(\theta) = A P_l^m(\cos\theta)}$, $P_l^m(x) = (-1)^m(1-x^2)^{m/2}\left(\frac{d}{dx}\right)^m P_l(x)$

and $P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l$ $\left(P_0(x) = 1,\ P_1(x) = \frac{1}{2}\frac{d}{dx}(x^2-1) = x,\ P_2(x) = \frac{1}{2}(3x^2-1)\right)$

if m is odd $P_l^m(\cos\theta)$ (is always a polynomial in $\cos\theta$) multiplied by $\sin\theta$ $\sqrt{1-\cos^2\theta}$
if m is even $P_l^m(\cos\theta)$ is just polynomial in $\cos\theta$

• l must be non-negative real integer, $l!$, only makes sense for that $(-1!) = \infty$

$P_l^m(x) = (-1)^m(1-x^2)^{m/2}\left(\frac{d}{dx}\right)^m\left[\frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l\right]$ ← if $m > l$, the $\left(\frac{d}{dx}\right)^{m}$ will take the derivative till its 0 $\left(\left(\frac{d}{dx}\right)^3\left(\frac{d}{dx}\right)^2 x^4 = 0\right)$

SO:

$\boxed{l = 0, 1, 2, 3}$ and $m \leq l$, m can be negative (powers of derivatives will cancel)

$\boxed{m = -l, -l+1, \dots, -1, 0, 1, 2, l-1, l}$ ← $2l+1$ values for m
(# of neg num + 0 + # of pos nums)

Normalization:

$d\Omega \equiv \sin\theta\, d\theta\, d\phi$

↳ $\int |\psi|^2 r^2 \sin\theta\, dr\, d\theta\, d\phi = \int |R|^2 r^2 dr \int |Y|^2 d\Omega = 1$, you can normalize them separately

↳ $\boxed{Y_l^m(\theta,\phi) = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\, e^{im\phi} P_l^m(\cos\theta) \quad l = 0, 1, 2, 3,\ m = -l, -l+1, \dots, -1, 0, 1, \dots, l-1, l}$

↳ (they are automatically orthogonal) → $\int_0^{\pi}\int_0^{2\pi} \left[Y_l^m(\theta,\phi)\right]^* \left[Y_{l'}^{m'}(\theta,\phi)\right] \sin\theta\, d\theta\, d\phi = \delta_{ll'}\delta_{mm'}$

{Tables on page 137}

① $\tilde{9}_s$

Radial Equation

$V(r)$ only effects the radial part

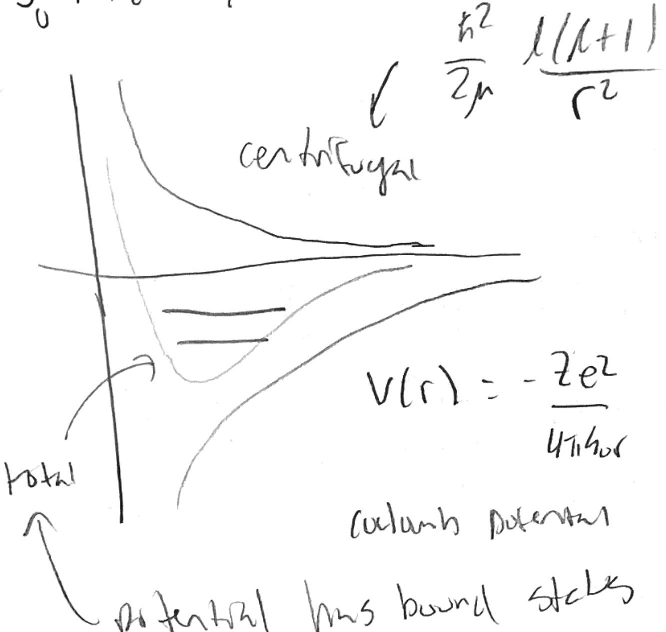
$\hookrightarrow \frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r) - E)R = l(l+1)R$

$\hookrightarrow$ let $u(r) = rR(r) \rightarrow$ $R = (u/r)$, $\frac{dR}{dr} = \frac{r\frac{du}{dr} - u}{r^2}$, $\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) = r\frac{d^2u}{dr^2}$

$\hookrightarrow -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \underbrace{\left[V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]}_{V_{eff}}u = Eu$ (completly identical to the Schrodinger eq in 1D

V_{eff}, contains a centrifugal term

$\int_0^\infty |u|^2 dr = 1$



The hydrogen atom

$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$ (potential energy of an electron from a proton at the center)

Radial equation:

$-\frac{\hbar^2}{2m_e}\frac{d^2u}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m_e}\frac{l(l+1)}{r^2}\right]u = Eu$

lets tidy up notation, $K \equiv \sqrt{-2m_eE}/\hbar$, for bound states $\rightarrow E = -|E|$

$\hookrightarrow \frac{1}{K^2}\frac{d^2u}{dr^2} = \left[1 - \frac{m_e e^2}{2\pi\epsilon_0\hbar^2}\frac{1}{K}\frac{1}{(Kr)} + \frac{l(l+1)}{(Kr)^2}\right]u$

define: $\rho = Kr$ and $\rho_0 \equiv \frac{m_e e^2}{2\pi\epsilon_0\hbar^2 K}$

$\hookrightarrow \boxed{\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]u}$ tidied up eq

[Asymtotic behavior of this diff eq]

as $\rho \to \infty \rightarrow \frac{d^2u}{d\rho^2} = u \rightarrow u(\rho) = Ae^{-\rho} + \cancel{Be^{\rho}}$ blows up as $\rho \to \infty$, $u(\rho) \sim Ae^{-\rho}$

as $\rho \to 0 \rightarrow \frac{d^2u}{d\rho^2} = \frac{l(l+1)}{\rho^2}u \xrightarrow{\text{general sol'n}} u(\rho) = C\rho^{l+1} + \cancel{D\rho^{-l}}$ as $\rho \to 0$ blows $\rightarrow$ $u(\rho) \sim C\rho^{l+1}$

$\hookrightarrow \boxed{u(\rho) = \rho^{l+1}e^{-\rho}v(\rho)}$ take derivits and plug into radial equation!

$$\boxed{\rho\frac{d^2v}{d\rho^2} + 2(l+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0}$$

Assume the solution $v(\rho)$ can be expressed as a power series in ρ

↳ $v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j \rightarrow \frac{dv}{d\rho} = \sum_{j=0}^{\infty} j c_j \rho^{j-1} = \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^j$

replace $j \to j+1$, doesnt have to start at $j=-1$ bec/ $j+1$ w/ $j=-1$ is 0 anyways!

↳ $\frac{d^2 v}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^{j-1}$

↳ <u>plugging in:</u> $\sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^j + 2(\ell+1) \sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^j$

$-2 \sum_{j=0}^{\infty} j c_j \rho^j + [\rho_0 - 2(\ell+1)] \sum c_j \rho^j = 0$

↳ can pull out sum and ρ^j so just need the coefficients:

$j(j+1) c_{j+1} + 2(\ell+1)(j+1) c_{j+1} - 2j c_j + [\rho_0 - 2(\ell+1)] c_j = 0$

↳ $\boxed{c_{j+1} = \left[\frac{2(j+\ell+1) - \rho_0}{(j+1)(j+2\ell+2)} \right] c_j}$, $v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$, c_j determines the coefficients & thus $v(\rho)$

↳ you start w/ $j=0$ and recursively find solutions

<u>Large j so large ρ, higher powers dominate</u>; $\rightarrow c_{j+1} \approx \frac{2j}{j(j+1)} c_j = \frac{2}{j+1} c_j$

$\rightarrow c_1 = \frac{2}{0+1} c_0 \rightarrow c_2 = \frac{2}{(1+1)} \frac{2}{(1+0)} c_0 \rightarrow c_3 = \frac{2}{(2+1)} \cdot \frac{2}{(1+1)} \frac{2}{(1+0)} c_0 \rightarrow c_4 = \frac{2}{\underset{4}{(3+1)}} \frac{2}{\underset{3}{(2+1)}} \cdot \frac{2}{\underset{2}{(1+1)}} \cdot \frac{2}{\underset{1}{1+0}} c_0$

↳ $\boxed{c_j \approx \frac{2^j}{j!} c_0}$ → lets say this is exact → $v(\rho) = c_0 \sum_{j=0} \frac{2^j}{j!} \rho^j = c_0 e^{2\rho}$

↳ then $u(\rho) = c_0 \rho^{\ell+1} e^{\rho}$ → the asymptotic behavior we dont want bec it blows up for large ρ

<u>Escaping the dilemma</u>

Series must terminate: $c_{N-1} \neq 0$ but $c_N = 0$, $v(\rho)$ a polynomial of order $(N-1)$, w/ $N-1$ roots and therefore the wave function has $N-1$ nodes

let $j = N-1$: $c_{N-1+1} = c_N = 0 = \frac{2(N-1+\ell+1)-\rho_0}{\sim} c_{N-1} \rightarrow 2(N+\ell) - \rho_0 = 0$

↳ $n \equiv N + \ell$ and then $\boxed{\rho_0 = 2n}$

But $\rho_0 = \frac{m_e e^2}{2\pi \varepsilon_0 \hbar^2 k}$ and $k = \frac{\sqrt{-2mE}}{\hbar} \rightarrow E = \frac{-m_e e^4}{8\pi^2 \varepsilon_0^2 \hbar^2 \rho_0^2}$

↳ $E_n = -\left[\frac{m_e}{2\hbar^2} \left(\frac{e^2}{4\pi\varepsilon_0} \right)^2 \right] \frac{1}{n^2} = \frac{E_1}{n^2}$, $n = 1, 2, 3, 4, 5, \ldots$ (Bohr formula)

...gen atom continued...

$\frac{m_e e^2}{2\pi\epsilon_0\hbar^2 k}$, $\rho_0 = 2n$ $\rightarrow$ $K = \left(\frac{m_e e^2}{4\pi\epsilon_0\hbar^2}\right)\frac{1}{n} = \frac{1}{an}$, $a \equiv \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$, Bohr radius

$\boxed{\rho = Kr = \frac{r}{an}}$

n = principle quantum number
l = azimuthal quantum number
m = magnetic quantum number

Wave function

$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\,Y_\ell^m(\theta,\phi)$, lets look at $R_{n\ell}(r)$

We defined: $u(r) = rR(r)$, but we solved for $u(r) = \rho^{\ell+1}e^{-\rho}v(\rho)$

$\hookrightarrow$ $\boxed{R_{n\ell}(r) = \frac{1}{r}\rho^{\ell+1}e^{-\rho}v(\rho)}$, $\boxed{v(\rho) = \sum_{j=0}^{\infty} c_j\rho^j,\ c_{j+1} = \frac{2(j+\ell+1-n)}{(j+1)(j+2\ell+2)}c_j}$

Quick side note

ground state: $E_1 = -\left[\frac{m_e}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right] = -13.6\,eV$ [binding energy of an electron in its ground state. (amount of energy to remove 1 electron) is 13.6 eV]

[What does $\psi_{n,\ell,m} = \psi_{1,0,0}$ look like?] $\rightarrow$ [if $n=1$, then from $n = N+\ell$ $\rightarrow$ $1 = N+\ell$ we need $N=1$, so we have c_0] $\rightarrow$ [$\ell=0$ then $m=0$ too so] $\rightarrow$ $\psi_{1,0,0} = R_{1,0}(r)\,Y_0^0$, $c_{0+1} = \frac{2(0)}{\sim} = 0$, $c_1 = 0$, truncates

n=0, everything 0, meaningless

$\hookrightarrow$ thus from $v(\rho) = c_0\rho^0 = c_0$ $\rightarrow$ $R_{1,0}(r) = \frac{1}{r}\frac{1}{\rho}e^{-\rho}c_0$, $\rho = \frac{r}{a\cdot 1}$

$\hookrightarrow$ $\boxed{R_{1,0} = \frac{c_0}{a}e^{-r/a}}$ $\rightarrow$ Normalize: $\int_0^\infty |R(r)|^2 r^2\,dr = \frac{|c_0|^2}{a^2}\int_0^\infty e^{-2r/a}r^2\,dr = |c_0|^2\frac{a}{4} = 1$ $\rightarrow$ $\boxed{|c_0| = \frac{2}{\sqrt{a}}}$

so $|c_0| = \frac{2}{\sqrt{a}}$, looking at table: $Y_0^0 = \frac{1}{\sqrt{4\pi}}$ $\Rightarrow$ $\boxed{\psi_{1,0,0}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}}$

First excited states ($\ell=0$, $m=0$) or ($\ell=1$ w/ $m=-1,0,+1$) all w/ $n=2$

For $\ell=0, n=2, m=0$ $\rightarrow$ $c_1 = -c_0$ and $c_2 = 0$ w/ $v(\rho) = \sum_{j=0}^{\infty} c_j\rho^j = c_0 - c_0\rho = c_0(1-\rho)$

$\hookrightarrow$ $R_{2,0}(r) = \frac{c_0}{2a}\left(1-\frac{r}{2a}\right)e^{-r/2a}$

For $\ell=1, n=2$, terminates immediately $\rightarrow$ $v(\rho) = c_0$ $\rightarrow$ $R_{2,1}(r) = \frac{c_0}{4a^2}\,r\,e^{-r/2a}$

[For arbitrary n the possible values of ℓ that are consistent w/ $n = N+\ell$] $\rightarrow$ $\ell = 0,1,2,\dots,n-1$
$\rightarrow$ for each ℓ there are $2\ell+1$ values of m

$\rightarrow$ the total degeneracy of each level is $d(n) = \sum_{\ell=0}^{n-1}(2\ell+1) = n^2$

Generalize the solution

$V(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$, defined by the recursion formula can be written:

$$V(\rho) = L^{2\ell+1}_{n-\ell-1}(2\rho) \quad \text{where} \quad \underset{\text{Associated Laguerre polynomial}}{L^p_q(x) \equiv (-1)^p \left(\frac{d}{dx}\right)^p L_{p+q}(x)}, \quad \underset{q^{th}\text{ laguerre Polynomial}}{L_q(x) \equiv \frac{e^x}{q!}\left(\frac{d}{dx}\right)^q (e^{-x}x^q)}$$

Finally

$$\psi_{n,\ell,m} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}}\; e^{-r/na}\left(\frac{2r}{na}\right)^{\ell}\left[L^{2\ell+1}_{n-\ell-1}(2r/na)\right] Y_\ell^m(\theta,\phi)$$

Visualization

- The number of radial nodes is $N-1$, or $n-\ell-1$
- m counts the number of nodes, real (or imaginary) part of ψ in ϕ dir
  - ↳ these nodes are planes on the z-axis on which the real or imag part of ψ vanishes
- $\ell-m$ gives # of nodes in the θ direction
  - ↳ cones about the z axis on which ψ vanishes

...mple Infinite Spherical Well

$$V(r) = \begin{cases} 0 & r \leq a \\ \infty & r > a \end{cases}$$

after separating the Schrodinger equation and defining $u(r) = rR(r)$ you get:

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu$$

Inside well $V=0$ so:

$$\frac{d^2u}{dr^2} = \left[\frac{l(l+1)}{r^2} - k^2\right]u \quad , \quad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

if $l = 0 \rightarrow \frac{d^2u}{dr^2} = -k^2 u$

$u(r) = A\sin(kr) + B\cos(kr)$

$R(r) = A\frac{\sin}{r} + B\frac{\cos}{r}$, then let $r \to 0$

$\frac{\sin}{r} = \frac{0}{0}$ and $\frac{\cos}{r} = \frac{1}{0} = \infty$

$\hookrightarrow R(r) = \frac{u}{r} \rightarrow$ plug boundary $u(0) = 0$ → in reality $0 = 0 + B \cdot 1 \rightarrow B = 0$

$\hookrightarrow u(a) = 0 \rightarrow \sin(ka) = 0 \rightarrow ka = N\pi$

$\hookrightarrow E_{N0} = \frac{N^2\pi^2\hbar^2}{2ma^2} \quad , \quad u_{N0} = \sqrt{\frac{2}{a}}\sin\left(\frac{N\pi r}{a}\right)$

general solution

$u(r) = Arj_l(kr) + Brn_l(kr)$

$$\begin{cases} j_l(x) \equiv (-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l \frac{\sin(x)}{x} & \leftarrow \text{Bessel function} \\ n_l(x) \equiv -(-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l \frac{\cos(x)}{x} & \leftarrow \text{Neumann function} \end{cases}$$

Bessel functions are finite at origin, while neumann blow up:

$\hookrightarrow R(r) = Aj_l(kr) \quad (B=0)$

Then $j_l(ka) = 0$ from $R(a) = 0$

$\hookrightarrow \boxed{k = \frac{1}{a}\beta_{Nl}}$ ← zero's for the bessel function (has to be computed numerically)

$\hookrightarrow \boxed{E_{Nl} = \frac{\hbar^2}{2ma^2}\beta_{Nl}^2}$ $\rightarrow \psi_{nlm}(r,\theta,\phi) = A_{nl}\, j_l\!\left(\beta_{Nl}\frac{r}{a}\right)Y_l^m(\theta,\phi)$

Generalized Statistical Approach

Chapter 1: [learned how to calculate the probability that a particle would be found in a specific location. And how to determine expectation value of any observable]

$P_{ab} = \int_a^b |\Psi|^2 dx$

$\rightarrow \langle Q \rangle = \int \Psi^* \hat{Q} \Psi dx$

Seperated SE: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$, $\hat{H}\psi = E\psi$

Chapter 2: [learned how to find the possible outcomes for Energy, and their probabilities.]

$\Psi(x,t) = \sum c_n \psi_n(x) e^{-iE_nt/\hbar}$ ← solutions are linear combos

$\Psi(x,0) = \sum c_n \psi_n(x)$, $|c_n|^2$ probability that a measurement of the energy returns E_n

↳ $\sum |c_n|^2 = 1$, $\langle H \rangle = \sum |c_n|^2 E_n$

[Fourier's Trick for reference] → $\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$ $\xrightarrow{\text{mult each side by } \psi_m^* \text{ and integrate}}$ $\int \psi_m^* \Psi(x,0) dx = \sum_{n=1}^{\infty} c_n \underbrace{\int \psi_m^* \psi_n dx}_{\text{orthonormal so } \delta_{mn}}$

$n \neq m \Rightarrow 0$
$n = m \Rightarrow 1$

↳ $\boxed{c_m = \int \psi_m^* \Psi(x,0) dx}$

The goal of this chapter is to figure out the possible results of any measurement, and their probabilities

What does this have to do w/ square integrable / normalizable ??

$\int \psi_m^* \psi_n dx = \delta_{mn}$

The beginning

- We have an observable $Q(x,p)$, we measure it on a particle in state $\Psi(x,t)$

↳ since its an observable then its hermitian and... → $\langle Q \rangle = \langle Q \rangle^*$, [expectation value has to be real] and [we defined the inner product like so] → $\langle f | g \rangle = \int_a^b f^*(x) g(x) dx$

[if ψ_n is complete the orthonormality holds]

[↳from the definition] → $\langle g | f \rangle = \langle f | g \rangle^*$

If $\langle Q \rangle = \int \psi^* \hat{Q} \psi dx = \langle \psi | \hat{Q} \psi \rangle$

putting together w/ real observables, $\langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle$ (hermitian definition)

(REVIEW!!!)

- If $\hat{Q}$ is descrete, the probability of getting a particular eigenvalue q_n associated w/ the associated orthonormalized eigenfunction f_n (like ψ_n) → $c_n = \langle f_n | \Psi \rangle$ (just like for $\hat{H}\psi = E\psi$)

orthonormal the generated · eigen value

[As before the eigen functions of an observable operator are complete, so you can do lin combo of them] → $\Psi(x,t) = \sum c_n f_n(x)$

[↳ fourier's trick exploiting their orthonormality] → $c_n(t) = \langle f_n | \Psi \rangle = \int f_n(x)^* \Psi(x,t) dx$

like $\psi_n(x)$ which is orthonormalized from $\hat{Q}\Psi = q\Psi$

c_n tells you how much f_n is contained in Ψ and given that a measurement has to return one of the eigenvalues, q_n of $\hat{Q}$

$|c_n|^2$ is the probability that a particle which is now in the state Ψ will in the state f_n subsequent to a measurement of Q"

[Quick recap so I understand] $\rightarrow$ $\Psi(x,t)$ is made up of liner combos of $f_n(x)$, these are orthonormalized with coefficients $c_n(t)$

↳ they can be found from $\hat{Q}\Psi(x,t) = q\,\Psi(x,t)$, solutions to this eqn, f_n and the liner combos w/ c_n to make a general solution,

↳ $|c_n|^2$ is the probability that a measurement of Q would yield q_n $\{\hat{Q} f_n = q_n f_n\}$

Some math

$$\sum |c_n|^2 = 1 \xrightarrow{\text{follows}} \text{from normalization} \rightarrow 1 = \langle \Psi | \Psi \rangle = \left\langle \left(\sum c_{n'} f_{n'}\right) \middle| \left(\sum c_n f_n\right) \right\rangle$$

take out constant but complex conjugate!

$$= \sum_{n'} \sum_{n} c_{n'}^* c_n \underbrace{\langle f_{n'} | f_n \rangle}_{\text{orthonormal set}} = \sum_{n'} \sum_{n} c_{n'}^* c_n \delta_{nn'} = \sum_n c_n^* c_n = \sum |c_n|^2$$

[Similarly for Q] $\rightarrow$ $\langle Q \rangle = \sum q_n |c_n|^2$

$\langle H \rangle = \sum E_n |c_n|^2$ ← for concept recall

proof $\rightarrow$ $\langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle = \left\langle \left(\sum_{n'} c_{n'} f_{n'}\right) \middle| \left(\hat{Q} \sum_n c_n f_n\right) \right\rangle$, $\hat{Q} f_n = q_n f_n$

$$↳ \langle Q \rangle = \sum_{n'} \sum_{n} c_{n'}^* c_n q_n \langle f_{n'} | f_n \rangle = \sum_{n'} \sum_{n} c_{n'}^* c_n q_n \delta_{nn'} = \sum_n q_n |c_n|^2$$

ex) A particle in the delta function well $V(x) = -\alpha\delta(x)$ what is the probability its momentum would yield a value more than $\boxed{p_0 = m\alpha/\hbar}$

split up integral

$$\Psi(x,t) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} e^{-iEt/\hbar} \rightarrow \Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \frac{\sqrt{m\alpha}}{\hbar} e^{-iEt/\hbar} \int_{-\infty}^{\infty} e^{-ipx/\hbar} e^{-m\alpha|x|/\hbar^2} dx$$

$$= \sqrt{\frac{2}{\pi}} \frac{p_0^{3/2} e^{-iEt/\hbar}}{p^2 + p_0^2}$$

$\rightarrow$ the probability is then $\rightarrow$ $\frac{2}{\pi} p_0^3 \int_{p_0}^{\infty} \frac{1}{(p^2+p_0^2)^2} dp = \frac{1}{\pi} \left[\frac{p p_0}{p^2 + p_0^2} + \tan^{-1}\left(\frac{p}{p_0}\right) \right]_{p_0}^{\infty}$

$$= \frac{1}{4} - \frac{1}{2\pi} = \boxed{0.0908}$$

mitian Operators

ets say you have an observable Q (like H, p, x etc..)

Expectation value $\langle Q \rangle = \int \Psi^* \hat{Q} \Psi \, dx = \langle \Psi | \hat{Q} \Psi \rangle$

↳ [the outcome of a measurement real so the complex conjugate of a real number is the same] → $\langle Q \rangle = \langle Q \rangle^*$

↓ but the reversed order has to be equal

Recall: $\langle g | f \rangle = \langle f | g \rangle^*$ (reverses order) → $\langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle$

Operators representing observables must have this property, its called hermitian.

Let's check this, is the momentum operator Hermitian?

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

integration by parts

if they are square integrable they must be zero at the boundary

$\langle f | \hat{Q} g \rangle = \langle Q^\dagger f | g \rangle$ $\quad \boxed{\int_{-\infty}^{\infty} f^* \hat{Q} g \, dx = \int_{-\infty}^{\infty} (\hat{Q}^\dagger f)^* g \, dx}$

a hermitian operator, is equal to its hermitian conjugate: $\hat{Q} = Q^\dagger$

Determinate States

• ordinarily if you measure an observable Q on an ensemble of identically prepared systems all in the same state Ψ, you don't get the same result

↳ Could we prepare a state such that every measurement of Q is certain to return the same value (call it q)

$\sigma^2 \equiv \langle (\Delta Q)^2 \rangle = \langle (Q - \langle Q \rangle)^2 \rangle$, $\Delta Q = Q - \langle Q \rangle$ how far the measurement is from $\langle Q \rangle$ IDK why

* if every measurement gives q then $\langle Q \rangle = q$

$\sigma^2 = \langle \Psi | (\hat{Q} - q)^2 \Psi \rangle$ = do the hermitian thing on just one $(\hat{Q} - q)$ = $\langle (\hat{Q} - q) \Psi | (\hat{Q} - q) \Psi \rangle = 0$

→ inner product of a vector w/ itself, has to be 0 bc
→ we know the RHS its $\sigma^2 = 0$ if its determinate (no spread)
→ the only vector whos dot product w/ itself is 0 is the 0 vector so!

$\hat{Q} \Psi = q \Psi$ eigen function

$(\hat{Q} - q) \Psi = 0 \rightarrow \boxed{\hat{Q} \Psi = q \Psi}$

Chapter 3 (Recasting the Theory)

Quantum theory is based on wave functions and operators!

State of system is represented by its wave function

Observables are represented by operators

a vector $|\alpha\rangle \to \vec{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_N \end{bmatrix}$

inner product $\langle \alpha | \beta \rangle = a_1^* b_1 + a_2^* b_2 + \dots + a_N^* b_N$

[Linear transformations are represented by matrices] $\to$ $|\beta\rangle = \hat{T}|\alpha\rangle \to b = Ta \begin{pmatrix} t_{11} & t_{12} & \cdots & t_{1N} \\ t_{21} & t_{22} & \cdots & t_{2N} \\ \vdots & \vdots & & \\ t_{N1} & t_{N2} & & t_{NN} \end{pmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix}$

A condition of quantum is $\int |\Psi|^2 = 1$, this says Ψ has to be square-integrable. These functions (set of functions) live in whats called a Hilbert Space.

satisfies all cond for an inner product

Inner product $\to$ $\langle f | g \rangle \equiv \int_a^b f^*(x) g(x)\, dx$, if f and g are square-int

Swarz-inequality $\to$ $\left| \int_a^b f^* g\, dx \right| \le \sqrt{\int_a^b |f|^2 dx \int_a^b |g|^2 dx}$

Notice: $\langle g | f \rangle = \langle f | g \rangle^*$ and $\langle f | f \rangle = \int_a^b |f|^2 dx$

Normalization: $\langle f_m | f_n \rangle = \delta_{mn}$

- a set of functions is complete if any other function (in Hilbert Space) can be expressed as a linear combo of them

Completeness: $f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$

$\hookrightarrow$ if set $\{ f_n(x) \}$ are orthonormal, $c_n = \langle f_n | f \rangle = \int_a^b \psi_n^* \psi(x,0) dx$

ψ_n $\psi(x,0)$

Note $\langle c\psi | \chi \rangle = c^* \langle \psi | \chi \rangle$

∠ uncertainty Principle

from $\sigma^2 = \langle (\hat{Q} - \langle Q\rangle)^2 \rangle$ ← square instead of absolute value
↳ distance from the mean

$$\sigma_A^2 = \langle (\hat{A} - \langle A\rangle)\Psi \,|\, (\hat{A} - \langle A\rangle)\Psi \rangle = \langle f|f\rangle$$

$$\sigma_B^2 = \langle (\hat{B} - \langle B\rangle)\Psi \,|\, (\hat{B} - \langle B\rangle)\Psi \rangle = \langle g|g\rangle$$

We will use the Schwarz inequality, derived elsewhere:

↳ $|a\cdot b|^2 \le a^2 b^2 \rightarrow |u\cdot v| \le |u||v|$

Quick Proof

↳ $|u+v|^2 = (u+v)\cdot(u+v) = u\cdot u + v\cdot v + 2u\cdot v = \underbrace{|u|^2 + |v|^2}_{\text{add this to each side of the original inequality}} + 2(u\cdot v)$ ← think about a triangle

$|u|^2 + |v|^2 + 2u\cdot v \le |u|^2 + |v|^2 + 2|u||v| = (|u| + |v|)^2$

↳ $|u+v|^2 \le (|u| + |v|)^2 \rightarrow |u+v| \le |u| + |v|$ (the length of the sum of two vectors is no more than the sum of lengths of the vectors)

Recast in terms of QM

$$\sigma_A^2 \sigma_B^2 = \underbrace{\langle f|f\rangle}_{\text{inner product, } |f|^2}\underbrace{\langle g|g\rangle}_{|g|^2} \ge |\langle f|g\rangle|^2$$

Now take a look at complex numbers

$|z|^2 = Re(z)^2 + Im(z)^2 \ge Im(z)^2$

↳ let $z = a + ib \rightarrow z - z^* = a + ib - a + ib = 2ib \rightarrow \frac{1}{2i}(z - z^*) = b = Im(z)$

↳ $|z|^2 \ge \left[\frac{1}{2i}(z - z^*)\right]^2$ with $\underbrace{\sigma_A^2\sigma_B^2}_{} = \underbrace{\langle f|f\rangle\langle g|g\rangle}_{\sigma_A^2\sigma_B^2} \ge |\underbrace{\langle f|g\rangle}_{z}|^2$

$\langle f|g\rangle^*$

$\langle Q\rangle = \langle Q\rangle^*$ ← flips

$\langle \Psi|\hat{Q}\Psi\rangle$
$= \langle \hat{Q}\Psi|\Psi\rangle$
$\hat{Q}^\dagger = \hat{Q}$

they are hermitian (real observables)

↳ $\sigma_A^2\sigma_B^2 \ge \left(\frac{1}{2i}\left[\langle f|g\rangle - \langle g|f\rangle\right]\right)^2$

$$\langle f|g\rangle = \langle (\hat{A} - \langle A\rangle)\Psi \,|\, (\hat{B} - \langle B\rangle)\Psi\rangle = \langle \Psi|(\hat{A} - \langle A\rangle)(\hat{B} - \langle B\rangle)\Psi\rangle$$

$$= \langle \Psi|(\hat{A}\hat{B} - \hat{A}\langle B\rangle - \hat{B}\langle A\rangle + \langle A\rangle\langle B\rangle)\Psi\rangle$$

$$= \langle \Psi|\hat{A}\hat{B}\Psi\rangle - \langle B\rangle\langle \Psi|\hat{A}\Psi\rangle - \langle A\rangle\langle \Psi|\hat{B}\Psi\rangle + \langle A\rangle\langle B\rangle\overbrace{\langle \Psi|\Psi\rangle}^{1}$$

$$= \langle \hat{A}\hat{B}\rangle - \langle B\rangle\langle A\rangle - \langle A\rangle\langle B\rangle + \langle A\rangle\langle B\rangle = \langle \hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle$$

← numbers not operators they can be in any order

$\langle f|g\rangle = \langle \hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle$

Now for $\langle g|f\rangle = \langle \hat{B}\hat{A}\rangle - \langle A\rangle\langle B\rangle$ ← flips

plug into here

$\langle f|g\rangle - \langle g|f\rangle = \langle \hat{A}\hat{B}\rangle - \langle \hat{B}\hat{A}\rangle$

$\langle \Psi|\hat{A}\hat{B}\Psi\rangle - \langle \Psi|\hat{B}\hat{A}\Psi\rangle = \langle \Psi|\underbrace{(\hat{A}\hat{B} - \hat{B}\hat{A})}_{[\hat{A}\hat{B}]}\Psi\rangle$

$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$

$$\sigma_A^2\sigma_B^2 \ge \left(\frac{1}{2i}\langle [\hat{A}, \hat{B}]\rangle\right)^2$$

ex $\hat{A} = x$, $\hat{B} = -i\hbar\frac{d}{dx}$ $\rightarrow [\hat{x}, \hat{p}] = i\hbar \rightarrow \sigma_A^2\sigma_B^2 \ge \left(\frac{1}{2i}i\hbar\right)^2 = \left(\frac{\hbar}{2}\right)^2$

$$\boxed{\sigma_x\sigma_p \ge \frac{\hbar}{2}}$$

Minimum uncertainty wave packet

• make schwarz inequality equal

↳ $\sigma_A^2 \sigma_B^2 = \langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2$ ← become equal when $g(x) = c\, f(x)$

↳ from $Re(z)^2 + Im(z)^2 \geq IM(z)^2$ → $Re(z) = 0$ ← equality, $z = \langle f|g\rangle$

$Re(c \langle f|f\rangle) = 0$ → $g(x) = \underbrace{ia}_{\text{some imaginary constant}} f(x)$

c ↑ imaginary, $\langle f|f\rangle$ real

↳ $g\Psi = c f \Psi$ → $\left(-i\hbar \frac{d}{dx} - \langle p\rangle\right)\Psi = ia\,(x - \langle x\rangle)\Psi$ (differential equation)

↳ $\Psi(x) = A e^{-a(x-\langle x\rangle)^2/2\hbar}\, e^{i\langle p\rangle x/\hbar}$ (gaussian is min uncertainty)

Energy - Time Uncertainty

$\Delta x \Delta p \geq \frac{\hbar}{2}$, Δx (the uncertainty) is loose notation for the standard deviation of the results of repeated measurements on identically prepared systems

(often paired with $\Delta t \Delta E \geq \frac{\hbar}{2}$) Δt isn't the standard deviation of a collection of time measurements. its the time it takes the system to change "substantially"

↳ as a measure → $\frac{d}{dt}\langle Q\rangle = \frac{d}{dt}\langle \Psi|\hat{Q}\Psi\rangle = \langle \frac{\partial \Psi}{\partial t}|\hat{Q}\Psi\rangle + \langle \Psi|\frac{\partial}{\partial t}(\hat{Q}\Psi)\rangle$ ← product rule again

$\frac{d}{dt}\langle Q\rangle = \langle \frac{\partial \Psi}{\partial t}|\hat{Q}\Psi\rangle + \langle \Psi|\frac{\partial \hat{Q}}{\partial t}\Psi\rangle + \langle \Psi|\hat{Q}\frac{\partial \Psi}{\partial t}\rangle$ and $i\hbar\frac{\partial \Psi}{\partial t} = \hat{H}\Psi$

$\hat{H}$ is hermitian!

minus from complex conjugate

↳ $\frac{d}{dt}\langle Q\rangle = -\frac{1}{i\hbar}\langle \hat{H}\Psi|\hat{Q}\Psi\rangle + \langle\frac{\partial \hat{Q}}{\partial t}\rangle + \frac{1}{i\hbar}\langle \Psi|\hat{Q}\hat{H}\Psi\rangle$

$= \frac{-1}{i\hbar}\langle \Psi|\hat{Q}\hat{H}\Psi\rangle - \frac{1}{i\hbar}\langle \Psi|\hat{H}\hat{Q}\Psi\rangle + \langle\frac{\partial \hat{Q}}{\partial t}\rangle$

$= \frac{-1}{i\hbar}\langle[\hat{H},\hat{Q}]\rangle + \langle\frac{\partial \hat{Q}}{\partial t}\rangle$ ← most the time $\frac{\partial \hat{Q}}{\partial t} = 0$, operators usually have no t dependence

ex) $Q = \frac{1}{2}m(\omega(t))^2 x^2$ spring constant changing due to t

[Go back to generalized uncertainty principle] → [with these operators H and Q] → $\sigma_H^2 \sigma_Q^2 \geq \left(\frac{1}{2i}\langle[\hat{H},\hat{Q}]\rangle\right)^2$, lets say Q has no t dependence

↳ $\sigma_H^2 \sigma_Q^2 = \left(\frac{1}{2i}\frac{\hbar}{i}\frac{d\langle Q\rangle}{dt}\right)^2 = \left(\frac{\hbar}{2}\right)^2\left(\frac{d\langle Q\rangle}{dt}\right)^2$ → $\boxed{\sigma_H \sigma_Q \geq \frac{\hbar}{2}\left|\frac{d\langle Q\rangle}{dt}\right|}$

define $\Delta E \equiv \sigma_H$ and

$\Delta t = \frac{\sigma_Q}{|d\langle Q\rangle/dt|}$ } $\Delta E \Delta t \geq \frac{\hbar}{2}$

$\sigma_Q = \left|\frac{d\langle Q\rangle}{dt}\right|\Delta t$ ← amount of time it takes the expectation value Q to change by one standard deviation

ertainty Principle Examples

xample 3.5

- if you have a stationary state, for which the energy is uniquely determined, all the expectation values are constant in time

↳ $|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{iEt/\hbar}\psi e^{-iEt/\hbar} = \psi^*\psi = |\psi(x)|^2$

↳ $\Delta E = 0$ and $\Delta t = \infty$

↳ to make something happen you have to have a linear combo of stationary states, (cross terms)

Lets say $\Psi(x,t) = a\underset{\psi_1(x)}{\psi_1} e^{-iE_1 t/\hbar} + b\psi_2 e^{-iE_2 t/\hbar}$

$|\Psi(x,t)|^2 = a^2\psi_1^2 + b^2\psi_2^2 + 2ab\psi_1\psi_2\cos\left(\frac{E_2 - E_1}{\hbar}t\right)$

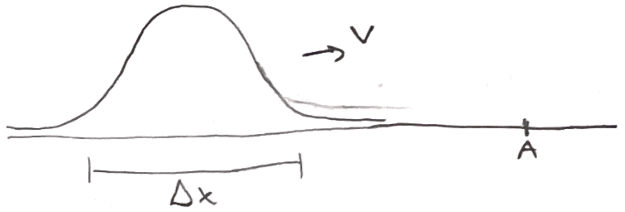
$\underbrace{\frac{E_2 - E_1}{\hbar}}_{\Delta E}\underbrace{\tau}_{\Delta t} = 2\pi$ (Period)

$\boxed{\Delta E\Delta t = 2\pi\hbar} \geq \hbar/2$

Example 3.6

- let Δt be the time it takes a free particle wave packet to pass a particular point.

Qualitatively: $\Delta t = \frac{\Delta x}{v} = \frac{m}{p}\Delta x$



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

$\Delta E\Delta t = \frac{p\Delta p}{m}\frac{m\Delta x}{p} = \Delta x\Delta p \geq \hbar/2$

- The Δ particle lasts about 10^{-23} s before decaying.
- If you make histogram of all the measurements of mass, you get a kind of bell shaped curve centered at $1232\ MeV/c^2$ w/ a width of $120\ MeV/c^2$.

↳ why does the measurement come out higher and sometimes lower?

let Δt be the lifetime of a particle (measure of how long it takes a sys to change)

$\Delta E\Delta t = \left(\frac{120}{2}MeV\right)\left(10^{-23}s\right) = 6\cdot 10^{-22}\ MeV\,s$

example

$\Psi(x,0) = a\psi_1 + b\psi_2$

$\Psi(x,t) = a\psi_1 e^{-iE_1 t/\hbar} + b\psi_2 e^{-iE_2 t/\hbar}$

$\hookrightarrow |\Psi|^2 = a^2\psi_1^2 + b^2\psi_2^2 + 2ab\,\psi_1\psi_2 \cos\left(\frac{E_1 - E_2}{\hbar} t\right)$

Find the uncertainty with $\Delta E \Delta t \geq \hbar/2$ and $b = 2a$

First: $\Psi(x,0) = \underset{c_1}{a}\psi_1 + \underset{c_2}{2a}\psi_2$ since its complete $\psi(x,0) = \sum c_n \psi_n$, $\sum |c_n|^2 = 1$

$\hookrightarrow$ $a^2 + 4a^2 = 1 \rightarrow a = 1/\sqrt{5}$

let: $\Delta t = \text{period} = \frac{2\pi}{\omega} = \frac{2\pi\hbar}{|E_1 - E_2|}$

$\Delta E = \sigma_H = \sqrt{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}$, remember $\hat{H}\psi = E\psi$

$\hat{H}^2\psi = \hat{H}\hat{H}\psi = \hat{H}(E\psi) = E(\underbrace{\hat{H}\psi}_{E\psi}) = E^2\psi$

$\langle \hat{H} \rangle = \sum |c_n|^2 E_n$ and $\langle \hat{H}^2 \rangle = \sum |c_n|^2 E_n^2$

$= \frac{1}{5}E_1^2 + \frac{4}{5}E_2^2$

$= \frac{1}{5}E_1 + \frac{4}{5}E_2$

$\hookrightarrow \langle \hat{H} \rangle^2 = \frac{1}{25}(E_1 + 4E_2)^2$ and $\langle \hat{H}^2 \rangle = \frac{1}{5}(E_1^2 + 4E_2^2)$

$= \frac{1}{25}(E_1^2 + 8E_1E_2 + E_2^2)$

$\sigma_H^2 = \frac{1}{5}E_1^2 + \frac{4}{5}E_2^2 - \frac{E_1^2}{25} - \frac{8}{25}E_1E_2 - \frac{1}{25}E_2^2 = \frac{4}{25}(E_1 - E_2)^2$

$\sigma_H = \frac{2}{5}(E_1 - E_2)$

$\Delta t \Delta E = \frac{4\pi}{5}\hbar \geq \frac{\hbar}{2}$