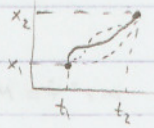
Quantum Mechanics 4/3/2007

$m\vec{a} = m\ddot{\vec{r}} = \vec{F}$ spherical $x = r\sin\theta\cos\varphi$ $y = r\sin\theta\sin\varphi$ $z = r\cos\theta$

$$S = \int_{t_1}^{t_2} L(\vec{q}, \dot{\vec{q}}, t)\, dt$$



trajectory is one that minimizes S

number $x \xrightarrow{f}$ number $f(x)$ function $F \xrightarrow{S}$ number $S[F]$

Basic variations calc.

$$S = \int_{t_1}^{t_2} F(x, \dot{x}, \ddot{x}, \dots, t)\, dt$$

$x \to \underset{\text{true trajectory}}{x} + \underset{\text{small variation}}{\delta x}$

$$S' = \int_{t_1}^{t_2} F(x + \delta x, \dot{x} + \delta\dot{x}, \dots t)\, dt$$

$$S' = S + \int_{t_1}^{t_2} \left(\frac{\partial F}{\partial x}\delta x + \frac{\partial F}{\partial \dot{x}}\delta\dot{x} + \frac{\partial F}{\partial \ddot{x}}\delta\ddot{x} + \dots \right) dt$$

$\delta S = S' - S \to 0$ if we are at true trajectory

$$0 = \int \Big[\frac{\partial F}{\partial x}\delta x + \overbrace{\frac{d}{dt}\left(\frac{\partial F}{\partial \dot{x}}\delta x\right) - \frac{d}{dt}\left(\frac{\partial F}{\partial \dot{x}}\right)\delta x}^{\frac{\partial F}{\partial \dot{x}}\delta\dot{x}} \dots \Big] dt$$

$$\delta S = 0 = \int \left(\frac{\partial F}{\partial x} - \frac{d}{dt}\left(\frac{\partial F}{\partial \dot{x}}\right) \right) \delta x\, dt + \frac{\partial F}{\partial \dot{x}} \underset{0}{\cancel{\delta x}} \Big|_{t_1}^{t_2}$$

$\delta x(t_1) = \delta x(t_2) = 0$

$$\therefore \boxed{\frac{d}{dt}\left(\frac{\partial F}{\partial \dot{x}}\right) = \frac{\partial F}{\partial x}}$$ Euler–Lagrange Eq.

if include 2nd derivative: $\frac{\partial F}{\partial x} - \frac{d}{dt}\left(\frac{\partial F}{\partial \dot{x}}\right) + \frac{d^2}{dt^2}\left(\frac{\partial F}{\partial \ddot{x}}\right) = 0$

$L(\underbrace{x, y, z}_{\vec{q}}, \underbrace{\dot{x}, \dot{y}, \dot{z}}_{\dot{\vec{q}}}, t)$ q_i $i = 1, 2, 3$: x, y, z $q_p \to$ different particle

$$S = \int_{t_1}^{t_2} L(\vec{q}, \dot{\vec{q}}, t)\, dt \to \text{action} \qquad \delta S = 0 \to \text{Hamilton's principle}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

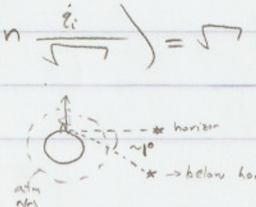
$E = A e^{i\omega t + i\vec{k}\cdot\vec{r}}$ $I = EE^* = |A|^2$ $k = \frac{2\pi}{\lambda}$

Fermat's principle $\varphi = \int \vec{k} \cdot d\vec{r} = \min$ for path of light

$$\int \frac{2\pi}{\lambda} dl = \int \frac{2\pi\nu}{c/n(\vec{r})} dl \qquad \varphi = \int_1^2 n(\vec{r})\, dl = \min = \int n(\vec{r}) \sqrt{\frac{dx^2}{dt^2} + \frac{dy^2}{dt^2} + \frac{dz^2}{dt^2}}\, dt$$

$$L = n(\vec{r})\sqrt{\dot{x}^2 + \dot{y}^2 + \dot{z}^2} \qquad \therefore \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i}$$

$$\frac{d}{dt}\left(n \frac{\dot{q}_i}{\sqrt{}}\right) = \sqrt{}\, \frac{\partial n}{\partial q_i}$$ if $\frac{\partial n}{\partial q_i} = 0$ $\therefore \frac{d}{dt}\left(\frac{\dot{q}_i}{\sqrt{}}\right) = 0 \Rightarrow \dot{q}_i = \text{constant}$



can see stars below horizon due to bending of light

$\to$ HW show $\theta \sim 1°$

cylindrical $x = r\cos\varphi$ $y = r\sin\varphi$ $L = \frac{m}{2}\dot{x}^2 + \frac{m}{2}\dot{y}^2$ Cartesian

$\dot{x} = \dot{r}\cos\varphi - r\sin\varphi\,\dot{\varphi}$ $\dot{y} = \dot{r}\sin\varphi + r\cos\varphi\,\dot{\varphi}$

$\boxed{L = \frac{m}{2}\dot{r}^2 + \frac{m r^2 \dot{\varphi}^2}{2}}$ Polar

$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\varphi}}\right) = \frac{d}{dt}\left(m r^2 \dot{\varphi}\right) = \frac{\partial L}{\partial \varphi} = 0 \quad \therefore \quad m r^2 \dot{\varphi} = M = \text{constant}$

$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}}\right) = \frac{d}{dt}\left(m\dot{r}\right) = \frac{\partial L}{\partial r} = m r \dot{\varphi}^2 \qquad m\ddot{r} = m r \dot{\varphi}^2$

$S = \int_{t_1}^{t_2} L(\vec{q},\dot{\vec{q}},t)\,dt \qquad L' = L + \frac{d}{dt}\left(f(\vec{q},t)\right)$ does not change equation of motion

$S' = S + \int_{t_1}^{t_2} \frac{d}{dt}\left(f(\vec{q},t)\right) dt = S + \underbrace{f(\vec{q}_2,t_2) - f(\vec{q}_1,t_1)}_{\text{fixed values}} \qquad \delta S' = \delta S$

$L(\dot{\vec{r}}^2)$ uniform isotropic $S = \int L(\dot{\vec{r}}^2)\,dt \qquad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_i}\right) = 0$

$\frac{d}{dt}\left(\frac{\partial L}{\partial v^2} 2\dot{r}_i\right) = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_i}\right) \qquad \frac{\partial L}{\partial \dot{r}_i} = \frac{\partial L}{\partial v^2}\frac{d v^2}{d\dot{r}_i} = \frac{\partial L}{\partial v^2} 2 r_i$

$\therefore \quad \frac{\partial L}{\partial v^2} 2 r_i = \text{constant} = p_i \qquad \dot{r}_i = \frac{p_i}{2\frac{\partial L}{\partial v^2}}$

$\sum_i r_i^2 = v^2 = \sum_i \left(\frac{p_i}{2\frac{\partial L}{\partial v^2}}\right)^2 \qquad v^2 = \text{constant} \qquad \dot{r}_i = \text{const}$

$\left((\vec{v},\vec{\varepsilon}) = \vec{v}\cdot\vec{\varepsilon}\right)$

$L = L\left((\vec{v}+\vec{\varepsilon})^2\right) = L(v^2) + \frac{\partial L}{\partial v^2} 2(\vec{v}\cdot\vec{\varepsilon})$

vel of frame of reference ($\varepsilon \ll v$)
Galilean transf

Since equation of motion don't change

$\frac{\partial L}{\partial v^2} 2(\vec{v}\cdot\vec{\varepsilon}) = \frac{d}{dt}\left(f(\vec{q},t)\right)$

$\frac{\partial L}{\partial v^2} 2(\dot{\vec{r}}\cdot\vec{\varepsilon}) = \frac{d}{dt}\left(f(\vec{r},t)\right) \qquad \therefore \frac{\partial L}{\partial v^2} = \text{constant} \qquad L = \frac{m}{2}v^2$

$L = \frac{m}{2}(\vec{v}+\vec{\varepsilon})^2 = \frac{m v^2}{2} + \underbrace{m(\dot{\vec{r}}\cdot\vec{\varepsilon}) + \frac{m}{2}(\vec{\varepsilon}\cdot\vec{\varepsilon})}$

$\frac{d}{dt}\left(m(\vec{r}\cdot\vec{\varepsilon}) + \frac{m}{2}(\vec{\varepsilon}\cdot\vec{\varepsilon})t\right)$

Action invariance transformation $\rightarrow$ existance of symmetry $\rightarrow$ integral of motion

4/5/2007

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}$$

action invariant transformation → existance of symmetry → integrals of motion

$$L' = L + \frac{d}{dt}(f(q,t)) \longrightarrow \underline{\text{inertial ref. frames}} \rightarrow V_i$$

$$L(\vec{r},\dot{\vec{r}},t) = L(\vec{r},\dot{\vec{r}},t+\delta t) = L(\vec{r},\dot{\vec{r}},t) + \frac{\partial L}{\partial t}\delta t = \underbrace{\left(1+\delta t\frac{\partial}{\partial t}\right)}L$$

require $\frac{\partial L}{\partial t} = 0$ to hold translation in time

operator $\hat{T}(\delta t) = \left(1 + \delta t \frac{\partial}{\partial t}\right)$ translation in time

summation notation

$$\frac{dL}{dt} = \frac{\partial L}{\partial t} + \underbrace{\frac{\partial L}{\partial r_i}}_{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_i}\right)}\dot{r}_i + \frac{\partial L}{\partial \dot{r}_i}\ddot{r}_i = \frac{\partial L}{\partial t} + \underbrace{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_i}\right)\dot{r}_i + \frac{\partial L}{\partial \dot{r}_i}\ddot{r}_i}_{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_i}\dot{r}_i\right)}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_i}\dot{r}_i - L\right) = -\frac{\partial L}{\partial t}$$

if $\frac{\partial L}{\partial t} = 0$ → invariant wrt time translation

$$\rightarrow \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i - L = E$$

$$L = \frac{1}{2}a_{ik}(\vec{q})\dot{q}_i\dot{q}_k + b_k(\vec{q})\dot{q}_k - U(\vec{q})$$ generic form of L $\left(L = \frac{1}{2}m\dot{r}^2 - U(\vec{r})\right)$

$$E = \underbrace{\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i - L}_{(p\dot{q}_i - L)} \qquad \dot{q}_i\frac{\partial L}{\partial \dot{q}_i} = a_{ik}\dot{q}_i\dot{q}_k + b_k\dot{q}_k \qquad \frac{\partial L}{\partial \dot{q}_m} = \frac{\partial}{\partial \dot{q}_m}\left(\frac{1}{2}a_{ik}\dot{q}_i\dot{q}_k + b_k\dot{q}_k\right)$$

$$\frac{\partial L}{\partial \dot{q}_m} = \frac{1}{2}a_{ik}\underbrace{\frac{\partial \dot{q}_i}{\partial \dot{q}_m}}_{\delta_{im}}\dot{q}_k + \frac{1}{2}a_{ik}\dot{q}_i\frac{\partial \dot{q}_k}{\partial \dot{q}_m} + b_k\frac{\partial \dot{q}_k}{\partial \dot{q}_m} = \frac{1}{2}a_{ik}\dot{q}_k\delta_{im} + \frac{1}{2}a_{ik}\dot{q}_i\delta_{km} + b_k\delta_{km}$$

$$= \underbrace{\frac{1}{2}a_{mk}\dot{q}_k + \frac{1}{2}a_{im}\dot{q}_i}_{\text{making symmetric \& add up}} + b_m \qquad \therefore \boxed{E = \frac{1}{2}a_{ik}\dot{q}_i\dot{q}_k + U(\vec{q})}$$

Translation in space $\vec{r}_s \rightarrow \vec{r}_s + \vec{\varepsilon}$, $\dot{\vec{r}}_s \rightarrow \dot{\vec{r}}_s$ s: particle (multiple particles)

$$\delta L = L(\vec{r}_s+\vec{\varepsilon}, \dot{\vec{r}}_s, t) - L(\vec{r}_s, \dot{\vec{r}}_s, t) = \sum_s\left(\underbrace{\frac{\partial L}{\partial \vec{r}_s}}_{\nabla_s L}\cdot\vec{\varepsilon}\right) = 0 \quad \text{if invariant}$$

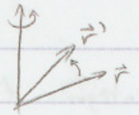
operator $\hat{T}(\vec{\varepsilon}) = \left(1 + \vec{\varepsilon}\sum_s\frac{\partial}{\partial \vec{r}_s}\right)$

$$\sum_s \vec{\varepsilon}\cdot\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{r}}_s}\right) = \frac{d}{dt}\left(\vec{\varepsilon}\cdot\sum_s\frac{\partial L}{\partial \dot{\vec{r}}_s}\right) = 0$$

$\vec{r}_s \rightarrow \vec{r}_s + \vec{\varepsilon}$ $\quad \delta L = 0 \quad \rightarrow \quad \vec{\varepsilon}\cdot\sum_s\frac{\partial L}{\partial \dot{\vec{r}}_s} = \vec{\varepsilon}\cdot\sum_s\vec{P}_s = P_\varepsilon$ momentum conservation

$\boxed{\vec{p} = \frac{\partial L}{\partial \dot{\vec{r}}}}$ generalized momentum

Rotation $\delta\vec{\varphi}$



$$\delta\vec{r}_s = [\delta\vec{\varphi}\times\vec{r}_s] \qquad e_{ikl} \quad e_{123}=1 \quad e_{321}=-1$$

$$\delta\dot{\vec{r}}_s = [\delta\vec{\varphi}\times\dot{\vec{r}}_s]$$

$$\delta L = \sum_s\left(\frac{\partial L}{\partial\vec{r}_s}\delta\vec{r}_s + \frac{\partial L}{\partial\dot{\vec{r}}_s}\delta\dot{\vec{r}}_s\right) = \sum_s\left(\underbrace{\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\vec{r}}_s}\right)}_{\frac{d\vec{p}_s}{dt}}\cdot(\delta\vec{\varphi}\times\vec{r}_s) + \vec{p}_s\cdot(\delta\vec{\varphi}\times\dot{\vec{r}}_s)\right)$$

$$= \sum_s\left(\delta\vec{\varphi}\cdot(\vec{r}_s\times\dot{\vec{p}}_s) + \delta\vec{\varphi}\cdot(\dot{\vec{r}}_s\times\vec{p}_s)\right) = \delta\vec{\varphi}\cdot\frac{d}{dt}\underbrace{\sum_s(\vec{r}_s\times\vec{p}_s)}_{\text{angular momentum}}$$

$$M_\varphi = \sum_s M_\varphi = \sum_s(\vec{r}_s\times\vec{p}_s)_\varphi \qquad \text{conservation of angular momentum}$$

Noether's theorem – future HW

$$\vec{p} = \frac{\partial L}{\partial\dot{\vec{q}}} \qquad \frac{d\vec{p}}{dt} = \frac{\partial L}{\partial\vec{q}}$$

Hamilton – Jacobi

$$L = L(q,\dot{q},t) \qquad dL = \frac{\partial L}{\partial t}dt + \underbrace{\frac{\partial L}{\partial q}}_{\dot{p}}dq + \underbrace{\frac{\partial L}{\partial\dot{q}}}_{p}d\dot{q} = \frac{\partial L}{\partial t}dt + \dot{p}\,\delta q + p\,\delta\dot{q}$$

$$p\,\delta\dot{q} = d(p\dot{q}) - \dot{q}\,\delta p \qquad dL = \frac{\partial L}{\partial t}dt + \dot{p}\,dq + d(p\dot{q}) - \dot{q}\,dp$$

$$d(p\dot{q}-L) = -\frac{\partial L}{\partial t}dt - \dot{p}\,\delta q + \dot{q}\,\delta p = dH \qquad \boxed{\dot{q} = \frac{\partial H}{\partial p} \quad \dot{p} = -\frac{\partial H}{\partial q}}$$

Hamiltonian $\boxed{H(q,p,t) = p\dot{q} - L}$ function of 3 indep variable not an energy

1) take $L(q,\dot{q},t)$ 2) $p = \frac{\partial L}{\partial\dot{q}} \Rightarrow \dot{q} = \dot{q}(q,p,t)$ 3) $H = p\dot{q}(q,p,t) - L(q,\dot{q}(q,p,t),t)$

Particle in EM field

$$L = \frac{1}{2}mv^2 - e\phi(\vec{r}) + \frac{e}{c}(\vec{v}\cdot\vec{A}) \qquad P_k = \frac{\partial L}{\partial v_k} = mv_k + \frac{e}{c}A_k \quad \text{generalized momentum}$$

$$v_k = \frac{P_k - \frac{e}{c}A_k}{m} \qquad H = p_k\left(\frac{P_k - \frac{e}{c}A_k}{m}\right) - L$$

$$H(p,r,t) = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + e\phi$$

$$\boxed{\dot{q} = \frac{\partial H}{\partial p} \quad \dot{p} = -\frac{\partial H}{\partial q}} \rightarrow \text{Hamilton's Canonical Eqs.} \qquad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$$

$$\frac{dH}{dt} = -\frac{\partial L}{\partial t} - \dot{p}\frac{dq}{dt} + \dot{q}\frac{dp}{dt} = -\frac{\partial L}{\partial t} \qquad \frac{dH}{dt} = -\frac{\partial L}{\partial t} = \frac{\partial H}{\partial t}$$

$\vec{r}_s' = \vec{r}_s + \vec{\varepsilon}$ $\quad \vec{p}_s' = \vec{p}_s$

$$H = H + \sum_s \left(\underbrace{\frac{\partial H}{\partial \vec{r}_s}}_{-\dot{\vec{p}}_s} \cdot \vec{\varepsilon}\right) = H - \vec{\varepsilon} \cdot \sum_s \dot{\vec{p}}_s \qquad dH = 0 \Rightarrow \frac{d}{dt}\left(\vec{\varepsilon} \cdot \sum_s \vec{p}_s\right) = 0$$

$\vec{P}_\varepsilon = \vec{\varepsilon} \cdot \sum_s \vec{p}_s = \text{const}$

arbitrary function $f(q,p,t)$ $\qquad \frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial p}\dot{p} + \frac{\partial f}{\partial q}\dot{q}$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} \underbrace{- \frac{\partial f}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial f}{\partial q}\frac{\partial H}{\partial p}} \qquad \boxed{\frac{df}{dt} = \frac{\partial f}{\partial t} + \{H, f\}}$$

Poisson bracket $\{H, f\} = \sum_s \left(\frac{\partial H}{\partial \vec{p}_s} \cdot \frac{\partial f}{\partial \vec{r}_s} - \frac{\partial H}{\partial \vec{r}_s} \cdot \frac{\partial f}{\partial \vec{p}_s}\right)$

$\hookrightarrow \frac{\partial H}{\partial p_x}\frac{\partial f}{\partial r_x} + \frac{\partial H}{\partial p_y}\frac{\partial f}{\partial r_y} + \dots$

if $\frac{\partial f}{\partial t} = 0$ $\qquad \frac{df}{dt} = \{H, f\}$ $\qquad$ if f is integral of motion $\{H, f\} = 0$

if $f = H$ $\qquad \frac{dH}{dt} = \frac{\partial H}{\partial t}$ $\qquad$ since $\{H, H\} = 0$

Poisson bracket properties $\qquad \{f(p,q), g(p,q)\} = \frac{\partial f}{\partial p}\frac{\partial g}{\partial q} - \frac{\partial f}{\partial q}\frac{\partial g}{\partial p}$

1) $\{f, g\} = -\{g, f\}$

2) $\{f, \text{const}\} = 0$ $\qquad$ 3) $\{f_1 f_2, g\} = f_1\{f_2, g\} + f_2\{f_1, g\}$

4) $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$ $\quad$ Jacobi identity

if g, f are integral of motion $\qquad \frac{\partial g}{\partial t} + \{H, g\} = 0 \qquad \frac{\partial f}{\partial t} + \{H, f\} = 0$

can show that $\{f, g\}$ is also an integral of motion (using Jacobi identity)

$\{f, r_k\} = \frac{\partial f}{\partial p_i}\overbrace{\frac{\partial r_k}{\partial r_i}}^{\delta_{ik}} - \frac{\partial f}{\partial r_i}\cancel{\frac{\partial r_k}{\partial p_i}}^{0}$ indep. variables

$$\boxed{\begin{array}{lll} \{f, r_k\} = \frac{\partial f}{\partial p_k} & \{f, p_k\} = -\frac{\partial f}{\partial r_k} & \\ \{r_i, r_k\} = 0 & \{p_i, p_k\} = 0 & \{p_i, r_k\} = \delta_{ik} \end{array}}$$

for $\vec{M} = \vec{r} \times \vec{p}$ $\qquad M_i = e_{ijk} r_j p_k$

$\{M_i, r_j\} = \frac{\partial}{\partial p_j}(e_{ink} r_n p_k) = e_{ink} r_n \delta_{kj} = e_{inj} r_n = -e_{ijn} r_n$

$$\boxed{\begin{array}{ll} \{M_i, r_j\} = -e_{ijk} r_k & \{M_i, p_j\} = -e_{ijk} p_k \\ \{M_i, M_j\} = -e_{ijk} M_k & \end{array}}$$

Ex: $\underbrace{\frac{dM_x}{dt} = 0 \quad \frac{dM_y}{dt} = 0}_{\text{integrals of motion}} \Rightarrow M_z = \text{const.}$ (using Jacobi identity)

$\frac{dM_z}{dt} = 0 \quad \frac{dp_y}{dt} = 0 \Rightarrow p_z = \text{const.}$

$\frac{df}{dt} = \{H, f\}$ (if $\frac{\partial f}{\partial t} = 0$) $\qquad \frac{\partial f}{\partial \varphi} = \{\vec{M}, f\}$

$f(\vec{r}, \vec{p}) \qquad f(\vec{r} + \delta\vec{r}, \vec{p}) = f(\vec{r}, \vec{p}) + \delta\vec{r} \cdot \frac{\partial f}{\partial \vec{r}} = f(\vec{r}, \vec{p}) + \delta\vec{r} \cdot \{\vec{p}, f\}$

momentum is generator of small translations

$\frac{\partial f}{\partial \vec{r}} = \{\vec{p}, f\} \qquad \frac{\partial f}{\partial \vec{p}} = -\{\vec{r}, f\}$ $\quad$ $-\vec{r}$ is generator of translations in $\vec{p}$

$\frac{\partial f}{\partial \varphi} = \{\vec{M}, f\}$ angular momentum is generator of rotations

$\frac{df}{dt} = \{H, f\}$ (if $\frac{\partial f}{\partial t} = 0$) Hamiltonian is generator of translations in time

---

$f(p(t), q(t))$ $\quad f|_{t=0} = f(p(0), q(0))$

$f(t) = f(0) + t\frac{f^{(1)}}{1!} + t^2\frac{f^{(2)}}{2!} + \dots t^n \frac{f^{(n)}}{n!}$ $\qquad \frac{df^{(1)}}{dt} = \{H, f^{(1)}\} = \{H, \{H, f\}\}$

$\frac{df}{dt} = \{H, f\}$ $\qquad f(t) = f(0) + t\{H, f\} + \frac{1}{2}t^2\{H, \{H, f\}\} + \dots$

$H = \frac{p^2}{2m} - max$ $\qquad x(t) = x(0) + t\frac{p(0)}{m} + \frac{t^2}{2}a + 0$

$\{H, x\} = \frac{\partial H}{\partial p_x} = \frac{p}{m}$ $\qquad \{H, \{H, x\}\} = \{H, \frac{p}{m}\} = a$

$p(t) = p(0) + t\,ma$ $\qquad \{H, p\} = -\frac{\partial H}{\partial x} = ma$

$f(q, p) = e^{t\hat{H}} f(q, p)|_{t=0}$ $\qquad e^{t\hat{H}} = 1 + \frac{t}{1!}\{H, \_\} + \frac{t^2}{2!}\{H, \{H, \_\}\} + \dots$

4/10/2007

$Q_i = Q_i(q, p, t)$ $\quad P_i = P_i(q, p, t)$

new coords.

$\delta \int_{t_1}^{t_2} L\,dt = 0 \Rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = \frac{\partial L}{\partial q}$

variational principle

$L = p\dot{q} - H(q, p, t) = \Lambda(q, p, \dot{q}, \dot{p}, t)$

$\frac{d}{dt}\left(\frac{\partial \Lambda}{\partial \dot{q}}\right) - \frac{\partial \Lambda}{\partial q} = 0 \Rightarrow \frac{d}{dt}(p) + \frac{\partial H}{\partial q} = 0 \Rightarrow \dot{p} = -\frac{\partial H}{\partial q}$ as before

$\frac{d}{dt}\left(\frac{\partial \Lambda}{\partial \dot{p}}\right) - \frac{\partial \Lambda}{\partial p} = 0 \rightarrow \dot{q} = \frac{\partial H}{\partial p}$ as before

$\int \Lambda\,dt \rightarrow \int (p\,dq - H\,dt) = \underbrace{\int (P\,dQ - H'dt)}_{\text{new variables}} + \int dF$

full diff. of some function $\quad \int L\,dt \rightarrow \int (L + \frac{df}{dt})\,dt$

$dF = p\,dq - P\,dQ + (H' - H)\,dt = dF(q, Q, t)$ generating function

$p = \frac{\partial F}{\partial q}$ $\quad P = -\frac{\partial F}{\partial Q}$ $\quad H' = H + \frac{\partial F}{\partial t}$

$Q(q,p,t) \longrightarrow P(q,p,t) \longrightarrow H(Q, P, t)$

Meaning of p, q is ~lost $\quad \begin{matrix} Q = p \\ P = -q \end{matrix}$ satisfies eqns

---

$\{f, g\}_{p,q} = \{f, g\}_{P,Q}$ — invariant don't depend on ref. frame

---

$\{Q_i, Q_k\} = \{P_i, P_k\} = 0$ $\qquad \{P_i, Q_k\} = \delta_{ik}$

canonical conjugate variables

Uses for generating function

1) $H \to H + \delta H^{(1)}$ first order pertubation

$\to H + \delta H^{(>1)}$ using generator function ex: $\underset{(1)}{\text{rot.}}$, $\underset{(1)}{\text{vib.}}$, $\underset{(>1)}{\text{coupling between}}$ rot. + vib.

2) Explicitly account for symmetry

3) Can set $H' \to 0$

4) Adiabatic invariants theory (small changes) ex slow growth of BH with planets around it

More on (3) $H' = H + \frac{\partial F}{\partial t}$

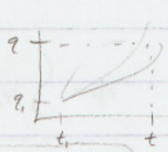
Hamilton-Jacobi theory

find S so that $H' = H + \frac{\partial S}{\partial t} = 0$ $\quad \underbrace{\dot{Q} = \frac{\partial H'}{\partial P} = 0 \quad \dot{P} = -\frac{\partial H'}{\partial Q} = 0}$ trivial eqns of motion

solutions: $Q = \text{const}$ $\quad P = \text{const}$ variables are called action and angle

$$dS(q, Q{=}\text{const}, t) = p\,dq - P\,dQ + (H' - H)\,dt = p\,dq - H\,dt$$

$$\frac{dS}{dt} = p\dot{q} - H = L \qquad S = \int_{t_1}^{t} L\,dt \quad \text{action}$$



$$\boxed{\frac{\partial S}{\partial q} = p \qquad H = -\frac{\partial S}{\partial t}} \qquad \boxed{H\Big(q_1, q_2, \ldots, \underbrace{\frac{\partial S}{\partial q_1}, \frac{\partial S}{\partial q_2}, \ldots}_{P_1, P_2, \ldots}, t\Big) + \frac{\partial S}{\partial t} = 0}$$

Ex: $H = \frac{1}{2m}p^2 + m\frac{x^2}{2}$ $\qquad \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + \frac{m}{2}x^2 + \frac{\partial S}{\partial t} = 0$

$dS = \sum_i p_i\,dq_i - H\,dt$ (multiple particles) $\qquad S = \int \sum_i p_i\,dq_i - E(t - t_0)$ if $\frac{\partial H}{\partial t} = 0$ $\quad H \to E$ energy

Quantum Mechanics

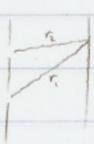
Balmer 1885 $\quad \lambda = \frac{n^2}{n^2 - 2^2}\, 3645.6\,\text{Å}$ $\quad$ also Bohr (1913) $\quad E_n = -\left(\frac{qe}{4\pi\epsilon_0}\right)^2 \frac{m}{2\hbar^2 n^2}$

$E_n - E_{n'} = \frac{hc}{\lambda}$

Planck $\quad I(\omega) = \frac{\hbar\omega^3}{\pi^2 c^2}\left(e^{-\frac{\hbar\omega}{kT}} - 1\right)^{-1}$

photon $\quad E = \hbar\omega = h\nu \qquad k = \frac{2\pi}{\lambda} = \frac{\omega}{c} \qquad E = pc \qquad k = \frac{p}{\hbar}$

(1924) de Broglie electrons $\quad \omega = \frac{E}{\hbar} \quad k = \frac{p}{\hbar}$ electrons as waves



$E = A e^{i(k\cdot r - \omega t)}$

$I = E^* E = |A|^2 \qquad E = A e^{i(k\cdot r_1 - \omega t)} + A e^{i(k\cdot r_2 - \omega t)}$

$$I = 2|A|^2\left(1 + \cos(k(r_1 - r_2))\right) = 4|A|^2 \cos^2\left(\frac{k\Delta r}{2}\right)$$

$$E = A e^{i(\vec{p}\cdot\vec{r} - Et)\frac{1}{\hbar}} = A e^{\frac{i}{\hbar}\underbrace{\left(\int \vec{p}\,d\vec{r} - E\,dt\right)}_{\text{action } S}}$$

$\hbar \to 0$

Geometric Optics

Fermat's principle $\int \vec{k}\cdot d\vec{r} = \min$

$k = \frac{2\pi}{\lambda}$ $\lambda \ll \ell$ (scale length)

$\psi = a e^{i\frac{S}{\hbar}}$ particle as wave $\hbar = 1.055 \times 10^{-27}$

$\psi^* \psi \to$ interpret this as a probability Born 1926

$\psi(x) = \int \psi(x')\, \underbrace{\delta(x'-x)}_{\text{wave function with determined coordinate}}\, dx'$ superposition principle

differential probability function $\frac{dP}{dx} = \psi_{(x)}^* \psi_{(x)} = \int \psi^*_{(x'')}\, \delta(x''-x)\, \delta(x'-x)\, \psi(x')\, dx'\, dx''$

$\Phi = \frac{dP}{dx}$ $\hat{\Phi} = \delta(x'-x)\,\delta(x''-x)$

for any measurement $\underbrace{\Phi}_{\text{observable}} = \int \psi^* \underbrace{\hat{\Phi}_{(x',x'')}}_{\text{operator}} \psi\, dx'\, dx''$

$\psi = c_1 \psi_1 + c_2 \psi_2$

configuration space

$\psi = \sum_{x'} \underbrace{\psi_{x'}}_{\text{coeff.}} \underbrace{|x'\rangle}_{\text{state}} = \sum_{p'} \varphi_{p'} |p'\rangle$

$|\psi\rangle$ ket $\Phi = \int \psi_x^* |x\rangle^* \hat{\Phi}_x \psi_x |x\rangle\, dx$ $\Phi = \int \psi_p^* |p\rangle^* \hat{\Phi}_p \psi_p |p\rangle\, dp$

$\Phi = \langle \psi | \hat{\Phi} | \psi \rangle$ indep of basis/coordinates

$\psi = c_1 \psi_{1(t)} + \psi_{2(t)}$ evolution with time must be linear $\frac{d\psi}{dt} = \hat{L}\psi$ (not $\hat{L}\psi^n$ $n \neq 1$)

$\int_{-\infty}^{\infty} \psi^*_{(x)} \psi_{(x)}\, dx = 1$ normal $\langle \psi | \psi \rangle = 1$ scalar/inner product

$|\psi\rangle = \sum_f A_f |f\rangle \to$ obeys linear algebra

Hilbert space

$\langle \psi_1 | \psi_2 \rangle =$ a number $|\psi_1\rangle\langle \psi_2| =$ an operator

$|\psi_1\rangle = a_{11}|1\rangle + b_{12}|2\rangle$ $|\psi_2\rangle = a_{21}|1\rangle + b_{22}|2\rangle$ $\langle \psi_1 | \psi_2 \rangle = (a_{11}\ b_{12})\begin{pmatrix} a_{21} \\ b_{22} \end{pmatrix} = a_{11}a_{21} + b_{12}b_{22}$

$|\psi_1\rangle\langle \psi_2| = \begin{pmatrix} a_{21} \\ b_{22} \end{pmatrix}(a_{11}\ b_{12}) = \begin{pmatrix} a_{21}a_{11} & a_{21}b_{12} \\ b_{22}a_{11} & b_{22}b_{12} \end{pmatrix}$

$\langle \psi_n | \psi_n \rangle = 1$ $\sum |a_n|^2 = 1$ $|a_n|^2 =$ probability to find system in state n

4/12/2007

$\langle\psi|\psi\rangle = 1 = \sum |a_n|^2$ $\quad\langle\psi| = \sum a_n^* \langle\psi_n|$

$1 = \sum a_n^* \langle\psi_n|\psi\rangle$ $\quad a_n = \langle\psi_n|\psi\rangle = \langle\psi_n|\sum_m a_m|\psi_m\rangle = \sum_m a_m \langle\psi_n|\psi_m\rangle$

$\therefore \langle\psi_n|\psi_m\rangle = \delta_{nm}$ orthogonal

$\bar{f} = \sum f_n \underbrace{|a_n|^2}_{\text{prob. to get } f_n} = \langle\psi|\hat{f}|\psi\rangle = \sum f_n a_n \langle\psi|\psi_n\rangle = \sum \langle\psi|f_n a_n|\psi_n\rangle$

$\hat{f}|\psi\rangle = \hat{f}\sum a_n|\psi_n\rangle = \sum_n a_n \hat{f}|\psi_n\rangle$ $\quad\therefore \hat{f}|\psi_n\rangle = f_n|\psi_n\rangle$ eigenvector, eigenvalue

$\bar{f} = \bar{f}^* = \int \psi^* \hat{f}\psi\, dq = \int \psi\, \hat{f}^*\psi^*\, dq = \int \hat{f}^*\psi^*\psi\, dq$

transposed operator: $\int \psi\, \hat{f}\varphi\, dq = \int (\tilde{\hat{f}}\psi)\varphi\, dq$ $\quad\therefore \hat{f}^* = \tilde{\hat{f}}$ $\quad \hat{f} = \tilde{\hat{f}}^* = \hat{f}^+$

self-adjoint / hermitian → real observables

$f^* = (\langle\psi|\hat{f}|\psi\rangle)^+ = \langle\psi|\hat{f}^+|\psi\rangle = \langle\psi|\hat{f}|\psi\rangle = f$

Degeneracy + Multiple observables

$\hat{f}|\psi_m\rangle = f_m|\psi_m\rangle$ $\quad \hat{f}|\psi_n\rangle = f_n|\psi_n\rangle$ $\quad \langle\psi_m|\cdot$

$\langle\psi_m|\hat{f}^+ = f_m\langle\psi_m|$ $\quad \cdot|\psi_n\rangle \rightarrow \langle\psi_m|\hat{f}^+|\psi_n\rangle = f_m\langle\psi_m|\psi_n\rangle$ $\quad \langle\psi_m|\hat{f}|\psi_n\rangle = f_n\langle\psi_m|\psi_n\rangle$

$\langle\psi_m|\psi_n\rangle = \begin{cases} 1 & m=n \\ 0 & m\neq n \end{cases} = \delta_{mn}$ $\quad\therefore (f_m - f_n)\langle\psi_m|\psi_n\rangle = 0$ if $\hat{f} = \hat{f}^+$

$\hat{f}|\psi_n\rangle = f_n|\psi_n\rangle$ $\quad \hat{g}|\psi_n\rangle = g_n|\psi_n\rangle$

$\hat{f}\hat{g}|\psi_n\rangle = \hat{f}g_n|\psi_n\rangle = f_n g_n|\psi_n\rangle = g_n f_n|\psi_n\rangle = \hat{g}\hat{f}|\psi_n\rangle$

$(\hat{f}\hat{g} - \hat{g}\hat{f})|\psi_n\rangle = 0$ $\quad \{\hat{f},\hat{g}\} = 0$ comutator $\quad$ can measure both observables

$\hat{P}_{nm} = |\psi_n\rangle\langle\psi_m|$ $\quad \hat{P}_{nm}|\psi\rangle = |\psi_n\rangle\langle\psi_m|\psi\rangle = a_m|\psi_n\rangle$ $\quad |\psi\rangle = \sum a_m|\psi_m\rangle$

projection operator $\quad$ projects state m to state n

$\sum_n |\psi_n\rangle\langle\psi_n| = \hat{I}$ $\quad \hat{I}|\psi\rangle = |\psi\rangle$ $\quad \sum_n |\psi_n\rangle\langle\psi_n|\psi\rangle = \sum_n a_n|\psi_n\rangle = |\psi\rangle$

closed relationship

$\hat{f}|\psi_n\rangle = f_n|\psi_n\rangle$ $\quad \sum_n \hat{f}|\psi_n\rangle\langle\psi_n| = \sum_n f_n|\psi_n\rangle\langle\psi_n|$ $\quad \hat{f}\hat{I} = \sum_n |\psi_n\rangle f_n\langle\psi_n| = \hat{f}$

spectral decomposition

– can make operator if you know f_n, ψ_n, $n=1,2,\ldots$

discrete $\rightarrow$ continuous

$|\psi\rangle = \sum_n a_n|\psi_n\rangle \rightarrow |\psi\rangle = \int a_f|\psi_f\rangle\, df$

$\hat{x}|x\rangle = x|x\rangle$ $\quad x_1 \neq x_2$ $\quad \langle x_1|x_2\rangle = 0$ $\quad \hat{I} = \sum_{x_1} |x_1\rangle\langle x_1| \rightarrow \int |x_1\rangle\langle x_1|\, dx_1 = \hat{I}$

$\hat{I}|x_2\rangle = |x_2\rangle = \int |x_1\rangle\langle x_1|x_2\rangle\, dx_1$ $\quad\therefore \langle x_1|x_2\rangle = \delta(x_1 - x_2)$

$\langle\psi_{f'}|\psi_f\rangle = \delta(f - f')$ for continuous

$\psi = a e^{i\frac{S}{\hbar}}$ form of wave function

$\frac{\partial\psi}{\partial t} = \frac{i}{\hbar}\frac{\partial S}{\partial t}\psi$ in geometric optics limit (small $\hbar$)

↳ only one to give linear in time $\frac{\partial\psi}{\partial t}\propto\psi$

$\frac{\partial S}{\partial t} = -H(\vec r,\vec p,t)$ ∴ $\boxed{\hat H|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle}$ Schrödinger Eqn.

$-i\hbar\frac{\partial}{\partial t}\langle\psi| = \langle\psi|\hat H^+$ $\quad$ $i\hbar\langle\psi|\frac{\partial}{\partial t}|\psi\rangle = \langle\psi|\hat H|\psi\rangle$

$i\hbar\left(\langle\psi|(\frac{\partial}{\partial t}|\psi\rangle) + (\frac{\partial}{\partial t}\langle\psi|)|\psi\rangle\right)$ $\quad$ $-i\hbar\left(\frac{\partial}{\partial t}\langle\psi|\right)|\psi\rangle = \langle\psi|H^+|\psi\rangle$

$i\hbar\frac{\partial}{\partial t}\underbrace{\langle\psi|\psi\rangle}_{1} = \langle\psi|\underbrace{\hat H - \hat H^+}|\psi\rangle$

$\hat H = \hat H^+$ hermitian

$\bar f = \langle\psi|\hat f|\psi\rangle$ $\quad$ $\dot{\bar f} = \frac{d\bar f}{dt} = \underbrace{\langle\dot\psi|}_{\langle\psi|\frac{i}{\hbar}\hat H}\hat f|\psi\rangle + \langle\psi|\frac{\partial\hat f}{\partial t}|\psi\rangle + \langle\psi|\hat f\underbrace{|\dot\psi\rangle}_{-\frac{i}{\hbar}\hat H|\psi\rangle}$

$\langle\psi|\frac{\partial\hat f}{\partial t} + \frac{i}{\hbar}(\hat H\hat f - \hat f\hat H)|\psi\rangle$ $\quad$ $\boxed{\dot{\hat f} = \frac{\partial\hat f}{\partial t} + \frac{i}{\hbar}\{\hat H,\hat f\}}$

Classical: $\frac{df}{dt} = \frac{\partial f}{\partial t} + \{H,f\}$

$\{g,f\}\leftrightarrow\frac{i}{\hbar}\{\hat g,\hat f\}$

Classical: $\frac{\partial f}{\partial\vec r} = \{\vec p, f\}$ $\quad$ $\{\vec p, H\} = \frac{\partial H}{\partial\vec r}$

QM. $\frac{i}{\hbar}\{\hat p,\hat H\} = \frac{\partial H}{\partial r}$ $\quad$ $\{\hat p,\hat H\} = -i\hbar\frac{\partial}{\partial\vec r}\hat H$

$\hat p\hat H - \hat H\hat p = -i\hbar\frac{\partial}{\partial\vec r}\hat H \implies \boxed{\hat p = -i\hbar\frac{\partial}{\partial\vec r}}$ Momentum operator

Clas: $\frac{\partial f}{\partial\vec p} = -\{\vec r, f\}$ $\quad$ $\{\vec r, H\} = -\frac{\partial H}{\partial\vec p}$ $\xrightarrow{QM}$ $\{\hat{\vec r},\hat H\} = i\hbar\frac{\partial\hat H}{\partial\vec p}$

$(\hat r\cdot\hat H - \hat H\cdot\hat r)|\psi\rangle = \left(i\hbar\frac{\partial\hat H}{\partial p}\right)|\psi\rangle$ $\quad$ $\hat r\hat H|\psi\rangle = (\hat r(\hat H))|\psi\rangle + \hat r(\hat H(|\psi\rangle))$ ∴ $\boxed{\hat r = i\hbar\frac{\partial}{\partial\vec p}}$ Position operator

$\frac{\partial H}{\partial\vec\varphi} = \{\vec M, H\} \xrightarrow{QM} \{\hat M,\hat H\} = -i\hbar\frac{\partial H}{\partial\varphi}$ $\quad$ $\boxed{\hat M = -i\hbar\frac{\partial}{\partial\varphi}}$

CM $\{r_i,r_k\}=0$ $\quad$ QM $\{\hat r_i,\hat r_k\}=0$ $\quad$ $\{\hat p_i,\hat p_k\}=0$ $\quad$ $\{\hat p_i,\hat r_k\} = -i\hbar\delta_{ik}$

$\{\hat M_i,\hat r_j\} = i\hbar e_{ijk}\hat r_k$ $\quad$ $\{\hat M_i,\hat p_j\} = i\hbar e_{ijk}\hat p_k$ $\quad$ $\{\hat M_i,\hat M_j\} = i\hbar e_{ijk}\hat M_k$

$\{\hat{\vec M}, \underbrace{|\vec M|^2}_{\text{scalar}}\} = 0$

$rHf = Hrf + \{r,H\}f = Hrf + i\hbar\frac{\partial H}{\partial p}f$

→ if $r = i\hbar\frac{\partial}{\partial p}$: $rHf = H\,i\hbar\frac{\partial f}{\partial p} + i\hbar\frac{\partial H}{\partial p}f = i\hbar\frac{\partial}{\partial p}(Hf)$

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{r}) = -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial \vec{r}}\right)^2$$

$$\psi = a(\vec{r},t)\, e^{\frac{i}{\hbar}S(\vec{r},t)} \qquad i\hbar\frac{\partial}{\partial t}\left(a e^{i\frac{S}{\hbar}}\right) = -\frac{\hbar^2}{2m}\nabla^2\left(a e^{i\frac{S}{\hbar}}\right) + U a e^{i\frac{S}{\hbar}}$$

$$i\hbar\frac{\partial a}{\partial t} - a\frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m}\Delta a - \frac{i\hbar}{m}(\nabla a\cdot\nabla S) - \frac{\hbar^2}{2m}a\left(\frac{i}{\hbar}\Delta S - \frac{(\nabla S)^2}{\hbar^2}\right) + Ua$$

$\nabla^2 a$ (I think)

this brings all data on

similar to Navier-Stoke's eq.

real $\quad \frac{\partial S}{\partial t}a - \frac{\hbar^2}{2m}\Delta a + \frac{(\nabla S)^2}{2m}a + Ua = 0 \Longrightarrow \frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + U = \frac{\hbar^2}{2m}\frac{\Delta a}{a}$

CM: $\frac{\partial S}{\partial r} = p$

imag. $\quad \frac{\partial a}{\partial t} + \nabla a\cdot\frac{\nabla S}{m} + \frac{a}{2}\nabla\left(\frac{\nabla S}{m}\right) = 0 \xrightarrow{\times 2a} \frac{\partial a^2}{\partial t} + \nabla\left(\underbrace{a^2\frac{\nabla S}{m}}_{\vec{J}}\right) = 0 \qquad a^2\frac{\nabla S}{m} = \vec{J}$

equivalent to continuity (in probability)

$$\boxed{\vec{J} = \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)}$$

4/17/2007

$\dot{\hat{f}} = \frac{\partial\hat{f}}{\partial t} + \frac{i}{\hbar}\{\hat{H},\hat{f}\}$ Evolution in time of operator

$\hat{f} = \hat{H} \qquad \frac{\partial\hat{H}}{\partial t} = 0 \qquad \dot{\hat{f}} = 0 \qquad \hat{H}|\psi\rangle = E|\psi\rangle \rightarrow E_n, |\psi_n\rangle$

Classic limit $\quad a e^{\frac{i}{\hbar}S} = a e^{\frac{i}{\hbar}(S_0(r) - E(t-t_0))}$

$|\psi_n\rangle_{t_0}$ time part

$i\hbar\frac{\partial|\psi_n\rangle}{\partial t} = \hat{H}|\psi_n\rangle = E_n|\psi_n\rangle \qquad |\psi_n\rangle_t = e^{-\frac{i}{\hbar}E_n(t-t_0)}|\psi_n\rangle_{t=t_0} \qquad \omega_n = \frac{E_n}{\hbar}$

Operators $\longleftrightarrow$ Matrices

$\bar{f} = \langle\psi|\hat{f}|\psi\rangle \qquad |\psi\rangle = \sum a_n|\psi_n\rangle_t \qquad \bar{f} = \sum_{nm} a_n^* a_m \underbrace{e^{i\frac{E_n - E_m}{\hbar}t}\overbrace{\langle\psi_n|\hat{f}|\psi_m\rangle_{t=0}}^{f_{nm}}}_{f_{nm}(t)}$

$f_{nm}(t)$ matrix element for transition

$\omega_{nm} = \frac{E_n - E_m}{\hbar}$ transition frequency

dependance on time drops out if f is such that $\langle\psi_n|f|\psi_m\rangle_{t=0} \propto \delta_{nm}$ integral of motion ?

$$(\dot{\hat{f}})_{nm} = \frac{d}{dt}\left(e^{i\omega_{nm}t}f_{nm}\right) = e^{i\omega_{nm}t}\, i\omega_n f_{nm}$$

$\bar{f}^* = \sum_{nm} a_n a_m^* e^{-\frac{i}{\hbar}(E_n - E_m)t}f_{nm}^* \qquad n\leftrightarrow m \qquad \sum_{mn} a_m a_n^* e^{\frac{i}{\hbar}(E_m - E_n)t} f_{mn}^* \qquad \therefore f_{nm} = f_{mn}^*$

$\therefore f_{nm} = f_{nm}^{+}$

$f_{nm} = \langle\psi_n|\hat{f}|\psi_m\rangle \qquad \langle\psi_n|\psi_m\rangle = \delta_{nm} \qquad \hat{f}|\psi_m\rangle = \sum_k f_{km}|\psi_k\rangle$

$$\langle\psi_n|\hat{f}|\psi_m\rangle = \sum_k f_{km}\langle\psi_n|\psi_k\rangle = \sum_k f_{km}\delta_{nk} = f_{nm}$$

$$\hat{f}\cdot\hat{g}|\psi_n\rangle = \hat{f}(\hat{g}|\psi_n\rangle) = \hat{f}\sum_k g_{kn}|\psi_k\rangle = \sum_k g_{kn}\hat{f}|\psi_k\rangle = \sum_k g_{kn}\sum_m f_{mn}|\psi_m\rangle$$

$(\hat{f}\hat{g})_{mn} = \sum_k f_{mk}g_{kn}$ matrix product

$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle \qquad |\psi\rangle = \sum_m c_m |\psi_m\rangle$

$\hat{f}|\psi\rangle = f|\psi\rangle \rightarrow \sum c_m \hat{f}|\psi_m\rangle = f\sum c_m|\psi_m\rangle \qquad \langle\psi_n|$

$\sum_m c_m f_{nm} = \sum_m f c_m \delta_{nm} \qquad \boxed{\sum_m (f_{nm} - \delta_{nm} f) c_m = 0}$ can be solved to find eigenvalues c_m

eigenvalue f_k which belongs to spectrum

eigenvector $|\phi_k\rangle$

$|\phi_k\rangle = \sum_m u_{mk}|\psi_m\rangle$ energy eigenstates

$\langle\phi_i|\phi_k\rangle = \delta_{ik} = \sum_{jm}\langle\psi_j|u_{ij}^* u_{mk}|\psi_m\rangle = \sum_{jm} u_{ij}^* u_{mk}\delta_{jm} = \sum_j u_{ij}^* u_{jk} = \underline{u^+ u = 1}$ unit matrix

$u^+u = 1 \qquad uu^+ = 1 \qquad \underline{u^+ = u^{-1}}$ unitary matrix

$\hookrightarrow$ changes you from one basis to another

$|\phi\rangle = u|\psi\rangle \qquad \langle\psi|\hat{f}'|\psi\rangle$

$\langle\phi|\hat{f}|\phi\rangle = \langle\psi|u^+\hat{f}u|\psi\rangle \qquad \hat{f}' = u^+\hat{f}u = u^{-1}\hat{f}u$

Trace $\quad Tr(\hat{g}) = \sum_i \langle\psi_i|\hat{g}|\psi_i\rangle = \sum_i g_{ii}$ sum of diagonal

$\sum_{klj} u_{ij}^* g_{ik} u_{lk}\delta_{lj} = \sum_i g_{ii}$ trace is same regardless of basis

$\hat{g}\hat{f}\hat{l} \rightarrow u^{-1}\hat{g}\underbrace{uu^{-1}}_{1}\hat{f}\underbrace{uu^{-1}}_{1}\hat{l}u \rightarrow$ invariant

unitary operator $\hat{u} = e^{i\hat{R}} \qquad \hat{R}^+ = \hat{R} \qquad e^{i\hat{R}} = 1 + i\hat{R} - \hat{R}^2 + \ldots$

$\hat{u}^+ = e^{-i\hat{R}^+} = e^{-i\hat{R}} \qquad \hat{u}^+\hat{u} = \hat{u}\hat{u}^+ = e^{-i\hat{R}}e^{i\hat{R}} = 1 \qquad u^+ = u^{-1}$

$\hat{f}' = u^{-1}\hat{f}u = e^{-i\hat{R}} f e^{i\hat{R}}$

first order in expansion $\quad \hat{f}' = (1 - i\hat{R} + \ldots)\hat{f}(1 + i\hat{R} + \ldots)$

$\hat{f}' = \hat{f} - i\hat{R}\hat{f} + \hat{f}i\hat{R} + O(\hat{R}^2) = \hat{f} + \{\hat{f}, i\hat{R}\} + O(\hat{R}^2)$

general answer: $\quad \hat{f}' = \hat{f} + \{\hat{f}, i\hat{R}\} + \frac{1}{2}\{\{\hat{f}, i\hat{R}\}, i\hat{R}\} + \ldots$

for energy $\quad i\hbar\frac{\partial}{\partial t}|\psi_n\rangle = \hat{H}|\psi_n\rangle = E_n|\psi_n\rangle \quad$ if $\frac{\partial\hat{H}}{\partial t} = 0$

$|\psi\rangle_t = \sum_j c_j e^{-\frac{i}{\hbar}E_j(t-t_0)}|\psi_j\rangle_{t=t_0} = \sum_j c_j e^{-\frac{i}{\hbar}E_j(t-t_0)}|E_j\rangle = \sum_j c_j e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}|E_j\rangle$

$|\psi\rangle_t = \underbrace{e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}}_{\hat{u}(t,t_0)}|\psi\rangle_{t=t_0}$

evolution in time is going from one basis to another

$\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$ is called propagator

$|\psi\rangle_t = \sum c_j e^{-\frac{i}{\hbar}E_j(t-t_0)} |E_j\rangle \qquad c_j = \langle E_j|\psi\rangle \longrightarrow \sum_j \langle E_j|\psi\rangle e^{-\frac{i}{\hbar}E_j(t-t_0)} |E_j\rangle$

$= \sum_j \underbrace{|E_j\rangle e^{\frac{i}{\hbar}E_j(t-t_0)} \langle E_j|}_{\text{spectral decomposition of propagator}} \psi\rangle \qquad |\psi\rangle_t = \hat{U}(t,t_0)|\psi\rangle_{t_0}$

$\bar{f} = {}_t\langle\psi|\hat{f}|\psi\rangle_t = {}_{t_0}\langle\psi| U^{-1}_{(t,t_0)} f\, U_{(t,t_0)} |\psi\rangle_{t_0}$

now the time dependance is on operator, not on basis

$\hat{f}(t) = U^{-1}_{(t,t_0)} \hat{f}_{(t_0)} U_{(t,t_0)} = e^{\frac{i}{\hbar}\hat{H}(t-t_0)} \hat{f} e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$ same as $e^{i\hat{R}}\hat{f}e^{-i\hat{R}}$

$\hat{f}(t) = \hat{f} - \{\hat{f}, \frac{i}{\hbar}\hat{H}(t-t_0)\} + \frac{1}{2!}\{\{f, \frac{i}{\hbar}\hat{H}(t-t_0)\}, \frac{i}{\hbar}\hat{H}(t-t_0)\} + \dots$

Classical: $f(t) = f(0) + \frac{t}{1!}\{H,f\} + \frac{t^2}{2!}\{H,\{H,f\}\} + \dots \qquad \underset{CM}{\{H,f\}} \rightarrow \underset{QM}{\frac{i}{\hbar}\{\hat{H},\hat{f}\}}$

$\frac{d}{dt}\hat{f}(t) = \frac{i}{\hbar}\hat{H}\, e^{\frac{i}{\hbar}\hat{H}(t-t_0)} \hat{f}_{(t_0)} e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} + e^{i\sim} \hat{f}_{t_0} \underbrace{-\frac{i\hat{H}}{\hbar} e^{-i\sim}}_{\text{commute}}$

$= \frac{i}{\hbar}\hat{H}\hat{f} - \frac{i}{\hbar}\hat{f}\hat{H} \qquad \therefore \quad \frac{d\hat{f}}{dt} = \frac{i}{\hbar}\{\hat{H},\hat{f}\}$ with $\frac{\partial f}{\partial t} = 0$

Momentum

$\hat{p} = -i\hbar\frac{\partial}{\partial \vec{r}} = -i\hbar\nabla$ geometrical optics (CM limit) $\quad \langle\vec{r}|\psi\rangle = a e^{iS/\hbar} \qquad S = \int(\vec{p}\,d\vec{r} - H\,dt)$

$\frac{\partial S}{\partial t} = -H \qquad \frac{\partial S}{\partial \vec{r}} = \vec{p}$

CM limit $a \rightarrow$ const $\quad \langle\vec{r}|\hat{p}|\psi\rangle = \cancel{-i}\hbar\frac{\cancel{i}}{\hbar}\underbrace{\frac{\partial S}{\partial \vec{r}}}_{\vec{p}}\langle\vec{r}|\psi\rangle$

$\hat{p}|\vec{p}\rangle = \vec{p}'|\vec{p}\rangle \qquad |\vec{p}\rangle = \sum_{\vec{r}'} \langle\vec{r}'|\vec{p}\rangle|\vec{r}'\rangle$ ..... actually integral

$-i\hbar\frac{\partial}{\partial\vec{r}}\langle\vec{r}|\vec{p}\rangle = \vec{p}\underbrace{\langle\vec{r}|\vec{p}\rangle}_{\text{functions of coordinates}} \qquad \langle\vec{r}|\vec{p}\rangle = \text{const}_{(p)}\, e^{\frac{i}{\hbar}\vec{p}\vec{r}}$

projection of $\vec{p}$ onto $\vec{r}$ space (coordinate space)

$\delta(\vec{p}'-\vec{p}) = \langle\vec{p}'|\vec{p}\rangle = \delta(p_x'-p_x)\,\delta(p_y'-p_y)\,\delta(p_z'-p_z)$

$\langle\vec{p}'|\vec{p}\rangle = \int \langle\vec{p}'|\vec{r}\rangle\langle\vec{r}|\vec{p}\rangle d^3\vec{r} \qquad \int|\vec{r}\rangle\langle\vec{r}|\,d^3\vec{r} = 1$

$= |\text{const}_p|^2 \int e^{-\frac{i}{\hbar}\vec{p}'\vec{r}} e^{\frac{i}{\hbar}\vec{p}\vec{r}} d^3\vec{r} \qquad \boxed{\int_{-\infty}^{\infty} e^{i(p_x-p_x')\frac{x}{\hbar}}dx = 2\pi\,\delta(p_x-p_x')\,\hbar}$

$= \underbrace{|\text{const}_p|^2(2\pi\hbar)^3}_{=1}\delta(\vec{p}-\vec{p}')$

$\therefore \quad \boxed{\langle\vec{r}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\frac{\vec{p}\cdot\vec{r}}{\hbar}}}$

$$|\psi\rangle = \int \underbrace{\langle \vec r|\psi\rangle}_{\psi(\vec r)} |\vec r\rangle\, d^3\vec r$$

now in momentum space $\qquad |\psi\rangle = \int \overbrace{a_{\vec p}}^{\text{wave function in } \vec p \text{ space}} |\vec p\rangle\, d^3\vec p \qquad \langle \vec r|\cdot$

$$\underbrace{\langle \vec r|\psi\rangle}_{\psi(\vec r)} = \int a_{\vec p} \langle \vec r|\vec p\rangle\, d^3\vec p$$

$$\psi(\vec r) = \int a_{\vec p} \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\vec p\vec r}\, d^3\vec p$$ to get $a_{\vec p}$ $\rightarrow$ inverse Fourier transform

$$\int \psi(\vec r) e^{-\frac{i}{\hbar}\vec p'\vec r}\, d^3\vec r = \int a_{\vec p}\, d^3\vec p \underbrace{\int e^{\frac{i}{\hbar}(\vec p-\vec p')\vec r}\, d^3\vec r}_{(2\pi\hbar)^3 \delta(\vec p-\vec p')} \frac{1}{(2\pi\hbar)^{3/2}} = (2\pi\hbar)^{3/2} a_{\vec p'}$$

$$\boxed{a_{\vec p} = \langle \vec p|\psi\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \int \langle \vec r|\psi\rangle e^{-\frac{i}{\hbar}\vec p\vec r}\, d^3\vec r}$$

$$\overline{\vec r} = \langle \psi|\hat r|\psi\rangle = \int \langle \psi| \underbrace{\vec r\rangle \vec r \langle \vec r}_{\text{spectral decomposition}}|\psi\rangle\, d^3\vec r$$

$$\overline{\vec p} = \int \langle \psi| \underbrace{\vec r\rangle \overbrace{-i\hbar\frac{\partial}{\partial \vec r}}^{\hat p} \langle \vec r}_{\hat p \text{ as 'matrix' (in r coordinate space)}}|\psi\rangle\, d^3\vec r$$

$$\langle \vec p|\psi\rangle = \int \langle \vec r|\psi\rangle e^{-\frac{i}{\hbar}\vec p\vec r} \frac{1}{(2\pi\hbar)^{3/2}}\, d^3\vec r \qquad \langle \vec r|\psi\rangle = \int \langle \vec p|\psi\rangle e^{\frac{i}{\hbar}\vec p\vec r} \frac{d^3\vec p}{(2\pi\hbar)^{3/2}}$$

$$\overline{\vec p} = \int d^3\vec r \underbrace{\int \langle \psi|\vec p'\rangle e^{-\frac{i}{\hbar}\vec p'\vec r} \frac{d^3\vec p'}{(2\pi\hbar)^{3/2}}}_{\langle \psi|\vec r\rangle} \underbrace{\left(-i\hbar\frac{\partial}{\partial \vec r}\right)}_{\hat p} \underbrace{\int \langle \vec p|\psi\rangle e^{\frac{i\vec p\vec r}{\hbar}} \frac{d^3\vec p}{(2\pi\hbar)^{3/2}}}_{\langle \vec r|\psi\rangle}$$

$$= \int \langle \psi|\vec p'\rangle \vec p \langle \vec p|\psi\rangle\, d^3\vec p\, d^3\vec p' \underbrace{\int e^{\frac{i}{\hbar}(\vec p-\vec p')\vec r} \frac{d^3\vec r}{(2\pi\hbar)^3}}_{\delta(\vec p-\vec p')} = \int \langle \psi|\vec p\rangle \vec p \langle \vec p|\psi\rangle\, d^3\vec p$$

in r space $\qquad \hat r \rightarrow \vec r \qquad \hat{\vec p} \rightarrow -i\hbar\frac{\partial}{\partial \vec r} \qquad$ acting on $\langle \vec r|\psi\rangle$

in p space $\qquad \hat{\vec r} \rightarrow i\hbar\frac{\partial}{\partial \vec p} \qquad \hat p \rightarrow \vec p \qquad$ acting on $\langle \vec p|\psi\rangle$

$$\{\hat p_i, \hat r_k\} = -i\hbar\, \delta_{ik}$$

$$-\hat r_k(\hat p_i) = -i\hbar\, \delta_{ik}$$

4/19/2007

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

$$\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} \qquad |\psi\rangle_t = \hat{U}|\psi\rangle_{t_0}$$

small translation $\hat{T}_{\vec{a}}\, f(\vec{r}) = f(\vec{r}+\vec{a})$

$$f(\vec{r}+\vec{a}) = f(\vec{r}) + \underbrace{\vec{a}\cdot\frac{\partial f}{\partial \vec{r}}}_{\left(\sum_k a_k \frac{\partial f}{\partial r_k}\right)} + \dots + \frac{1}{2!}a_k a_j \frac{\partial^2 f}{\partial r_k \partial r_j} + \dots \qquad \hat{p} = -i\hbar\frac{\partial}{\partial \vec{r}}$$

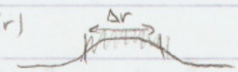
$$\vec{a}\cdot\frac{\partial}{\partial\vec{r}} = \left(\vec{a}\cdot -i\hbar\frac{\partial}{\partial\vec{r}}\right)\frac{i}{\hbar} = \frac{i}{\hbar}(\vec{a}\cdot\hat{\vec{p}}) \qquad \hat{T}_a f(\vec{r}) = e^{\frac{i}{\hbar}\vec{a}\cdot\hat{\vec{p}}} f(\vec{r})$$

$$\hat{T}_a = e^{\frac{i}{\hbar}\vec{a}\cdot\hat{\vec{p}}} \qquad \hat{p}|\psi\rangle = -i\hbar\frac{\partial}{\partial\vec{r}}|\psi\rangle$$

$$\langle\vec{p}|\psi\rangle = \int \underbrace{\langle r|\psi\rangle}_{\psi(r)} e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\frac{d^3\vec{r}}{(2\pi\hbar)^{3/2}}$$

$$\psi(\vec{r}) = \delta(\vec{r}-\vec{r}\,') \longrightarrow \psi(\vec{p}) = e^{-i\frac{\vec{p}\cdot\vec{r}\,'}{\hbar}}\frac{1}{(2\pi\hbar)^{3/2}}$$

$\psi^*_{(p)}\psi_{(p)}$ = constant $\rightarrow$ same probability everywhere



$$\frac{p\,\Delta r}{\hbar}\sim 1 \qquad p \gg \frac{\hbar}{\Delta r} \rightarrow \langle p|\psi\rangle \rightarrow 0$$

$$\Delta p \sim \frac{\hbar}{\Delta r}$$

sin/cos waves oscillate rapidly and average to zero

Wegl's theorem

$$\bar{x} = \int \psi^*_{(x)}\, x\, \psi_{(x)}\, dx \qquad \bar{p} = \int \psi^*_{(x)}\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x)\, dx$$

$x \rightarrow x' + \bar{x}$

$$\int \psi^*(x'+\bar{x})\,(x'+\bar{x})\,\psi(x'+\bar{x})\,dx' \quad \rightarrow \text{can choose origin so that } \bar{x}=0$$

$\psi_{(x)} \rightarrow \psi'_{(x)} e^{i\frac{p_0 x}{\hbar}}$

$$\bar{p} = \int \psi'^*_{(x)} e^{-i\frac{p_0 x}{\hbar}}\left(\underbrace{-i\hbar\frac{\partial\psi'}{\partial x}}_{\hat{p}\psi'} e^{i\frac{p_0 x}{\hbar}} - \underbrace{i\hbar\frac{\partial}{\partial x}\left(e^{i\frac{p_0 x}{\hbar}}\right)\psi'}_{p_0\psi'}\right)dx$$

$$\bar{p} = \int \psi'^*\hat{p}\,\psi\, dx + \bar{p} \quad \rightarrow \quad \bar{p} = 0$$

this corresponds to being in particle's reference frame

$$\delta x = \sqrt{\overline{(x-\bar{x})^2}} \qquad \delta p = \sqrt{\overline{(p-\bar{p})^2}}$$

can set $\bar{x} = \bar{p} = 0$ as shown above

consider $$\int_{-\infty}^{\infty}\left|\alpha x\psi + \frac{\partial}{\partial x}\psi\right|^2 dx > 0 \qquad \int\left(\alpha x\psi^* + \frac{\partial}{\partial x}\psi^*\right)\left(\alpha x\psi + \frac{\partial}{\partial x}\psi\right)dx$$

$$= \alpha^2\underbrace{\int\psi^* x^2\psi\, dx}_{\delta x^2} + \alpha\int\underbrace{\left(x\psi^*\frac{\partial\psi}{\partial x} + x\frac{\partial\psi^*}{\partial x}\psi\right)}_{\frac{d}{dx}(x\psi^*\psi) - \psi^*\psi - x\psi^*\frac{d\psi}{dx}}dx + \int\frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x}dx$$

$\psi \rightarrow 0$ as $x \rightarrow \infty$

integrate by parts $\quad -\int\psi^*\underbrace{\frac{\partial^2\psi}{\partial x^2}}_{(i\frac{\partial}{\partial x})^2}dx$

$$= \alpha^2\,\delta x^2 - \alpha + \frac{\delta p^2}{\hbar^2} > 0$$

$\alpha^2 \delta x^2 - \alpha + \frac{\delta p^2}{\hbar^2} > 0$ $\qquad 1 - \frac{\delta x^2 \delta p^2}{\hbar^2} \geq 0$ $\quad \alpha$ has no roots

$\Rightarrow \boxed{\delta x \, \delta p \geq \hbar}$ Heisenberg Uncertainty principle

---

$\hat{H}|\psi\rangle = E|\psi\rangle$ $\qquad$ spectral decomposition of $\hat{H}$ $\quad \sum |r\rangle \hat{H} \langle r|$ or $\sum |p\rangle \hat{H} \langle p|$

$E|\psi\rangle = \sum |r\rangle \hat{H} \langle r|\psi\rangle \quad \langle r| \cdot \rightarrow \quad E \underbrace{\langle r|\psi\rangle}_{\psi(r)} = \hat{H} \underbrace{\langle r|\psi\rangle}_{\psi(r)}$

or $E \underbrace{\langle p|\psi\rangle}_{\psi(p)} = \hat{H} \underbrace{\langle p|\psi\rangle}_{\psi(p)}$

$\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{r}) \rightarrow \hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + U(r)$ $\quad$ or $\quad \hat{H} = \frac{p^2}{2m} + U\left(i\hbar \frac{\partial}{\partial p}\right)$

he uses Δ

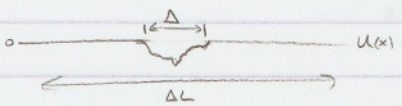
$U(r) = 0 \qquad \hat{H} = \frac{-\hbar^2}{2m}\nabla^2 \qquad \frac{-\hbar^2}{2m}\nabla^2\psi = E\psi \qquad \{\hat{H}, \hat{p}\} = 0$

$\psi_{\vec{p}}(\vec{r}) = A e^{+i\frac{\vec{p}\cdot\vec{r}}{\hbar}}$ parameter $\quad$ where $E = \frac{p^2}{2m}$ $\quad$ degenerate $|\vec{p}| \rightarrow$ same E $\quad$ (no direction)

$\int \psi^*_{p'} \psi_p \, d^3\vec{r} = \delta(\vec{p}' - \vec{p}) \rightarrow A = \frac{1}{(2\pi\hbar)^{3/2}}$ normalization

$\psi_{\vec{p}}(\vec{r},t) = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\underbrace{\left(\vec{p}\cdot\vec{r} - E_p(t-t_0)\right)}_{S}}$ $\quad$ with $\frac{E_p}{\hbar} = \omega \quad \frac{\vec{p}}{\hbar} = \vec{k} \quad \frac{p}{\hbar} = \frac{2\pi}{\lambda}$

dispersion relation (unless $E = pc$)



consider broad region $\Delta L >> \Delta$ much larger than Δ

to first order particle ignores $U(x)$

Now say $U(x) = -G\,\delta(x)$ $\qquad$ scale of solution is larger than scale of potential

$\{\hat{H}, \hat{p}\} \neq 0 \qquad E\psi = \frac{-\hbar^2}{2m}\nabla^2\psi - G\,\delta(x)\psi$

unbound states $E > 0 \qquad \psi = A_1 e^{ikx} - A_2 e^{-ikx}$ $\quad$ waves moving right + left

parity transformation $\hat{P}$ $\quad x \rightarrow -x \qquad \{\hat{H}, \hat{P}\} = 0 \qquad \delta(-x) = \delta(x) \Rightarrow \psi = C_1 \cos kx + C_2 \sin kx$

$$\psi = \begin{cases} C_1 \cos kx + C_2 \sin kx & x \geq 0 \\ C_3 \cos kx + C_4 \sin kx & x \leq 0 \end{cases}$$

$\lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} E\psi \, dx = \int_{-\epsilon}^{\epsilon} \left(\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} - G\,\delta(x)\psi\right) dx$

$0 = \frac{-\hbar^2}{2m}\left(\left.\frac{d\psi}{dx}\right|_{+\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon}\right) - G\psi(0)\underbrace{\int_{-\epsilon}^{\epsilon}\delta(x)\,dx}_{1}$

$\left.\frac{d\psi}{dx}\right|_{+\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon} = -\frac{G\,2m}{\hbar^2}\psi(0)$ $\qquad$ boundary conditions $\qquad \psi|_{+\epsilon} = \psi|_{-\epsilon}$

From b.c.s $C_1 = C_3 = C$ $\qquad$ C, S arbitrary constants

$$C_2 k - C_4 k = -\frac{2mG}{\hbar^2} C \qquad C_4 - C_2 = \frac{2mG}{\hbar^2 k} C \qquad \begin{aligned} C_4 &= S + \frac{mG}{\hbar^2 k} C \\ C_2 &= S - \frac{mG}{\hbar^2 k} C \end{aligned}$$

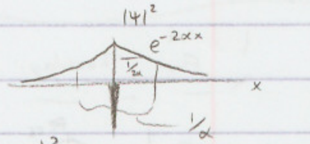
$$\psi = C \begin{cases} \cos kx - \frac{mG}{\hbar^2 k}\sin kx \\ \cos kx + \frac{mG}{\hbar^2 k}\sin kx \end{cases} + S \begin{cases} \sin kx & x \geq 0 \\ \sin kx & x \leq 0 \end{cases}$$

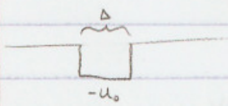
$$\therefore \quad \psi = \underbrace{C\left(\cos kx - \frac{mG}{\hbar^2 k}\sin k|x|\right)}_{\psi_e} + \underbrace{S \sin kx}_{\psi_o} \qquad \begin{aligned} \hat{P}\psi_o &= -\psi_o \\ \hat{P}\psi_e &= \psi_e \end{aligned}$$

$E<0$

$$\psi = C \begin{cases} e^{-\alpha x} & x>0 \\ e^{+\alpha x} & x<0 \end{cases} \qquad E = \frac{-\hbar^2}{2m}\alpha^2 \qquad \alpha = \frac{\sqrt{2m(-E)}}{\hbar}$$

b.c. s : $\quad C(-\alpha) - C\alpha = \frac{-G2m}{\hbar^2} C \qquad \alpha = \frac{mG}{\hbar^2}$





$$\int -G\,\delta(x)\,dx = -G \rightarrow -U_0\Delta$$

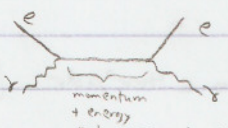
$$\frac{1}{\alpha} = \frac{\hbar^2}{mG}$$

as $G\uparrow$ $\frac{1}{\alpha}\downarrow$ more localized

$$\underbrace{\frac{1}{\alpha} = \frac{\hbar^2}{mU_0\Delta} \gg \Delta}$$ $\rightarrow$ based on initial approximations

as $U_0\uparrow$ $\quad \frac{\hbar^2}{mU_0\Delta^2} = 1$ $\quad$ deep well $\rightarrow$ you will get a new energy level

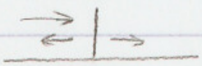
$$U_0 > \frac{\hbar^2}{m\Delta^2}$$



Compton effect

QED diagram

$\rightarrow$ virtual state (short lived)



$$E\psi = \frac{-\hbar^2}{2m}\nabla^2\psi + G\,\delta(x)\,\psi$$

$\psi_1 = C_1 e^{ikx}$ incoming $\qquad \psi_2 = C_2 e^{-ikx}$ reflected $\qquad \frac{\hbar^2 k^2}{2m} = E \quad \therefore$ same k for this problem

$\psi_3 = C_3 e^{ikx}$ transmitted

$$\frac{\partial |\psi|^2}{\partial t} + \nabla\cdot\vec{J} = 0 \qquad \vec{J} = \frac{1}{2m}\left(\psi^*\hat{p}\psi + \psi\hat{p}^*\psi^*\right)$$ flow of probability

$$\vec{J} = \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right) \qquad J_1 = \frac{i\hbar}{2m}\left(C_1 e^{ikx}(-ik)C_1^* e^{-ik} - C_1^* e^{-ikx}(ik)C_1 e^{ikx}\right)$$

$$J_1 = \frac{\hbar k}{m}|C_1|^2$$

$$\frac{\hbar k}{m}|C_1|^2 - \frac{\hbar k}{m}|C_2|^2 = \frac{\hbar k}{m}|C_3|^2$$

$$|C_1|^2 = |C_2|^2 + |C_3|^2$$

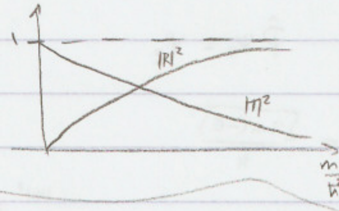
$C_1 = 1$ set $\quad C_2 = R$ reflection coefficient $\quad C_3 = T$ transmission coefficient

$$1 = |R|^2 + |T|^2$$

$$\psi_I = e^{ikx} + R e^{-ikx} \qquad \psi_{II} = T e^{ikx} \qquad 1 + R = T$$

$$T + R = 1 - i \frac{2mG}{\hbar^2 k} T$$ with derivative b.c.

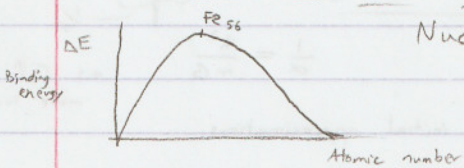
$$\therefore \quad T = \frac{1}{1 + i\frac{mG}{\hbar^2 k}} \qquad R = \frac{-i\frac{mG}{\hbar^2 k}}{1 + i\frac{mG}{\hbar^2 k}} \qquad |T|^2 = \frac{1}{1 + \left(\frac{mG}{\hbar^2 k}\right)^2} \qquad |R|^2 = \frac{\left(\frac{mG}{\hbar^2 k}\right)^2}{1 + \left(\frac{mG}{\hbar^2 k}\right)^2}$$



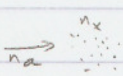
4/24/2007

For Thursday: read 5.7 harmonic oscillator with operators
5.9.3

Nuclear reactions



$4H \to He_4 \qquad \Delta mc^2 \simeq 26.7$ MeV



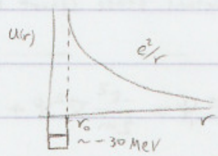
$\frac{\text{rate}}{\text{volume}} = n_a n_x \sigma v = r \qquad Q = \Delta mc^2$

$$\Delta E = Q n_a n_x \langle \sigma v \rangle$$ thermally averaged

production rate per unit mass $\boxed{\epsilon = \frac{Qr}{\rho}} \qquad dL = \epsilon\, dm = \epsilon\, 4\pi r^2 \rho\, dr \quad \left[\frac{\text{erg}}{\text{s}}\right]$

Classical look:

proton size $r_0 \sim 10^{-13}$ cm from $m_p e r_0 \sim \hbar$



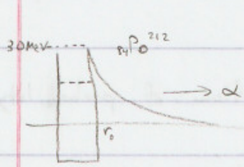
$$\frac{e^2}{r_0} = \underbrace{\frac{e^2}{m_e c^2}}_{\text{classical radius of } e^-} \frac{m_e c^2}{r_0} \sim 0.5 \text{ MeV } (2.8) \sim 1.4 \text{ MeV}$$

$r_e = 2.818 \times 10^{-13}$ cm

Sun center $\sim 2 \times 10^7$ K $\to 2$ keV

10^4 K ~ 1 eV

$\frac{E_c}{kT} \sim 10^3 \longrightarrow$ fusion wont happen classically $\qquad e^{-10^3} \propto$ # of fusion reactions



$\longrightarrow \alpha$ (9 MeV) $\qquad \alpha$-decay

Quantum Mechanical approach to nuclear reactions

Semiclassical Approximation

WKB Method

$\lambda < L$ (characteristic size) geometric optics limit

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right)\psi(x) = E\,\psi(x) \qquad \psi(x) = \langle x|\psi\rangle$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (E - U(x))\psi = 0 \qquad \psi = a\,e^{i\frac{S}{\hbar}} = e^{\frac{i}{\hbar}\left(S + \frac{\hbar}{i}\ln a\right)}$$

$$\psi = e^{\frac{i}{\hbar}\left(\underset{\sim S}{\sigma_0} + \frac{\hbar}{i}\underset{\sim \ln a}{\sigma_1} + \left(\frac{\hbar}{i}\right)^2\sigma_2 + \dots\right)} = e^{\frac{i}{\hbar}\sigma}$$

$$\frac{1}{2m}\sigma'^2 - \frac{i\hbar}{2m}\sigma'' = E - U(x) \qquad \frac{1}{2m}\sigma'^2 - (E - U(x)) = \frac{i\hbar}{2m}\sigma''$$

$\hbar \to 0 \quad \sigma \to \sigma_0 \qquad \frac{1}{2m}\sigma_0'^2 = E - U(x) \qquad \boxed{\sigma_0 = \pm\int \underbrace{\sqrt{2m(E - U(x))}}_{p(x)}\,dx}$

$\sigma_0 \to S = -Et \pm \int p\,dx$

Applicability: $\frac{1}{2m}\sigma_0'^2 \gg \left|\frac{i\hbar}{2m}\sigma''\right|$

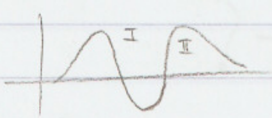
$$\hbar\left|\frac{\sigma''}{\sigma'^2}\right| \ll 1 \qquad \left|\frac{d}{dx}\left(\frac{\hbar}{\sigma'}\right)\right| \ll 1 \quad \sigma' = p \qquad \boxed{\left|\frac{d}{dx}\left(\frac{\hbar}{p}\right)\right| = \left|\frac{d\lambda}{dx}\right| \ll 1} \qquad \lambda \ll L$$

$$\frac{-\hbar}{p^2}\sqrt{2m}\frac{d}{dx}(E-U)^{1/2} = \boxed{\left|\frac{\hbar m}{p^3}F\right| \ll 1} \qquad F = -\frac{dU}{dx}$$

$$\frac{1}{2m}\left(\sigma_0' + \frac{\hbar}{i}\sigma_1'\right)^2 - (E - U) = \frac{i\hbar}{2m}\sigma_0'' \qquad \sigma_1' = -\frac{\sigma_0''}{2\sigma_0'} = \frac{-p'}{2p}$$

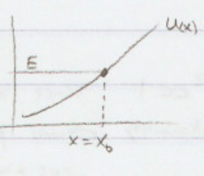
$$\boxed{\sigma_1 = -\frac{1}{2}\ln p} \qquad \psi = \frac{c_1}{\sqrt{p}}e^{\frac{i}{\hbar}\int p\,dx} + \frac{c_2}{\sqrt{p}}e^{-\frac{i}{\hbar}\int p\,dx} \qquad p = \sqrt{2m(E - U(x))}$$

$|\psi|^2 = \frac{c}{p}$ ← depends on how much time it spends in that state



in II: $\psi = \frac{c_1'}{\sqrt{|p|}}e^{-\frac{1}{\hbar}\int |p|\,dx} + \frac{c_2'}{\sqrt{|p|}}e^{\frac{1}{\hbar}\int |p|\,dx}$

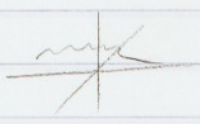
as long as $\left|\frac{d\lambda}{dx}\right| \ll 1$ holds



$E = U(x_0)$ reflection point

$$E - U(x) = \underbrace{E - U(x_0)}_{0} + \overset{-\frac{\partial U}{\partial x}}{F}(x - x_0) = F(x - x_0)$$

$$\therefore \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E + Fx)\psi = 0$$

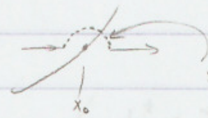


this provides boundary conditions

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

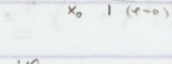
$$\psi = A\frac{1}{\sqrt{\pi}}\int_0^\infty \cos\left(\frac{u^3}{3} - u\xi\right)du \quad \text{with} \quad \xi = \left(\frac{2mF}{\hbar^2}\right)^{1/3}\left(x + \frac{E}{F}\right)$$

$$c_1' \to c_1'(c_1, c_2)$$



$x = x_0 + \rho e^{i\varphi}$ to avoid trap at reflection point

$$\frac{1}{\sqrt[4]{2m|F_0|(x - x_0)}}\, e^{\frac{i}{\hbar}\int\sqrt{2m|F|(x-x_0)}\,dx}$$

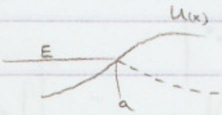


$$= \frac{1}{(2m|F_0|)^{1/4}\cancel{\rho}\, e^{i\varphi/4}}\, e^{\frac{i}{\hbar}\int\sqrt{2m|F_0|\rho}\, e^{i\frac{\varphi}{2}}\underbrace{\rho e^{i\varphi}d i\varphi}_{dx}}$$

$\longrightarrow e^{-i\frac{\pi}{4}}$ factor when going from one region to another

Generalized rule

$$\frac{c}{2\sqrt{p}}\, e^{-\frac{1}{\hbar}\left|\int_a^x p\,dx\right|}$$ $U(x) > E$ forbidden region

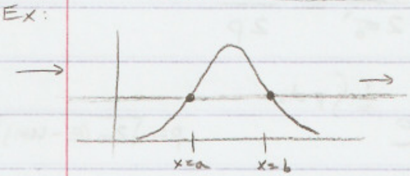


$$\longrightarrow \frac{c}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\left|\int_a^x p\,dx\right| - \frac{\pi}{4}\right)$$ $U(x) < E$ allowed region

same c

2 waves traveling in two directions

Ex:



$$\frac{c}{\sqrt{p}}\, e^{\frac{i}{\hbar}\int_b^x p\,dx + \frac{i\pi}{4}} = \psi(x) \quad x > b$$ start with end

$$\psi(x) = \frac{c}{\sqrt{p}}\, e^{\frac{1}{\hbar}\int_a^b |p|\,dx - \frac{1}{\hbar}\int_a^x |p|\,dx}$$

$$\psi(x) = \frac{c}{\sqrt{p}}\, e^{\frac{1}{\hbar}\int_x^b |p|\,dx}$$ for $a < x < b$

$$\int_x^b |p| = -\int_b^x = -\left(\int_b^a + \int_a^x\right) = \int_a^b - \int_a^x$$

$$2\frac{c}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_x^a p\,dx - \frac{\pi}{4}\right)e^{\frac{1}{\hbar}\int_a^b |p|\,dx} = \psi \quad x < a$$ 2 waves $\rightleftarrows$

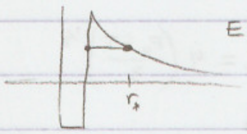
$$T = \exp\left(-\frac{2}{\hbar}\int_a^b |p|\,dx\right)$$ penetration probability is T^2

$T^2 \ll 1$ since here $R = 1$

applicability requires perfect reflection

$\cos x = c_1 e^{ix} + c_1 e^{-ix}$

$P^{1/2} = e^{\frac{i}{\hbar}\int_a^b p\,dr}$ probability$^{1/2}$



$E = \frac{p^2}{2m} + \frac{Z_1 Z_2 e^2}{r}$ $\frac{p^2}{2m} = E - \frac{Z_1 Z_2 e^2}{r}$ $p = \sqrt{2m}\, i \sqrt{\frac{Z_1 Z_2 e^2}{r} - E}$

$r_* = \frac{Z_1 Z_2 e^2}{E} \Longrightarrow p(r_*) = 0$

$$P^{1/2} = \exp\left\{-\frac{\sqrt{2mE}}{\hbar}\int_{r_0}^{r_*}\sqrt{\frac{r_*}{r}-1}\,dr\right\}$$ approx $r_0 \sim 0$

$$= \exp\left\{-2\sqrt{\frac{m}{2E}}\,\frac{e^2}{\hbar}Z_1Z_2\underbrace{\int_0^1\sqrt{\frac{1}{x}-1}\,dx}_{\pi/2}\right\} = \exp\left\{-\pi\sqrt{\frac{mc^2}{2E}}\,\underbrace{\frac{e^2}{\hbar c}}_{\alpha}Z_1Z_2\right\}$$

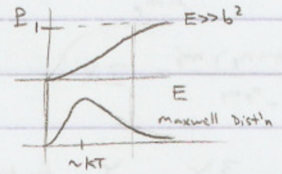
m – reduced mass

H: $\frac{m_p}{2}$

He_4: $2m_p$

$P = e^{-2\pi\sqrt{\frac{mc^2}{2E}}\,\alpha Z_1 Z_2}$ propability density to penetrate coulomb barrier $\alpha = \frac{1}{137}$

$b = 2\pi\alpha Z_1 Z_2\sqrt{\frac{mc^2}{2}}$ $P = e^{-b/E^{1/2}}$



$\langle\sigma v\rangle = ?$ $p \to \lambda \sim \frac{\hbar}{p}$ $\sigma \propto \pi\lambda^2$ in geometric limit (beam)

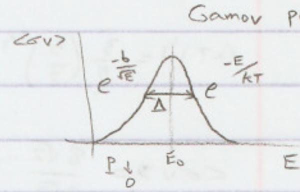
$\sigma \propto \pi\frac{\hbar^2}{p^2} \sim \frac{1}{E}$ ignoring interactions (penetrations) → only due to localization

$\sigma \propto S(E)\,\frac{1}{E}\,e^{-b/E^{1/2}}$

slowly varying function   penetration

$f(E)\,dE = \frac{2}{\sqrt{\pi}}\,\frac{E}{kT}\,e^{-E/kT}\,\frac{dE}{(kT)^{1/2}}$

Gamow peak (1928) (for α-decay initially)



$$\langle\sigma v\rangle = \int \sigma(E)\,v(E)\,f(E)\,dE = \frac{8}{m\pi}(kT)^{-3/2}\int_0^\infty S(E)\,e^{-\frac{E}{kT}}\,e^{-\frac{b}{\sqrt{E}}}\,dE$$

$\frac{\Delta}{E_0} \ll 1$ $e^{-\frac{E}{kT}-\frac{b}{\sqrt{E}}} = e^{-f(E)}$ $f(E) = \frac{E}{kT} + \frac{b}{\sqrt{E}}$

$\left.\frac{\partial f}{\partial E}\right|_{E_0} = 0 = \frac{1}{kT} - \frac{1}{2}\frac{b}{E_0^{3/2}}$ $E_0 = \left(\frac{bkT}{2}\right)^{2/3}$ $\left.\frac{\partial^2 f}{\partial E^2}\right|_{E_0} = \frac{b}{2}\,\frac{3}{2}\,E_0^{-5/2}$

$$\therefore\ e^{-f(E)} = e^{-f(E_0) - \underbrace{\left.\frac{df}{dE}\right|_{E_0}\cancel{(E-E_0)}}_{0\ \text{by choice}} - \frac{1}{2!}\frac{d^2f}{dE^2}(E-E_0)^2}$$ → Saddle point method to evaluate integral

$$\langle\sigma v\rangle \propto \int S(E)\,e^{-\frac{3E_0}{kT}}\,e^{-\frac{(E-E_0)^2}{(\Delta/2)^2}}\,dE\,(kT)^{-3/2}$$ $\Delta = 4\left(\frac{E_0 kT}{3}\right)^{1/2}$

$$\langle\sigma v\rangle = \left(\frac{8}{\pi m}\right)^{1/2} S(E_0)\,\frac{\Delta(T)}{2}(kT)^{-3/2}\sqrt{\pi}\,e^{-3E_0/kT}$$

4/26/2007

$dL = \epsilon\, dm = \epsilon 4\pi r^2 \rho\, dr$ $\quad \epsilon : \left[\frac{erg}{s\cdot g}\right]$

$\epsilon = n_x n_a \langle \sigma v \rangle \frac{Q}{\rho}$

$\langle \sigma v \rangle = \left(\frac{8}{\pi m}\right)^{1/2} S(E_0) \frac{\Delta}{2} (kT)^{-3/2} \sqrt{\pi}\, e^{-\frac{3E_0}{kT}}$

$E_0 = \left(\frac{bkT}{2}\right)^{2/3} \quad \Delta = 4\left(\frac{E_0 kT}{3}\right)^{1/2}$

$\frac{\Delta}{E_0} = \frac{4}{\sqrt{3}}\left(\frac{2\sqrt{kT}}{b}\right)^{1/3} \quad b = 2\pi\alpha Z_1 Z_2 \left(\frac{mc^2}{2}\right)^{1/2} \quad m = \frac{m_1 m_2}{m_1 + m_2}$

tunneling energy $E_t \sim b^2$ $\quad kT \sim \varepsilon b^2 \quad \varepsilon \sim 10^{-6}$ only small amount can tunnel

$\eta = \frac{3E_0}{kT} = \frac{3}{2^{2/3}} \frac{b^{2/3}}{(kT)^{1/3}} = \left(\frac{T_*}{T}\right)^{1/3} \quad T_* = \frac{3^3}{4} b^2 \propto Z_1^2 Z_2^2\, mc^2$

H + H $\quad T_* \sim (1e \cdot 1e)^2 \frac{m_H}{2}$ $\qquad$ He + He $\quad T_{*_{He}} \sim (2e\cdot 2e)^2 \frac{4m_H}{2} = 4^3 T_{*_H} = 64 T_{*_H}$

pressure $\quad P = \sum_i n_i kT = \frac{\rho}{\mu m_p} kT \qquad \frac{1}{\mu} = \sum_i \frac{n_i m_p}{\rho}$

H: $\quad n_e = n_p \qquad \frac{(n_i + n_p) m_p}{\underbrace{n_p m_p}_{\rho}} = 2X \qquad$ X: fraction by mass

He: $\quad \frac{\overset{e^-}{2n} + \overset{\alpha}{n}}{n(4m_p)} m_p = \frac{3}{4} Y \qquad$ Y: fraction of He by mass

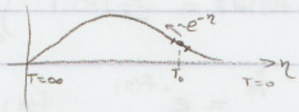
Metals: $\quad \frac{Zn + n}{nAm_p} m_p = \frac{Z+1}{A} \sim \frac{1}{2} Z \qquad \frac{1}{\mu} = 2X + \frac{3}{4} Y + \frac{1}{2} Z$

$\mu = \frac{1}{2} \to 2$
X=1 $\quad$ Z=1

change in $\mu \to$ less pressure
compensated by small increase in temperature

$(kT)^{1/3} = \frac{3}{\eta}\left(\frac{b}{2}\right)^{2/3} \qquad \Delta (kT)^{-3/2} = \frac{\Delta}{E_0} \frac{E_0}{kT} \frac{1}{(kT)^{1/2}}$

$\langle \sigma v \rangle = \frac{8\sqrt{2}}{9\sqrt{3}} \frac{S(E_0)}{\sqrt{m}\, b} \eta^2 e^{-\eta}$



$\langle \sigma v \rangle_T = \langle \sigma v \rangle_{T_0} \left(\frac{\eta}{\eta_0}\right)^2 e^{-\eta + \eta_0} \qquad \eta_0 = \left(\frac{T_*}{T_0}\right)^{1/3}$

$e^{-\eta+\eta_0} = e^{\eta_0(1 - \eta/\eta_0)} = e^{-\eta_0 \ln(1 - (1 - \eta/\eta_0))} \qquad \ln(1-\varepsilon) = -\varepsilon$

η is close to η_0 $\qquad = e^{-\eta_0 \ln(\eta/\eta_0)} = \left(\frac{\eta}{\eta_0}\right)^{-\eta_0}$

$\langle \sigma v \rangle_T = \langle \sigma v \rangle_{T_0} \left(\frac{\eta}{\eta_0}\right)^{2-\eta_0} = \langle \sigma v \rangle_{T_0} \left(\frac{T}{T_0}\right)^{\frac{\eta_0 - 2}{3}} \qquad \underline{n = \frac{\eta_0 - 2}{3} \quad \eta = \left(\frac{T_*}{T_0}\right)^{1/3}}$

H + H: $\quad n = 4.5$ (p-p chain) $\qquad$ He + He: $\quad n \simeq 16$ $\qquad$ C: $\quad n \sim 30$

$\epsilon = n_x n_a \frac{Q}{\rho} \langle \sigma v \rangle_{T_0} \left(\frac{T}{T_0}\right)^n = \underbrace{\frac{n_x n_a}{\rho^2} Q \langle \sigma v \rangle_{T_0}}_{\epsilon_0} \cdot \rho \left(\frac{T}{T_0}\right)^n \qquad \boxed{\epsilon = \epsilon_0 \rho \left(\frac{T}{T_0}\right)^n}$

changes with material and T_0

p-p chain $\quad p + p \rightarrow D + e^+ + \nu_e$

ν_e: (0.26 MeV) $\sigma_\nu \sim 10^{-44}\ cm^2$ escapes E is lost

e^+: (1.18 MeV) combines with e^- to make γ $\quad \sigma_T \sim 6.6 \times 10^{-24}\ cm^2$

$D + p \rightarrow He^3 + \gamma$ (5.49 MeV)

$He^3 + He^3 \rightarrow He^4 + 2p$ (12.86 MeV) $\qquad Q = 26.2$ MeV

$T \gtrsim 10^7 K$

if $T \gtrsim 2\times10^7 K$

$He^3 + He^4 \rightarrow Be^7 + \gamma$ (1.59 MeV)

$Be^7 + p \rightarrow B^8 + \gamma$ (0.13 MeV) $\qquad Q = 19.27$ MeV

$B^8 \rightarrow Be^8 + e^+ + \nu_e$ (7.2 MeV) $\qquad$ loss Q, but occurs slightly faster

$Be^8 \rightarrow 2He^4$ (0.09 MeV)

$$\frac{dn_i}{dt} = -\overbrace{n_i n_a \langle\sigma v\rangle}^{\frac{1}{\tau_a}\ \text{time scale}} + \underbrace{\ldots}_{\text{creation terms}} \qquad \frac{dn_j}{dt} = \ldots$$

Strong interactions happen quickly, weak are slow $\qquad \frac{dn_D}{dt} = 0 \quad \frac{dn_{He^3}}{dt} = 0$ strong reactions

the slowest drives evolution

p+p uses weak interaction

$p + p \rightarrow p + \underbrace{n + e^+ + \nu_e} \rightarrow D + e^+ + \nu_e$

$E_\nu \ll M_{Z,W^\pm} \qquad \sigma_\nu \sim E_\nu$

CNO cycle (catalytic)

$C^{12} + p \rightarrow N^{13} + \gamma$

$N^{13} \rightarrow C^{13} + e^+ + \nu_e$ (slowest)

$C^{13} + p \rightarrow N^{14} + \gamma$

$N^{14} + p \rightarrow O^{15} + \gamma$

$O^{15} \rightarrow N^{15} + e^+ + \nu_e$

$N^{15} + p \rightarrow C^{12} + He^4$ $\qquad N^{15} + p \rightarrow O^{16} + \gamma \qquad O^{16} + p \rightarrow F^{17} + \gamma$

$F^{17} \rightarrow O^{17} + e^+ + \nu_e \qquad O^{17} + p \rightarrow N^{14} + He^4$

$\epsilon_{CNO} \sim T^{20}$

$$\epsilon = \epsilon_0 \rho^\alpha \left(\frac{T}{T_0}\right)^n$$

p-p $\alpha = 1$ $n = 4$ $M \lesssim M_\odot$

CNO $\alpha = 1$ $n = 20$ $M > M_\odot$

$T \sim 10^8 K$

$He^4 + He^4 \rightleftharpoons Be^8 \qquad Be^8 + He^4 \rightarrow C^{12} + \gamma \qquad C^{12} + He^4 \rightarrow O^{16} + \gamma$

need 3 He^4 close together $\qquad$ triple-alpha process $\quad \alpha = 2 \quad n = 44$

so $\epsilon \propto \rho^2$

$T > 2\times10^8 K$

$$C^{12} + C^{12} \rightarrow \begin{cases} Na^{23} + H \\ Ne^{20} + He^4 \\ Mg^{23} + n \\ Mg^{24} + \gamma \end{cases} \qquad O^{16} + O^{16} \rightarrow \begin{cases} S^{32} + \gamma \\ P^{31} + H \\ S^{31} + n \\ Si^{28} + He^4 \\ Mg^{24} + 2He^4 \end{cases}$$

In reality, e^- shields p → screening effect (a sketch)

$$\nabla^2 \phi \propto \underbrace{e\,\delta(r)}_{\text{proton}} + n_e e^{-\frac{\phi}{kT}}$$

if T is large ($kT \gg \phi$) screening is small

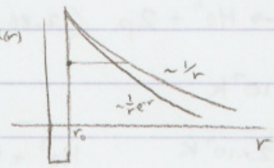
(so far we ignored screening)

Yukawa potential

$$\phi \propto \frac{e}{r} e^{\frac{-r}{\lambda_D}}$$

λ_D: Debye length

$$\frac{Ze^2}{\lambda_D} \frac{4\pi}{3} \lambda_D^3 \underset{\downarrow \atop Zn}{n_e} \sim kT \qquad \lambda_D = \left(\frac{kT}{4\pi n Z^2 e^2}\right)^{1/2}$$



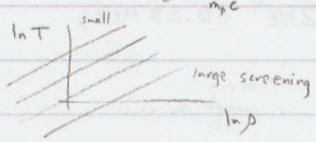
λ_D – large ⟹ (screening small) wrt. r_0

∴ $r_0 \ll \lambda_D$ → small perturbation can be added due to screening effect

if $\lambda_D \lesssim r_0$ need to resolve the problem

$$r_0 \sim \frac{\hbar}{m_p c} A^{1/3}$$

$$r_0 \simeq \lambda_D \simeq \left(\frac{kT}{4\pi Z^2 e^2 \left(\frac{\rho}{A m_p}\right)}\right)^{1/2}$$



n_e separation $a \sim n^{-1/3}$ classical if $a \gg$ quantum localization dimension

$$p \sim \frac{\hbar}{a} \sim \hbar n^{1/3} \qquad E \sim \frac{p^2}{2m} \sim \frac{\hbar^2 n^{2/3}}{2m} \leftarrow E_F \text{ Fermi energy}$$

if $T \to 0$ states fill up to Fermi Energy

$$\mathcal{E}_F \simeq E_F n = \frac{\hbar^2 n^{5/3}}{2m}$$

pressure $P = \mathcal{E}$ this can support star

Pycnonuclear reactions – if protons are degenerate and $T \sim 0K$ (or at least $\ll E_F$)

→ have high kinetic energy and can penetrate barrier and fuse

not common; perhaps occur in supernova

5/1/2007

Angular Momentum

$$\{\hat{x}_i, \hat{p}_j\} = i\hbar\, \delta_{ij}\, \hat{I}$$ — unity operator

$$\frac{\partial \hat{H}}{\partial t} = 0 \qquad H|\Psi\rangle = E|\Psi\rangle \qquad E_i,\ |\Psi_i\rangle = |E_i\rangle$$

translate system along $\vec{\alpha}$

$(\hat{\vec{p}} \cdot \vec{\alpha})\vec{\alpha}$ → projection of momentum along $\vec{\alpha}$ $\qquad \{\hat{H}, (\hat{\vec{p}}\cdot\vec{\alpha})\vec{\alpha}\} = 0$

Spherical symmetry: $\{\hat{H}, \hat{p}_i\} \neq 0$

$$\hat{L}_z \qquad \hat{L}^2 \qquad \{\hat{H}, \hat{L}_z\} = 0 \qquad \{\hat{H}, \hat{L}^2\} = 0$$

$\hat{L} = \hat{r} \times \hat{p} \qquad \hat{L}_i = e_{ik\ell}\, \hat{r}_k \hat{p}_\ell$

$\{\hat{L}_i, \hat{L}_k\} = i\hbar\, e_{ik\ell} \hat{L}_\ell \qquad \{\hat{L}_i, \hat{p}_k\} = i\hbar\, e_{ik\ell}\, \hat{p}_\ell \qquad \{\hat{L}_i, \hat{x}_k\} = i\hbar\, e_{ik\ell}\, \hat{x}_\ell$

$\{\hat{L}_i, \hat{L}^2\} = 0 \qquad \{\hat{L}_i, \hat{r}^2\} = 0 \qquad \{\hat{L}_i, \hat{p}^2\} = 0$ spherical sym.

$x = r\sin\theta\cos\varphi \qquad y = r\sin\theta\sin\varphi \qquad z = r\cos\theta$

$\langle \vec{r} | \hat{L}_z | \psi\rangle = \hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\varphi}$

$\hat{L}_x = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)$

$\hat{L}_y = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)$

$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)$

$\langle \vec{r} | \hat{L}_z | \psi\rangle = -i\hbar\frac{\partial\psi}{\partial\varphi} = \mu\psi$ ...eigenvalue $\qquad \psi = \langle \vec{r} | \psi\rangle$

$\psi = f(r,\theta)\, e^{\frac{i}{\hbar}\mu\varphi} \qquad \psi(r,\theta,\varphi+2\pi) = \psi(r,\theta,\varphi)$ experimentally required in Stern-Gerlach experiment

$e^{\frac{i}{\hbar}\mu 2\pi} = 1 \implies \mu = \hbar m \quad m = \pm\text{integer} \qquad \langle \vec{r} | m\rangle = f(r,\theta)\, e^{im\varphi}$

$\hat{L}_z |m\rangle = \hbar m |m\rangle$

$\hat{L}_+ = \hat{L}_x + i\hat{L}_y \qquad \hat{L}_- = \hat{L}_x - i\hat{L}_y$

$\{\hat{L}_+, \hat{L}_z\} = \underbrace{\{\hat{L}_x, \hat{L}_z\}}_{-i\hbar\hat{L}_y} + i\underbrace{\{\hat{L}_y, \hat{L}_z\}}_{i\hbar\hat{L}_x} = -\hbar(\hat{L}_x + i\hat{L}_y) = \boxed{-\hbar\hat{L}_+ = \{\hat{L}_+, \hat{L}_z\} \quad \{\hat{L}_-, \hat{L}_z\} = \hbar\hat{L}_-}$

$\hat{L}_+\hat{L}_z - \hat{L}_z\hat{L}_+ = -\hbar\hat{L}_+ \qquad \hat{L}_z\hat{L}_+ = \hat{L}_+(\hat{L}_z + \hbar\hat{I})$

$\hat{L}_z|\psi\rangle = \hbar m|\psi\rangle = \hbar m|m\rangle \qquad \hat{L}_z\hat{L}_+|m\rangle = \hat{L}_+(\hat{L}_z + \hbar\hat{I})|m\rangle = \hat{L}_+(\hbar m + \hbar)|m\rangle$

$\hat{L}_z\underline{\hat{L}_+|m\rangle} = \hbar(m+1)\hat{L}_+|m\rangle \qquad \hat{L}_z\hat{L}_-|m\rangle = \hbar(m-1)\hat{L}_-|m\rangle$

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

$\{\hat{L}_+, \hat{L}_-\} = 2\hbar\hat{L}_z \qquad \hat{L}_x = \frac{1}{2}(\hat{L}_+ + \hat{L}_-) \quad \hat{L}_y = \frac{1}{2i}(\hat{L}_+ - \hat{L}_-)$

$\hat{H}|\psi\rangle = E|\psi\rangle \qquad \hat{L}_z|\psi\rangle = \hbar m|\psi\rangle \qquad \hat{L}^2|\psi\rangle = \lambda|\psi\rangle$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = \hat{L}_+\hat{L}_- + \hat{L}_z^2 - \hbar\hat{L}_z = \hat{L}_-\hat{L}_+ + \hat{L}_z^2 + \hbar\hat{L}_z$$

$\hat{L}_z|\lambda m\rangle = \hbar m|\lambda m\rangle \qquad \hat{L}^2|\lambda m\rangle = \lambda|\lambda m\rangle \qquad \{\hat{L}_+, \underbrace{\hat{L}^2}_{\text{scalar}}\} = 0$

$\hat{L}_+\hat{L}^2|\lambda m\rangle = \lambda\hat{L}_+|\lambda m\rangle = \hat{L}^2\hat{L}_+|\lambda m\rangle$

$\hat{L}_+|\lambda m\rangle$ has same eigenvalue λ
OR $\hat{L}_+|\lambda m\rangle = 0$

$\hat{L}_+|\lambda, m\rangle = \text{const}\,|\lambda, m+1\rangle$

$\hat{L}^2 - \hat{L}_z^2 = \hat{L}_x^2 + \hat{L}_y^2$ always positive $\langle\lambda m|\hat{L}^2 - \hat{L}_z^2|\lambda m\rangle \geq 0 \qquad \lambda^2 - \hbar^2 m^2 \geq 0$

maximum value for $m \to l$

$\hat{L}_+|\lambda l\rangle = 0 \qquad m = -l, \ldots, -2, -1, 0, 1, 2, \ldots, l$

$2l+1$ states

$$\hat{L}^2|\lambda l\rangle = (\hat{L}_-\hat{L}_+ + \hat{L}_z^2 + \hbar\hat{L}_z)|\lambda l\rangle = 0 + \hbar^2 l^2|\lambda l\rangle + \hbar^2 l|\lambda l\rangle = \hbar^2 l(l+1)|\lambda m\rangle$$

$$\therefore \boxed{\lambda = \hbar^2 l(l+1) \qquad m = [-l, \ldots, l]}$$

$$-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)\psi_{lm}(\theta)e^{im\varphi} = \hbar^2 l(l+1)\psi_{lm}(\theta)e^{im\varphi}$$

$\psi_{lm} = P_l^m(\cos\theta)$ — associated Legendre polinomials $\quad 0 \leq m < l$

$P_l^m(x) = (1-x^2)^{m/2}\dfrac{d^m}{dx^m}P_l(x) \qquad \dfrac{d}{dx}\left[(1-x^2)\dfrac{dP_l}{dx}\right] + l(l+1)P_l = 0$

$\dfrac{d}{dx}\left[(1-x^2)\dfrac{dP_l^m}{dx}\right] + \left(l(l+1) - \dfrac{m^2}{1-x^2}\right)P_l^m = 0 \qquad \displaystyle\int_{-1}^{1}P_l(x)P_{l'}(x)\,dx = \frac{2\delta_{ll'}}{2l+1}$

$\displaystyle\int_{-1}^{1}P_l^m(x)P_{l'}^m(x)\,dx = \frac{2\delta_{ll'}}{2l+1}\frac{(l+m)!}{(l-m)!}$

for negative m: $\quad P_{l}^{-m}(x) = (-1)^m\dfrac{(l-m)!}{(l+m)!}P_l^m(x)$

$$Y_{lm}(\theta,\varphi) = \underbrace{i^l}_{\text{needed for right behavior under time inversion}}(-1)^{\frac{m+|m|}{2}}\left[\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2}P_l^{|m|}(\cos\theta)e^{im\varphi}$$

$\displaystyle\int_0^{2\pi}\int_0^{\pi}Y_{lm}^*(\theta,\varphi)Y_{l'm'}(\theta,\varphi)\sin\theta\,d\theta\,d\varphi = \delta_{ll'}\delta_{mm'} \qquad Y_{lm}^* = (-1)^{l-m}Y_{l,-m}$; in book: $Y_{lm}^* = (-1)^m Y_{l-m}$ not in book

$Y_{lm}(\pi-\theta, \varphi+\pi) = (-1)^l Y_{lm}(\theta,\varphi)$

$\hat{L}_\pm Y_{lm} = \hbar\left((l\mp m)(l+1\pm m)\right)^{1/2}Y_{l,m\pm1}$

$Y_{00} = \dfrac{1}{\sqrt{4\pi}} \qquad Y_{10} = i\sqrt{\dfrac{3}{4\pi}}\cos\theta \qquad Y_{1\pm1} = \mp i\sqrt{\dfrac{3}{8\pi}}\sin\theta\, e^{\pm i\varphi}$

$Y_{20} = \sqrt{\dfrac{5}{16\pi}}(1-3\cos^2\theta) \qquad Y_{2\pm1} = \pm\sqrt{\dfrac{15}{8\pi}}\cos\theta\sin\theta\, e^{\pm i\varphi}$

$Y_{2\pm2} = -\sqrt{\dfrac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\varphi}$

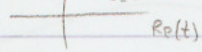
$\hat{L}_+ \,|\, l(l+1), l > = 0 \qquad \hat{L}_+ = \hbar e^{i\varphi}\left(\frac{\partial}{\partial\theta} + i\cot\theta \frac{\partial}{\partial\varphi}\right)$

$\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right) \underbrace{\chi_l(\theta)\, e^{il\varphi}}_{Y_{ll}(\theta,\varphi)} = 0 \qquad \frac{\partial\chi}{\partial\theta} - l\cot\theta\,\chi = 0 \qquad \chi = A\sin^l\theta$

$<\theta,\varphi \,|\, l(l+1), l> = \text{const } \sin^l\theta\, e^{il\varphi}$

$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l$ Rodrigues formula $\qquad f(z) = \frac{1}{2\pi i}\oint \frac{f(t)\,dt}{t-z}$ Cauchy's formula

$P_l(z) = \frac{1}{2^l}\frac{1}{2\pi i}\oint \frac{(t^2-1)^l}{(t-z)^{l+1}}\,dt$



$t = z + \sqrt{z^2-1}\, e^{-i\varphi}$ substitution $\qquad P_l(z) = \frac{1}{\pi}\int_0^\pi \left(z + \sqrt{z^2-1}\cos\varphi\right)^l d\varphi$ Laplace's integral

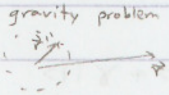
generating function $\qquad g(h,z) = \sum_{l=0}^{\infty} h^l P_l(z) = \frac{1}{\pi}\int_0^\pi \sum_{h=0}^{\infty} h^l \left(z+\sqrt{z^2-1}\cos\varphi\right)^l d\varphi$

$1 + x + x^2 + x^3 + \dots = \frac{1}{1-x} \qquad = \frac{1}{\pi}\int_0^\pi \frac{d\varphi}{1-hz-h\sqrt{z^2-1}\cos\varphi} = \frac{1}{\sqrt{1-2hz+h^2}}$

$\boxed{g(h,z) = \sum_{l=0}^{\infty} h^l P_l(z) = \frac{1}{\sqrt{1-2hz+h^2}}}$ generating function for Legendre polynomial

ex: $\frac{1}{|\vec r - \vec r\,'|} = \frac{1}{\sqrt{r^2+r'^2-2rr'\cos\theta}} = \frac{1}{r}\frac{1}{\sqrt{1+\left(\frac{r'}{r}\right)^2 - 2\frac{r'}{r}\cos\theta}} \qquad h = \frac{r'}{r} \quad z = \cos\theta$

gravity problem



$\frac{1}{|\vec r - \vec r\,'|} = \frac{1}{r}\sum_{l=0}^{\infty}\left(\frac{r'}{r}\right)^l P_l(\cos\theta)$ multiple expansion

if I had taken out r' (rather than r) it would be like being inside of a dist^n of masses

$\frac{\partial g}{\partial h} = \frac{z-h}{1-2hz+h^2}\, g \;\to\; (1-2hz+h^2)\frac{\partial g}{\partial h} = (z-h)\, g$

group equal power of h $\quad h^l: \; (l+1)P_{l+1} - 2zlP_l + (l-1)P_{l-1} = zP_l - P_{l-1}$

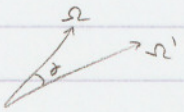
$(l+1)P_{l+1} - (2l+1)zP_l + lP_{l-1} = 0$

$h^l: \; (1-2hz+h^2)\frac{\partial g}{\partial z} = hg \qquad P_l' - 2zP_{l-1}' + P_{l-2}' = P_{l-1}'$

$P_{l+1}' - zP_l' = (l+1)P_l \qquad zP_l' - P_{l-1}' = lP_l \qquad P_{l+1}' - P_{l-1}' = (2l+1)P_l \qquad (z^2-1)P_l' = lzP_l - lP_{l-1}$

$$f(\overset{\theta,\varphi}{\Omega}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} B_{lm} Y_{lm}(\Omega) \qquad B_{lm} = \int Y^*_{lm}(\Omega) f(\Omega)\, d\Omega$$

$$\delta(\Omega-\Omega') = \sum_{lm} Y^*_{lm}(\Omega') Y_{lm}(\Omega)$$ addition theorem $$f(\Omega) = \int \delta(\Omega-\Omega') f(\Omega')\, d\Omega'$$



$$\cos\gamma = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi-\varphi')$$

$$\delta(\Omega-\Omega') = \sum_l \frac{2l+1}{4\pi} P_l(\cos\gamma)$$

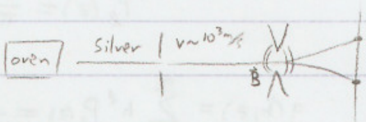
$$Y_{lm}(\Omega) = \sum_{m'=-l}^{l} C^l_{mm'} Y_{lm'}(\Omega')$$ → Clebsch-Gordan coefficients

rotation of reference frame
m states get mixed (not l)

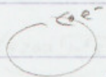
5/3/2007

Spin

Stern-Gerlach Experiment:



$F = evB$

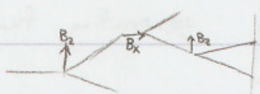


$$\tau \simeq evrB = \frac{e}{m}\underbrace{mvr}_{L}B$$ L — angular momentum

$$\vec{\mu} = \frac{e}{2m} g \vec{L}$$ magnetic moment
↳ Lande factor

$$\vec{F} = -\nabla U \qquad U = -\vec{\mu}\cdot\vec{B} \qquad \vec{F} = \nabla(\vec{\mu}\cdot\vec{B})$$

Apply B field again



$2l+1$ states in angular momentum (odd #)

spin: turn $2\pi \to -1$ turn $4\pi \to 1$ (back to same)

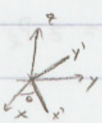
Atom $J = 1$ (units of $\hbar$)
$J_z = -1, 0, 1$

$$\hat{\mu} = \underbrace{\frac{e}{2m} g\hbar}_{\mu} \hat{I}$$ ← operator of angular momentum

$$\Psi = \alpha|-1\rangle + \beta|0\rangle + \gamma|1\rangle \qquad |\alpha|^2+|\beta|^2+|\gamma|^2 = 1$$

$$\hat{I}_z|1\rangle = 1\,|1\rangle \qquad \hat{I}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \{\hat{I}_j, \hat{I}_k\} = i e_{jkl} \hat{I}_l$$

$$\hat{I} = \hat{U}^+ \hat{I}' \hat{U} \qquad U^+ = U^{-1}$$ unitary transformation that relates one basis to another



$$x' = x\cos\theta - y\sin\theta \qquad y' = x\sin\theta + y\cos\theta \qquad z' = z \qquad \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

if $\theta \to \delta\theta \to 0$
$\cos\delta\theta \to 0$
$\sin\delta\theta \to \delta\theta$

$$= \left(\hat{1} - i\delta\theta\,\hat{I}_z'\right)\begin{pmatrix} x \\ y \\ z \end{pmatrix} \qquad I_z' = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

generator of infinitesimal rotations

$$\hat{I}_z'^{\,2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \hat{I}_z'^{\,2k} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\hat{I}_z'^{\,2k+1} = \hat{I}_z'$$

finite rotation

$$e^{-i\theta \hat{I}_z'} = \sum_{l=1}^{\infty} \frac{1}{l!}\left(-i\theta \hat{I}_z'\right)^l = \hat{1} + \hat{I}_z'(-i\sin\theta) + \hat{I}_z'^2(\cos\theta - 1)$$

$$\hat{I}_x' = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$ rotation around x, mixes y and z

can be obtained like $\hat{I}_z'$

$$\hat{I}_y' = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$ $\rightarrow$ can find with commutation relations

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} i & 0 & -i \\ -1 & 0 & -1 \\ 0 & -\sqrt{2}i & 0 \end{pmatrix} \qquad \hat{I} = \hat{U}^+ \hat{I}' \hat{U}$$

$$\hat{I}_z' \rightarrow \hat{I}_z$$

$$\hat{I}_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad \hat{I}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$2l+1 = 2n \Rightarrow l = n - \frac{1}{2}$ even dimensions of matrix

$\hat{I}_z|1/2\rangle = \frac{1}{2}|1/2\rangle \qquad \hat{I}_z|-1/2\rangle = -1/2\,|-1/2\rangle \qquad I_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2}\sigma_z$ Pauli matrix

$\hat{\vec{I}} = \frac{1}{2}\hat{\vec{\sigma}} \qquad \hat{\sigma}_j^+ = \hat{\sigma}_j \qquad \begin{pmatrix} a & c \\ d & b \end{pmatrix}^+ = \begin{pmatrix} a^* & d^* \\ c^* & b^* \end{pmatrix} = \begin{pmatrix} a & c \\ d & b \end{pmatrix}$

$a^* = a \qquad d^* = c \qquad c^* = d \qquad b^* = b$

$$\sigma = \begin{pmatrix} a & \rho e^{-i\varphi} \\ \rho e^{+i\varphi} & b \end{pmatrix}$$ $Det(\sigma)$, $Trace(\sigma)$ invariant

$Tr(\sigma_z) = 0 \quad \therefore \quad a = -b$

$Det(\sigma_z) = -1 \quad \therefore \quad -a^2 - \rho^2 = -1$

$$\sigma = \begin{pmatrix} \cos\chi & \sin\chi\, e^{-i\varphi} \\ \sin\chi\, e^{+i\varphi} & -\cos\chi \end{pmatrix}$$

$\left\{\frac{1}{2}\hat{\sigma}_j, \frac{1}{2}\hat{\sigma}_k\right\} = i\epsilon_{jkl}\frac{1}{2}\hat{\sigma}_l$

$$\boxed{\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{Pauli Matrices}}$$

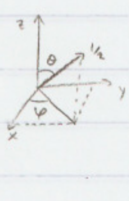
$\hat{\sigma}_x^2 = \hat{\sigma}_y^2 = \hat{\sigma}_z^2 = \hat{1} \qquad \hat{I}_x^2 + \hat{I}_y^2 + \hat{I}_z^2 = \left(\frac{1}{2}\hat{\sigma}_x\right)^2 + \left(\frac{1}{2}\hat{\sigma}_y\right)^2 + \left(\frac{1}{2}\hat{\sigma}_z\right)^2 = \frac{1}{4}\,3\,\hat{1} = \frac{1}{2}\left(\frac{1}{2}+1\right)\hat{1}$

$l(l+1)$

$\psi = \alpha|1/2\rangle + \beta|-1/2\rangle \qquad S = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \qquad |\alpha|^2 + |\beta|^2 = 1 \qquad \psi^*\psi =$

spinor

$S^+S = (\alpha^* \beta^*)\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 1$



$\langle S_z \rangle = \frac{1}{2}\cos\theta \qquad \langle S_y \rangle = \frac{1}{2}\sin\theta\sin\varphi \qquad \langle S_z \rangle = \frac{1}{2}\sin\theta\cos\varphi$

$\langle S_z \rangle = S^+ \frac{1}{2}\sigma_z S = (\alpha^* \beta^*)\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{1}{2}\left(|\alpha|^2 - |\beta|^2\right) = \frac{1}{2}\cos\theta$

arbitrary phase factors

$$|\alpha|^2+|\beta|^2=1 \qquad |\alpha|^2-|\beta|^2=\cos\theta \qquad \alpha=\cos\frac{\theta}{2}\,e^{i\psi} \qquad \beta=\sin\frac{\theta}{2}\,e^{i\phi}$$

$$\frac{1}{2}\sin\theta\sin\varphi=(\alpha^*\ \beta^*)\,\frac{1}{2}\begin{pmatrix}0&-i\\ i&0\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

$$e^{i\psi}=e^{i\left(\frac{\psi+\phi}{2}+\frac{\psi-\phi}{2}\right)}$$

$$e^{i\phi}=e^{i\left(\frac{\psi+\phi}{2}-\frac{\psi-\phi}{2}\right)}$$

$$\alpha=\cos\frac{\theta}{2}\,e^{i\varphi/2} \qquad \beta=\sin\frac{\theta}{2}\,e^{-i\varphi/2}$$

$$\boxed{S(\theta,\varphi)=\begin{pmatrix}\cos\frac{\theta}{2}e^{i\varphi/2}\\ \sin\frac{\theta}{2}e^{-i\varphi/2}\end{pmatrix}}$$ Spinor

$\varphi: 0\to 2\pi \qquad S(\theta,\varphi)\to -S(\theta,\varphi)$

$\Psi(r_1,r_2)=\psi_1(r_1)\psi_2(r_2)-\psi_1(r_2)\psi_2(r_1)$ antisymmetric

Spinor

$\langle\theta,\varphi|\frac{1}{2}\hat\sigma_z|\theta,\varphi\rangle \qquad |\theta,\varphi\rangle=\mathcal{U}|1/2\rangle$ spinor in z direction

$$\langle 1/2|\mathcal{U}^+\tfrac{1}{2}\hat\sigma_z\mathcal{U}|1/2\rangle$$

$$\mathcal{U}^+\tfrac{1}{2}\hat\sigma_z\mathcal{U}=\underbrace{\sin\theta\cos\varphi}_{u_x}\tfrac{1}{2}\hat\sigma_x+\tfrac{1}{2}\underbrace{\sin\theta\sin\varphi}_{u_y}\hat\sigma_y+\underbrace{\cos\theta}_{u_z}\tfrac{1}{2}\hat\sigma_z=\cdots$$

$$=\frac{1}{2}\begin{pmatrix}u_z & u_x-iu_y\\ u_x+iu_y & -u_z\end{pmatrix}=\frac{1}{2}\begin{pmatrix}\cos\theta & \sin\theta e^{-i\varphi}\\ \sin\theta e^{i\varphi} & -\cos\theta\end{pmatrix} \qquad \hat u^+\hat u=\hat u\hat u^+=\hat 1$$

$$\mathcal{U}=\begin{pmatrix}\cos\frac{\theta}{2} & -\sin\frac{\theta}{2}e^{+i\varphi}\\ \sin\frac{\theta}{2}e^{-i\varphi} & \cos\frac{\theta}{2}\end{pmatrix}e^{i\varphi/2}$$

$\mathcal{U}^+|\theta,\varphi\rangle=|1/2\rangle=\begin{pmatrix}1\\0\end{pmatrix} \longrightarrow$ this provives phase factor

$\theta \nearrow \vec n$ rotate around $\vec n$: $e^{-i\theta\,\vec n\cdot\frac{\hat{\vec\sigma}}{2}}$

$$\vec n\cdot\hat{\vec\sigma}=n_x\hat\sigma_x+n_y\hat\sigma_y+n_z\hat\sigma_z \qquad n_x^2+n_y^2+n_z^2=1$$

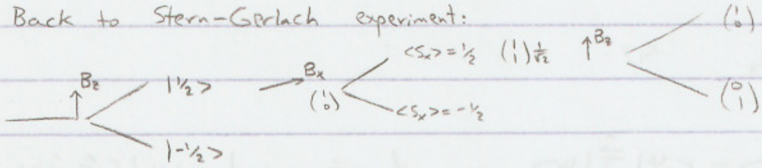
$$(\vec n\cdot\hat{\vec\sigma})^2=\underbrace{n_x^2\underset{\hat 1}{\hat\sigma_x^2}+n_y^2\underset{\hat 1}{\hat\sigma_y^2}+n_z^2\underset{\hat 1}{\hat\sigma_z^2}}_{\hat 1}+n_xn_y(\hat\sigma_x\hat\sigma_y+\hat\sigma_y\hat\sigma_x)+n_xn_z(\hat\sigma_x\hat\sigma_z+\hat\sigma_z\hat\sigma_x)+n_yn_z(\hat\sigma_y\hat\sigma_z+\hat\sigma_z\hat\sigma_y)$$

$$\sigma_x\sigma_y=\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&-i\\i&0\end{pmatrix}=\begin{pmatrix}i&0\\0&-i\end{pmatrix} \qquad \sigma_y\sigma_x=\begin{pmatrix}0&-i\\i&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}=\begin{pmatrix}-i&0\\0&i\end{pmatrix}$$

$$\boxed{\hat\sigma_i\hat\sigma_k+\hat\sigma_k\hat\sigma_i=2\delta_{ik}\hat 1}$$

$$e^{-i\theta\,\vec n\cdot\frac{\hat{\vec\sigma}}{2}}=\begin{pmatrix}\cos\frac{\theta}{2}-in_z\sin\frac{\theta}{2} & -(in_x+n_y)\sin\frac{\theta}{2}\\ (-in_x+n_y)\sin\frac{\theta}{2} & \cos\frac{\theta}{2}+in_z\sin\frac{\theta}{2}\end{pmatrix}$$

Back to Stern-Gerlach experiment:



$$\frac{1}{2}\underbrace{\begin{pmatrix}0&1\\1&0\end{pmatrix}}_{\sigma_x}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \frac{1}{2}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

spinor in x

$$\therefore \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \leftarrow \langle S_x\rangle = \tfrac{1}{2} \qquad \langle S_x\rangle = -\tfrac{1}{2} \rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

$$\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{2}\left[\begin{pmatrix}1\\1\end{pmatrix} + \begin{pmatrix}1\\-1\end{pmatrix}\right] \qquad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\left(\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\right)$$

5/8/2007

May 31 — QM presentation

Hamiltonian with magnetic field

$\hat{H} = \hat{H}_0 - \vec{\mu}\cdot\vec{B}$ includes motion of e^- and spin

small perturbation does not mix levels $\qquad H|\psi\rangle = E|\psi\rangle$

g - Lande factor $[0, \tfrac{5}{2}]$ (range)

$\langle|H|\rangle = E - \frac{e}{2m_e} g\hbar m|B|$

QM number

$\mu_B = \frac{e\hbar}{2m_e}$ Bohr magneton $\quad \mu_B = 9.27\times10^{-24}\ \mathrm{J\,T^{-1}}$

$= 5.79\times10^{-5}\ \frac{\mathrm{eV}}{\mathrm{T}} = 5.79\times10^{-9}\ \frac{\mathrm{eV}}{\mathrm{gauss}}$

$\Delta E_{sun} = 10^{-7}$ eV $\qquad B \sim 20$–40 gauss $\qquad \Delta\lambda \sim 1\mathrm{m}$?

1) Zeeman splitting

$\xrightarrow{B}$ $\underset{2}{=}$ $\rhd$ $\qquad \uparrow B$ $\underset{1}{-}$ $\rhd$ $\qquad$ Sun is complicated with convection zones

2) Zeeman line broadening
splitting of levels is small and unresolved for distant stars

3) Doppler imaging
star is moving

4) Synchrotron spectrum

5) Hanle effect $\qquad$ distortion of Faraday rotation

A-B chemically peculiar

system dominated by prominent B field such as dipole

Neutron star

○ ⟶ o $\qquad B \to 10^{11}$–10^{12} gauss $\qquad \mu B \sim$ a few keV $\to$ will ionize atoms

$\sim 10^4$ km $\qquad \sim$ km $\qquad$ no longer a small perturbation

Magnetars $\sim 10^{15}$ gauss $\to$ enough E to create e^-e^+ $\leftarrow$ QED

$\vec{F}_z = -\nabla(\vec{\mu}\cdot\vec{B}) \overset{?}{\doteq} -\mu \frac{\partial B}{\partial z}\hat{e}_z$ $\quad x, y?$

$\vec{\mu}\cdot\vec{B} = \frac{\mu}{\hbar}\vec{J}\cdot\vec{B}$ (angular moment) $\quad \langle \vec{J} \rangle = \langle \psi | \hat{\vec{J}} | \psi \rangle \quad \frac{d}{dt}\langle \vec{J} \rangle = \frac{1}{i\hbar}\langle \psi | \{\hat{\vec{J}}, \hat{H}\} | \psi \rangle$

$\{\hat{\vec{J}}, \hat{H}\} = -\frac{\mu}{\hbar}\{\hat{\vec{J}}, \hat{\vec{J}}\cdot\vec{B}\} \qquad \{\hat{J}_i, \hat{J}_k B_k\} = i\hbar\, e_{ikl}\hat{J}_l B_K$

$= -\frac{\mu}{\hbar}(i\hbar)\,\vec{B}\times\hat{\vec{J}} \qquad \frac{d}{dt}\langle\vec{J}\rangle = -\frac{\mu}{\hbar}\left[\vec{B}\times\langle\vec{J}\rangle\right]$

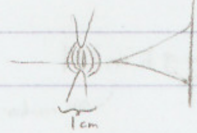
if $\vec{B} = (0,0,B)$ $\quad \frac{d\langle J_x\rangle}{dt} = \frac{\mu B}{\hbar}\langle J_y\rangle \quad \frac{d\langle J_y\rangle}{dt} = -\frac{\mu B}{\hbar}\langle J_x\rangle \quad \frac{d\langle J_z\rangle}{dt} = 0$

$\omega = \frac{\mu B}{\hbar}$ – Larmor frequency

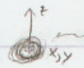
$\omega = \frac{(10^{-23}\frac{J}{T})(1T)\left(\frac{B}{1T}\right)}{10^{-34}\ J\cdot s} = 10^{11}\ Hz\left(\frac{B}{1T}\right)$

$V_T \sim 10^3\ m/s \quad \Delta \sim 1cm \rightarrow t \sim 10^{-5}\ sec$

$(10^{-5})(10^{11}) \sim 10^6$



$\therefore$ it averages out x,y components



10^6 times

$\therefore \quad \hat{H} = \hat{H}_0 - \mu_z B_z \qquad \langle\mu_x\rangle = \langle\mu_y\rangle = 0$

Hydrogen-like Atoms

Spherically symmetric potential $\qquad$ other atoms $\rightarrow$ add perturbation

$\hat{H} = \frac{1}{2m}\hat{p}^2 + V(r) + \delta V$ $\qquad$ nonperturbative effect: e^- are identical (Pauli exclusion)

e-e interactions, spin-orbit coupling, spin-spin coupling, (hyperfine splitting)

isotope separation (atom 'recoils' as e^- moves), e motion (non relativistic)

For now $\delta V = 0$

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right)\langle r|\psi\rangle = E\langle r|\psi\rangle$$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \underbrace{\frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial}{\partial\varphi^2}\right)}_{-\frac{1}{r^2}\frac{\hat{L}^2}{\hbar^2}}$$

$\{\hat{L}^2, \hat{p}^2\} = 0 \qquad \{\hat{L}^2, \hat{r}^2\} = 0$

E, l, m

$\hat{H}, \hat{L}^2, \hat{L}_z$

$\langle r|\psi\rangle = u(r)\, Y_{\ell m}(\theta,\varphi)$

$$\left(\frac{-\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\ell(\ell+1)\right) + (V(r)-E)\right) u_\ell(r)\, Y_{\ell m}(\theta,\varphi) = 0$$

no dependance on m

Estimates:

$V(r) = -\frac{Ze^2}{r}$ $\quad$ KE: $\frac{p^2}{2m_e} \sim \frac{\hbar^2}{m_e}\frac{1}{r^2} \sim \frac{Ze^2}{r}$ if e^- bound

$E \sim -\frac{Ze^2}{r} \sim -\frac{Z^2 m_e e^4}{\hbar^2} \sim m_e v^2$ $\quad$ $\therefore\ r \sim \frac{\hbar^2}{Ze^2 m_e} = \frac{1}{Z}\underbrace{\frac{\hbar^2}{m_e e^2}}_{a_0\text{ - Bohr radius}} = \frac{a_0}{Z}$

$\frac{v^2}{c^2} \sim Z^2\frac{e^4}{\hbar^2 c^2}$ $\qquad$ $\frac{v}{c} \sim Z\underbrace{\frac{e^2}{\hbar c}}_{\alpha = \frac{1}{137}}$ $\qquad$ $\frac{v}{c} \sim Z\alpha$ $\quad$ e^- not relativistic

$Z \sim 31,\ 28,\ 15$ (Ca, Ni, P) $\quad$ relativistic corrections important

not fine structure constant

$\alpha^2 = -\frac{8mE}{\hbar^2}$ $\qquad$ $\rho = \alpha r$ $\qquad$ $\lambda = \frac{2mZe^2}{\alpha\hbar^2}$

$\chi(\rho) = u_\ell(\rho/\alpha)$

$$\frac{1}{\rho^2}\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial\chi}{\partial\rho}\right) + \left(\frac{\lambda}{\rho} - \frac{1}{4} - \frac{\ell(\ell+1)}{\rho^2}\right)\chi = 0$$

if $\rho\to\infty$ $\qquad$ $\frac{d^2\chi}{d\rho^2} - \frac{1}{4}\chi = 0$ $\qquad$ $\chi = e^{-\rho/2}$ $\quad$ normalizable, non divergent so no $e^{+\rho/2}$ $\qquad$ BK 1

$\rho\to 0$ $\qquad$ $\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{d\chi}{d\rho}\right) = \frac{\ell(\ell+1)}{\rho^2}\chi$ $\qquad$ $\chi = \rho^s \Rightarrow s(s+1) = \ell(\ell+1)$ $\qquad$ BC 2

$\underline{s=\ell}$, $s = -\ell-1$

$\rho^{-\ell-1}\to\infty$ as $\rho\to 0$

$$\chi = \rho^\ell e^{-\rho/2}\cdot\sum_{k=0}^{\infty} c_k\rho^k$$

$c_{k+1} = \left(\frac{\ell+k+1-\lambda}{(k+1)(k+2\ell+2)}\right)c_k$ $\qquad$ for large k $\quad$ $c_{k+1} = \frac{1}{k}c_k \to \sum\frac{1}{k!}\rho^k = e^\rho$

but this makes χ divergent $\therefore$ must terminate series

$\to\ \lambda$ must be integer number n to terminate series

$\lambda = n$

$k = n-\ell-1 \geq 0$

$\therefore\ n \geq \ell+1$

$n = \lambda = \frac{2mZe^2}{\alpha\hbar^2} \to \alpha(n)$ $\qquad$ $\alpha^2 \to E_n$ $\qquad$ $E_n = -\frac{Z^2 me^4}{2n^2\hbar^2} = -\frac{Z^2}{n^2}R$

Rydberg 13.6 eV

$\rho = \underbrace{\frac{2Z}{na_0}}_{\alpha}r$ $\qquad$ $\sum_{k=0}^{n-\ell-1} c_k\rho^k = L_{n-\ell-1}^{2\ell+1}(\rho)$ — Associated Laguerre polynomials

$$u_{n\ell}(r) = \alpha^{3/2}\left(\frac{(n-\ell-1)}{2n((n+\ell)!)}\right)^{1/2} e^{\frac{-\alpha r}{2}}(\alpha r)^\ell L_{n-\ell-1}^{2\ell+1}(\alpha r)$$

$$L_n^k(x) = (-1)^k \frac{d^k}{dx^k} L_{n+k}(x)$$

Laguerre polynomials

Laguerre Polynomials

Generating function

$$g(x,z) = \frac{e^{-xz/(1-z)}}{1-z} = \sum_{n=0}^{\infty} L_n(x)\, z^n$$

$$L_n(x) = \frac{1}{2\pi i} \oint \frac{e^{\frac{-xz}{1-z}}}{(1-z)\, z^{n+1}}\, dz$$

$z^n \to |z|^n e^{i\theta n}$

$x y'' + (1-x) y' + n y = 0 \longrightarrow$ solution is $L_n(x)$

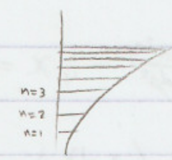
$z = 1 - \frac{x}{s} \qquad s = x + \frac{xz}{1-z} = \frac{x}{1-z}$

$$L_n(x) = \frac{e^x}{2\pi i} \oint \frac{s^n e^{-s}}{(s-x)^{n+1}}\, ds = e^x \frac{1}{n!} \frac{d^n}{dx^n}\left(x^n e^{-x}\right) = L_n(x)$$

$$L_n(x) = \sum_{s=0}^{n} (-1)^{n-s} \frac{n!\, x^{n-s}}{((n-s)!)^2\, s!}$$

5/17/2007

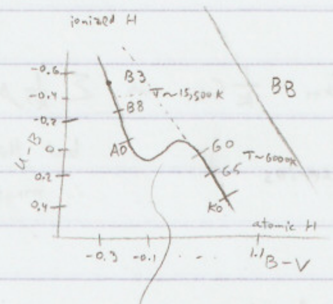
$$E_n = -\frac{Z^2 m e^4}{2n^2 \hbar^2} = -\frac{Z^2}{n^2} \underbrace{R_y}_{13.6\,eV} \qquad a_0 = \frac{\hbar^2}{me^2}$$



Lyman ($n=1 \to n'$) $\quad L_\alpha = 1216$ Å ($n=1 \to n=2$)

$L_\beta = 1025.18$ Å $\quad L_\gamma = 972.02$ Å $\quad$ limit: 911.267 Å ($n=1 \to n=\infty$)

Balmer series ($n=2 \to n'$) $\quad H_\alpha = 6563$ Å $\quad H_\beta = 4861$ Å $\quad$ limit: 3646 Å ($n=2 \to n=\infty$)



→ Balmer dip
enough E to produce Balmer series

$$u - B = 2.5 \log\left[\frac{\int S_{B_\nu} l_\nu\, d\nu}{\int S_{u_\nu} l_\nu\, d\nu}\right] + \text{const}$$

$$m_s = -2.5 \log\left[\int_0^\infty S_\nu l_\nu\, d\nu\right]$$

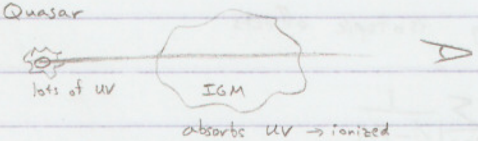
U: 3000 – 4000 Å

B: 3500 – 5500 Å

V: 4800 – 6500 Å

1965 Gunn-Peterson Effect

Quasar

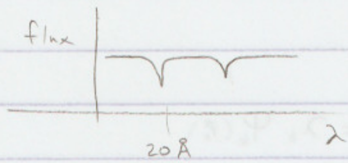


absorbs UV → ionized

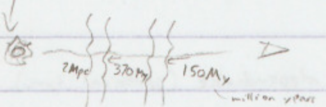
~2001 Becker $z = 6.28$, $z = 5.82$, $z = 5.99$ $z > 6$ → have neutral hydrogen there

Similarly for X-rays:

Mrk 421



absorption lines in keV range
→ inner e^- of Oxygen



2 filaments absorbing light → contains some of the missing baryonic matter
(CMB predicts more Ω_B than observed)

Real atoms Z protons Q electrons
$A = n + p$

$$\hat{H} = \underbrace{\frac{1}{2m_N}\hat{p}_N^2}_{\text{Nucleus}} + \underbrace{\frac{1}{2m_e}\sum_{i=1}^{Q}\hat{p}_i^2}_{\text{Electron motion}} + \underbrace{\sum_{i=1}^{Q}\frac{-Ze^2}{|\vec{r}_i - \vec{r}_N|}}_{e^- \leftrightarrow p \text{ interaction}} + \underbrace{\sum_{i<j}\frac{e^2}{|\vec{r}_i - \vec{r}_j|}}_{e^- \leftrightarrow e^- \text{ interaction}} \qquad \hat{P}_N = -i\hbar\vec{\nabla}_{\vec{r}_N} \qquad \hat{p}_i = -i\hbar\nabla_i$$

Missing: 1) Exchange

2) Relatistic e^- in high Z atoms $H = \sqrt{p^2c^2 + m^2c^4} = mc^2\sqrt{1 + \left(\frac{p}{mc}\right)^2} = mc^2 + \frac{p^2}{2m} + mc^2\left(\frac{p}{mc}\right)^4$

3) Isotopic shift is included (m_N) motion of nucleus because of e^- motion

4) Fine (e^- moving in E field of nucleus → B field) $\vec{l}\vec{s}$
Hyperfine splitting $\vec{s}\vec{s}$

5) QED Lamb shift charge polarizes vacuum (e^-e^+ pairs appearing)

Center of mass reference frame $\vec{R} = \frac{1}{M}\left[m_N\vec{r}_N + \sum_{i=1}^{Q} m_e\vec{r}_i\right]$

$M = m_N + Q m_e$ $\quad \mu = \frac{m_e m_N}{m_e + m_N}$ $\quad \vec{r}_{iN} = \vec{r}_i - \vec{r}_N$

$$\hat{H} = \underbrace{-\frac{\hbar^2}{2M}\nabla_R^2}_{\text{motion of atom as a whole}} - \frac{\hbar^2}{2\mu}\sum_{i=1}^{Q}\nabla_{r_{iN}}^2 - \underbrace{\frac{\hbar^2}{2m_N}\sum_{i\neq j}\left(\vec{\nabla}_{r_{iN}}\cdot\vec{\nabla}_{r_{jN}}\right)}_{\text{isotopic effect}} - Ze^2\sum_{i=1}^{\infty}\frac{1}{r_{iN}} + e^2\sum_{i<j}\frac{1}{|\vec{r}_{iN} - \vec{r}_{jN}|}$$

$\to 0$ $\qquad \Psi = \Psi_{cm}(\vec{R})\,\Psi(\vec{r}_{1N}, \vec{r}_{2N}, \ldots)$ $\qquad \Psi_{CM}(\vec{R}) = e^{i\frac{\vec{P}\cdot\vec{R}}{\hbar}}$

isotopic effects $\sim \frac{m}{A m_p} R_y \sim 10^{-4} R_y$
$\left(\frac{-\hbar^2}{2m_N} \sum_{i \neq j} \vec{\nabla}_{r_{iN}} \cdot \vec{\nabla}_{r_{jN}}\right)$

$r_{iN} \to r_i \quad \mu \to m$ (e^- mass) ignoring isotopic effects

$$\hat{H}^\circ = \frac{-\hbar^2}{2m} \sum_{i=1}^{Q} \nabla_{r_i}^2 - Ze^2 \sum_{i=1}^{Q} \frac{1}{|\vec{r}_i|} + e^2 \sum_{i<j} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$

Assume distribution of e^- is spherically symmetric
$\hookrightarrow$ Central field approximation

$$\Psi(\vec{r}_1, \vec{r}_2 \ldots) = \Psi(\vec{r}_1)\Psi(\vec{r}_2)\cdots$$

$$\frac{-\hbar^2}{2m} \nabla_k^2 \Psi_k(\vec{r}_k) + V(\vec{r}_k)\Psi_k(\vec{r}_k) = \lambda_k \Psi_k(\vec{r}_k)$$

$\Psi_k(\vec{r}_k) = U_{n\ell}(r_k) Y_{\ell m}(\theta_k, \varphi_k) \qquad \lambda_k = \lambda_k(n,\ell)$ no m dependance (spherical sym.)

$\Psi_k(\vec{r}_k) \longrightarrow$ called orbitals

Set of all orbitals with same $n\ell$ (different m) form electronic shell

But e^- are fermions: Slater determinant

$$\Psi = \frac{1}{\sqrt{Q!}} \begin{vmatrix} \Psi_1(r_1) & \Psi_2(r_1) & \Psi_3(r_1) & \cdots \\ \Psi_1(r_2) & \Psi_2(r_2) & \cdots & \Psi_n(r_2) \\ & & & \Psi_n(r_n) \end{vmatrix}$$

# of states for given electronic shell: $\underbrace{(2\ell+1)}_{m} \underset{\text{spin}}{2}$

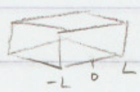
$\ell=0$	s	2
$\ell=1$	p	6
$\ell=2$	d	10
$\ell=3$	f	14

Thomas-Fermi Model

e^- distributed in system $\rho(\vec{r}) \qquad \nabla^2\Phi = -\frac{\rho}{\epsilon_0}$

electron gas $\to$ cool down $\longrightarrow$ farthest e^- in atom at fermi energy $\to$ just barely bound

atom is box



$k_x = n_x \frac{\pi}{L} \qquad n_x, n_y, n_z$ - integer $\qquad k_y = n_y \frac{\pi}{L} \qquad k_z = n_z \frac{\pi}{L}$

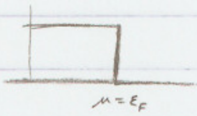
$$E = \frac{\hbar^2}{2m} k^2 = \frac{\hbar^2}{2m} \frac{\pi^2}{L^2} (\vec{n} \cdot \vec{n}) \qquad (n_x^2 + n_y^2 + n_z^2)^{1/2} < \frac{L}{\pi\hbar}(2mE)^{1/2}$$

$$\frac{4\pi}{3}(n_x^2 + n_y^2 + n_z^2)^{3/2} = \frac{4\pi}{3} \frac{L^3}{\pi^3 \hbar^3} (2mE)^{3/2} \quad \text{number of states}$$

density of states $\quad n(E) = \frac{1}{6\pi^2\hbar^3}(2mE)^{3/2} \longleftarrow \frac{\#}{(2L)^3} \leftarrow$ volume

Occupation # of Fermi-Dirac statistics

$$S(\varepsilon) = \left(e^{-\frac{\mu-\varepsilon}{kT}} + 1\right)^{-1}$$



spin degrees of freedom e^-: 2

$$N = \int \frac{dp_x\, dp_z\, dp_y\, dx\, dy\, dz}{(2\pi\hbar)^3} S(\varepsilon)\, g$$

$$N = Vg \int_0^{p_F} \frac{4\pi p^2\, dp}{(2\pi\hbar)^3} \qquad p_F^2 = 2m\varepsilon_F \qquad \underline{\frac{N}{V} = n(\varepsilon) = \frac{1}{6\pi^2\hbar^3}(2m\varepsilon_F)^{3/2} g}$$

to be bound $\varepsilon_F \le \phi$ ← main statement of Thomas-Fermi Model

$$n(\varepsilon) \to \frac{\rho}{e} = \frac{2}{6\pi^2\hbar^3}\left(2m(-e\phi(r))\right)^{3/2}$$

$$\nabla^2 \phi = -\frac{\rho}{\varepsilon_0} = -\frac{e}{3\pi^2\hbar^3\varepsilon_0}\left(-2me\phi\right)^{3/2}$$

$$\Phi = \frac{-4\pi\varepsilon_0 r}{Ze}\phi$$

$r \to 0$ $\Phi \to +1$ Coulomb field close to nucleus

$r \to \infty$ $\Phi \to 0$ if atom is neutral, e^- screen nucleus

$$\varepsilon = \frac{4r}{a_0}\left(\frac{2Z}{9\pi^2}\right)^{1/3} \qquad a_0 = \frac{\hbar^2}{me^2} \implies \frac{d^2\Phi}{d\varepsilon^2} = \varepsilon^{-1/2}\,\Phi^{3/2}$$

$$\Phi(\varepsilon) = \frac{1}{1 + 0.02747\varepsilon^{1/2} + \ldots}$$

scale $\phi(r)\left|\frac{d\phi}{dr}\right|^{-1} \gg n^{-1/3}$

$$\Rightarrow \left(\frac{\Phi}{\varepsilon}\right)^{3/2} \gg \left(\frac{4\pi}{Z}\right)^{1/3} \frac{d}{d\varepsilon}\left(\frac{\Phi}{\varepsilon}\right)$$ — applicability condition

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

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr}U_{nl}\right) - \left\{\frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2}\left(V(r) - \lambda_{nl}\right)\right\}U_{nl} = 0$$

$\lambda_{1s} < \lambda_{2s} < \lambda_{2p} < \lambda_{3s} < \lambda_{3p} < \lambda_{3d} < \lambda_{4s}$ independent from Z

except for $Z < 27$: $\lambda_{4s} < \lambda_{3d}$

H $1s$ He $1s^2$ Li $1s^2\,2s$ Be $1s^2\,2s^2$ B $1s^2\,2s^2\,2p$

spectroscopic notation

$$2\,{}^2P_{3/2}$$

principal QM # (n) — 2

multiplicity (2s+1) — superscript 2

orbital moment (l) — P

total angular momentum $(\vec{l} + \vec{s})$ — 3/2

l:	0	1	2	3	4
	S	P	D	F	G

Real atoms 5/22/2007

Approximation: Spherically Symmetric + Thomas-Fermi

Potential: self-consistent field approx

$$V(r) = -\frac{Ze^2}{r_k} + e^2 \sum_{i\neq k} \int \frac{|\Psi(\vec{r}_i)|^2}{|\vec{r}_i - \vec{r}_k|} d^3\vec{r}_i$$

~ density

$$\frac{-\hbar^2}{2m}\nabla_k^2 \Psi_k(\vec{r}_k) - \frac{Ze^2}{r_k}\Psi_k(r_k) + e^2 \sum_{i\neq j}\left\{\int \frac{|\Psi(r_i)|^2}{|\vec{r}_i - \vec{r}_k|} d^3\vec{r}_i\right\}\Psi_k = \lambda_k \Psi_k$$

need to solve iteratively

Hartree equations

Problems:

1) $\Psi = \Psi_1(r_1)\Psi_2(r_2) \ldots$ but should be represented by Slater Determinant: $\Psi = \frac{1}{\sqrt{Q!}}\left| \quad \right|$

2) Not spherically symmetric

make symmetric by averaging $\frac{1}{4\pi}\int \sum |\Psi_i|^2 d\Omega = \sum N_{n\ell} |U_{n\ell}(r)|^2$

$N_{n\ell}$: # e^- in shell

$$V(r) = -e^2 \sum_{n\ell} N_{n\ell}\left\{\frac{1}{r}\int_0^r r'^2 |U_{n\ell}(r')|^2 dr' + \int_r^\infty r' |U_{n\ell}(r')|^2 dr'\right\}$$

$$V_{exchange} = -e^2\left[\frac{3}{4\pi^2}\sum N_{n\ell} |u_{n\ell}(r)|^2\right]^{1/3}$$

Consider 2 e^- system

$$\Psi_a(1) = U_a(r_1)\chi_a(1) \qquad \chi_a(1) = \alpha \chi_+(1) + \beta \chi_-(2)$$

(a: state; 1: particle; χ_+: $+\frac{1}{2}$; χ_-: $-\frac{1}{2}$)

$$\Psi = \Psi_a(1)\Psi_b(2) - \Psi_a(2)\Psi_b(1)$$

$$\Phi_1 = \begin{vmatrix} u_a(r_1)\chi_+(1) & u_a(r_2)\chi_+(2) \\ u_b(r_1)\chi_+(1) & u_b(r_2)\chi_+(2) \end{vmatrix} \qquad \Phi_2 = \begin{vmatrix} u_a(r_1)\chi_+(1) & u_a(r_2)\chi_+(2) \\ u_b(r_1)\chi_-(1) & u_b(r_2)\chi_-(2) \end{vmatrix}$$

$$\Phi_3 = \begin{vmatrix} u_a(r_1)\chi_-(1) & \sim \\ u_b(r_1)\chi_+(1) & \sim \end{vmatrix} \qquad \Phi_4 = \begin{vmatrix} u_a(r_1)\chi_-(1) & u_a(r_2)\chi_-(2) \\ u_b(r_1)\chi_-(1) & u_b(r_2)\chi_-(2) \end{vmatrix}$$

$$\underset{m=1}{l=1} \rightarrow \phi_1 = \overbrace{\begin{vmatrix} u_a(r_1) & u_a(r_2) \\ u_b(r_1) & u_b(r_2) \end{vmatrix}}^{\mathcal{A}} \underbrace{\chi_+(1)\,\chi_+(2)}^{\text{symmetric}} \qquad \phi_4 = |\mathcal{A}|\,\chi_-(1)\,\chi_-(2) \quad \underset{m=-1}{l=1}$$

$$\frac{1}{\sqrt{2}}(\phi_2+\phi_3) = |\mathcal{A}|\,\frac{1}{\sqrt{2}}\left(\chi_+(1)\chi_-(2) + \chi_-(1)\chi_+(2)\right) \quad \underset{m=0}{l=1}$$

$$\frac{1}{\sqrt{2}}(\phi_2-\phi_3) = \left(u_a(r_1)u_b(r_2) + u_b(r_1)u_a(r_2)\right)\frac{1}{\sqrt{2}}\left(\chi_+(1)\,\chi_-(2) - \chi_-(1)\,\chi_+(2)\right) \quad \underset{m=0}{l=0}$$

$l=1$ triplet: radial part of wave function is antisymmetrical
spins symmetric

$l=0$ singlet: radial symmetric, spin antisymmetric

$\frac{e^2}{|r_1-r_2|}|\sim|^2 \rightarrow$ small if radial part is antisym
large if radial part is symmetric (antisym. spin)

n=2 --- s=0
n=1

He: larger n so overcomes repulsion and both e^- are in S-state
not necessarily so for higher Z atoms (lots of e^-)

n=2 $l=1$

B ↑ ex: $m=-1$

C ↑↑ → different m say $m=-1,0$ so that spins can be sym so that repulsion is small

N ↑↑↑ $m=-1,0,1$

O ↑↓ ↑↑ F, Ne ↑↓ ↑↓ ↑↓ Hund's rule

$\varphi_i = u_i(r_j)\chi_i(j)$ ϕ is antisym combination of $\varphi \rightarrow \phi = |\;|$ Slater Det

$\langle u_i|u_j\rangle = \delta_{ij}$

$$\langle\phi|\hat{H}|\phi\rangle = \langle\phi|\underbrace{\sum_{i=1}^{Q}\left\{-\frac{\hbar^2}{2m}\nabla_i^2 - \frac{Ze^2}{r_i}\right\}}_{\text{no } j \text{ coord}} + \sum_{i<j}\frac{e^2}{r_{ij}}|\phi\rangle$$

$$\sum_i \langle\varphi_i|F(i)|\varphi_i\rangle$$

$$\sum_{i<j}\Big\{\langle\varphi_i\varphi_j|G(i,j)|\varphi_i\varphi_j\rangle - \langle\varphi_i\varphi_j|G(i,j)|\varphi_j\varphi_i\rangle\Big\}$$

Apply variational principle for u (radial function) ⟹ equivalent Schrödinger Eq.

⟹ Hartree-Foch Eqns

All other effects can be found perturbatively

perturbatios — mix levels
— change levels

Spin-Orbit Interaction

$H = H_0 + \delta H$

Pressure broadening
→ levels change by presence of other atoms (external fields)

Order of Magnitude

$\vec{B} = -\frac{\vec{v}}{c} \times \vec{E}$ $\quad \vec{E} = -\frac{dU}{dr} \cdot \frac{\vec{r}}{r} \cdot \frac{1}{e}$ (U: potential)

$\vec{B} = \frac{1}{c}(\vec{v} \times \vec{r}) \frac{1}{r} \frac{dU}{dr} \frac{1}{e} \frac{m}{m} = \frac{\vec{l}}{mcre} \frac{dU}{dr}$ $\quad \vec{\mu} = -\frac{e}{mc}\vec{s}$ magnetic momentum

Classically: $\vec{\mu} = -\frac{1}{2}\frac{e}{mc}\vec{s}$ $\quad \frac{1}{2} \to$ will appear if you use Dirac equation so 2 errors cancel out

Classically:

$U_{int} = -\vec{\mu} \cdot \vec{B} = \frac{1}{2} \frac{1}{m^2c^2}(\vec{s} \cdot \vec{l}) \frac{1}{r} \frac{dU}{dr}$ correct result ↑

$\delta H_{(ls)} = \frac{1}{2} \frac{1}{m^2c^2}(\vec{s} \cdot \vec{l}) \frac{1}{r} \frac{dU}{dr}$

Fine splitting

$\delta H_{ss} = \frac{\mu_1 \mu_2}{r^3} = \frac{e}{mc} \frac{e}{Mc} \frac{\vec{s}_1 \cdot \vec{s}_2}{r^3}$

$\delta H_{ss} = \frac{m}{M}\left(\frac{e}{mc}\right)^2 \frac{(\vec{s}_1 \cdot \vec{s}_2)}{r^3}$ Hyperfine splitting

~20 times smaller than fine

Atom in EM field

$H = \frac{1}{2m}\left(\vec{p} - e\vec{A}\right)^2 + e\varphi$ Classically $\quad$ potential $(\vec{A}, \varphi)$ $\quad$ gauge transformation

$\varphi' = \varphi - \frac{\partial \chi}{\partial t}$ $\quad A' = A + \nabla\chi$ arbitrary transformation

QM: $\hat{H} = \frac{1}{2m}\left(\hat{\vec{p}} - e\vec{A}\right)^2 + e\varphi$

$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\vec{\nabla} - e\vec{A}\right)^2 \psi + e\varphi\psi$

Gauge Transformation: $\quad i\hbar \frac{\partial}{\partial t}\left(\psi e^{i\frac{e\chi}{\hbar}}\right)$ $\quad \psi \to \psi e^{i\frac{e\chi}{\hbar}}$ Schrödinger eqn. will stay the same

$H = \frac{1}{2m}\hat{p}^2 - \frac{e}{2m}\left(\hat{\vec{p}} \cdot \vec{A} + \vec{A} \cdot \hat{\vec{p}}\right) + \frac{e^2}{2m}(\vec{A} \cdot \vec{A}) + e\varphi$

$= \underbrace{\frac{1}{2m}\hat{p}^2 - \frac{e}{m}\vec{A}\hat{p} - \frac{e}{2m}\sum_{n}\{\hat{A}_n, \hat{p}_n\}}_{1\gamma \text{ process (photon)}} + \underbrace{\frac{e^2}{2m}(\vec{A} \cdot \vec{A})}_{\text{double photon process or } 2\gamma \text{ process (second order)}} + e\varphi$

(sum over components)

$1\gamma \quad \nu \sim 10^8 \, s^{-1} \qquad 2\gamma \quad \nu \sim 10 \, s^{-1}$

Consider pure, constant $\vec{B}$

$$\vec{A} = -\frac{\vec{r}\times\vec{B}}{2} \qquad A_i = -\frac{1}{2} e_{ik\ell}\, \hat{r}_k B_\ell$$

$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{e}{2m}\left((\vec{r}\times\vec{B})\cdot\hat{\vec{p}}\right) + \frac{e}{4m}\sum_n \left\{ \hat{P}_n, (\vec{r}\times\vec{B})_n \right\} + \frac{e^2}{8m}\left(\vec{r}\times\vec{B}\right)^2$$

$e_{ik\ell}\, r_k B_\ell P_i$

$-e_{\ell k i} B_\ell r_k P_i \rightarrow -(\vec{B}\cdot\vec{L})$

$L_\ell - e_{\ell k i} r_k P_i$

$\{P_n, e_{nk\ell}\, r_k B_\ell\}$

$e_{nk\ell} B_\ell \underbrace{\{P_n, r_k\}}_{\hbar \delta_{kn}} \qquad e_{nk\ell} B_\ell \delta_{kn} = 0$

$$\therefore \hat{H} = \frac{1}{2m}\hat{P}^2 - \frac{e}{2m}(\vec{B}\cdot\vec{L}) + \frac{e^2}{8m}(\vec{r}\times\vec{B})^2 - \underbrace{\frac{e}{m}(\vec{B}\cdot\vec{s})}_{\text{Dirac}}$$

$$\hat{H} = \frac{1}{2m}\hat{P}^2 - \frac{e}{2m}\left(\vec{B}\cdot\underbrace{(\vec{L}+2\vec{s})}_{\vec{J}+\vec{s}}\right) + \frac{e^2}{8m}(\vec{r}\times\vec{B})^2$$

$$\vec{J} = \vec{L} + \vec{s}$$

OoM estimate:

$$\frac{\langle\psi|\frac{e^2}{8\pi}(\vec{r}\times\vec{B})^2|\psi\rangle}{\langle\psi|\frac{e}{2m}(B\cdot L)|\psi\rangle} \simeq \frac{eB}{\hbar} r^2 \simeq 10^{-5}\frac{B}{1T}$$

$\sim Å$ (for r)

tesla

need huge B fields (neutron stars)

or need $(\vec{B}\cdot\vec{L})$ term to be forbidden transition

---

$$\hat{H} = \hat{H}_0 + \delta H$$

Choose basis: $\hat{H}_0|E\rangle = E|E\rangle \Rightarrow E_i, |E_i\rangle \qquad E_1 < E_2 < \ldots$

$\langle E_i|E_k\rangle = \delta_{ik}$ or $\delta(E_i - E_k)$

unperturbed

$$E_i = E_i^{(0)} + E_i^{(1)} + E_i^{(2)} + \ldots$$

$\frac{\delta H}{E_i - E_k} \qquad \delta H^2$

E_1, E_2

$$|E_i\rangle \rightarrow |E_i\rangle + \sum_k \underbrace{C_{ik}^{(1)}}_{\delta H}|E_k\rangle + \sum_k \underbrace{C_{ik}^{(2)}}_{\delta H^2}|E_k\rangle$$

$$\left(E_i + E_i^{(1)}\right)\left(|E_i\rangle + \sum_k C_{ik}^{(1)}|E_k\rangle\right) = \left(\hat{H}_0 + \delta\hat{H}\right)\left(|E_i\rangle + \sum_k C_{ik}^{(1)}|E_k\rangle\right)$$

$$\cancel{E_i|E_i\rangle} + E_i^{(1)}|E_i\rangle + E_i\sum_k C_{ik}^{(1)}|E_k\rangle + \underbrace{E_i^{(1)}\sum C_{ik}^{(1)}}_{2^{nd}\text{ order}} = \cancel{\hat{H}_0|E_i\rangle} + \delta\hat{H}|E_i\rangle + \sum_k C_{ik}^{(1)}\hat{H}_0|E_k\rangle$$

$$\sum_k C_{ik}^{(1)} E_k|E_k\rangle$$

$$E_i^{(1)}|E_i\rangle = \delta\hat{H}|E_i\rangle + \sum_{k\neq i} C_{ik}^{(1)}(E_k - E_i)|E_k\rangle$$

$$\langle E_i|\times \longrightarrow E_i^{(1)} = \langle E_i|\delta\hat{H}|E_i\rangle = \delta H_{ii}$$

$$\langle E_m|\times \longrightarrow 0 = \langle E_m|\delta\hat{H}|E_i\rangle + \underbrace{\sum_k C_{ik}^{(1)}(E_k - E_i)\overbrace{\langle E_m|E_k\rangle}^{\delta_{mk}}}_{C_{im}(E_m - E_i)}$$

$$\underset{m\neq i}{C_{im}} = -\frac{\delta\hat{H}_{mi}}{E_m - E_i} \qquad C_{ii} = 0$$

$$\frac{\delta H}{\Delta E} \sim 10^{-5}$$

Balmer transitions $E_i - E_n \sim 600\,nm$

$H\beta = 656\,nm$

fine structure 10^{-5} Z eV $\frac{100\,nm}{10^{-5}} \sim 10^{7}\,nm \sim 1\,cm$

hyperfine $20\,(1cm) \sim 20\,cm$

5/24/2007

Kathy talk: CO rotational emission

$n(H_2) > 10^3\ cm^{-3}$ $10^3 < n < 10^5$

CO is slow line so not present in high density

$\Delta J = 1$ conservation of momentum (with 1 photon)

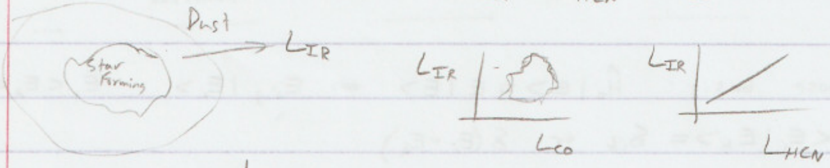
For high density : HCN ($J = 1 \to 0$) faster transition

CO – tracer of H_2 in galaxy

HCN – tracer of extreme densities of H_2

Cao + Solomon (ApJ 606, 271 (2004))

→ tried to correlate L_{IR} L_{HCN} L_{CO}



$$\frac{L_{IR}}{L_{HCN}} \sim \frac{L_{IR}}{M_{dense}} \sim \text{constant}$$

tracer to characterize SFR : $\frac{L_{HCN}}{L_{CO}} \propto \frac{SFR}{M_{\odot}}$

$\langle E_m | \delta\hat{H} | E_i \rangle = \delta H_{mi}$ $\frac{\delta H}{\Delta E} \sim 10^{-5}$

$$|E_i\rangle \to |E_i\rangle + \sum_k C_{ik}^{(1)} |E_k\rangle + \sum_k C_{ik}^{(2)} |E_k\rangle$$

$$E_i^{(2)} = \sum_{m \neq i} \frac{\delta H_{in}\, \delta H_{mi}}{E_m - E_i}$$

$$C_{ik}^{(2)} = \sum_{\substack{m \neq i \\ m \neq k}} \frac{\delta H_{km}\, \delta H_{mi}}{(E_i - E_k)(E_m - E_i)} - \frac{\delta H_{ki}\, \delta H_{ii}}{(E_i - E_k)(E_k - E_i)}$$

$$C_{ii}^{(2)} = \frac{1}{2} \sum_{m \neq i} \frac{\delta H_{im}\, \delta H_{mi}}{(E_m - E_i)(E_i - E_m)}$$

→ 2nd order effects

like $\Delta J = 2$ → forbidden transitions ?

low probability

$\hat{H}_0 | E_n^\alpha \rangle = E_n | E_n^\alpha \rangle \qquad \alpha = 1, 2, 3, \dots, g_n$ degeneracy

$\langle E_n^{\alpha'} | E_n^\alpha \rangle = \delta_{\alpha'\alpha}$

$|\psi_n\rangle = \sum_\alpha c_\alpha | E_n^\alpha \rangle \qquad (\hat{H}_0 + \delta\hat{H}) |\psi_n\rangle = (E_n + \delta E_n) |\psi_n\rangle$

$\sum_{\alpha=1}^{g_n} \langle E_n^\beta | \delta\hat{H} | E_n^\alpha \rangle c_\alpha = \delta E_n c_\beta \qquad [\delta H_n^{\alpha\beta}] \vec{C} = \delta E_n \vec{C}$ remove degeneracy

with $\vec{B}$ $\qquad \delta\hat{H} = -\frac{e}{m}(\vec{B}\cdot\vec{S}) \qquad \vec{S} = \frac{1}{2}\hbar\hat{\vec{\sigma}} \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\vec{B} = B(1,0,0) = B\hat{x}$

$$\delta H^{\alpha\beta} = -\underbrace{\frac{e}{m}\frac{\hbar}{2}}_{\mu_B} B \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

eigenvalues: $\begin{pmatrix} 0 & -\mu B \\ -\mu B & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \lambda \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$

$$\begin{vmatrix} -\lambda & -\mu B \\ -\mu B & -\lambda \end{vmatrix} = 0 \implies \lambda = \pm\mu B$$

$\begin{pmatrix} \mp\mu B & -\mu B \\ -\mu B & \mp\mu B \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$

$\lambda = +\mu B$: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ $\quad \langle S_z \rangle = 0 \rightarrow \langle \sim | \frac{1}{2}\hbar\hat{\sigma}_z | \sim \rangle$

$\langle S_x \rangle = 1 \qquad (1\ -1)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = (1\ -1)\begin{pmatrix} -1 \\ 1 \end{pmatrix} = -1-1 = -2$

$\lambda = -\mu B$: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ $\quad \langle S_x \rangle = 0$

$$\delta H = \sum_{i=1}^{a} \left(-\frac{e\hbar}{2m}(\vec{B}\cdot\vec{L}_i) - \frac{e\hbar}{m}(\vec{B}\cdot\vec{S}_i) \right) = -\frac{e\hbar}{2m}(\vec{B}\cdot\vec{L}) - \frac{e\hbar}{m}(\vec{B}\cdot\vec{S}) = -\mu_B [\vec{B}\cdot(\vec{J}+\vec{S})]$$

$\langle J, M | \delta\hat{H} | J, M \rangle \qquad \vec{B} = B\hat{z}$

$= -\mu B \ \langle J, M | (\hat{J}_z + \hat{S}_z) | J, M \rangle$

consider any vector $\quad \langle JM | V_z | JM \rangle = \beta \langle JM | J_z | JM \rangle \qquad \langle JM | \vec{V} - \beta\vec{J} | JM \rangle = 0$

$\quad V_y = \beta \quad J_y$

$\quad V_x = \beta \quad J_x$

with proper choice of β

5/29/2007

$\frac{p^2}{2m} \sim \frac{e^2}{r} \qquad p \sim \frac{\hbar}{r} \qquad \frac{\hbar^2}{mr^2} \sim \frac{e^2}{r} \quad \therefore \quad \underline{r \sim \frac{\hbar^2}{me^2}}$ Bohr radius

KE vs. PE $\qquad$ Heisenberg

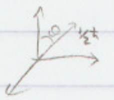
$\frac{e^2}{r} \sim mc^2$ gives you classical e^- radius

Fermi energy $\quad$ depends on n (density) $\qquad T \to 0 \quad p \to 0 \quad r \to \infty$

typical distance $n^{-1/3}$

$p \sim \frac{\hbar}{n^{-1/3}} \sim n^{1/3}\hbar \qquad \underline{\varepsilon_F = \frac{p^2}{2m} \sim \frac{n^{2/3}\hbar^2}{m}}$

Spinor

 $\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ $\quad |\alpha|^2+|\beta|^2=1$

$\sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix} \quad \hat{S}_z = \frac{\hbar}{2}\hat{\sigma}_z \quad \langle S_z\rangle = \langle\psi|\hat{S}_z|\psi\rangle$

$\langle S_z\rangle = \frac{1}{2}\hbar\cos\theta = \langle\psi|\hat{S}_z|\psi\rangle = \frac{\hbar}{2}\left(|\alpha|^2-|\beta|^2\right)$ $\quad |\alpha|^2-|\beta|^2=\cos\theta$

$\cos(\frac{\theta}{2}) \quad \sin(\frac{\theta}{2})$

$\cos^2 x-\sin^2 x=\cos 2x$

can add $e^{i\varphi_1}$, $e^{i\varphi_2}$ arbitrary phase factor

$\alpha=\cos(\frac{\theta}{2})e^{i\varphi/2} \quad \beta=\sin(\frac{\theta}{2})e^{-i\varphi/2}$

or: $\cos(\frac{\theta}{2})e^{i\varphi}$, $\sin(\frac{\theta}{2})$

$\vec{B}=B\hat{z} \qquad \delta H=-\mu B\,(J_z+S_z) \qquad \mu=\frac{e\hbar}{2m}$

ferro/para magnetism spin aligned to $\vec{B}$ → amplify field

diamagnetism → reduce field

perturbations $\quad \langle J,M|\,\delta H\,|J,M\rangle = -\mu B\,\langle J,M|\,J_z+S_z\,|J,M\rangle$

$\langle J,M|\,\vec{V}\,|J,M\rangle = \beta\,\langle\,|\vec{J}|\,\rangle$ $\quad$ doesnt matter what $\hat{z}$ axis is values will be related by rotation matrix

$\langle J,M|\,\vec{S}-(g-1)\vec{J}\,|J,M\rangle = 0$

$\langle J,M|\,\delta H\,|J,M\rangle = -\mu B\,\langle J,M\,|J_z+(g-1)J_z\,|J,M\rangle = -\mu B\,g(L,S,J)\underbrace{\langle J_z\rangle}_{M}$

$\langle\delta H\rangle = -\mu B\,\underbrace{g(L,S,J)}_{\text{Lande factor}}M$

$\langle|\vec{J}\cdot\underbrace{(\vec{J}+\vec{S})}_{g\vec{J}}|\rangle = g\langle|\vec{J}|^2\rangle = g\,J(J+1)$

$\hat{J}^2+\hat{J}\cdot\hat{S} = \hat{J}^2+(\hat{L}+\hat{S})\cdot\hat{S} = \hat{J}^2+\hat{L}\cdot\hat{S}+\hat{S}^2$

$J^2=(\hat{L}+\hat{S})^2 = L^2+S^2+2(\hat{L}\cdot\hat{S}) \qquad \frac{J(J+1)-L(L+1)-S(S+1)}{2} = \langle\hat{L}\cdot\hat{S}\rangle$

$g\,J(J+1) = J(J+1)+S(S+1)+\langle\hat{L}\cdot\hat{S}\rangle$

$\therefore \quad g(J,L,S) = \frac{3J(J+1)+S(S+1)-L(L+1)}{2\,J(J+1)}$

\# of levels: $2J+1$

distance between levels: $\propto Bg$

if you change $S \to S+1$, $L \to L+1$ } g unchanged — can remove this degeneracy with ↘

First effect in real atoms is exchange: spin $<$ antisym / sym, so orbital $<$ sym / antisym

leads to Hunds rules

Spin-Orbit:

$$\delta H_i = \frac{1}{2m^2c^2}\frac{\hbar^2}{r_i}\frac{dV(r_i)}{dr_i}\left(\hat{L}_i \cdot \hat{S}_i\right) = \xi(r_i)\left(\hat{L}_i \cdot \hat{S}_i\right)$$

$$\delta H_{LS} = \sum_{i=1}^{Q} \xi(r_i)\left(\vec{L}_i \cdot \vec{S}_i\right)$$

wont commute with L_i, S_i, L, S

but will with J^2, J_z

$$\downarrow$$

$$\sum_i \chi_i(L,S)(\vec{L}\cdot\vec{S})$$

$$\langle JSL | \delta H_{LS} | JSL\rangle = \underbrace{\Gamma(L,S,n)}_{\text{radial dependence}} \underbrace{\langle \sim | (\hat{L}\cdot\hat{S}) | \sim \rangle}_{\frac{1}{2}\left(J(J+1) - L(L+1) - S(S+1)\right)}$$

$(J+2)(J+1) - (J+1)J = 2(J+1)$

spacing between levels ?

fine structure — residual electrostatic attraction — exchange (electro static)

$$\hat{H} = \underbrace{\hat{H}_0}_{\text{spherically sym}} + \underbrace{\hat{H}_{ex}}_{\text{exchange effect + residual electrostatic energy}} + \delta\hat{H}_{LS}$$

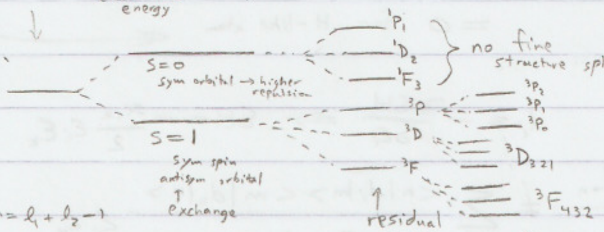
Thomas Fermi $\to V(r)$

$L=1$ 3 component transforms like vector

x, y, z : Y_{10}, Y_{11}, Y_{1-1}

$J = L + 0$

$n=3$ (2 e^-) $l_1 = 1$, $l_2 = 2$



$\uparrow l_2$ $\uparrow l_1$ $m = l_1 + l_2$

Lowering operator $m = l_1 + l_2 - 1$

$l_2 \downarrow \uparrow l_1$ $m = |l_2 - l_1|$

$\therefore L = 3, 2, 1$

F D P

F - states farther ~ sort of reasoning

C $1s^2 2s^2 2p^2$ — O $1s^2 2s^2 2p^4$

$2e^-$ on p — 2 missing e^- on p (2 holes)

ground state $S=1$ — $S=1$

$L = 2, 1, 0$

antisym orbital, need odd parity $\therefore L=1$

$^3P_{\underline{2}10}$ — ground state

$^3P_{21\underline{0}}$ — because of holes

$$\overbrace{\left(c_1 Y_{10} + c_2 Y_{1-1} + c_3 Y_{11}\right)}^{r_1}\overbrace{\left(c_1 Y_{10}' + c_2 Y_{1-1}' + c_3 Y_{11}'\right)}^{r_2}$$

9 terms → part will be $(\vec{r}_1 \cdot \vec{r}_2)$ 1 term

scalar product → no angle dependence

$\Rightarrow$ L=0 state

part will be vector 3 terms $(\vec{r}_1 \times \vec{r}_2)$

$\Rightarrow$ L=1 state

part will be tensor $\Rightarrow$ L=2 state

parity eigenvalue $(-1)^l$

6/1/2005

Perturbations due to external $\vec{E}$ field

$$H = H_0 + \underset{\substack{\text{exchange}\\ \text{+residual}\\ \text{E-field}}}{H_1} + \underset{\text{spin-orbit}}{\delta H_{SO}} + \underset{\substack{\text{B-field}\\ \sim B}}{\delta H_B} + \underset{\substack{\text{spin-spin}\\ \sim \frac{m_e}{m_p}\frac{1}{\alpha}}}{\delta H_{ss}} + \delta H_{\text{isotopic}} + \underset{\substack{\text{size of}\\ \text{nucleus}}}{\delta H_{\text{finite}}} + \delta H_{rel} + \delta H_{\substack{\text{rot.}\\ \text{vib.}}} + \underset{\text{van der Waals forces}}{\delta H_{\substack{\text{external}\\ \text{fields}}}}$$

spin-spin interaction $\rightarrow$ hyperfine splitting

$$\mu_N = g_p \frac{e}{2M} \underset{\text{spin of nucleus}}{I} \qquad \frac{M}{m_e} \sim 1840 \qquad g_p = 5.585 \qquad g_e = 2.00236$$

will have $\vec{I}\cdot\vec{L}$, $\vec{I}\cdot\vec{S}$ terms : $\hat{\vec{I}}\cdot\hat{\vec{J}}$

$$\hat{\vec{F}} = \hat{\vec{I}} + \hat{\vec{J}} \qquad F(F+1) - I(I+1) - J(J+1) \propto \delta H_{ss}$$

$$F^2 = I^2 + J^2 + 2(\vec{I}\cdot\vec{J}) \ldots$$

H $\quad {}^2S_{1/2}$ $\quad$ $F=1$ $\uparrow\uparrow$ $\quad$ 1420 MHz $\quad$ 21 cm

$J = 1/2$

(proton) $I = 1/2$ $\quad$ $F = 0$ $\uparrow\downarrow$ $\quad$ $\Delta E = 5.9 \times 10^{-6}$ eV $\quad$ lifetime 10^7 yrs

between $z = 6, 20$ should have lots of 21 cm radiation

redshifted to meter range $\rightarrow$ for pointing accuracy need large L $\quad \theta \sim \frac{\lambda}{L}$

$\rightarrow$ Square Kilometer Array

Electric field $\quad \vec{\mathcal{E}}$

$$\delta H = -\mathcal{E}\cdot q r\cos\theta = -\vec{\mathcal{E}}\cdot\vec{d}$$ dipole moment

$$\langle n l m | \delta H | n l m \rangle \qquad \int Y_{lm}^* \cos\theta \, Y_{lm}\, d\Omega$$

Parity, $\theta \rightarrow \pi - \theta$, $\phi \rightarrow \phi + \pi$ $\quad$ Y^*Y unchanged but $\cos\theta \rightarrow -\cos\theta$

$= 0$ for H-like atom

dipole moment

$$d_i = \alpha_{ik}\mathcal{E}_k$$

polarization tensor

$$d_i = -\frac{\partial \delta H}{\partial \mathcal{E}_i} \Rightarrow \delta H = -\frac{\alpha_{ik}}{2}\mathcal{E}_i\mathcal{E}_k$$

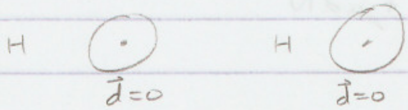
$$\Delta E^{(1)} = 0$$

$$\Delta E_n^{(2)} = \sum_{\substack{m\\ m\neq n}} \frac{\delta H_{nm}\,\delta H_{mn}}{E_n - E_m} = \sum_{\substack{m\\ m\neq n}} \frac{\langle n|d_i|m\rangle\langle m|d_k|n\rangle}{E_n - E_m}\mathcal{E}_i\mathcal{E}_k$$

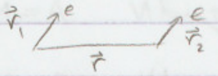
$$\alpha_{ik} = -2\sum_{\substack{m\\ m\neq n}} \frac{(d_i)_{nm}(d_k)_{mn}}{E_n - E_m}$$

$$\hat{\alpha}_{ik} = \alpha_n\delta_{ik} + \beta_n\left(\hat{J}_i\hat{J}_k + \hat{J}_k\hat{J}_i - \frac{2}{3}\delta_{ik}\hat{J}^2\right)$$

van der Waals force



$\rightarrow$ fluctuate $\vec{d}$ then can induce $\vec{E}$ fields and interact (polarize)



$$\delta H = \frac{e^2}{|\vec{r}|} + \frac{e^2}{|\vec{r}+\vec{r}_2-\vec{r}_1|} - \frac{e^2}{|\vec{r}+\vec{r}_2|} - \frac{e^2}{|\vec{r}-\vec{r}_1|}$$

$$\delta H = \frac{e^2}{r^3}\left\{ \vec{r}_1\cdot\vec{r}_2 - 3(\vec{r}_1\cdot\vec{r}_2)(\vec{r}_1\cdot\vec{r}_2) \right\} \qquad \propto \frac{1}{r^6} \text{ van der Waals forces}$$

$er_1 = d_1 \quad er_2 = d_2$

Important in
1) Cool stars $\quad \Delta E$ - broadening
2) Opacity $\quad H^- \quad E_{bind} = 0.75\text{ eV} \quad H + e \rightarrow H^-$ (polarizes H)
3) $\downarrow$

electron$_1$ elec$_2$
$|100\rangle \quad |100\rangle$

$\frac{\alpha}{r^3} \propto \langle 100_2\ 100_1 | \delta H | 100_1\ 100_2 \rangle = 0$ to first order?

$\langle 100_2 \underbrace{21m}_{\text{excited state}} | \delta H | 100_1\ 21m_1 \rangle \rightarrow$ mixing of states - some repulsive, some attractive

$\frac{1}{\sqrt{2}}\left(|100;21m\rangle + |21m;100\rangle\right) \qquad \frac{1}{\sqrt{2}}\left(|100;21m\rangle - |21m;100\rangle\right)$

$+\frac{\alpha_m}{r^3} \qquad\qquad -\frac{\alpha_m}{r^3}$

cool T : low crossection of forming H_2
higher T : more H_2 formed since can excite the H $\rightarrow$ form stars / fuel BH @ early times

---

Statistical

bring 2 volumes together $\quad$ Thermal Equilibrium
$T =$ constant $\quad P =$ constant $\quad$ Chemical potential $\mu =$ constant (energy penalty to add particle)

$V = \sum_i V_i \quad S = \sum_i S_i \quad N = \sum_i N_i \quad$ (additive)

1st law of Thermo

$$dE = \underbrace{TdS}_{\text{heat}} - \underbrace{PdV}_{\text{work done by system}} + \underbrace{\mu dN}_{\text{energy brought by adding particles}} \qquad E(S,V,N)$$

$\left(\frac{\partial E}{\partial S}\right)_{V,N} = T$ etc.

$E = \sum_i E_i = N f\left(\frac{S}{N}, \frac{V}{N}\right)$ $\quad$ 2 non-additive parameters

$P = P\left(T, \frac{V}{N}\right) \quad \mu = \mu\left(T, \frac{V}{N}\right)$ $\quad$ non-additive

$\underbrace{\frac{S}{N} = s\left(T, \frac{V}{N}\right)}_{\text{non-additive}}$

Enthalpy $H = E + PV$ $dH = TdS + VdP + \mu dN$

additive

$H = N f\left(P, \frac{S}{N}\right)$

Helmholtz Free Energy $A = E - TS$ $dA = -SdT - PdV + \mu dN$ $A = N f\left(T, \frac{V}{N}\right)$

Gibbs Free Energy $G = H - TS$ $dG = -SdT + VdP + \mu dN$ $G = N f(T, P)$

$\left(\frac{\partial G}{\partial N}\right)_{T,P} = \mu$ $\therefore$ $f(T,P)$ in G is μ $\Rightarrow$ $\boxed{G = N\mu(T,P)}$

Thermodynamical potential $\Omega = A - \mu N = A - G = E - H = -PV$

$d\Omega = -SdT - PdV - Nd\mu$ $\Omega = \Omega(T, \mu, V) = V f(T, \mu)$

$\boxed{\Omega = -V\, P(T,\mu)}$

$-\left(\frac{\partial \Omega}{\partial V}\right)_{T,\mu} = P = -\frac{\Omega}{V}$ $S = -\left(\frac{\partial \Omega}{\partial T}\right)_{V,\mu} = V\left(\frac{\partial P}{\partial T}\right)_{\mu}$ $s = \frac{S}{V} = \left(\frac{\partial P}{\partial T}\right)_{\mu}$

$N = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} = V\left(\frac{\partial P}{\partial \mu}\right)_{T}$ $n = \frac{N}{V} = \left(\frac{\partial P}{\partial \mu}\right)_{T}$

$\mu(n,T) \longrightarrow P(\mu,T) \longrightarrow P(n,T)$ eqn. of state

$C_V = \left(\frac{\partial E}{\partial T}\right)_{V,N} = T\left(\frac{\partial S}{\partial T}\right)_{V,N} = T\left.\frac{\partial(S,N)}{\partial(T,N)}\right|_{V}$

$\frac{\partial(v,w)}{\partial(x,y)} = \begin{vmatrix} \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} \end{vmatrix}$ Jacobian

1) $\frac{\partial(v,y)}{\partial(x,y)} = \left(\frac{\partial v}{\partial x}\right)_y$ 2) $\frac{\partial(v,w)}{\partial(x,y)} = -\frac{\partial(w,v)}{\partial(x,y)}$

3) $\frac{\partial(v,w)}{\partial(x,y)} = \frac{\partial(v,w)}{\partial(t,s)}\frac{\partial(t,s)}{\partial(x,y)}$

$C_V = T\,\dfrac{\frac{\partial(S,N)}{\partial(T,\mu)}}{\frac{\partial(T,N)}{\partial(T,\mu)}}$

$$C_V = T\,\frac{\left(\frac{\partial S}{\partial T}\right)_{\mu V}\left(\frac{\partial N}{\partial \mu}\right)_{TV} - \left(\frac{\partial S}{\partial \mu}\right)_{TV}\left(\frac{\partial N}{\partial T}\right)_{\mu V}}{\left(\frac{\partial N}{\partial \mu}\right)_T} = VT\left[\frac{\partial^2 P}{\partial T^2} - \frac{\partial^2 P}{\partial T\partial\mu}\Big/\frac{\partial^2 P}{\partial \mu^2}\right]$$

Simple Gas

probability density $\Psi(p) = f(p_x)f(p_y)f(p_z)$ $p^2 = p_x^2 + p_y^2 + p_z^2$

$\ln \Psi(p) = \ln f(p_x) + \ldots$

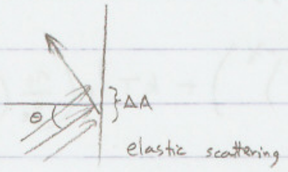
$\frac{\partial p}{\partial p_x} = \frac{1}{2}\frac{2p_x}{p} = \frac{p_x}{p}$

$\frac{1}{\Psi(p)}\frac{\partial \Psi(p)}{\partial p}\frac{\partial p}{\partial p_x} = \frac{1}{f(p_x)}\frac{\partial f}{\partial p_x}$

$\frac{1}{\Psi(p)}\frac{\partial \Psi(p)}{\partial p}\frac{1}{p} = \frac{1}{p_x}\frac{1}{f(p_x)}\frac{\partial f}{\partial p_x} = \frac{1}{p_y}\frac{1}{f(p_y)}\frac{\partial f}{\partial p_y} = \cdots = \alpha$ ($\Leftarrow$ const)

$\therefore$ $f = \sqrt{\frac{\alpha}{\pi}}\, e^{-\alpha p_x^2}$ $\Psi = \left(\frac{\alpha}{\pi}\right)^{3/2} e^{-\alpha p^2}$

$$dn(p) = \frac{N}{V}\left(\frac{\alpha}{\pi}\right)^{3/2} e^{-\alpha p^2}\, 4\pi p^2\, dp$$



$$\Delta p = 2p\cos\theta \qquad \Delta N = \Delta A \cos\theta\, v_p\, \Delta t\, \Delta n(p)$$

$$v_p = \frac{\partial \varepsilon_p}{\partial p} \qquad \varepsilon_p = mc^2 + \frac{p^2}{2m}$$

$$\Delta P = \frac{\Delta p\, \Delta N}{\Delta t\, \Delta A} = 2p\frac{\partial \varepsilon_p}{\partial p}\cos^2\theta\, \Delta n(\vec{p})$$

$$P = \int_0^\infty \frac{p}{3}\frac{\partial \varepsilon_p}{\partial p}\frac{N}{V}\left(\frac{\alpha}{\pi}\right)^{3/2} e^{-\alpha p^2}\, 4\pi p^2\, dp = \frac{N}{V}kT \implies \alpha = \frac{1}{2mkT}$$

$PV = NkT$ ← known back then

$$\underset{\substack{\downarrow \\ P(T,\mu)}}{VP} = \int_0^\infty \frac{p}{3}\frac{\partial \varepsilon_p}{\partial p}\underbrace{\frac{N}{V}\left(\frac{1}{2mkT\pi}\right)^{3/2}\frac{(2\pi\hbar)^3}{g}e^{\frac{mc^2}{kT}}}_{e^{\frac{\mu}{kT}}}e^{-\frac{\varepsilon_p}{kT}}\underbrace{g\frac{4\pi p^2\, dp\, dV}{(2\pi\hbar)^3}}_{\text{density of states}}$$

$g = 2s+1$ statistical weight due to degrees of freedom

$$\mu = kT\ln\left\{\left(\frac{2\pi\hbar^2}{mkT}\right)^{3/2}\frac{n}{g}\right\} + mc^2$$

$$PV = -\Omega = \int_0^\infty \frac{p}{3}\frac{\partial \varepsilon_p}{\partial p}\underbrace{e^{\frac{\mu-\varepsilon_p}{kT}}}_{\substack{\text{occupation} \\ \text{number } f(\varepsilon_p)}} g\frac{4\pi p^2\, dp\, dV}{(2\pi\hbar)^3}$$

$$f(\varepsilon_p) = \frac{1}{e^{-\frac{(\mu-\varepsilon_p)}{kT}}+0} \qquad \text{Maxwell–Boltzmann}$$

$$= \frac{1}{e^{-\frac{\mu-\varepsilon_p}{kT}}+1} \qquad \text{Fermi–Dirac} \qquad \mu=\varepsilon_p \qquad s = 1/2$$

$$= \frac{1}{e^{-\frac{\mu-\varepsilon_p}{kT}}-1} \qquad \text{Bose–Einstein} \qquad s=1$$

6/7/2007

$$P(\mu,T) = \int_0^\infty \frac{p^2}{3m}e^{\frac{\mu}{kT}}e^{-\frac{p^2}{2mkT}}g\frac{4\pi p^2\, dp}{(2\pi\hbar)^3} = kTg\underbrace{\frac{(2\pi mkT)^{3/2}}{(2\pi\hbar)^3}e^{\frac{\mu}{kT}}}_{} = nkT$$

$$\left(\frac{\partial P}{\partial \mu}\right)_T = n = g\left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2}e^{\mu/kT}$$

$$\left(\frac{\partial P}{\partial T}\right)_\mu = s = \frac{S}{V} = \left(\frac{5}{2}k - \frac{\mu}{T}\right)n \qquad \mu = kT\ln\left(\frac{n}{g}\left(\frac{2\pi\hbar^2}{mkT}\right)^{3/2}\right)$$

Saha Equation

$A \rightleftharpoons A^+ + e^-$ in thermodynamic equilibrium $T, P, \mu = \text{constant}$

$$kT \ln\left(n_0 \frac{1}{g_0}\left(\frac{mkT}{2\pi\hbar^2}\right)^{-3/2}\right) - \underbrace{\chi_I}_{\text{ionization potential}} = kT \ln\left(\frac{n_+}{g_+}\left(\frac{mkT}{2\pi\hbar^2}\right)^{-3/2}\right) + kT \ln\left(\frac{n_e}{g_e}\left(\frac{m_e kT}{2\pi\hbar^2}\right)^{-3/2}\right)$$

$$\frac{n_e n_+}{g_e g_+}\left(\frac{m_e kT}{2\pi\hbar^2}\right)^{-3/2} = \frac{n_0}{g_0} e^{-\frac{\chi_I}{kT}} \qquad g_e = 2$$

$$\boxed{\frac{n_+}{n_0} = \frac{g_+}{g_0}\frac{2}{n_e}\left(\frac{m_e kT}{2\pi\hbar^2}\right)^{3/2} e^{-\frac{\chi_I}{kT}}} \qquad \text{Saha Equation}$$

$$\frac{n_i}{n} = \frac{g_i e^{-\frac{E_i}{kT}}}{Z}$$

partition function $Z = \sum g_i e^{-\frac{E_i}{kT}}$

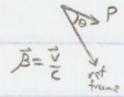
photons $h\nu$ $\quad E_i = i h\nu$ (i = # photons)

$$\bar{E} = \frac{\sum_i E_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} = -\frac{\partial}{\partial\beta}\ln \sum_i e^{-\beta i h\nu} \qquad \left(1 - e^{-\beta h\nu}\right)^{-1} \qquad 1 + q + q^2 + \dots = \frac{1}{1-q}$$

$$\bar{E} = \frac{h\nu}{e^{\frac{h\nu}{kT}} - 1} \qquad \text{Planck's spectrum} \qquad \mu = 0$$

photons readjusted in thermodynamics

Relativistic Quantum Mechanics



$$x' = \gamma(x - \beta ct) \qquad \gamma = \frac{1}{\sqrt{1-\beta^2}}$$
$$ct' = \gamma(ct - \beta x)$$

$$\underbrace{\vec{p} - \vec{p}\cdot\vec{\beta}\,\frac{\vec{\beta}}{\beta^2}}_{\vec{p}_\perp} + \underbrace{\vec{p}\cdot\vec{\beta}\,\frac{\vec{\beta}}{\beta^2}}_{\vec{p}_\parallel} = \vec{p}$$

$$\vec{p}\,' = \vec{p} - \vec{p}\cdot\vec{\beta}\,\frac{\vec{\beta}}{\beta^2} + \gamma\left[\vec{p}\cdot\vec{\beta}\,\frac{\vec{\beta}}{\beta^2} - \vec{\beta}\frac{E}{c}\right] \qquad \frac{E'}{c} = \gamma\left[\frac{E}{c} - \vec{p}\cdot\vec{\beta}\right]$$

photon $E = pc$

$$E' = \gamma(E - E\beta\cos\theta) \qquad \frac{E'}{E} = \frac{1 - \beta\cos\theta}{\sqrt{1-\beta^2}}$$

$$\frac{E}{E'} = \frac{\sqrt{1-\beta^2}}{1 - \beta\cos\theta} \qquad \text{relativistic doppler factor} \quad (E = h\nu) \qquad \theta = 0 \quad \frac{E}{E'} = \sqrt{\frac{1+\beta}{1-\beta}}$$

$$p^\mu = \left(\frac{E}{c}, \vec{p}\right) \qquad p_\mu = \left(\frac{E}{c}, -\vec{p}\right) \qquad p^\mu p_\mu = \frac{E^2}{c^2} - p^2 = m^2c^2$$

1) Superposition (came from interference of light)

$$|\psi\rangle = \sum \alpha_i |\psi_i\rangle$$

$$\hat{\lambda}|\psi\rangle = \lambda|\psi\rangle \qquad \hat{\lambda}|\psi_i\rangle = \lambda_i|\psi_i\rangle \qquad \langle\psi_j|\psi_i\rangle = 0$$

$$\langle\psi|\hat{\lambda}|\psi\rangle = \sum \lambda_i \underbrace{|\alpha_i|^2}_{\text{probability}} \qquad \hat{\vec{r}}|\psi\rangle = \vec{r}|\psi\rangle \qquad |\psi\rangle = \int \psi(r)|\vec{r}\rangle d^3\vec{r}$$

$$\langle\psi|\psi\rangle = \int |\psi|^2 d^3\vec{r} = 1 \qquad \rho = |\psi|^2$$

probability densative

2) Evolution operator $i\hbar \frac{\partial\psi}{\partial t} = \hat{H}\psi$ (from geometric limit)

$$\psi = a e^{i\frac{S}{\hbar}} \qquad S = \int p\,dr - Et$$

$$i\hbar \frac{\partial}{\partial t}|\psi|^2 = \psi^* \hat{H}\psi - (\hat{H}^*\psi^*)\psi \qquad \hat{H} = \hat{H}^+ \qquad \frac{\partial}{\partial t}\int |\psi|^2 d^3\vec{r} = 0$$

$E = H = \frac{p^2}{2m}$ $\quad i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi$ $\quad \vec{p} = -i\hbar\nabla$ $\quad$ not Lorentz invariant

$E = \sqrt{p^2c^2 + m^2c^4}$ $\quad i\hbar\frac{\partial}{\partial t}\psi = \sqrt{-\hbar^2c^2\nabla^2 + m^2c^4}\,\psi$ $\quad$ better, but might still not work

$E^2 = p^2c^2 + m^2c^4$ $\quad -\hbar^2\frac{\partial^2\psi}{\partial t^2} = (-\hbar^2c^2\nabla^2 + m^2c^4)\psi$ $\quad$ Klein-Gordon Eqn.

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{mc}{\hbar}\right)^2\right]\psi = \left[\frac{\partial}{\partial x_\mu}\frac{\partial}{\partial x^\mu} + \left(\frac{mc}{\hbar}\right)^2\right]\psi = 0$$

Lorentz invariant

but now $E = \pm\sqrt{\sim}$ didnt have $-$ solution before

$$\psi^*\frac{\partial}{\partial x_\mu}\frac{\partial}{\partial x^\mu}\psi - \psi\frac{\partial}{\partial x_\mu}\frac{\partial}{\partial x^\mu}\psi^* = 0$$

$$\underbrace{\frac{1}{c^2}\frac{\partial}{\partial t}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right)}_{\times\frac{i\hbar}{2m}\to\rho} - \nabla\cdot\underbrace{\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]}_{\times\frac{\hbar}{2im}\to\vec{j}} = 0 \quad \to \quad \frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0$$

but ρ can be negative

No spin

want linear equation in time $\longrightarrow$

Dirac Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(\frac{\hbar c}{i} \left(\alpha_x \frac{\partial}{\partial x} + \alpha_y \frac{\partial}{\partial y} + \alpha_z \frac{\partial}{\partial z} \right) + \beta m c^2 \right) \Psi$$

$(|\Psi|^2, \vec{J})$?

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_n \end{pmatrix} \qquad \alpha, \beta \to \text{matrices } N \times N$$

To work must satisfy $\left\{ \begin{array}{l} \text{1) Lorentz invariant} \\ \text{2) Continuity equation} \\ \text{3) } E^2 = p^2c^2 + m^2c^4 \end{array} \right.$

$$-\hbar^2 \frac{\partial^2 \Psi}{\partial t^2} = \left[-\hbar^2 c^2 \sum_{kj} \frac{\alpha_k \alpha_j + \alpha_j \alpha_k}{2} \frac{\partial^2 \Psi}{\partial x^k \partial x^j} + \frac{\hbar m c^3}{i} \sum_k \left(\alpha_k \beta + \beta \alpha_k \right) \frac{\partial \Psi}{\partial x^k} + \beta^2 m^2 c^4 \right] \Psi$$

Equivalent to Klein-Gordon

$$\therefore \quad \alpha_j \alpha_k + \alpha_k \alpha_j = 2\delta_{jk} \qquad \alpha_j \beta + \beta \alpha_j = 0 \qquad \alpha_j^2 = \beta^2 = 1$$

eigenvalues should be ± 1

$$\alpha_j = -\beta \alpha_j \beta$$

$$\mathrm{Tr}(\alpha) = -\mathrm{Tr}(\alpha) = 0$$

4 dimensional matrices

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$\sigma_i \to$ Pauli matrix $\quad 1 \to \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad 0 \to \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

$$\Psi = (\Psi_1, \Psi_2, \Psi_3, \Psi_4)$$

$$i\hbar \Psi^+ \frac{\partial \Psi}{\partial t} = \frac{\hbar c}{i} \sum_k \Psi^+ \alpha_k \frac{\partial \Psi}{\partial x^k} + mc^2 \Psi^+ \beta \Psi \qquad (1)$$

$$-i\hbar \left(\frac{\partial \Psi^+}{\partial t} \right) \Psi = -\frac{\hbar c}{i} \frac{\partial \Psi^+}{\partial x^k} \alpha_k \Psi + mc^2 \Psi^+ \beta \Psi \qquad (2)$$

$(1) - (2)$: $\quad i\hbar \frac{\partial}{\partial t}(\Psi^+ \Psi) = \frac{\hbar c}{i} \sum_k \frac{\partial}{\partial x^k} (\Psi^+ \alpha_k \Psi)$

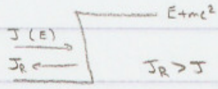
$$\rho = \Psi^+ \Psi \qquad J^k = c \Psi^+ \alpha^k \Psi \qquad (\rho, \vec{J}) \qquad \frac{\partial}{\partial x^\mu} J^\mu = 0$$

$c\hat{\alpha} \equiv$ operator of velocity

$p = 0 \quad i\hbar \frac{\partial \Psi}{\partial t} = \beta m c^2 \Psi \qquad \Psi_1 = e^{-\frac{imc^2}{\hbar} t} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \Psi_2 = e^{-\frac{imc^2}{\hbar} t} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad E = mc^2$

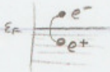
$\Psi_3 = e^{+\frac{imc^2}{\hbar} t} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad \Psi_4 = e^{+\frac{imc^2}{\hbar} t} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad \underline{E = -mc^2}$

even if you ignore negative energy states, Lorentz transformation brings it back



$J_R > J$ apparent paradox, more reflected than incident

Dirac eqn predicts:



positive hole (positron)

Lamb shift predicted by Dirac equation (with negative energy states)