01/12/2010 Time Independent Perturbation Theory: Nondegenerate Case

$H|n\rangle = E_n|n\rangle$

$H = H_0 + \lambda V$

$H_0$ - exactly solvable

$V$ - perturbation

$0 \leq \lambda \leq 1$ bookkeeping parameter.

$$H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$$

$$|n\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$$

$$(H_0 + \lambda V)|n\rangle = E_n|n\rangle$$

$$(H_0 + \lambda V)(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots) = (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots)(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots)$$

Must hold for each order of $\lambda$.

$\lambda^0$ order: $\quad H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$

$\lambda^1$ order: $\quad H_0|n^{(1)}\rangle + V|n^{(0)}\rangle = E_n^{(0)}|n^{(1)}\rangle + E_n^{(1)}|n^{(0)}\rangle$

$\lambda^2$ order: $\quad H_0|n^{(2)}\rangle + V|n^{(1)}\rangle = E_n^{(0)}|n^{(2)}\rangle + E_n^{(1)}|n^{(1)}\rangle + E_n^{(2)}|n^{(0)}\rangle$

$\lambda^i$ order: $\quad H_0|n^{(i)}\rangle + V|n^{(i-1)}\rangle = E_n^{(0)}|n^{(i)}\rangle + E_n^{(1)}|n^{(i-1)}\rangle + E_n^{(2)}|n^{(i-2)}\rangle + \cdots + E_n^{(i)}|n^{(0)}\rangle$

$(i \geq 1)$

Look at $H_0|n^{(1)}\rangle + V|n^{(0)}\rangle = E_n^{(0)}|n^{(1)}\rangle + E_n^{(1)}|n^{(0)}\rangle$

Multiply by $\langle n^{(0)}|$.

$$\underbrace{\langle n^{(0)}|H_0|n^{(1)}\rangle}_{E_n^{(0)}\langle n^{(0)}|n^{(1)}\rangle} + \langle n^{(0)}|V|n^{(0)}\rangle = E_n^{(0)}\langle n^{(0)}|n^{(1)}\rangle + E_n^{(1)}\underbrace{\langle n^{(0)}|n^{(0)}\rangle}_{=1}$$

$$\Rightarrow \boxed{E_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle}$$

Likewise, for $i^{th}$ order

$$\underbrace{\langle n^{(0)}|H_0|n^{(i)}\rangle}_{E_n^{(0)}\langle n^{(0)}|n^{(i)}\rangle} + \langle n^{(0)}|V|n^{(i-1)}\rangle = \cancel{E_n^{(0)}\langle n^{(0)}|n^{(i)}\rangle} + E_n^{(1)}\langle n^{(0)}|n^{(i-1)}\rangle + \cdots + E_n^{(i)}\langle n^{(0)}|n^{(0)}\rangle$$

If $\langle n^{(0)}|n^{(i)}\rangle = \delta_{i0}$,

$$\boxed{E_n^{(i)} = \langle n^{(0)}|V|n^{(i-1)}\rangle}$$

Need to find $|n^{(i)}\rangle$.

$$\sum_k |k^{(0)}\rangle\langle k^{(0)}| = 1$$ (Closure relation for exactly solvable problem)

$$|n^{(i)}\rangle = \sum_{k\neq n} |k^{(0)}\rangle\langle k^{(0)}|n^{(i)}\rangle \qquad (i = 1, 2, 3, \ldots)$$

If $k = n$, $\langle k^{(0)}|n^{(i)}\rangle = \delta_{i0}$

$$\sum_k |k^{(0)}\rangle\langle k^{(0)}| = 1 = |n^{(0)}\rangle\langle n^{(0)}| + \sum_{k\neq 0}|k^{(0)}\rangle\langle k^{(0)}|$$ Check!

So $(k \neq n)$

$$\underbrace{\langle k^{(0)} | H_0 | n^{(i)} \rangle}_{E_k^{(0)} \langle k^{(0)} | n^{(i)} \rangle} + \langle k^{(0)} | V | n^{(i-1)} \rangle = E_n^{(0)} \langle k^{(0)} | n^{(i)} \rangle + E_n^{(1)} \langle k^{(0)} | n^{(i-1)} \rangle + \cdots + E_n^{(i-1)} \langle k^{(0)} | n^{(1)} \rangle + E_n^{(i)} \underbrace{\langle k^{(0)} | n^{(0)} \rangle}_{=0}$$

If $E_k^{(0)} \neq E_n^{(0)}$ (nondegenerate)

$$\langle k^{(0)} | n^{(i)} \rangle = \frac{1}{E_n^{(0)} - E_k^{(0)}} \left( \langle k^{(0)} | V | n^{(i-1)} \rangle - E_n^{(1)} \langle k^{(0)} | n^{(i-1)} \rangle - \cdots - E_n^{(i-1)} \langle k^{(0)} | n^{(1)} \rangle \right)$$

$$E_n^{(1)} = \langle n^{(0)} | V | n^{(0)} \rangle$$

$$\langle k^{(0)} | n^{(1)} \rangle = \frac{1}{E_n^{(0)} - E_k^{(0)}} \langle k^{(0)} | V | n^{(0)} \rangle$$

Up to first order in $\lambda$, we find

$$\boxed{|n\rangle = |n^{(0)}\rangle + \lambda \sum_{k \neq n} |k^{(0)}\rangle \left( \frac{1}{E_n^{(0)} - E_k^{(0)}} \right) \langle k^{(0)} | V | n^{(0)} \rangle}$$

$$\boxed{E_n = E_n^{(0)} + \lambda \langle n^{(0)} | V | n^{(0)} \rangle}$$

01/14/2010 Examples of Perturbation Method

$$(H_0 + \lambda V)|n\rangle = E_n|n\rangle$$

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

$$|n\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \ldots$$

$$H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$$

$i^{th}$ order $(i \geq 1) \rightarrow$ $E_n^{(i)} = \langle n^{(0)}|V|n^{(i-1)}\rangle$

$$|n^{(i)}\rangle = \sum_{k \neq n} |k^{(0)}\rangle\langle k^{(0)}|n^{(i)}\rangle$$

$$\langle k^{(0)}|n^{(i)}\rangle = \frac{1}{E_n^{(0)} - E_k^{(0)}}\left(\langle k^{(0)}|V|n^{(i-1)}\rangle - E_n^{(1)}\langle k^{(0)}|n^{(i-1)}\rangle - \ldots - E_n^{(i-1)}\langle k^{(0)}|n^{(1)}\rangle\right)$$

$$E_n = E_n^{(0)} + \lambda\langle n^{(0)}|V|n^{(0)}\rangle$$

$$|n\rangle = |n^{(0)}\rangle + \lambda\sum_{k \neq n} \frac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}|k^{(0)}\rangle$$

What is $E_n^{(2)}$ and $|n^{(2)}\rangle$?

$$E_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle$$

$$= \langle n^{(0)}|V|\sum_{k \neq n}|k^{(0)}\rangle\frac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}$$

$$\boxed{E_n^{(2)} = \sum_{k \neq n}\frac{|\langle n^{(0)}|V|k^{(0)}\rangle|^2}{E_n^{(0)} - E_k^{(0)}}}$$

$$\langle k^{(0)}|n^{(2)}\rangle = \frac{1}{E_n^{(0)}-E_k^{(0)}}\left(\langle k^{(0)}|V|n^{(1)}\rangle - E_n^{(1)}\langle k^{(0)}|n^{(1)}\rangle - E_n^{(2)}\underbrace{\cancel{\langle k^{(0)}|n^{(0)}\rangle}}_{\to 0}\right)$$

$$= \frac{1}{E_n^{(0)}-E_k^{(0)}}\left(\langle k^{(0)}|V|\sum_{l\neq n}|l^{(0)}\rangle\frac{\langle l^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)}-E_l^{(0)}}\right.$$

$$\left. - \langle n^{(0)}|V|n^{(0)}\rangle\langle k^{(0)}|\sum_{l\neq n}|l^{(0)}\rangle\frac{\langle l^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)}-E_l^{(0)}}\right)$$

$$\boxed{|n^{(2)}\rangle = \sum_{k\neq n}\sum_{l\neq n}\left(\frac{1}{E_n^{(0)}-E_k^{(0)}}\right)\left(\frac{1}{E_n^{(0)}-E_l^{(0)}}\right)\left(\langle k^{(0)}|V|l^{(0)}\rangle\langle l^{0}|V|n^{(0)}\rangle\right)|k^{(0)}\rangle - \sum_{k\neq n}|k^{(0)}\rangle\frac{\langle n^{(0)}|V|n^{(0)}\rangle\langle k^{(0)}|V|n^{(0)}\rangle}{(E_n^{(0)}-E_k^{(0)})^2}}$$

Wavefunction Renormalization

$$\langle n^{(0)}|n^{(0)}\rangle = 1$$

$$\langle n|n\rangle \neq 1$$

Define normalized state $|n\rangle_N = Z_n^{1/2}|n\rangle$ so ${}_N\langle n|n\rangle_N = 1$.

$$\langle n|n\rangle = \frac{1}{Z_n}$$

$$Z_n^{-1} = \langle n|n\rangle = 1 + \lambda^2\sum_{k\neq n}\frac{|\langle k^{(0)}|V|n^{(0)}\rangle|^2}{(E_n^{(0)}-E_k^{(0)})^2} + \cdots > 1$$

$$\Rightarrow Z_n < 1$$

$$Z_n \approx 1 - \lambda^2\sum_{k\neq n}\frac{|\langle k^{(0)}|V|n^{(0)}\rangle|^2}{(E_n^{(0)}-E_k^{(0)})^2} < 1 \qquad \left(\frac{1}{1+\delta}\approx 1-\delta+\ldots\right)$$

$$= \frac{\partial}{\partial E_n^{(0)}}\left(E_n^{(0)} + \lambda\langle n^{(0)}|V|n^{(0)}\rangle + \lambda^2\sum_{k\neq n}\frac{|\langle k^{(0)}|V|n^{(0)}\rangle|^2}{(E_n^{(0)}-E_k^{(0)})} + \cdots\right)$$

Example: Stark Effect in Hydrogen-Like Atom.

Hydrogen-Like → Single unpaired electron determines properties of atom.

Want nondegenerate → must restrict to only ground state.

$$H_0 = \frac{p^2}{2m} - \frac{Ze^2}{r} \qquad \text{(Coulomb Potential)}$$

$$V = -e\vec{\mathcal{E}} \cdot \vec{r} \qquad \text{(electric field applied to atom)}$$

$$\vec{\mathcal{E}} = \mathcal{E}\hat{z} \rightarrow V = -e\mathcal{E}\hat{z} \qquad (e<0)$$

Treat V as a perturbation.

We consider only the ground state $|n\ell m\rangle = |100\rangle$.

$$E_{100} = E_{100}^{(0)} + E_{100}^{(1)} + E_{100}^{(2)} + \cdots$$

$$E_{100}^{(1)} = \langle 100^{(0)}| -e\mathcal{E}z | 100^{(0)}\rangle$$

$$= -e\mathcal{E} \langle 100^{(0)}| z | 100^{(0)}\rangle$$

$$= -e\mathcal{E} \int d^3r \, |\psi_{100}(r,\theta,\phi)|^2 z$$

$= 0$ because $\psi_{100}$ has even parity, and $z$ is odd.

Must go to second order shift. → Quadratic Stark Effect.

$$E_{100}^{(2)} = e^2 \mathcal{E}^2 \sum_{n\ell m \neq 100} \frac{|\langle n\ell m^{(0)}|z|100^{(0)}\rangle|^2}{E_{100}^{(0)} - E_{n\ell m}^{(0)}}$$

$$\langle n\ell m^{(0)}|z|100^{(0)}\rangle = \int d^3r \underbrace{\psi_{n\ell m}^{*}(r,\theta,\phi)}_{R_{n\ell}(r)\,Y_{\ell m}^{*}(\theta,\phi)} (r\cos(\theta)) \underbrace{\psi_{100}(r,\theta,\phi)}_{R_{10}(r)\,Y_{00}(\theta,\phi)}$$

$$= \int r^2 dr\, R_{n\ell}(r)\, r\, R_{10}(r) \int d\Omega\, Y_{\ell m}^{*}(\theta,\phi) \underbrace{\cos(\theta)\sqrt{\frac{1}{4\pi}}}_{\frac{1}{\sqrt{3}} Y_{10}(\theta,\phi)}$$

$$\int d\Omega\, Y_{\ell m}^{*}(\theta,\phi) \frac{1}{\sqrt{3}} Y_{10}(\theta,\phi) = \frac{1}{\sqrt{3}} \delta_{\ell 1}\, \delta_{m0}$$

$$\langle n\ell m^{(0)}|z|100^{(0)}\rangle = \frac{1}{\sqrt{3}} \delta_{\ell 1}\, \delta_{m0} \int r^3 dr\, R_{n\ell}(r)\, R_{10}(r)$$

$z$ is a tensor operator $T_{(q=0)}^{(k=1)}$

Like adding angular momentum

$\ell = 0,\ k = 1 \rightarrow \ell_{tot} = 1$ (we find $\delta_{\ell 1}$)

$m_1 = 0,\ q = 0 \rightarrow m_{tot} = 0$ (we find $\delta_{m0}$)

01/19/2010

Time Independent Perturbation Theory: Degenerate Case

$$H_0 = \frac{p^2}{2m} - \frac{Ze^2}{r}$$

$$V = -e\mathcal{E}z$$

Found energy shift last time. What about the wave function?

$$|100\rangle = |100^{(0)}\rangle - e\mathcal{E}\sum_{nlm\neq 100} \frac{|\langle nlm^{(0)}|z|100^{(0)}\rangle|^2}{E_{100}^{(0)} - E_{nlm}^{(0)}} |nlm^{(0)}\rangle + \cdots$$

Sakurai 5.7: Find electric polarizability of hydrogen atom.

$$D = \langle 100|ez|100\rangle$$

$$= e\cancelto{0}{\langle 100^{(0)}|z|100^{(0)}\rangle} - 2e^2\mathcal{E}\sum_{nlm\neq 100}\frac{|\langle nlm^{(0)}|z|100^{(0)}\rangle|^2}{E_{100}^{(0)} - E_{nlm}^{(0)}} + \cdots$$

Polarizability: $\alpha = \left.\frac{\partial D}{\partial \mathcal{E}}\right|_{\mathcal{E}=0}$

$$\alpha = -2e^2\sum_{nlm\neq 100}\frac{|\langle nlm^{(0)}|z|100^{(0)}\rangle|^2}{E_{100}^{(0)} - E_{nlm}^{(0)}}$$

$$\boxed{\alpha = -2\frac{E_{100}^{(2)}}{|\vec{\mathcal{E}}|^2}}$$

$$\boxed{E_{100}^{(2)} = -\frac{\alpha}{2}|\vec{\mathcal{E}}|^2}$$

$$E_{nlm}^{(0)} = \frac{-e^2}{2a_0 n^2}$$

$$-2e^2\sum\frac{|\langle nlm^{(0)}|z|100^{(0)}\rangle|^2}{E_{100}^{(0)} - E_{nlm}^{(0)}} \leq \frac{-2e^2}{E_{100}^{(0)} - E_{2lm}^{(0)}} \underbrace{\sum_{nlm\neq 100}|\langle nlm^{(0)}|z|100^{(0)}\rangle|^2}$$

$$\underbrace{\sum_{nlm}|\langle nlm^{(0)}|z|100^{(0)}\rangle|^2 - \cancelto{0}{|\langle 100^{(0)}|z|100^{(0)}\rangle|^2}}$$

$$\underbrace{\sum_{nlm}\langle 100^{(0)}|z|nlm^{(0)}\rangle\langle nlm^{(0)}|z|100^{(0)}\rangle}$$

$$= \langle 100^{(0)}|z^2|100^{(0)}\rangle$$

$$\langle 100^{(0)} | z^2 | 100^{(0)} \rangle = \frac{1}{3} \langle 100^{(0)} | r^2 | 100^{(0)} \rangle$$

$$\langle r^2 \rangle_{n\ell m} = \frac{a_0^2 n^2}{2 Z^2} \left( 5n^2 + 1 - 3\ell(\ell+1) \right)$$

$$E_{100}^{(0)} - E_{n\ell m}^{(0)} = \frac{-3e^2}{8a_0}$$

$$\Rightarrow \quad \alpha \leq \frac{16 a_0}{3} \cdot \frac{1}{3} \frac{a_0^2}{2} (5+1)$$

$$\boxed{\alpha \leq \frac{16 a_0^3}{3} \sim 5.3 a_0^3}$$

Dalgarmo + Lewis result $-$ $\alpha = 4.5 a_0^3$

Consider an excited state $\rightarrow$ $|200\rangle$

$$|200\rangle = |200^{(0)}\rangle - e\mathcal{E} \sum_{n\ell m \neq 200} \frac{\langle n\ell m^{(0)} | z | 200^{(0)} \rangle}{E_{200}^{(0)} - E_{n\ell m}^{(0)}} |n\ell m^{(0)}\rangle + \dots$$

$$\langle 210^{(0)} | z | 200^{(0)} \rangle \neq 0$$

$$\text{but} \quad E_{200}^{(0)} - E_{210}^{(0)} = 0 \quad \Rightarrow \quad \text{PROBLEM!}$$

$n=2$ states in hydrogen (Stark effect)

$$\ell = 1 \begin{cases} m=+1 & - \; |2P_1\rangle \\ m=0 & \quad |2P_0\rangle \\ m=-1 & \quad |2P_{-1}\rangle \end{cases}$$

$$\ell = 0 \quad - \; |2S_0\rangle$$

$$E_{2\ell m} = \frac{-e^2}{8a_0}$$

$$\langle 2\ell' m' | V | 2\ell m \rangle = \left( \begin{array}{cc|cc} 0 & \langle 2S_0 | V | 2P_0 \rangle & 0 & 0 \\ \langle 2P_0 | V | 2S_0 \rangle & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right).$$

Diagonalize V.

$$V \doteq \langle 2S_0|V|2P_0\rangle \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{(relevant } 2\times 2 \text{ matrix)}$$

Secular equation $\to \det\begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix} = \lambda^2 - 1 = 0$

$$\lambda = \pm 1$$

$$\lambda = +1 \to |+\rangle = \frac{1}{\sqrt{2}}\left(|2S_0\rangle + |2P_0\rangle\right)$$

$$\lambda = -1 \to |-\rangle = \frac{1}{\sqrt{2}}\left(|2S_0\rangle - |2P_0\rangle\right)$$

$\langle +|V|+\rangle$
$\langle -|V|-\rangle$ gives first order energy shift

$\to$ Linear Stark Effect.

$$\langle 2S_0|V|2P_0\rangle = \langle 2P_0|V|2S_0\rangle$$

$$= -e\mathcal{E} \int d^3r\, \psi^*_{200}(r,\theta,\phi)\, r\cos(\theta)\, \psi_{210}(r,\theta,\phi)$$

$$= -e\mathcal{E}\left(\int r^2 dr\, R_{20}(r)\, r\, R_{21}(r)\right)\underbrace{\left(\int d\Omega \cos(\theta)\, Y^*_{00}(\theta,\phi)\, Y_{10}(\theta,\phi)\right)}_{\frac{\sqrt{3}}{4\pi}\int d\cos(\theta)\cos^2(\theta)\int d\phi \;=\; \frac{1}{\sqrt{3}}}$$

$$\langle 2S_0|V|2P_0\rangle = \frac{-e\mathcal{E}}{\sqrt{3}}\left(\int dr\, r^3 R_{20}(r) R_{21}(r)\right)$$

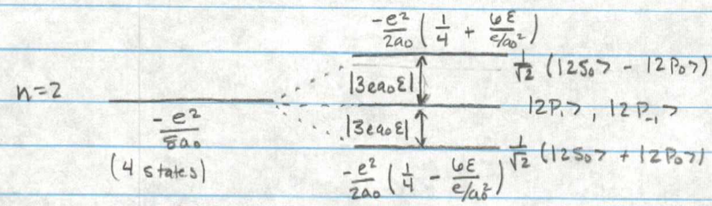
$$\langle 2S_0|V|2P_0\rangle = \frac{-e\mathcal{E}}{\sqrt{3}\,a_0}\left(\frac{1}{2a_0}\right)^3 \int_0^\infty dr\, r^4 \left(2 - \frac{r}{a_0}\right) e^{-r/a_0}$$

$$\boxed{\langle 2S_0|V|2P_0\rangle = 3ea_0\mathcal{E}}$$

$\langle + | V | + \rangle \rightarrow \Delta E_+ = 3 e a_0 \mathcal{E} \qquad \left( |+\rangle = \frac{1}{\sqrt{2}} \left( |2S_0\rangle + |2P_0\rangle \right) \right)$

$(e < 0)$

$\langle - | V | - \rangle \rightarrow \Delta E_- = -3 e a_0 \mathcal{E} \qquad \left( |-\rangle = \frac{1}{\sqrt{2}} \left( |2S_0\rangle - |2P_0\rangle \right) \right)$




$$\left| \frac{e}{a_0^2} \right| = 5.15 \times 10^9 \ \mathrm{V/cm}$$

Two State Problem

$$H = \underbrace{\begin{pmatrix} E_1^{(0)} & 0 \\ 0 & E_2^{(0)} \end{pmatrix}}_{H_0} + \lambda \underbrace{\begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix}}_{V}$$

Suppose $\quad V_{11} = V_{22} = 0 \quad$ and $\quad V_{12} = V_{21}^* \quad$ from Hermiticity

then

$$H = \begin{pmatrix} E_1^{(0)} & \lambda V_{12} \\ \lambda V_{12}^* & E_2^{(0)} \end{pmatrix}$$

Exact Solution:

$$\det \begin{pmatrix} E_1^{(0)} - \alpha & \lambda V_{12} \\ \lambda V_{12}^* & E_2^{(0)} - \alpha \end{pmatrix} = 0$$

$$\alpha^2 - \left(E_1^{(0)} + E_2^{(0)}\right)\alpha + E_1^{(0)} E_2^{(0)} - \lambda^2 |V_{12}|^2 = 0$$

$$E_{\substack{1+ \\ 2-}} = \frac{E_1^{(0)} + E_2^{(0)}}{2} \pm \sqrt{\frac{\left(E_1^{(0)} - E_2^{(0)}\right)^2}{4} + \lambda^2 |V_{12}|^2}$$

$$= \frac{E_1^{(0)} + E_2^{(0)}}{2} \pm \frac{\left|E_1^{(0)} - E_2^{(0)}\right|}{2} \sqrt{1 + \left(\frac{2\lambda |V_{12}|}{E_1^{(0)} - E_2^{(0)}}\right)^2}$$

If $E_1^{(0)} \neq E_2^{(0)}$ (non degenerate case) and $\lambda |V_{12}| << |E_1^{(0)} - E_2^{(0)}|$

$$\sqrt{1+\epsilon} \sim 1 + \frac{1}{2}\epsilon - \frac{\epsilon^2}{8} + \cdots$$

$$E_1 = E_1^{(0)} + \frac{\lambda^2 |V_{12}|^2}{(E_1^{(0)} - E_2^{(0)})} + \cdots$$

$$E_2 = E_2^{(0)} + \frac{\lambda^2 |V_{12}|^2}{E_2^{(0)} - E_1^{(0)}} + \cdots$$

If $E_1^{(0)} = E_2^{(0)}$ (degenerate case) then

$$E_{1,2} = E^{(0)} \pm \lambda |V_{12}|$$

01/21/2010 Hydrogen Atom: Fine Structure

$$H_0 = \frac{\vec{p}^2}{2m} - \frac{e^2}{r}$$

$$E_n^{(0)} = \frac{-e^2}{2a_0 n^2} \qquad a_0 = \frac{\hbar^2}{me^2}$$

$$E_n^{(0)} = \frac{-1}{2n^2} mc^2 \left(\frac{e^2}{\hbar c}\right)^2 \qquad \frac{e^2}{\hbar c} = \alpha \approx \frac{1}{137}$$ Fine structure constant

$$E_n^{(0)} = \frac{-1}{2} mc^2 \alpha^2 \left(\frac{1}{n^2}\right)$$

$$M_p c^2 \sim 1\ \text{GeV} = 10^9\ \text{eV}$$

$$m_e c^2 \sim .5\ \text{MeV} = \tfrac{1}{2}\times 10^6\ \text{eV} \sim \frac{1}{2000} M_p c^2$$

$$E_n^{(0)} \approx -13.6\ \text{eV}\left(\frac{1}{n^2}\right)$$

$E=0$ ———— $E_\infty^{(0)}$

$E_3^{(0)} = -1.5\text{eV}$ ———— $n=3$ $l=2, l=1, l=0$

$E_2^{(0)} = -3.4\text{eV}$ ———— $n=2$ $l=0, l=1$

$E_1^{(0)} = -13.6\text{eV}$ ———— $n=1$ $l=0$

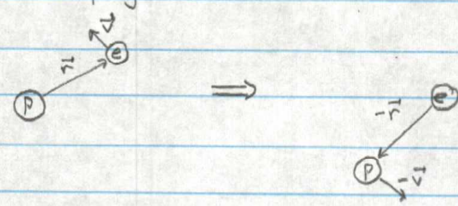
$$V_{Stark} = -e\,\mathcal{E}\,z$$

$H_0$ neglects spin and relativistic kinematics.

$\rightarrow$ Fine structure of H spectrum $(\sim\alpha^4)$

$$\boxed{V = V_{spin\text{-}orbit} + V_{rel.\ kin.}}$$

## I. Spin-Orbit Coupling




Proton creates "current loop" → Magnetic field

$$V_{so} = -\vec{\mu} \cdot \vec{B}$$

$\vec{\mu}$: due to $e^-$ spin; $\vec{B}$: due to $e^-$ orbital motion

$$\vec{B} = \frac{-e}{c} \frac{(-\vec{r}) \times (-\vec{v})}{r^3} \qquad \text{(Biot-Savart Law)}$$

$$= \frac{-e}{mc} \frac{\vec{L}}{r^3} \qquad (\vec{L} = \vec{r} \times m\vec{v})$$

$$\vec{\mu} = \frac{e}{mc} \vec{S} = \frac{g}{2} \frac{e}{mc} \vec{S} \qquad (g = 2 \text{ for electron})$$

$$V_{so} = \frac{e^2}{2(mc)^2 r^3} \vec{S} \cdot \vec{L} \sim \frac{e^2}{m^2c^2} \underbrace{\left(\frac{me^2}{\hbar^2}\right)}_{1/a_0}{}^3 \hbar^2$$

$2$: $e^-$ in non-inertial frame, Thomas precession factor

$$= mc^2 \left(\frac{e^2}{\hbar c}\right)^4 = mc^2 \alpha^4$$

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

$$j = \begin{cases} l + \frac{1}{2} \\ l - \frac{1}{2} \end{cases}$$

$nL_j$ – Spectroscopic notation

$n=1,\ l=0,\ j=1/2 \rightarrow 1s_{1/2}$

$n=2,\ l=0 \rightarrow j=1/2 \qquad 2s_{1/2}$

$\qquad l=1 \rightarrow j=3/2,\ 1/2 \qquad 2p_{3/2},\ 2p_{1/2}$

II Relativistic Kinematics

$$T = \sqrt{p^2c^2 + m^2c^4} - mc^2 \qquad \text{relativistic kinetic energy}$$

$$= mc^2\sqrt{1 + \frac{p^2}{m^2c^2}} - mc^2$$

$$(1+\epsilon)^n \sim 1 + n\epsilon + n(n-1)\frac{1}{2!}\epsilon^2 + \cdots$$

$$T = mc^2\left(1 + \frac{p^2}{2m^2c^2} + \frac{-p^4}{8m^4c^4} + \cdots\right) - mc^2$$

$$T = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \cdots$$

$$V_{RK} = \frac{-1}{2mc^2}\left(\frac{p^2}{2m}\right)^2 \qquad \left(H_0 = \frac{p^2}{2m} - \frac{e^2}{r}\right)$$

$$= \frac{-1}{2mc^2}\left(\underset{\sim \alpha^2 mc^2}{H_0} + \frac{e^2}{r}\right)^2 \sim mc^2\alpha^4$$

$$E_{RK}^{(1)} = \frac{-1}{2mc^2}\langle nls;jm|\left(H_0 + \frac{e^2}{r}\right)\left(H_0 + \frac{e^2}{r}\right)|nls;jm\rangle$$

$$= \frac{-1}{2mc^2}\left(\left(E_n^{(0)}\right)^2 + 2E_n^{(0)}e^2\left\langle\frac{1}{r}\right\rangle_{nl} + e^4\left\langle\frac{1}{r^2}\right\rangle_{nl}\right)$$

$$= \frac{-1}{2mc^2}\left(\left(\frac{m c^2\alpha^2}{2n^2}\right)^2 + \underbrace{2\left(\frac{-mc^2\alpha^2}{2n^2}\right)e^2\left(\frac{1}{a_0 n^2}\right)}_{-2e^2\left(\frac{mc^2\alpha^2}{2n^4}\right)\left(\frac{me^2}{\hbar^2}\right) = \frac{-(mc^2)^2\alpha^4}{n^4}} + e^4\left(\frac{1}{a_0^2 n^3(l+\frac{1}{2})}\right)\right)$$

Pg 455

$$\frac{e^4}{a_0^2 n^3(l+\frac{1}{2})} = \frac{(mc^2)^2\alpha^4}{n^3(l+\frac{1}{2})}$$

$$E_{RK}^{(1)} = \frac{-mc^2\alpha^4}{2}\left(\frac{1}{4n^4} - \frac{1}{n^4} + \frac{1}{n^3(l+\frac{1}{2})}\right)$$

$$\boxed{E_{RK}^{(1)} = \frac{-mc^2\alpha^4}{2}\left(\frac{1}{n^3(l+\frac{1}{2})} - \frac{3}{4n^4}\right)}$$

01/26/2010

## Zeeman Effect

From last time

$$V = \underbrace{\frac{-1}{2mc^2}\left(\frac{\vec{P}}{2m}\right)^2}_{RK} + \underbrace{\frac{e^2}{2m^2c^2r^3}\vec{S}\cdot\vec{L}}_{SO} \quad \sim mc^2\alpha^4$$

$$E_{RK}^{(1)} = \frac{-mc^2\alpha^4}{2}\left(\frac{1}{n^3(\ell+1/2)} - \frac{3}{4n^4}\right)$$

What is $E_{SO}^{(1)} = ?$

$$V_{SO} = \frac{e^2}{4m^2c^2r^3}(J^2 - S^2 - L^2) \qquad \left(\vec{S}\cdot\vec{L} = \tfrac{1}{2}(J^2 - L^2 - S^2)\right)$$

$$E_{SO}^{(1)} = \frac{e^2}{4m^2c^2} \langle n\ell s;jm| \frac{J^2 - S^2 - L^2}{r^3} |n\ell s;jm\rangle$$

$$= \frac{e^2}{4m^2c^2}\left\langle\frac{1}{r^3}\right\rangle_{n\ell}\left(j(j+1) - \ell(\ell+1) - \frac{3}{4}\right)\hbar^2 \qquad (s = 1/2)$$

$$\left\langle\frac{1}{r^3}\right\rangle_{n\ell} = \int_0^\infty dr\, r^2 (R_{n\ell}(r))^2 \frac{1}{r^3} = \frac{1}{a_0^3 n^3 \ell(\ell+\frac{1}{2})(\ell+1)}$$

$$E_{SO}^{(1)} = \underbrace{\frac{1}{4}\left(\frac{e^2}{m^2c^2}\right)\left(\frac{mc^2}{\hbar^2}\right)^3\hbar^2}_{mc^2\alpha^4}\left(\frac{1}{n^3(\ell)(\ell+\frac{1}{2})(\ell+1)}\right)\left(j(j+1) - \ell(\ell+1) - \frac{3}{4}\right)$$

$$j = \ell + \tfrac{1}{2} \text{ or } \ell - \tfrac{1}{2}$$

Lande's Interval Rule

$$E_{SO}^{(1)} = \frac{1}{4}mc^2\alpha^4\left(\frac{1}{n^3(\ell)(\ell+1/2)(\ell+1)}\right)\begin{cases}\ell & j = \ell + 1/2 \\ -\ell - 1 & j = \ell - 1/2\end{cases}$$

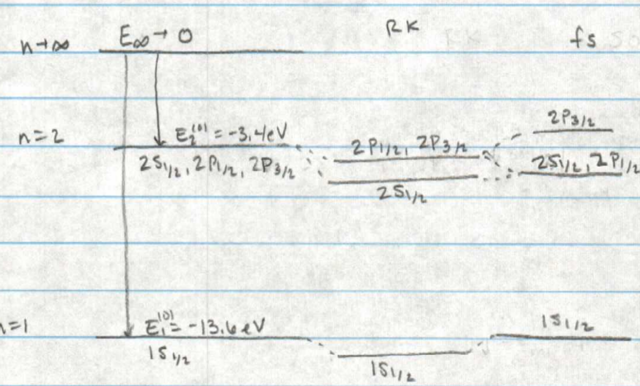
$$E_{fs}^{(1)} = E_{RK}^{(1)} + E_{SO}^{(1)}$$

$$E_{fs} = \frac{-mc^2\alpha^4}{2}\left(\frac{1}{n^3(\ell+1/2)} - \frac{3}{4n^4}\right) + \frac{1}{4}mc^2\alpha^4 \frac{1}{n^3\ell(\ell+1/2)(\ell+1)} \begin{cases} \ell & j=\ell+1/2 \\ -\ell-1 & j=\ell-1/2 \end{cases}$$

Write $j = \ell + 1/2 \rightarrow \ell = j - 1/2$

$j = \ell - 1/2 \rightarrow \ell = j + 1/2$

$$\boxed{E_{fs}^{(1)} = \frac{-mc^2\alpha^4}{2n^3}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right)}$$ for both $\Rightarrow$ independent of $\ell$.




| | $E_n^{(0)}$ $(mc^2\alpha^2)$ | $E_{RK}^{(1)}$ $(mc^2\alpha^4)$ | $E_{SO}^{(1)}$ $(mc^2\alpha^4)$ | $E_{fs}^{(1)}$ $(mc^2\alpha^4)$ |
|---|---|---|---|---|
| $1S_{1/2}$ | $-1/2$ | $-5/8$ | $1/2$ | $-1/8$ |
| $2S_{1/2}$ | $-1/8$ | $-13/128$ | $1/16$ | $-5/128$ |
| $2P_{1/2}$ | $-1/8$ | $-7/384$ | $-1/48$ | $-5/128$ |
| $2P_{3/2}$ | $-1/8$ | $-7/384$ | $1/96$ | $-1/128$ |

$\rightarrow$ Lamb shift $\sim mc^2\alpha^5$

$\uparrow$

Birth of QED

Quantum field theory

Now Zeeman effect . . .

$$H_0 = \frac{\vec{p}^{\,2}}{2m_e} - \frac{e^2}{r}$$

$$H_{fs} = \frac{e^2}{2m_e^2c^2r^3}\,\vec{S}\cdot\vec{L} - \frac{\vec{p}^{\,4}}{8m_e^3c^2}$$

$$H_B = \frac{-eB}{2m_ec}\,(L_z + \underset{\uparrow\, g=2 \text{ for } e^-}{2}S_z) \qquad \vec{B} = B\hat{z}$$

$$E_B^{(1)} = \frac{-eB}{2m_ec}\,\langle nls;jm|\underbrace{(L_z+2S_z)}_{J_z+S_z}|nls;jm\rangle$$

$$= \frac{-eB}{2m_ec}\left(m\hbar + \langle nls;jm|S_z|nls;jm\rangle\right)$$

Change basis using Clebsch-Goldan coefficients

$$|nls;jm\rangle = \sum_{m_s} \underbrace{\langle nls;\, m_l=m-m_s,\, m_s|nls;jm\rangle}_{CG}\,|nls;\, m_l=m-m_s,\, m_s\rangle$$

where $j = l+\frac{1}{2}$ or $l-\frac{1}{2}$

$$\langle nls;jm|S_z|nls;jm\rangle = \sum_{m_s'}\sum_{m_s}\left(\langle nls;\, m-m_s',\, m_s'|nls;jm\rangle\right)^* \overbrace{\left(\langle nls;\, m-m_s',\, m_s'|S_z|nls;\, m-m_s,\, m_s\rangle\right)}^{\hbar m_s\,\delta_{m_s,m_s'}}$$
$$*\left(\langle nls;\, m-m_s,\, m_s|nls;jm\rangle\right)$$

$$= \sum_{m_s}\left|\langle nls;\, m-m_s,\, m_s|nls;jm\rangle\right|^2 \hbar m_s$$

$$\langle nls;jm|S_z|nls;jm\rangle = \frac{\hbar}{2}\left|\langle nls;\, m-\tfrac{1}{2},\, \tfrac{1}{2}|nls;jm\rangle\right|^2 - \frac{\hbar}{2}\left|\langle nls;\, m+\tfrac{1}{2},\, -\tfrac{1}{2}|nls;jm\rangle\right|^2$$

$\langle nls; m_\ell m_s | nls; jm \rangle$

$m_s = \pm \frac{1}{2}$

| $j \backslash m_s$ | $\frac{1}{2}$ | $-\frac{1}{2}$ |
|---|---|---|
| $\ell + 1/2$ | $\sqrt{\frac{\ell+m+1/2}{2\ell+1}}$ | $\sqrt{\frac{\ell-m+1/2}{2\ell+1}}$ |
| $\ell - 1/2$ | $-\sqrt{\frac{\ell-m+1/2}{2\ell+1}}$ | $\sqrt{\frac{\ell+m+1/2}{2\ell+1}}$ |

(pg 214)

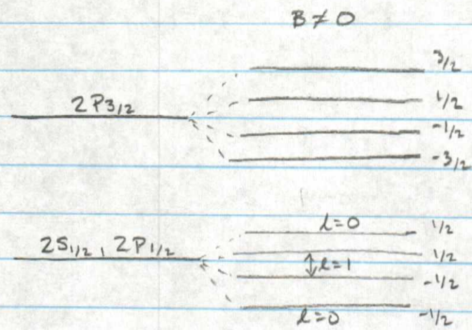
$$|j = \ell \pm \tfrac{1}{2}, m\rangle = \pm\sqrt{\frac{\ell \pm m + \frac{1}{2}}{2\ell+1}}\, |m_\ell = m - 1/2, m_s = 1/2\rangle$$
$$+ \sqrt{\frac{\ell \mp m + \frac{1}{2}}{2\ell+1}}\, |m_\ell = m + \tfrac{1}{2}, m_s = -\tfrac{1}{2}\rangle$$

$$\Rightarrow \langle nls; jm | S_z | nls; jm\rangle = \begin{cases} \frac{\hbar}{2}\left(\frac{\ell+m+\frac{1}{2}}{2\ell+1} - \frac{\ell-m+\frac{1}{2}}{2\ell+1}\right) & j = \ell + \frac{1}{2} \\ \frac{\hbar}{2}\left(\frac{\ell-m+\frac{1}{2}}{2\ell+1} - \frac{\ell+m+\frac{1}{2}}{2\ell+1}\right. & j = \ell - \frac{1}{2} \end{cases}$$

$$= \begin{cases} \frac{m\hbar}{2\ell+1} & j = \ell + \frac{1}{2} \\ \frac{-m\hbar}{2\ell+1} & j = \ell - \frac{1}{2} \end{cases}$$

$$\boxed{E_B^{(1)} = \frac{-eB}{2m_e c}\hbar m\left(1 \pm \frac{1}{2\ell+1}\right) \quad \text{for} \quad j = \ell \pm \tfrac{1}{2}}$$

m states are split.



B≠0
2P3/2
3/2
1/2
-1/2
-3/2
2S1/2 , 2P1/2
l=0
1/2
1/2
l=1
-1/2
l=0
-1/2

01/25/2010 <u>Variational Methods</u>

First, finish Zeeman effect

$$L_z + 2S_z = J_z + S_z \qquad \vec{J} = \vec{L} + \vec{S}$$

Need to compute $\langle S_z \rangle$

Wigner - Eckart Theorem

$$\langle \alpha', j'm' | T_q^{(k)} | \alpha, jm \rangle = \underbrace{\langle jk; mq | jk; j'm' \rangle}_{\text{CG coefficient}} \frac{\langle \alpha', j' || T^{(k)} || \alpha, j \rangle}{\sqrt{2j+1}}$$

$$m' = m + q$$

The double bar matrix element is independent of $m, m', q$

Projection Theorem

$j = j'$ , $k = 1$ case of Wigner - Eckart Theorem

$$T_q^{(1)} = V_q \qquad \text{vector}$$

$$\langle \alpha'; jm' | V_q | \alpha; jm \rangle = \frac{\langle \alpha'; jm | \vec{J} \cdot \vec{V} | \alpha jm \rangle}{\hbar^2 j(j+1)} \langle jm' | J_q | jm \rangle$$

$$\frac{\langle jm' | S_q | jm \rangle}{\langle jm' | J_q | jm \rangle} = \frac{\langle j || \vec{S} || j \rangle}{\langle j || \vec{J} || j \rangle}$$

$$= \frac{\langle \vec{S} \cdot \vec{J} \rangle_j}{\langle \vec{J}^2 \rangle_j}$$

$$\vec{S} \cdot \vec{J} = \underbrace{S_0 J_0}_{S_z J_z} \underbrace{- S_+ J_- - S_- J_+}_{S_x J_x + S_y J_y \, ?}$$

$$\langle jm | \underbrace{\vec{S} \cdot \vec{J}}_{\text{scalar}} | jm \rangle = C_{jm} \langle j || \vec{S} || j \rangle$$

actually independent of $m$

$$\langle jm | \vec{J}^2 | jm \rangle = c_j \langle j || \vec{J} || j \rangle$$

Now apply to find $\langle S_z \rangle_{jm}$

$$\frac{\langle jm | S_z | jm \rangle}{\langle jm | J_z | jm \rangle} = \frac{\langle \vec{S} \cdot \vec{J} \rangle_j}{\langle \vec{J}^2 \rangle_j} = \frac{\langle \vec{S} \cdot \vec{J} \rangle_j}{\hbar^2 j(j+1)}$$

$$\langle jm | J_z | jm \rangle = m\hbar$$

$$\langle S_z \rangle_{jm} = \langle \vec{S} \cdot \vec{J} \rangle_j \frac{m}{\hbar j(j+1)}$$

$$\vec{S} \cdot \vec{J} = \frac{1}{2} ( \vec{J}^2 + \vec{S}^2 - \vec{L}^2 )$$

$$\langle S_z \rangle_{jm} = \frac{m}{2\hbar j(j+1)} \langle \vec{J}^2 + \vec{S}^2 - \vec{L}^2 \rangle_j$$

$$j = \begin{cases} l + \frac{1}{2} \\ l - \frac{1}{2} \end{cases}$$

$$\langle S_z \rangle_{l \pm \frac{1}{2}, m} = \frac{m\hbar}{2} \frac{1}{(l \pm \frac{1}{2})(l \pm \frac{1}{2} + 1)} \left( (l \pm \tfrac{1}{2})(l \pm \tfrac{1}{2} + 1) + \frac{3}{4} - l(l+1) \right)$$

$$= m\hbar \begin{cases} \dfrac{l + 3/2}{(2l+1)(l + 3/2)} \\ \dfrac{-(l - 1/2)}{(2l+1)(l - 1/2)} \end{cases}$$

$$\langle S_z \rangle_{jm} = \begin{cases} \dfrac{m\hbar}{2l+1} & j = l + \frac{1}{2} \\ \dfrac{-m\hbar}{2l+1} & j = l - \frac{1}{2} \end{cases}$$

Now to variational method.

$$\bar{H} = \frac{\langle\tilde{0}|H|\tilde{0}\rangle}{\langle\tilde{0}|\tilde{0}\rangle} \geq E_0 \quad \text{where } |\tilde{0}\rangle \text{ is a trial ket.}$$

Proof: $\quad |\tilde{0}\rangle = \sum |k\rangle\langle k|\tilde{0}\rangle$

where $\quad H|k\rangle = E_k|k\rangle \quad$ (eigenstates of the Hamiltonian)

$$\bar{H} = \frac{\sum |\langle k|\tilde{0}\rangle|^2 E_k}{\sum|\langle k|\tilde{0}\rangle|^2}$$

By definition, $E_0 \leq E_k$, so

$$\bar{H} = \frac{\sum|\langle k|\tilde{0}\rangle|^2 E_k}{\sum|\langle k|\tilde{0}\rangle|^2} \geq \frac{\cancel{\sum|\langle k|\tilde{0}\rangle|^2} E_0}{\cancel{\sum|\langle k|\tilde{0}\rangle|^2}} = E_0$$

Description of Method

1. Choose (judiciously) a trial wave function that contains a whole bunch of free parameters $\lambda_i$

$$\psi = \psi(\lambda_1, \lambda_2, \ldots)$$

2. Vary the parameters $\lambda_i$ until the expectation value of $H$ is minimized.

$$\frac{\partial \bar{H}}{\partial \lambda_i} = 0 \quad \text{for all } \lambda_i \quad i = 1, 2, \ldots$$

3. Substitute the optimum values of $\lambda_i$ into the expression for $\bar{H}$ and $\psi$.

Example: Anharmonic Oscillator in 1D

$$H = \frac{p^2}{2m} + cx^4$$

1. Choose ground state of simple harmonic oscillator

$$\psi = \lambda^{\frac{1}{2}} \pi^{-\frac{1}{4}} e^{-\lambda^2 x^2/2}$$

$$\bar{H} = \lambda \pi^{-1/2} \int_{-\infty}^{\infty} dx \; e^{-\lambda^2 x^2/2} \left( -\frac{\hbar^2}{2m} \partial_x^2 + cx^4 \right) e^{-\lambda^2 x^2/2}$$

$$= \lambda \pi^{-1/2} \int_{-\infty}^{\infty} dx \left( \frac{-\hbar^2}{2m} (\lambda^4 x^2 - \lambda^2) + cx^4 \right) e^{-\lambda^2 x^2}$$

$$\int_{-\infty}^{\infty} dx \; x^{2n} e^{-\lambda^2 x^2} = \begin{cases} \sqrt{\frac{\pi}{\lambda}} & n = 0 \\ \frac{(2n-1)!! \sqrt{\pi}}{2^n \lambda^{2n+1}} & n = 1, 2, \ldots \end{cases}$$

$$\bar{H} = \frac{\hbar^2 \lambda^2}{4m} + \frac{3c}{4\lambda^4}$$

2. $$\frac{d\bar{H}}{d\lambda} = \frac{\hbar^2 \lambda}{2m} - \frac{3c}{\lambda^5} = 0$$

$$\lambda^6 = \frac{3c(2m)}{\hbar^2} = \frac{6mc}{\hbar^2}$$

$$\lambda = \left( \frac{6mc}{\hbar^2} \right)^{1/6}$$

3. $$\bar{H}_{min} = \frac{\hbar^2}{4m} \left( \frac{6mc}{\hbar^2} \right)^{1/3} + \frac{3c}{4} \left( \frac{\hbar^2}{6mc} \right)^{2/3}$$

$$\bar{H}_{min} = \frac{3}{4} 3^{1/3} \left( \frac{\hbar^2}{2m} \right)^{2/3} c^{1/3} \approx 1.082 \left( \frac{\hbar^2}{2m} \right)^{2/3} c^{1/3}$$

Numerical computation $\rightarrow$ $\bar{H}_{min} = 1.060 \left( \frac{\hbar^2}{2m} \right)^{2/3} c^{1/3}$

02/02/2010 **Time-Dependent Potentials: The Interaction Picture**

$$H = H_0 + V(t)$$

$$H_0 |n\rangle = E_n |n\rangle$$

At $t=0$, $|\alpha\rangle = \sum_n c_n(0) |n\rangle$

In Schrödinger picture, for $t>0$

$$|\alpha, t\rangle_S = \sum_n \underset{\substack{\uparrow \\ \text{from } V(t)}}{c_n(t)} \, \underset{\substack{\uparrow \\ \text{from } H_0}}{e^{-iE_n t/\hbar}} |n\rangle$$

$$i\hbar \partial_t |\alpha, t\rangle_S = (H_0 + V(t)) |\alpha, t\rangle_S$$

For $n^{th}$ term

$$\left(i\hbar \frac{\partial c_n}{\partial t}\right) e^{-iE_n t/\hbar} |n\rangle + \cancel{E_n c_n(t) e^{-iE_n t/\hbar}} |n\rangle = \cancel{E_n c_n(t) e^{-iE_n t/\hbar}} |n\rangle + V(t) c_n(t) e^{-iE_n t/\hbar} |n\rangle$$

$$i\hbar \frac{\partial c_n}{\partial t} |n\rangle = V(t) c_n(t) |n\rangle$$

Define
$$\left.\begin{aligned} |\alpha, t\rangle_I &= e^{iH_0 t/\hbar} |\alpha, t\rangle_S \\ A_I(t) &= e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar} \end{aligned}\right\} \text{Interaction Picture (Intermediate Picture)}$$

Compare to Heisenberg Picture

$$|\alpha\rangle_H = e^{iHt/\hbar} |\alpha, t\rangle_S$$

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

(full Hamiltonian where interaction picture uses only $H_0$)

$$i\hbar \partial_t |\alpha, t\rangle_I = i\hbar \partial_t \left( e^{iH_0 t/\hbar} |\alpha, t\rangle_S \right)$$

$$= -H_0 e^{iH_0 t/\hbar} |\alpha, t\rangle_S + e^{iH_0 t/\hbar} \underbrace{(H_0 + V(t))|\alpha, t\rangle_S}_{\text{from Schrödinger equation}}$$

$$[H_0, e^{iH_0 t/\hbar}] = 0$$

$$\Rightarrow \quad i\hbar \partial_t |\alpha, t\rangle_I = \overbrace{e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar}}^{V_I(t)} \underbrace{|\alpha, t\rangle_I}_{|\alpha, t\rangle_S}$$

$$\boxed{i\hbar \partial_t |\alpha, t\rangle_I = V_I(t) |\alpha, t\rangle_I}$$

$$\frac{dA_I}{dt} = \frac{iH_0}{\hbar} A_I(t) - A_I(t) \left( \frac{iH_0}{\hbar} \right)$$

$$\boxed{\frac{dA_I}{dt} = \frac{1}{i\hbar} [A_I, H_0]}$$

Heisenberg Picture $\rightarrow \quad \dfrac{dA_H}{dt} = \dfrac{1}{i\hbar} [A_H, H]$

$$\boxed{|\alpha, t\rangle_I = \sum_n c_n(t) |n\rangle}$$

Look for $c_n(t)$

$$i\hbar \partial_t (\langle n|\alpha, t\rangle_I) = \langle n| V_I(t) \underset{\uparrow \atop \sum |m\rangle\langle m|}{} |\alpha, t\rangle_I$$

$$i\hbar \partial_t (\langle n|\alpha, t\rangle_I) = \sum \langle n| V_I(t) |m\rangle \langle n|\alpha, t\rangle_I$$

Because $\langle n|\alpha, t\rangle_I = c_n(t)$ and

$$\langle n| V_I(t) |m\rangle = \langle n| e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar} |m\rangle$$

$$= e^{i(E_n - E_m)t/\hbar} \underbrace{\langle n| V(t) |m\rangle}_{V_{nm}(t)}$$

$$i\hbar\,\partial_t c_n(t) = \sum_m V_{nm}(t)\, e^{i\omega_{nm}t}\, c_m(t)$$

$$\omega_{nm} = \frac{E_n - E_m}{\hbar} \qquad (\omega_{nm} = -\omega_{mn})$$

$$i\hbar \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \\ \vdots \\ \dot{c}_n \end{pmatrix} = \begin{pmatrix} V_{11}(t) & V_{12}(t)e^{i\omega_{12}t} & \cdots \\ V_{21}(t)e^{i\omega_{21}t} & V_{22}(t) & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix}$$

Example: Time-Dependent Two State Problem

$$H_0 = E_1 |1\rangle\langle 1| + E_2 |2\rangle\langle 2| \qquad (E_2 > E_1)$$

$$V(t) = \gamma e^{i\omega t} |1\rangle\langle 2| + \gamma e^{-i\omega t} |2\rangle\langle 1| \qquad (\gamma, \omega \text{ are real and positive})$$

One example of this problem is Spin Magnetic Resonance

$$H = -\vec{\mu}\cdot\vec{B} \qquad \left(\vec{\mu} = \frac{e}{m_e c}\vec{S}\right)$$

$$\vec{B} = B_0\hat{z} + B_1(\hat{x}\cos(\omega t) + \hat{y}\sin(\omega t))$$

$$H = H_0 + V(t)$$

$$H_0 = -\frac{e\hbar B_0}{2m_e c}\left(|+\rangle\langle +| - |-\rangle\langle -|\right)$$

$$V(t) = \frac{-e\hbar B_1}{2m_e c}\left(\cos(\omega t)\left(|+\rangle\langle -| + |-\rangle\langle +|\right) + \sin(\omega t)\left(-i|+\rangle\langle -| + i|-\rangle\langle +|\right)\right)$$

$$V(t) = \frac{-e\hbar B_1}{2m_e c} e^{-i\omega t} |+\rangle\langle -| - \frac{e\hbar B_1}{2m_e c} e^{i\omega t} |-\rangle\langle +|$$

$$|+\rangle \to |2\rangle \qquad (e < 0,\ E_+ > E_-)$$

$$|-\rangle \to |1\rangle$$

$$\omega_{21} = \frac{|e| B_0}{m_e c} = \frac{E_+ - E_-}{\hbar}$$

$$i\hbar \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \end{pmatrix} = \begin{pmatrix} 0 & \gamma e^{i\omega t} e^{i\omega_{12} t} \\ \gamma e^{-i\omega t} e^{i\omega_{21} t} & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$i\hbar \frac{d}{dt} c_1(t) = \gamma e^{i(\omega - \omega_{21})t} c_2(t)$$

$$i\hbar \frac{d}{dt} c_2(t) = \gamma e^{-i(\omega - \omega_{21})t} c_1(t)$$

Define $\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} e^{i(\omega - \omega_{21})t/2} a_1 \\ e^{-i(\omega - \omega_{21})t/2} a_2 \end{pmatrix}$

$$\ddot{a}_1 = -\left( \frac{\gamma^2}{\hbar^2} + \frac{(\omega - \omega_{21})^2}{4} \right) a_1$$

$$\ddot{a}_2 = -\left( \frac{\gamma^2}{\hbar^2} + \frac{(\omega - \omega_{21})^2}{4} \right) a_2$$

From $\frac{i(\omega - \omega_{21})}{2} a_1 + \dot{a}_1 = \frac{\gamma}{i\hbar} a_2$

$$\frac{-i(\omega - \omega_{21})}{2} a_2 + \dot{a}_2 = \frac{\gamma}{i\hbar} a_1$$

Suppose $c_1(0) = 1$

then $c_2(t) = \dfrac{\gamma}{i\hbar\left( \frac{\gamma^2}{\hbar^2} + \frac{(\omega - \omega_{21})^2}{4} \right)^{1/2}} e^{-i(\omega - \omega_{21})t/2} \sin\left( \left( \frac{\gamma^2}{\hbar^2} + \frac{(\omega - \omega_{21})^2}{4} \right)^{1/2} t \right)$

$$|c_2(t)|^2 = \frac{(\gamma/\hbar)^2}{\left( \frac{\gamma^2}{\hbar^2} \right) + \frac{(\omega - \omega_{21})^2}{4}} \sin^2\left( \left( \frac{\gamma^2}{\hbar^2} + \frac{(\omega - \omega_{21})^2}{4} \right)^{1/2} t \right)$$

$$|c_1(t)|^2 = 1 - |c_2(t)|^2$$

02/04/2010 For problem 2 HW#3

$$\vec{A} = \frac{1}{2}\vec{B}\times\vec{r}$$

$$\vec{A}^2 = \frac{1}{4}\left(r^2B^2 - (\vec{r}\cdot\vec{B})^2\right)$$

## Time-Dependent Perturbation Theory

$$|\alpha, t\rangle_S = U(t,t_0)\,|\alpha, t_0\rangle_S$$

$$|\alpha, t\rangle_I = U_I(t,t_0)\,|\alpha, t_0\rangle_I \qquad (U_I(t_0,t_0) = \mathbb{I})$$

$$i\hbar\frac{\partial}{\partial t}|\alpha, t\rangle_S = H|\alpha, t\rangle_S$$

$$i\hbar\frac{\partial}{\partial t}|\alpha, t\rangle_I = V_I(t)\,|\alpha, t\rangle_I$$

$$|\alpha, t\rangle_I = e^{iH_0t/\hbar}\,|\alpha, t\rangle_S$$

$$V_I(t) = e^{iH_0t/\hbar}\,V(t)\,e^{iH_0t/\hbar}$$

$$\boxed{i\hbar\frac{\partial}{\partial t}U_I(t,t_0) = V_I(t)\,U_I(t,t_0)}$$

Schrödinger → $i\hbar\frac{\partial}{\partial t}U(t,t_0) = H\,U(t,t_0)$

$$dU_I(t,t_0) = \frac{1}{i\hbar}V_I(t)\,U_I(t,t_0)\,dt$$

Integrate both sides from $t_0$ to $t$

$$\int_{t_0}^{t} dU_I(t,t_0) = \int_{t_0}^{t}\frac{1}{i\hbar}V_I(t)\,U_I(t,t_0)\,dt$$

$$U_I(t,t_0) - \underbrace{U_I(t_0,t_0)}_{1} = \frac{-i}{\hbar}\int_{t_0}^{t}V_I(t)\,U_I(t,t_0)\,dt$$

Dyson Series

$$U_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} V_I(t')\,dt' + \left(\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, V_I(t')\,V_I(t'') + \cdots$$

$$-\left(\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt' \int_{t_0}^{t''} \cdots \int_{t_1}^{t^{(n-1)}} dt^{(n)}\, V_I(t')\,V_I(t'') \cdots V_I(t^{(n)})$$

$$+ \cdots$$

Suppose $|\alpha, t_0\rangle = |i\rangle$, then

$$|\alpha, t\rangle_I = U_I(t,t_0)\,|i\rangle$$

$$= \sum_n |n\rangle \underbrace{\langle n| U_I(t,t_0)|i\rangle}_{C_n(t)}$$

$$C_n(t) = \langle n| U_I(t,t_0)|i\rangle$$

$$= \langle n|\left(1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, V_I(t') + \cdots\right)|i\rangle$$

$$= \underbrace{\langle n|i\rangle}_{\delta_{ni}} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \langle n|V_I(t')|i\rangle + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t}\int_{t_0}^{t'} dt''dt'\, \langle n|V_I(t')V_I(t'')|i\rangle + \cdots$$

$$C_n(t) = C_n^{(0)}(t) + C_n^{(1)}(t) + C_n^{(2)}(t) + \cdots$$

$$C_n^{(0)}(t) = \delta_{ni} \quad \text{(time independent)}$$

$$C_n^{(1)}(t) = \frac{-i}{\hbar}\int_{t_0}^{t} dt'\, \langle n|V_I(t')|i\rangle$$

$$= \frac{-i}{\hbar}\int_{t_0}^{t} dt'\, \langle n| e^{iH_0t'/\hbar}\, V(t')\, e^{-iH_0t'/\hbar}|i\rangle$$

$$\boxed{C_n^{(1)}(t) = \frac{-i}{\hbar}\int_{t_0}^{t} dt'\, e^{i(E_n-E_i)t'/\hbar}\, \langle n|V(t')|i\rangle}$$

$$\omega_{ni} = \frac{E_n - E_i}{\hbar} \qquad \langle n | V(t) | i \rangle = V_{ni}(t)$$

$$\boxed{C_n^{(1)}(t) = \frac{-i}{\hbar}\int_{t_0}^{t} dt' \, e^{i\omega_{ni}t'} V_{ni}(t')}$$

For second order, insert closure relation between $V_I(t') V_I(t'')$

$$\boxed{C_n^{(2)}(t) = \left(\frac{-i}{\hbar}\right)^2 \sum_m \int_{t_0}^{t}\int_{t_0}^{t'} dt'' \, dt' \, e^{i\omega_{nm}t'} V_{nm}(t') \, e^{i\omega_{mi}t''} V_{mi}(t'')}$$

Transition Probability

$$(n \neq i)$$

$$P(i \to n) = |C_n(t)|^2 = |C_n^{(1)}(t) + C_n^{(2)}(t) + \cdots|^2 \qquad (C_{n\neq i}^{(0)}(t) = 0)$$

Example: Two State Problem

$$V(t) = \gamma e^{i\omega t} |1\rangle\langle 2| + \gamma e^{-i\omega t} |2\rangle\langle 1|$$

$|i\rangle = |1\rangle \; (t=0)$ Find $C_2$.

$$C_2^{(1)}(t) = \frac{-i}{\hbar}\int_0^t dt' \, e^{i\omega_{21}t'} V_{21}(t')$$

$$= \frac{-i}{\hbar}\int_0^t dt' \, \gamma e^{-i(\omega-\omega_{21})t'}$$

$$= \frac{\gamma}{\hbar}\left(e^{-i(\omega-\omega_{21})t} - 1\right)\frac{1}{\omega-\omega_{21}}$$

$$|C_2^{(1)}(t)|^2 = C_2^{(1)}(t) \cdot \left(C_2^{(1)}(t)\right)^*$$

$$= \left(\frac{\gamma}{\hbar}\right)^2 \frac{1}{(\omega-\omega_{21})^2}\left(1 + 1 - e^{-i(\omega-\omega_{21})t} - e^{i(\omega-\omega_{21})t}\right)$$

$$= \left(\frac{\gamma}{\hbar}\right)^2 \frac{2(1-\cos((\omega-\omega_{21})t))}{(\omega-\omega_{21})^2}$$

$$\boxed{|C_2^{(1)}(t)|^2 = \left(\frac{\gamma}{\hbar}\right)^2 \frac{4}{(\omega-\omega_{21})^2} \sin^2\left(\frac{(\omega-\omega_{21})t}{2}\right)}$$

Compare to Rabi's formula from last time

$$|c_2(t)|^2 = \frac{(\gamma/\hbar)^2}{\left(\frac{\gamma}{\hbar}\right)^2 + \frac{(\omega-\omega_{21})^2}{4}} \sin^2\left(\sqrt{\left(\frac{\gamma}{\hbar}\right)^2 + \frac{(\omega-\omega_{21})^2}{4}}\; t\right)$$

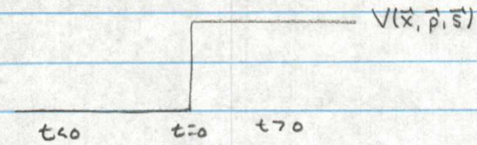
Expanded to first order, we find $|c_2^{(1)}(t)|^2$.

Resonance at $\omega = \omega_{21}$ (see pg 322)

02/09/2010

## Interactions with the Classical Radiation Field

Example: Constant Perturbation




$$C_n^{(0)}(t) = C_n^{(0)}(0) = \delta_{ni}$$

$$C_n^{(1)}(t) = \frac{-i}{\hbar}\int_0^t dt' \, e^{i\omega_{ni}t'} V_{ni}$$

$$= \frac{-i}{\hbar} V_{ni} \int_0^t dt' \, e^{i\omega_{ni}t'} \qquad \omega_{ni} = \frac{1}{\hbar}(E_n - E_i)$$

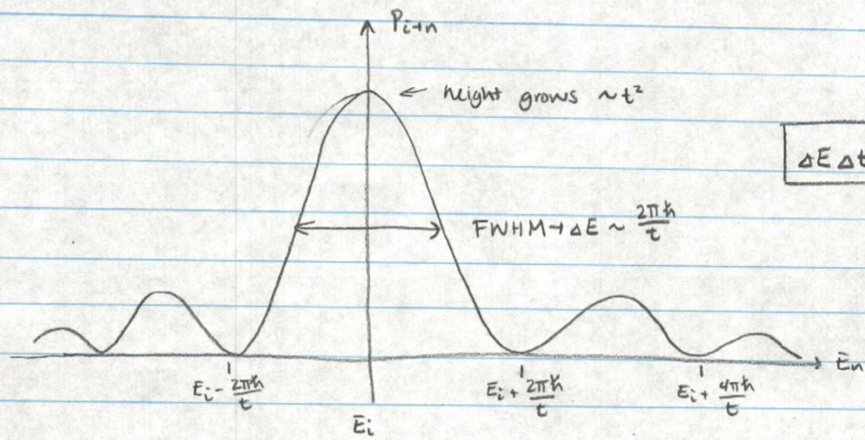
$$= \frac{-i}{\hbar} V_{ni} \left( \frac{1}{i\omega_{ni}} \left( e^{i\omega_{ni}t} - 1 \right) \right)$$

$$C_n^{(1)}(t) = \frac{+V_{ni}}{\hbar\omega_{ni}} \left( 1 - e^{i\omega_{ni}t} \right)$$

$$|C_n^{(1)}(t)|^2 = P_{i\to n}(t) = C_n^{(1)}(t)\, C_n^{(1)*}(t)$$

$$= \frac{|V_{ni}|^2}{\hbar^2\omega_{ni}^2} \left( 4\sin^2(\omega_{ni}t/2) \right)$$

$$= \left( \frac{\sin\left( \frac{E_n - E_i}{2\hbar} t \right)}{\left( \frac{E_n - E_i}{2} \right)} \right)^2 |V_{ni}|^2$$




$$\boxed{\Delta E \, \Delta t \sim \hbar}$$

$$\sum_{n\ (E_n \approx E_i)} |C_n^{(1)}(t)|^2 \longrightarrow \int dE_n \underset{\substack{\uparrow \\ \text{density of states}}}{\rho(E_n)} |C_n^{(1)}(t)|^2$$

$$= 4 \int dE_n \sin^2\left(\frac{E_n - E_i}{2\hbar} t\right) |V_{ni}|^2 \frac{1}{(E_n - E_i)^2} \rho(E_n)$$

At large $t$, $\dfrac{\sin^2\left(\frac{E_n - E_i}{2\hbar} t\right)}{(E_n - E_i)^2}$ acts like $\delta(E_n - E_i)$

$$\lim_{\alpha \to \infty} \frac{1}{\pi} \frac{\sin^2(\alpha x)}{\alpha x^2} = \delta(x)$$

$$\lim_{t \to \infty} \frac{1}{(E_n - E_i)^2} \sin^2\left(\frac{E_n - E_i}{2\hbar} t\right) = \frac{\pi t}{2\hbar} \delta(E_n - E_i)$$

$$\lim_{t \to \infty} \int dE_n \rho(E_n) |C_n^{(1)}(t)|^2 = \frac{2\pi}{\hbar} \overline{|V_{ni}|^2} \rho(E_n) t \Big|_{E_n \approx E_i}$$

Rate of transition

$$\frac{d}{dt}\left(\sum_n |C_n^{(1)}(t)|^2\right) = \text{constant}$$

<u>Fermi's Golden Rule</u>:

Transition rate $i \to [n]$

$$W_{i \to [n]} = \frac{2\pi}{\hbar} \overline{|V_{ni}|^2} \rho(E_n) \Big|_{E_n \approx E_i}$$

$[n]$ - group of final states with energy similar to $i$.

Up to $2^{nd}$ order $\overline{|V_{ni}|^2} \to \overline{\left|V_{ni} + \sum_m \frac{V_{nm} V_{mi}}{E_i - E_m}\right|^2}$

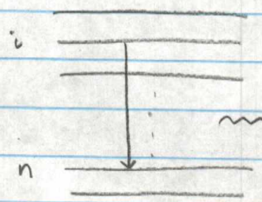
Harmonic Perturbation

$$V(t) = V(\vec{x}, \vec{p}, \vec{s})\, e^{\mp i\omega t}$$

$$W_{i \to [n] \pm \gamma} = \frac{2\pi}{\hbar} \left| \overline{V_{n\mp\gamma, i}} \right|^2 \rho(E_n \mp \hbar\omega) \Big|_{E_n \pm \hbar\omega \approx E_i}$$

emit/absorb a photon

Example: Spontaneous Emission




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

$$= \frac{\vec{p}^{\,2}}{2m} \underbrace{- \frac{e}{mc} \vec{A}(\vec{r}, t) \cdot \vec{p}}_{V(t)} + \frac{e^2 \vec{A}^2}{2mc^2} + e\phi$$

(classical field)

$$\vec{A}(\vec{r}, t) = A_0 \vec{\epsilon}\, e^{-i(\vec{k}\cdot\vec{r} - \omega t)}$$

polarization of $\gamma$

$$\text{Single photon energy density} = \frac{\hbar\omega}{V} = \frac{1}{8\pi}\left(|\vec{E}|^2 + |\vec{B}|^2\right)$$

$$= \frac{1}{8\pi}\left(\left|-\frac{1}{c}\frac{\partial \vec{A}}{\partial t}\right|^2 + |\nabla \times \vec{A}|^2\right)$$

$$\left|\frac{-1}{c}\frac{\partial \vec{A}}{\partial t}\right|^2 = \left|\frac{-1}{c} A_0 \vec{\epsilon}(i\omega)\, e^{-i(\vec{k}\cdot\vec{r} - \omega t)}\right|^2$$

$$|\nabla \times \vec{A}|^2 = \left| -i A_0\, \vec{k} \times \vec{\epsilon}\, e^{-i(\vec{k}\cdot\vec{r} - \omega t)} \right|^2$$

$$(\vec{k} \times \vec{\epsilon}) \cdot (\vec{k} \times \epsilon)^* = \vec{k}^2\, \vec{\epsilon} \cdot \vec{\epsilon}^* - \cancel{|\vec{k} \cdot \vec{\epsilon}|^2}$$

0 transverse wave

$$\sum_{\lambda=1}^{2} \vec{\epsilon} \cdot \vec{\epsilon}^* = 2 \qquad \frac{\omega}{k} = c$$

$$\Rightarrow \frac{\hbar\omega}{V} = \frac{1}{8\pi}\left(|E|^2 + |B|^2\right) = \frac{\omega^2 |A_0|^2}{2\pi c^2}$$

$$A_0 = \sqrt{\frac{2\pi c^2 \hbar}{\omega V}}$$

$$V(t) = \underbrace{\left(\frac{-e}{mc}\sqrt{\frac{2\pi c^2 \hbar}{\omega V}}\; e^{-i(\vec{k}\cdot\vec{r})}\;\vec{\epsilon}\cdot\vec{p}\right)}_{V(\vec{r},\vec{p},\vec{\epsilon})} e^{i\omega t}$$

Transition rate

$$\Gamma_{i\to n+\gamma} = \frac{2\pi}{\hbar}\int dE_\gamma\, \rho(E_\gamma)\,|\langle n|\,V(\vec{r},\vec{p},\vec{\epsilon})\,|i\rangle|^2\, \delta(E_n + E_\gamma - E_i)$$

$$dE_\gamma\, \rho(E_\gamma) = d^3 n_\gamma = dn_x\, dn_y\, dn_z = \left(\frac{L}{2\pi}\right)^3 d^3 k$$

$$k_x = \frac{2\pi n_x}{L} \quad \text{etc.} \qquad V = L^3$$

$$\left(\frac{L}{2\pi}\right)^3 d^3 k = \frac{V}{(2\pi)^3}\, k^2 dk\, d\Omega_k$$

$$= \frac{V}{(2\pi c)^3}\,\omega^2 d\omega\, d\Omega_k$$

$$= \frac{V}{(2\pi\hbar c)^3}\,(\hbar\omega)^2\, \underbrace{d(\hbar\omega)}_{dE_\gamma}\, d\Omega_k$$

$$\rightarrow \rho(E_\gamma) = \frac{V}{(2\pi\hbar c)^3}\,(\hbar\omega)^2\, d\Omega_k$$

$$\Gamma_{i\to n+\gamma} = \frac{2\pi}{\hbar}\int d\Omega_k\, d(\hbar\omega)\, \frac{V(\hbar\omega)^2}{(2\pi\hbar c)^3}\, \frac{e^2}{m^2c^2}\left(\frac{2\pi c^2 \hbar}{\omega V}\right)\left|\langle n|\, e^{-i\vec{k}\cdot\vec{r}}\,\vec{\epsilon}\cdot\vec{p}\,|i\rangle\right|^2 \delta(E_n + \hbar\omega - E_i)$$

$$= \frac{\alpha}{2\pi}\int d\Omega_k\, \frac{E_i - E_n}{\hbar c}\left|\frac{1}{mc}\langle n|\, e^{-i\vec{k}\cdot\vec{r}}\,\vec{\epsilon}\cdot\vec{p}\,|i\rangle\right|^2$$

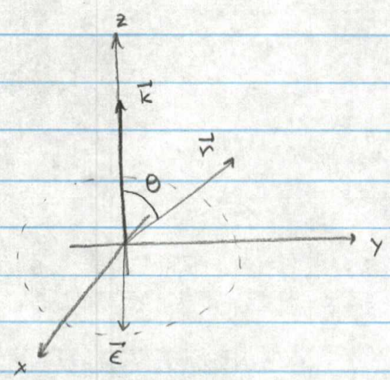
$$\alpha = \frac{e^2}{\hbar c}$$

02/11/2010 Energy Shift and Decay Width

Spontaneous Emission

$$\begin{array}{l} i \ \text{———} \\ \quad \downarrow \ \rightsquigarrow \gamma \\ n \ \text{———} \end{array}$$

$$\Gamma_{i\to n+\gamma} = \frac{\alpha}{2\pi} \int d\Omega_k \, \frac{E_i - E_n}{\hbar\omega} \left| \frac{1}{mc} \langle n | e^{-i\vec{k}\cdot\vec{r}} \, \vec{\epsilon}\cdot\vec{p} \, | i \rangle \right|^2$$




$$\vec{k}\cdot\vec{r} \sim \frac{\langle \vec{r} \rangle}{\lambda} \sim \frac{1\,\text{Å}}{100-1000\,\text{Å}} \ll 1$$

$$\to \ e^{-i\vec{k}\cdot\vec{r}} \sim 1 - i\vec{k}\cdot\vec{r} + \frac{1}{2}(-i\vec{k}\cdot\vec{r})^2 \sim 1 \qquad (\vec{k}\cdot\vec{r} \ll 1)$$

Dipole approximation

$$\langle n | \vec{\epsilon}\cdot\vec{p} | i \rangle = \frac{m}{i\hbar} \vec{\epsilon} \cdot \langle n | [\vec{r}, H_0] | i \rangle$$

$$\vec{p} = m \frac{d\vec{r}}{dt} = m \frac{1}{i\hbar} [\vec{r}, H_0]$$

$$\to \Gamma_{i\to n+\gamma} = \frac{\alpha}{2\pi} \int d\Omega_k \, \frac{E_i - E_n}{\hbar} \left| \frac{1}{mc} \langle n | \vec{\epsilon}\cdot\vec{p} | i \rangle \right|^2$$

$$\langle n | [\vec{r}, H_0] | i \rangle = \langle n | \vec{r} H_0 - H_0 \vec{r} | i \rangle = (E_i - E_n) \langle n | \vec{r} | i \rangle$$

$$\sum_{pol} |\vec{\epsilon} \langle n | \vec{r} | i \rangle|^2 = |\epsilon_x \langle n | x | i \rangle|^2 + |\epsilon_y \langle n | y | i \rangle|^2$$

$$= |\langle n | x | i \rangle|^2 + |\langle n | y | i \rangle|^2 \qquad (\epsilon_i \epsilon_i^* = 1)$$

$$= |\langle n | \vec{r} | i \rangle|^2 - |\langle n | z | i \rangle|^2$$

$$z = \frac{\vec{k}\cdot\vec{r}}{|\vec{k}|} = \frac{\cos(\theta)}{|\vec{k}|}$$

$$|\langle n|\vec{r}|i\rangle|^2 - |\langle n|z|i\rangle|^2 = |\langle n|\vec{r}|i\rangle|^2 (1-\cos^2(\theta)) = |\langle n|\vec{r}|i\rangle|^2 \sin^2(\theta)$$

$$\omega_{in} = \frac{E_i - E_n}{\hbar}$$

$$\rightarrow \Gamma_{i\to n+r} = \frac{\alpha}{2\pi c^2}\int d\Omega_k \; \omega_{in}^3 \; |\langle n|\vec{r}|i\rangle|^2 \sin^2(\theta)$$

$$= \frac{\alpha}{2\pi c^2}\,\omega_{in}^3\,|\langle n|\vec{r}|i\rangle|^2 \left(\frac{8\pi}{3}\right)$$

$$= \frac{4e^2}{3\hbar c^3}\,\omega_{in}^3\,|\langle n|\vec{r}|i\rangle|^2$$

Jackson pg 665 Eq. 14.22 ($2^{nd}$ Edition)

Total power radiated by an accelerated charge.

$$P = \frac{2e^2\vec{a}^{\,2}}{3c^3} = \frac{2e^2(r\omega^2)^2}{3c^3}$$

$$P\cdot\tau = \frac{\hbar\omega}{2} \qquad \tau - \text{half lifetime}$$

$$\Gamma = \frac{1}{\tau} = \frac{P}{\hbar\omega/2}$$

$$\Gamma = \frac{4e^2\omega^3}{3\hbar c^3}\,r^2 \qquad \text{Classical correspondence.}$$

Example: $2p \rightarrow 1s$ Transition in Hydrogen-like Atom

$$\Gamma_{2p\to 1s} = \frac{4}{3}\,\frac{e^2}{\hbar c^3}\,\omega^3\,|\langle 1s|\vec{r}|2p\rangle|^2$$

$$\omega = \frac{E_{2p}-E_{1s}}{\hbar} = \frac{3}{8}\left(\frac{mc^2}{\hbar}\right) Z^2\alpha^2$$

$$E_{1s} = \frac{-Z^2}{2}mc^2\alpha^2 \qquad E_{2p} = \frac{-Z^2}{8}mc^2\alpha^2$$

$$\langle 100|\vec{r}|21m\rangle = \frac{1}{\sqrt{3}}\left(\frac{-\hat{x}+i\hat{y}}{\sqrt{2}}\delta_{m1} + \frac{\hat{x}+i\hat{y}}{\sqrt{2}}\delta_{m-1} + \hat{z}\,\delta_{m0}\right)\int_0^\infty dr\, r^3 R_{10}(r) R_{21}(r)$$

$$\int_0^\infty dr\, r^3 R_{10}(r)\, R_{21}(r) = \frac{1}{\sqrt{6}}\left(\frac{Z}{a_0}\right)^4 \int_0^\infty dr\, r^4 e^{-3Zr/2a_0}$$

$$= 4\sqrt{6}\left(\frac{2}{3}\right)^5 \frac{a_0}{Z}$$

$$\bar{\Gamma}_{2p\to 1s+\gamma} = \frac{1}{3}\sum_m \Gamma_{2p\to 1s+\gamma} = \frac{2^{17}}{3^{11}}\,\frac{e^2\omega^3}{\hbar c^3}\left(\frac{a_0}{Z}\right)^2$$

$$a_0 = \frac{\hbar}{me^2} \qquad \omega = \frac{3}{8}\left(\frac{mc^2}{\hbar}\right)Z^2\alpha^2 \qquad \alpha = \frac{e^2}{\hbar c}$$

$$\boxed{\bar{\Gamma}_{2p\to 1s+\gamma} = \left(\frac{2}{3}\right)^8 \frac{mc^2}{\hbar}\,\alpha^5 Z^4}$$

$$\bar{\Gamma}_{2p\to 1s+\gamma} \approx 6\times 10^8\, Z^4\ /s$$

$$\tau = \frac{1}{\Gamma} \approx 1.6\times 10^{-9}\, Z^{-4}\ s$$

$$\lim_{\epsilon\to 0}\frac{1}{x+i\epsilon} = P\frac{1}{x} - i\pi\delta(x) \qquad P\frac{1}{x} \to \text{principle value of } \frac{1}{x}$$

Real part of energy shift → level shift

Imaginary part of energy shift → decay width - allows spontaneous emission

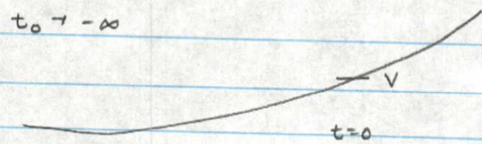
$$n\neq i \quad c_n^{(1)} = \frac{V_{ni}}{E_n - E_i}\left(1 - e^{i\omega_{ni}t}\right)$$

$$c_i^{(1)} = ?$$

Slow-turn-on Method (Adiabatic Approximation)

$$V \to e^{\eta t}\, V \qquad (0<\eta<1)$$

After calculation, $\eta \to 0$




$n \neq i$

$$C_n^{(1)}(t) = \frac{-i}{\hbar} V_{ni} \lim_{t_0 \to -\infty} \int_{t_0}^{t} dt' \, e^{\eta t'} e^{i\omega_{ni} t'}$$

$$= \frac{-i}{\hbar} V_{ni} \frac{e^{\eta t + i\omega_{ni} t}}{\eta + i\omega_{ni}}$$

$$|C_n(t)|^2 \approx \frac{|V_{ni}|^2}{\hbar^2} \frac{e^{2\eta t}}{\eta^2 + \omega_{ni}^2}$$

$$\frac{d}{dt}|C_n(t)|^2 \approx \frac{2|V_{ni}|^2}{\hbar^2} \frac{\eta e^{2\eta t}}{\eta^2 + \omega_{ni}^2}$$

$$\lim_{\eta \to 0} \frac{\eta}{\eta^2 + \omega_{ni}^2} = \pi \, \delta(\omega_{ni}) = \pi \hbar \, \delta(E_n - E_i)$$

$$\frac{d}{dt}|C_n(t)|^2 = W_{i\to n} \approx \frac{2\pi}{\hbar} |V_{ni}|^2 \delta(E_n - E_i)$$ Fermi's Golden Rule.

$$C_i^{(0)}(t) = 1$$

$$C_i^{(1)}(t) = \frac{-i}{\hbar} V_{ii} \frac{e^{\eta t}}{\eta}$$

$$C_i^{(2)}(t) = \left(\frac{-i}{\hbar}\right)^2 |V_{ii}|^2 \frac{e^{2\eta t}}{2\eta^2} + \left(\frac{-i}{\hbar}\right) \sum_{m\neq i} \frac{|V_{mi}|^2 e^{2\eta t}}{2\eta(E_i - E_m + i\hbar\eta)}$$

$$C_i(t) = C_i^{(0)}(t) + C_i^{(1)}(t) + C_i^{(2)}(t) + \cdots$$

$$\frac{\dot{c}_i}{c_i} = \frac{-i}{\hbar} V_{ii} + \left(\frac{-i}{\hbar}\right) \sum_{m\neq i} \frac{|V_{mi}|^2}{E_i - E_m + i\hbar\eta} = \frac{i}{\hbar} \Delta_i$$

$$\boxed{C_i(t) = e^{-i\Delta_i t/\hbar}}$$

$$e^{-i\Delta_i t/\hbar} = e^{-i\mathrm{Re}(\Delta_i) t/\hbar} \, e^{-\mathrm{Im}(\Delta_i) t/\hbar}$$

$$\Delta_i = \mathrm{Re}(\Delta_i) + i \, \mathrm{Im}(\Delta_i)$$

$$\mathrm{Im}(\Delta_i^{(2)}) = -\pi \sum_{m\neq i} |V_{mi}|^2 \delta(E_i - E_m) < 0 \Rightarrow \boxed{\frac{\Gamma_i}{\hbar} = \frac{-2}{\hbar} \mathrm{Im}(\Delta_i)}$$

Decay width

02/18/2010 **Permutation Symmetry and Symmetrization Postulate**

Example: Two identical particles, mass m, in 1D box

$$V(x) = \begin{cases} 0 & 0 \le x \le a \\ \infty & \text{else} \end{cases}$$

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

$$H = H_1(x_1) + H_2(x_2)$$

$$H\psi(x_1, x_2) = E\psi(x_1, x_2)$$

$$\psi_{n_1 n_2}(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2) \qquad \text{(Hartree)}$$

$$E_{n_1 n_2} = E_{n_1} + E_{n_2} = \frac{\pi^2\hbar^2}{2ma^2}(n_1^2 + n_2^2)$$

Ground State $\rightarrow$ $n_1 = n_2 = 1$

$$\psi_{11}(x_1, x_2) = \psi_1(x_1)\psi_1(x_2) = \psi_1(x_2)\psi_1(x_1)$$

Symmetric under permutation of particles.

Excited states $\rightarrow$ $n_1 = 1, n_2 = 2$ or $n_1 = 2, n_2 = 1$

$$\psi_1(x_1)\psi_2(x_2) \neq \psi_1(x_2)\psi_2(x_1)$$

In general $\psi_{n_1}(x_1)\psi_{n_2}(x_2) \neq \psi_{n_1}(x_2)\psi_{n_2}(x_1)$ when $n_1 \neq n_2$

$P_{12}$ : two particle exchange operator

$$P_{12} \psi_{n_1 n_2}(x_1, x_2) = \psi_{n_1 n_2}(x_2, x_1)$$

$$[H, P_{12}] = 0$$

$P_{12}^2 = I \rightarrow$ two eigenvalues $\pm 1$

$+1 \rightarrow$ boson system - integer spin system $(\gamma, \pi, He^4)$

$-1 \rightarrow$ fermion system - half-integer spin system $(e^-, p^+, \mu, \nu)$

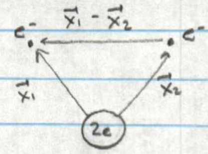
Hartree - Fock

$$P_{12} = +1 \rightarrow \quad \psi^{(S)}_{n_1 n_2} = \frac{1}{\sqrt{2}}\left(\psi_{n_1}(x_1)\psi_{n_2}(x_2) + \psi_{n_1}(x_2)\psi_{n_2}(x_1)\right)$$

$$P_{12} = -1 \rightarrow \quad \psi^{(A)}_{n_1 n_2} = \frac{1}{\sqrt{2}}\left(\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)\right)$$

02/23/2010 Two Electron System

Example: Hamiltonian of Helium Atom




$$r_1 = |\vec{x}_1| \qquad r_2 = |\vec{x}_2| \qquad r_{12} = |\vec{x}_1 - \vec{x}_2|$$

$$H = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_{12}}$$

↑ repulsion of 2 electrons

$$\Psi(\vec{x}_1, \vec{x}_2) = \phi_{space}(\vec{x}_1, \vec{x}_2)\, \chi_{spin}(m_1, m_2)$$

$$P_{12} = -1 \qquad \text{(fermion system)}$$

$$P_{12} = P_{12}^{(space)} P_{12}^{(spin)}$$

Spin wavefunction

$$\frac{1}{2} \otimes \frac{1}{2} = \begin{cases} 1 \text{ (triplet)} & \begin{cases} |\uparrow\uparrow\rangle \rightarrow \chi_{++} \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \rightarrow \frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{-+}) \\ |\downarrow\downarrow\rangle \rightarrow \chi_{--} \end{cases} \\ 0 \text{ (singlet)} & \left\{ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \rightarrow \frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+}) \right. \end{cases}$$

$$P_{12}^{(spin)} = \begin{cases} +1 & \text{triplet} \\ -1 & \text{singlet} \end{cases}$$

Space wavefunction

Neglect the repulsion term

$$\phi(\vec{x}_1, \vec{x}_2) = \psi_{100}(\vec{x}_1)\, \psi_{100}(\vec{x}_2)$$

$$E^{ground} = -\underbrace{\left(\frac{mc^2\alpha^2}{2}\right)}_{13.6\,eV} Z^2$$

$$E_1^{ground} = (-13.6\,eV)(4) \qquad E_2^{ground} = (-13.6\,eV)(4)$$

$$E_{tot}^{ground} = -108.8\,eV$$

$$E_{experimental}^{ground} = -78.975\,eV \rightarrow \text{Can't neglect repulsion term!}$$

Treat it as a perturbation.

$$H_0 = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2}$$

$$V = \frac{e^2}{r_{12}}$$

$$\Psi(\vec{x}_1, \vec{x}_2) = \psi_{100}(x_1)\, \psi_{100}(x_2) \left(\frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+})\right) \qquad E_0^{(0)} = -108.8\,eV$$

$$P_{12}\, \Psi(\vec{x}_1, \vec{x}_2) = -\Psi(\vec{x}_1, \vec{x}_2)$$

First order perturbation

$$E_0^{(1)} = \langle \psi_{1s}(1)\, \psi_{1s}(2)\, \chi_{singlet} | \frac{e^2}{r_{12}} | \psi_{1s}(1)\, \psi_{1s}(2)\, \chi_{singlet} \rangle$$

$$= \langle \psi_{1s}(1)\, \psi_{1s}(2) | \frac{e^2}{r_{12}} | \psi_{1s}(1)\, \psi_{1s}(2) \rangle$$

$$= \int d^3x_1\, d^3x_2\, \psi_{100}^*(\vec{x}_1)\, \psi_{100}^*(\vec{x}_2) \frac{e^2}{|\vec{x}_1 - \vec{x}_2|} \psi_{100}(\vec{x}_1)\, \psi_{100}(\vec{x}_2)$$

$$\psi_{100}(\vec{x}_1) = R_{10}(r_1)\, Y_0^0(\theta_1,\phi_1) = \frac{1}{\sqrt{4\pi}}\left(\frac{Z}{a_0}\right)^{3/2} 2\cdot e^{-Zr_1/a_0}$$

$$\psi_{100}(\vec{x}_2) = \frac{1}{\sqrt{4\pi}}\left(\frac{Z}{a_0}\right)^{3/2} 2\cdot e^{-Zr_2/a_0}$$

$$\boxed{\psi_{100}(\vec{x}_1)\,\psi_{100}(\vec{x}_2) = \frac{Z^3}{\pi a_0^3}\, e^{-Z(r_1+r_2)/a_0}}$$

$$\frac{1}{|\vec{x}_1-\vec{x}_2|} = \frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos(\gamma)}}$$ $\gamma$ - angle between $\vec{x}_1$ and $\vec{x}_2$

$$= \sum \frac{r_<^{\ell}}{r_>^{\ell+1}} P_\ell(\cos(\gamma))$$ (Like in Jackson)

$$= \sum_\ell \sum_m \frac{r_<^{\ell}}{r_>^{\ell+1}} \frac{4\pi}{2\ell+1} Y_{\ell m}^*(\theta_1,\phi_1)\, Y_{\ell m}(\theta_2,\phi_2)$$

$$E_0^{(1)} = \left(\frac{Z^3}{\pi a_0^3}\right)^2 e^2 \sum_{\ell,m} \frac{4\pi}{2\ell+1}\int r_1^2\,dr_1\, d\cos(\theta_1)\, d\phi_1\, r_2^2\,dr_2\, d\cos(\theta_2)\, d\phi_2 \left(e^{-2Z(r_1+r_2)/a_0}\right)\left(\frac{r_<^{\ell}}{r_>^{\ell+1}}\right)\left(Y_{\ell m}^*(\theta_1,\phi_1)\, Y_{\ell m}(\theta_2,\phi_2)\right)$$

$$\int d\cos(\theta_1)\, d\phi_1\, Y_{\ell m}^*(\theta_1,\phi_1) = \sqrt{4\pi}\,\delta_{\ell 0}\,\delta_{m0}$$

$$E_0^{(1)} = \left(\frac{Z^3}{\pi a_0^3}\right)^2 e^2 (4\pi)^2 \int r_1^2\,dr_1\, r^2\,dr_2 \left(e^{-2Z(r_1+r_2)/a_0}\frac{1}{r_>}\right)$$

$$= \left(\frac{4Z^3 e}{a_0^3}\right)^2 \left(\int_0^\infty\int_0^{r_1} r_2^2\,dr_2\, r_1^2\,dr_1 \left(e^{-2Z(r_1+r_2)/a_0}\frac{1}{r_1}\right) + \int_0^\infty\int_{r_1}^\infty r_2^2\,dr_2\, r_1^2\,dr_1\left(e^{-2Z(r_1+r_2)/a_0}\frac{1}{r_2}\right)\right)$$

$$= \left(\frac{4Z^3 e}{a_0^3}\right)^2 \left(\int_0^\infty dr_1\, r_1\, e^{-2Z(r_1)/a_0}\int_0^{r_1} dr_2\, r_2^2\, e^{-2Zr_2/a_0} + \int_0^\infty dr_1\, r_1^2 e^{-2Z(r_1)/a_0}\int_{r_1}^\infty dr_2\, r_2\, e^{-2Zr_2/a_0}\right)$$

$$\int dx\, x^2 e^{\alpha x} = e^{\alpha x}\left(\frac{x^2}{\alpha} - \frac{2x}{\alpha^2} + \frac{2}{\alpha^3}\right)$$

$$\int dx\, x^3 e^{\alpha x} = e^{\alpha x}\left(\frac{x^3}{\alpha} - \frac{3x^2}{\alpha^2} + \frac{6x}{\alpha^3} - \frac{6}{\alpha^4}\right)\Big|_0^\infty = +\frac{6}{\alpha^4}$$

$$\alpha = \frac{-2Z}{a_0}$$

$$= \left(\frac{4Z^3 e}{a_0^3}\right)^2 \left(\frac{5}{128}\frac{a_0^5}{Z^5}\right)$$

$$E_0^{(1)} = \frac{5Z}{8}\left(\frac{e^2}{a_0}\right)$$

$Z=2$ for Helium

$$E_0^{(1)} = \frac{5}{2}\underbrace{\left(\frac{e^2}{2a_0}\right)}_{\frac{1}{2}mc^2\alpha^2 = 13.6\,eV} = \frac{5}{2}(13.6\,eV) = 34\,eV$$

$$\rightarrow \boxed{E^{ground} = -108.8\,eV + 34\,eV = -74.8\,eV}$$

Try using variational method

$$\phi_{trial}(\vec{x}_1, \vec{x}_2) = \frac{Z_{eff}^3}{\pi a_0^3} e^{-Z_{eff}(r_1+r_2)/a_0}$$

$Z_{eff}$ - effective nuclear charge due to screening.
→ variational parameter.

$$\langle H \rangle = \underbrace{\left\langle \frac{p_1^2}{2m} - \frac{Ze^2}{r_1} \right\rangle}_{\left\langle \frac{p_1^2}{2m} - \frac{Z_{eff}e^2}{r_1} \right\rangle + \left\langle \frac{(Z_{eff}-Z)e^2}{r_1} \right\rangle} + \left\langle \frac{p_2^2}{2m} - \frac{Ze^2}{r_2} \right\rangle + \underbrace{\left\langle \frac{e^2}{r_{12}} \right\rangle}_{\text{already did this}}$$

All of these are known!

$$\langle H \rangle = \left(-\underbrace{\left(\frac{mc^2\alpha^2}{2}\right)}_{\frac{e^2}{2a_0}} Z_{eff}^2 + (Z_{eff}-Z)e^2 \overbrace{\left\langle \frac{1}{r_1} \right\rangle}^{\frac{Z_{eff}}{a_0}}\right)(2) + \frac{5}{8}Z_{eff}\left(\frac{e^2}{a_0}\right)$$

$$= \left(Z_{eff}^2 - 2ZZ_{eff} + \frac{5}{8}Z_{eff}\right)\left(\frac{e^2}{a_0}\right)$$

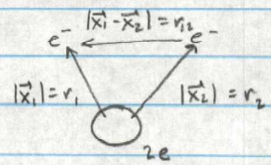
$$\frac{\partial\langle H\rangle}{\partial Z_{eff}} = 0 = \left(\frac{e^2}{a_0}\right)\left(2Z_{eff} - 2Z + \frac{5}{8}\right)$$

$$Z_{eff} = Z - \frac{5}{16} = 2 - \frac{5}{16} = \frac{27}{16} \approx 1.6875$$

$$\boxed{\langle H \rangle\big|_{Z_{eff}=1.6875} = -77.5\,eV}$$

02/25/2010

## Helium Atom




$$H = H_0 + V$$

$$H_0 = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2}$$

$$V = \frac{e^2}{r_{12}}$$

$$\Psi_0(\vec{x}_1, \vec{x}_2) = \psi_{100}(\vec{x}_1)\,\psi_{100}(\vec{x}_2)\,\chi_{singlet} \qquad \left(\chi_{singlet} = \frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+})\right)$$

$$\Psi_1^S(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}}\left(\psi_{100}(\vec{x}_1)\,\psi_{2\ell m}(\vec{x}_2) + \psi_{2\ell m}(\vec{x}_1)\,\psi_{100}(\vec{x}_2)\right)\chi_{singlet}$$

$$\Psi_1^T(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}}\left(\psi_{100}(\vec{x}_1)\,\psi_{2\ell m}(\vec{x}_2) - \psi_{2\ell m}(\vec{x}_1)\,\psi_{100}(\vec{x}_2)\right)\chi_{triplet}$$

$$\chi_{triplet} = \begin{cases} \chi_{++} \\ \frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{-+}) \\ \chi_{--} \end{cases}$$

$$\Delta E_\ell^{(S,T)} = \frac{1}{2} e^2 \int d^3x_1\, d^3x_2 \left(\psi_{100}(\vec{x}_1)\,\psi_{2\ell m}(\vec{x}_2) \pm \psi_{2\ell m}(\vec{x}_1)\,\psi_{100}(\vec{x}_2)\right)^* * \left(\frac{1}{|\vec{x}_1 - \vec{x}_2|}\right)\left(\psi_{100}(\vec{x}_1)\,\psi_{2\ell m}(\vec{x}_2) \pm \psi_{2\ell m}(\vec{x}_1)\,\psi_{100}(\vec{x}_2)\right)$$

$$= \underbrace{e^2 \int d^3x_1\, d^3x_2 \frac{|\psi_{100}(\vec{x}_1)|^2\,|\psi_{2\ell m}(\vec{x}_2)|^2}{|\vec{x}_1 - \vec{x}_2|}}_{\text{positive}}$$

$$\pm \underbrace{e^2 \int d^3x_1\, d^3x_2\, \psi_{100}^*(\vec{x}_1)\,\psi_{2\ell m}^*(\vec{x}_2)\,\frac{1}{|\vec{x}_1 - \vec{x}_2|}\,\psi_{2\ell m}(\vec{x}_1)\,\psi_{100}(\vec{x}_2)}_{\text{positive}}$$

$$\Delta E^S > \Delta E^T$$

Look at second term.

$$\Delta E_\ell^{S,T} = I_\ell \pm J_\ell \qquad (\text{Not } I_{\ell m} \pm J_{\ell m} \text{ because } [V, L_z] = 0 \text{ + m doesn't matter})$$

$$J_1 = e^2 \int d^3x_1\, d^3x_2\, \psi^*_{100}(\vec{x}_1)\, \psi^*_{210}(\vec{x}_2) \frac{1}{|\vec{x}_1 - \vec{x}_2|} \psi_{210}(\vec{x}_1)\, \psi_{100}(\vec{x}_2)$$

$$\psi_{100}(r,\theta,\phi) = R_{10}(r)\, Y_{00}(\theta,\phi) = \frac{1}{\sqrt{4\pi}} \left(2\left(\frac{2}{a_0}\right)^{3/2} e^{-2r/a_0}\right)$$

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi}} \left(\frac{2}{a_0}\right)^{3/2} e^{-2r/a_0}$$

$$\psi_{210}(r,\theta,\phi) = \overset{z=1}{R_{21}}(r)\, Y_{10}(\theta,\phi)$$

(Take $z=1$ because the $\psi_{100}$ $e^-$ screens the nucleus)

$$\psi_{210}(r,\theta,\phi) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{2a_0}\right)^{5/2} r\, e^{-r/a_0} \cos(\theta)$$

$$J_1 = \frac{e^2}{(2\pi)^2 a_0^8} \left( \int d^3x_1\, d^3x_2\, e^{-5r_1/2a_0}\, r_1 \cos(\theta_1)\, e^{-5r_2/2a_0}\, r_2 \cos(\theta_2) \frac{1}{|\vec{x}_1 - \vec{x}_2|} \right)$$

$$\frac{1}{|\vec{x}_1 - \vec{x}_2|} = \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\gamma)}} = \sum \frac{r_<^\ell}{r_>^{\ell+1}} P_\ell(\cos(\gamma))$$

$$= \sum_{\ell,m} \frac{4\pi}{2\ell+1} \frac{r_<^\ell}{r_>^{\ell+1}} Y^*_{\ell m}(\theta_1,\phi_1)\, Y_{\ell m}(\theta_2,\phi_2)$$

$$\int d\Omega_1\, Y^*_{\ell m}(\theta_1,\phi_1) \cos(\theta_1) = \int d\Omega_1\, Y^*_{\ell m}(\theta_1,\phi_1) \sqrt{\frac{4\pi}{3}}\, Y_{10}(\theta_1,\phi_1)$$

$$= \sqrt{\frac{4\pi}{3}} \int d\Omega_1\, Y^*_{\ell m}(\theta_1,\phi_1)\, Y_{10}(\theta_1,\phi_1)$$

$$= \sqrt{\frac{4\pi}{3}}\, \delta_{\ell 1}\, \delta_{m0}$$

Same for $d\Omega_2$

$$J_1 = \frac{e^2}{(2\pi)^2 a_0^8} \left(\frac{4\pi}{3}\right)\left(\frac{4\pi}{3}\right) \int_0^\infty \int_0^\infty dr_2\, dr_1\, r_1^3 r_2^3\, e^{-5r_1/2a_0} \frac{r_<}{r_>^2}\, e^{-5r_2/2a_0}$$

$$= \frac{e^2}{(2\pi)^2 a_0^8} \left(\frac{4\pi}{3}\right)^2 \left( \int_0^\infty \int_0^{r_1} dr_2\, dr_1\, r_1 r_2^4\, e^{-5r_1/2a_0}\, e^{-5r_2/2a_0} \right.$$

$$\left. + \int_0^\infty \int_{r_1}^\infty dr_2\, dr_1\, r_1^4 r_2\, e^{-5(r_1+r_2)/2a_0} \right)$$

$$K = \int_0^{r_1} dr_2 \frac{1}{r_1^2} r_2^4 e^{-5r_2/2a_0} + \int_{r_1}^{\infty} dr_2\, r_1 r_2 e^{-5r_2/2a_0}$$

$$= \frac{1}{r_1^2} \int_0^{r_1} dr_2\, r_2^4 e^{-5r_2/2a_0} + r_1 \int_{r_1}^{\infty} dr_2\, r_2 e^{-5r_2/2a_0}$$

$$= \frac{1}{r_1^2} \left( \cancel{\frac{-2a_0}{5} r_1^4 e^{-5r_1/2a_0}} + \frac{8a_0}{5} \left( e^{-5r_1/2a_0} \left( -\frac{2a_0}{5} r_1^3 - 3\left(\frac{2a_0}{5}\right)^2 r_1^2 - 6\left(\frac{2a_0}{5}\right)^3 r_1 - 6\left(\frac{2a_0}{5}\right)^4 \right) + 6\left(\frac{2a_0}{5}\right)^4 \right) \right.$$

$$\left. + r_1 \left( e^{-5r_1/2a_0} \left( \cancel{\frac{2a_0}{5} r_1} + \left(\frac{2a_0}{5}\right)^2 \right) \right) \right)$$

$$J_1 = \frac{e^2}{(2\pi)^2 a_0^8} \left(\frac{4\pi}{3}\right)^2 \left( -\int_0^{\infty} dr_1 \left( e^{-5r_1/a_0} \left( \frac{2a_0}{5} r_1^4 + 3\left(\frac{2a_0}{5}\right)^2 r_1^3 + 6\left(\frac{2a_0}{5}\right)^3 r_1^2 + 6\left(\frac{2a_0}{5}\right)^4 r_1 \right) \right) \left(\frac{8a_0}{5}\right) \right.$$

$$\left. + \frac{8a_0}{5} \int_0^{\infty} dr_1\, e^{-5r_1/a_0} r_1 \left( 6\left(\frac{2a_0}{5}\right)^4 \right) + \int_0^{\infty} dr_1\, r_1^4 e^{-5r_1/a_0} \left(\frac{2a_0}{5}\right)^2 \right)$$

$$= \frac{e^2}{(2\pi)^2 a_0^8} \left(\frac{4\pi}{3}\right)^2 \left( -\frac{2a_0}{5} \frac{6a_0}{5} \int_0^{\infty} dr_1\, r_1^4 e^{-5r_1/a_0} \right.$$

$$- \frac{24a_0}{5} \left(\frac{2a_0}{5}\right)^2 \int_0^{\infty} dr_1\, r_1^3 e^{-5r_1/a_0}$$

$$- \frac{48a_0}{5} \left(\frac{2a_0}{5}\right)^3 \int_0^{\infty} dr_1\, r_1^2 e^{-5r_1/a_0}$$

$$- \frac{48a_0}{5} \left(\frac{2a_0}{5}\right)^4 \int_0^{\infty} dr_1\, r_1 e^{-5r_1/a_0}$$

$$\left. + \frac{48a_0}{5} \left(\frac{2a_0}{5}\right)^4 \int_0^{\infty} dr_1\, r_1 e^{-5r_1/a_0} \right)$$

$$\int_0^{\infty} dr\, r^n e^{-\lambda r} = \frac{n!}{\lambda^{n+1}} \qquad (\lambda = -5/a_0)$$

$$= \frac{e^2}{(2\pi)^2 a_0^8} \left(\frac{4\pi}{3}\right)^2 \left( \left(\frac{a_0}{5}\right)^7 \left( (-12)\,4! - (24)(4)(3!) - 48(2^3)(2!) - 48(2^4) + (48)(2^4)(2^2) \right) \right.$$

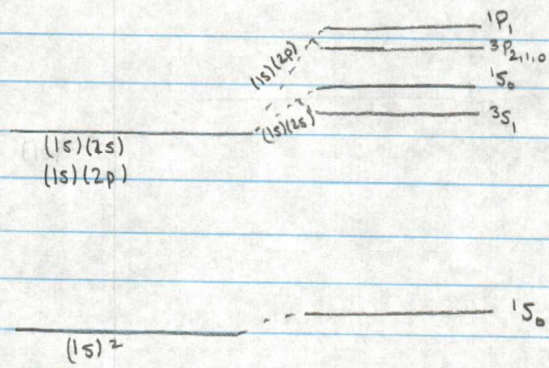
$$-288 - 576 - 768 + \underbrace{48(2^4)(3)}_{2304}$$

$$J_1 = \frac{e^2}{(2\pi)^2 a_0^8} \left(\frac{4\pi}{3}\right)^2 \frac{672}{5^7} a_0^7 > 0$$

$$\boxed{J_1 = \frac{(2^8)(7)}{3\,(5^7)} \left(\frac{e^2}{2a_0}\right) \approx .00745\ Ry}$$

$$13.6\ eV = 1\ Ry$$

$$\Delta E_\ell^S = I_\ell + J_\ell > \Delta E_\ell^T = I_\ell - J_\ell$$

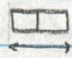
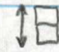



$^{2S+1}L_J$

Singlet is always the higher state.

V has no spin dependence. But because of the wavefunction symmetry, it makes a difference.

03/02/2010 **Permutation Symmetry and Young Tableaux**

 symmetric  antisymmetric

Two electron system

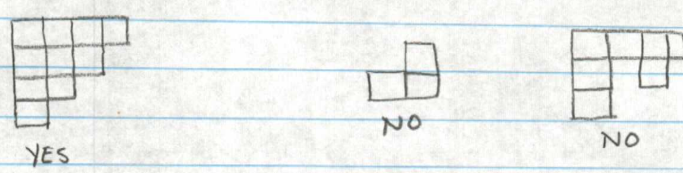
$\chi_{triplet} \begin{cases} \uparrow\uparrow \\ \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ \downarrow\downarrow \end{cases} \leftrightarrow$ 

$\chi_{singlet} \ \{ \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) \leftrightarrow$ 

Rules for Young Tableaux Technique

1. A box ☐ represents a particle (or object) and the label inside the box (eg. $\boxed{1}$, $\boxed{2}$) represents the state of the particle.

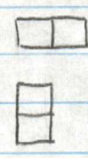
2. Boxes always added to the right and down



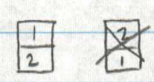

3. To count the dimensionality of a tableaux, do not decrease the label going from the left to the right. Increase the label going from up to down
   (Purpose is to remove double counting)

For example

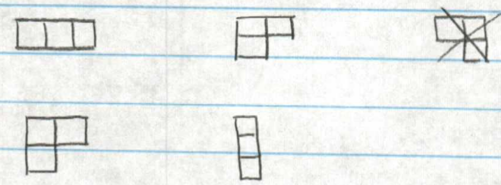
1. $\boxed{1} \leftrightarrow \uparrow$
   $\boxed{2} \leftrightarrow \downarrow$

2. 

3. $\boxed{1\,|\,1}$ $\boxed{1\,|\,2}$ $\boxed{2\,|\,2}$ $\cancel{\boxed{2\,|\,1}}$

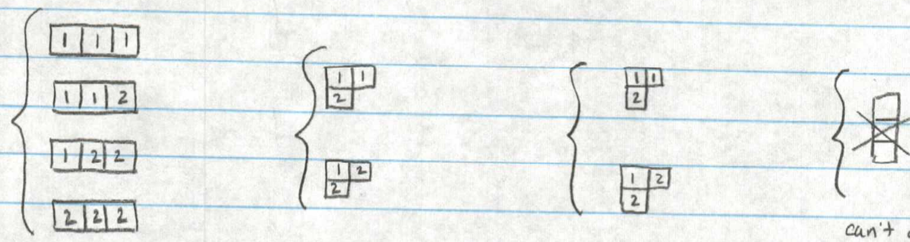


Example: Three Electron System



(from $2e^-$ triplet)

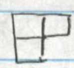
(from $2e^-$ singlet)



quartet $\{4\}$ doublet $\{2\}$ doublet $\{2\}$ can't do this

$$\tfrac{1}{2} \otimes \tfrac{1}{2} = 1 \oplus 0$$

$$\begin{aligned}\tfrac{1}{2} \otimes \tfrac{1}{2} \otimes \tfrac{1}{2} = (1 \oplus 0) \otimes \tfrac{1}{2} &= \left(1 \otimes \tfrac{1}{2}\right) \oplus \left(0 \otimes \tfrac{1}{2}\right) \\ &= \left(\tfrac{3}{2} \oplus \tfrac{1}{2}\right) \oplus \left(\tfrac{1}{2}\right) \\ &= \{4\} + \{2\} + \{2\}\end{aligned}$$

 mixed symmetry - depends on if it came from the triplet or the singlet.

Example: Two Quark System (Mesons)

$$\left.\begin{array}{l} \boxed{1} = u \\ \boxed{2} = d \\ \boxed{3} = s \end{array}\right\} \square = \{3\}$$

$$\square \otimes \square = \begin{array}{|c|c|}\hline \ & \ \\ \hline\end{array} \oplus \begin{array}{|c|}\hline \ \\ \hline \ \\ \hline\end{array} \qquad (\{3\} \otimes \{3\})$$

Sextet $\{6\}$:

$$\left\{\begin{array}{l}
\begin{array}{|c|c|}\hline 1&1\\ \hline\end{array} \\
\begin{array}{|c|c|}\hline 1&2\\ \hline\end{array} \\
\begin{array}{|c|c|}\hline 1&3\\ \hline\end{array} \\
\begin{array}{|c|c|}\hline 2&2\\ \hline\end{array} \\
\begin{array}{|c|c|}\hline 2&3\\ \hline\end{array} \\
\begin{array}{|c|c|}\hline 3&3\\ \hline\end{array}
\end{array}\right.$$

triplet $\{3\}$:

$$\left\{\begin{array}{l}
\begin{array}{|c|}\hline 1\\ \hline 2\\ \hline\end{array} \\
\begin{array}{|c|}\hline 1\\ \hline 3\\ \hline\end{array} \\
\begin{array}{|c|}\hline 2\\ \hline 3\\ \hline\end{array}
\end{array}\right.$$

$$\{3\} \otimes \{3\} = \{6\} + \{3^*\}$$

$$\begin{array}{|c|}\hline 1\\ \hline 2\\ \hline 3\\ \hline\end{array} = \{1\}$$

Example: Three Quark System (Baryons)

$$\left(\begin{array}{|c|c|}\hline \ & \ \\ \hline\end{array} \oplus \begin{array}{|c|}\hline \ \\ \hline \ \\ \hline\end{array}\right) \otimes \square = \left(\begin{array}{|c|c|}\hline \ & \ \\ \hline\end{array} \otimes \square\right) \oplus \left(\begin{array}{|c|}\hline \ \\ \hline \ \\ \hline\end{array} \otimes \square\right)$$

$$= \left(\begin{array}{|c|c|c|}\hline \ & \ & \ \\ \hline\end{array} \oplus \begin{array}{|c|c|}\hline \ & \ \\ \hline \ \\ \cline{1-1}\end{array}\right) \oplus \left(\begin{array}{|c|c|}\hline \ & \ \\ \hline \ \\ \cline{1-1}\end{array} \oplus \begin{array}{|c|}\hline \ \\ \hline \ \\ \hline \ \\ \hline\end{array}\right)$$

$\{10\}$ decuplet:

$$\left\{\begin{array}{l}
\begin{array}{|c|c|c|}\hline 1&1&1\\ \hline\end{array} \\
\begin{array}{|c|c|c|}\hline 1&1&2\\ \hline\end{array} \\
\begin{array}{|c|c|c|}\hline 1&1&3\\ \hline\end{array} \\
\begin{array}{|c|c|c|}\hline 1&2&2\\ \hline\end{array} \\
\begin{array}{|c|c|c|}\hline 1&2&3\\ \hline\end{array} \\
\begin{array}{|c|c|c|}\hline 1&3&3\\ \hline\end{array} \\
\begin{array}{|c|c|c|}\hline 2&2&3\\ \hline\end{array} \\
\begin{array}{|c|c|c|}\hline 2&2&2\\ \hline\end{array} \\
\begin{array}{|c|c|c|}\hline 2&3&3\\ \hline\end{array} \quad \begin{array}{|c|c|c|}\hline 3&3&3\\ \hline\end{array}
\end{array}\right.$$

$\{8\}$ octet:

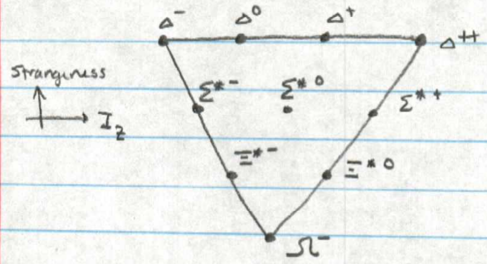
$$\left\{\begin{array}{ll}
\begin{array}{|c|c|}\hline 1&1\\ \hline 2\\ \cline{1-1}\end{array} & \begin{array}{|c|c|}\hline 2&2\\ \hline 3\\ \cline{1-1}\end{array} \\
\begin{array}{|c|c|}\hline 1&1\\ \hline 3\\ \cline{1-1}\end{array} & \begin{array}{|c|c|}\hline 2&3\\ \hline 3\\ \cline{1-1}\end{array} \\
\begin{array}{|c|c|}\hline 1&2\\ \hline 2\\ \cline{1-1}\end{array} & \\
\begin{array}{|c|c|}\hline 1&2\\ \hline 3\\ \cline{1-1}\end{array} & \\
\begin{array}{|c|c|}\hline 1&3\\ \hline 2\\ \cline{1-1}\end{array} & \\
\begin{array}{|c|c|}\hline 1&3\\ \hline 3\\ \cline{1-1}\end{array} &
\end{array}\right.$$

$\{1\}$ singlet:

$$\left\{\begin{array}{|c|}\hline 1\\ \hline 2\\ \hline 3\\ \hline\end{array}\right.$$

27 states!

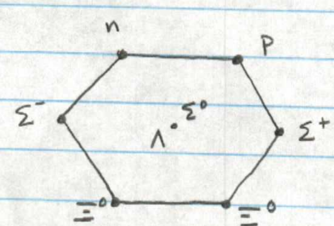
$$\{10\} + \{8\}_S + \{8\}_A + \{1\}$$




decuplet

(Gell-Mann and 8-Fold Way)

$\Omega^-$ predicted from this




octet


singlet

Example: Three $j=1$ Objects

$$\{10\} \rightarrow \underbrace{\{7\}}_{j=3} \oplus \underbrace{\{3\}}_{j=1}$$

$$\{8\} \rightarrow \underbrace{\{5\}}_{j=2} \oplus \underbrace{\{3\}}_{j=1}$$

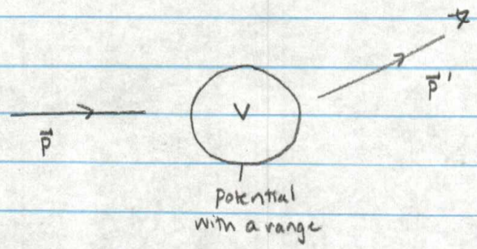
$$\{1\} - j=0$$

$$\{7\} \oplus \{3\} \oplus \{5\} \oplus \{3\} \oplus \{5\} \oplus \{3\} \oplus \{1\}$$

$j=1$ can be fully symmetric or mixed symmetry.

Not an irreducible representation.

03/04/2010 Lippmann-Schwinger Equation




Elastic scattering $\Rightarrow$ $|\vec{p}| = |\vec{p}\,'|$

$$H_0 = \frac{\vec{p}^{\,2}}{2m}$$

$$V = V(\vec{x}) \quad \text{(local potential)}$$

Asymptotically, $H_0 |\phi\rangle = E|\phi\rangle \rightarrow (E - H_0)|\phi\rangle = 0$

However, the true equation is

$$H|\psi\rangle = E|\psi\rangle \qquad \text{(same } E\text{)}$$

$$\boxed{(H_0 + V)|\psi\rangle = E|\psi\rangle}$$

$$(E - H_0)|\psi\rangle = V|\psi\rangle$$

What is $|\psi\rangle$?

$$\boxed{|\psi\rangle = |\phi\rangle + \frac{1}{E - H_0} V|\psi\rangle} \qquad \text{(homogeneous + particular solution)}$$

To avoid singularities

$$\boxed{|\psi^{(\pm)}\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\epsilon} V|\psi^{(\pm)}\rangle}$$

Position representation of L-S equation

$$\langle\vec{x}|\psi^{(\pm)}\rangle = \langle\vec{x}|\phi\rangle + \int d^3x' \langle\vec{x}|\frac{1}{E-H_0\pm i\epsilon}|\vec{x}'\rangle\langle\vec{x}'|V|\psi^{(\pm)}\rangle$$

$\int d^3x'' |\vec{x}''\rangle\langle\vec{x}''|$

$\langle\vec{x}'|V|\vec{x}''\rangle = V(\vec{x}')\,\delta(\vec{x}'-\vec{x}'')$

Green's function

$$G_\pm(\vec{x},\vec{x}') \equiv \frac{\hbar^2}{2m}\langle\vec{x}|\frac{1}{E-H_0\pm i\epsilon}|\vec{x}'\rangle$$

Derivation given eq. 7.1.12 - 7.1.16

$$G_\pm(\vec{x},\vec{x}') = \frac{-1}{4\pi}\frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} \qquad \left(k=\frac{\sqrt{2mE}}{\hbar}\right)$$

$$\langle\vec{x}|\psi^{(\pm)}\rangle = \langle\vec{x}|\phi\rangle - \frac{m}{2\pi\hbar^2}\int d^3x' \frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} V(\vec{x}')\langle\vec{x}'|\psi^{(\pm)}\rangle \qquad (7.1.22)$$

$\vec{x}'$ - positions in the local region of the potential

$\vec{x}$ - position of detector.

Long-range approximation. $\rightarrow |\vec{x}| \gg |\vec{x}'|$

$r=|\vec{x}| \qquad r'=|\vec{x}'| \qquad \alpha$ - angle between $\vec{x}$ and $\vec{x}'$

$$|\vec{x}-\vec{x}'| = \sqrt{(\vec{x}-\vec{x}')^2} = \sqrt{r^2-2rr'\cos(\alpha)+r'^2}$$

$$= r\sqrt{1-2\frac{r'}{r}\cos(\alpha)+\left(\frac{r'}{r}\right)^2}$$

$$\approx r\left(1-\frac{r'}{r}\cos(\alpha)\right) \qquad \left(\frac{r'}{r}\ll 1\right)$$

$$= r - \underbrace{r'\cos(\alpha)}_{\text{projection of } \vec{x}' \text{ onto } \vec{x}} = r - \hat{r}\cdot\vec{x}'$$

$$e^{\pm ik|\vec{x}-\vec{x}'|} \approx e^{\pm ikr} e^{\mp ik\hat{r}\cdot\vec{x}'} = e^{\pm ikr} e^{\mp i\vec{k}'\cdot\vec{x}'} \qquad (\vec{k}' = k\hat{r})$$

$$\langle\vec{x}|\psi^{(\pm)}\rangle \approx \langle\vec{x}|\phi\rangle - \frac{m}{2\pi\hbar^2}\frac{e^{\pm ikr}}{r}\int d^3x'\, e^{\mp i\vec{k}'\cdot\vec{x}'} V(\vec{x}')\langle\vec{x}'|\psi^{(\pm)}\rangle$$

$$H_0|\phi\rangle = \frac{\hbar^2k^2}{2m}|\phi\rangle$$

$$|\phi\rangle = |\vec{k}\rangle \qquad \vec{p}|\phi\rangle = \hbar\vec{k}|\phi\rangle \quad \text{(relabeling)}$$

$$\langle\vec{x}|\phi\rangle = \langle\vec{x}|\vec{k}\rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{x}}$$

$$\langle\vec{x}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{x}/\hbar} \quad \text{(last semester)}$$

$$\langle\vec{x}|\psi^{(\pm)}\rangle \xrightarrow{r\text{ large}} \frac{1}{(2\pi)^{3/2}}\left(e^{i\vec{k}\cdot\vec{x}} + \frac{e^{\pm ikr}}{r} f_\pm(\vec{k}',\vec{k})\right)$$

$$f_\pm(\vec{k}',\vec{k}) = -\frac{m}{2\pi\hbar^2}(2\pi)^3\int d^3x' \underbrace{\frac{e^{\mp i\vec{k}'\cdot\vec{x}'}}{(2\pi)^{3/2}}}_{\langle\pm\vec{k}'|\vec{x}'\rangle} \underbrace{V(\vec{x}')\langle\vec{x}'|\psi^{(\pm)}\rangle}_{\langle\vec{x}'|V|\psi^{(\pm)}\rangle}$$

$$\boxed{f_\pm(\vec{k}',\vec{k}) = \frac{-4\pi^2 m}{\hbar^2}\langle\pm\vec{k}'|V|\psi^{(\pm)}\rangle} \qquad \text{Scattering Amplitude}$$

We find a plane wave + outgoing spherical wave

$$\boxed{\begin{array}{c} \langle\vec{x}|\psi^{(+)}\rangle \xrightarrow{r\text{ large}} \frac{1}{(2\pi)^{3/2}}\left(e^{i\vec{k}\cdot\vec{x}} + \frac{e^{ikr}}{r} f_+(\vec{k}',\vec{k})\right) \\ \text{where } f_+(\vec{k}',\vec{k}) = \frac{-4\pi^2 m}{\hbar^2}\langle\vec{k}'|V|\psi^{(+)}\rangle \end{array}}$$

$$\phi_{\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} \qquad \psi^{sc}_{\vec{k}}(\vec{x}) = \frac{e^{ikr}}{r} f_+(\vec{k}',\vec{k})$$

$$i\hbar\,\partial_t \psi(\vec{x},t) = \frac{-\hbar^2}{2m}\nabla^2\psi(\vec{x},t) + V(\vec{x})\psi(\vec{x},t)$$

$$\rightarrow \quad \partial_t \rho + \nabla\cdot\vec{j} = 0$$

$$\rho = |\psi|^2$$

$$\vec{j} = \frac{\hbar}{2im}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$$

$$\vec{j}_{inc} = \frac{\hbar}{2im}\left(\phi_{\vec{k}}^*\nabla\phi_{\vec{k}} - (\nabla\phi_{\vec{k}}^*)\phi_{\vec{k}}\right)$$

$$= \frac{\hbar}{2im}\left(\phi_{\vec{k}}^*(i\vec{k})\phi_{\vec{k}} - (-i\vec{k})\phi_{\vec{k}}^*\phi_{\vec{k}}\right)$$

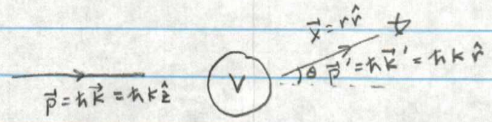
$$\boxed{\vec{j}_{inc} = \frac{\hbar\vec{k}}{m} = \frac{\hbar k}{m}\hat{z}}$$

$$\vec{j}_{sc} = \frac{\hbar}{2im}\left(\psi_{\vec{k}}^{sc*}\nabla\psi_{\vec{k}}^{sc} - (\nabla\psi_{\vec{k}}^{sc*})\psi_{\vec{k}}^{sc}\right)$$

$$\nabla = \underset{\uparrow}{\hat{r}\frac{\partial}{\partial r}} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\varphi}\frac{1}{r\sin(\theta)}\frac{\partial}{\partial\varphi}$$

this term dominates when $r$ is large.

03/09/2010 Born Approximation




$$\langle \vec{x} | \psi^{(+)} \rangle \xrightarrow{\text{large } r} \frac{1}{(2\pi)^{3/2}} \Big( \underbrace{e^{i\vec{k}\cdot\vec{x}}}_{\phi_{\vec{k}}(\vec{x})} + \underbrace{\frac{e^{ikr}}{r} f_+(\vec{k}',\vec{k})}_{\psi_{\vec{k}}^{sc}(\vec{x})} \Big)$$

where $\quad f_+(\vec{k}',\vec{k}) = \frac{-4\pi^2 m}{\hbar^2} \langle \vec{k}' | V | \psi^{(+)} \rangle$

Time dependent Schrödinger equation

$$i\hbar \partial_t \psi = \frac{-\hbar^2}{2m} \nabla^2 \psi + V(\vec{x}) \psi$$

$$\Rightarrow \quad \partial_t \rho + \nabla \cdot \vec{j} = 0$$

$$\rho = |\psi(\vec{x},t)|^2$$

$$\vec{j} = \frac{\hbar}{2im} \left( \psi^* \nabla \psi - \nabla \psi^* \psi \right)$$

$$\vec{j}_{inc} = \frac{\hbar \vec{k}}{m} = \frac{\hbar k}{m} \hat{z}$$

$$\vec{j}_{sc} = \frac{\hbar}{2im} \left( \psi_{\vec{k}}^{sc*} \nabla \psi_{\vec{k}}^{sc} - \nabla \psi_{\vec{k}}^{sc*} \psi_{\vec{k}}^{sc} \right)$$

$$\nabla = \underset{\uparrow}{\hat{r} \frac{\partial}{\partial r}} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\varphi} \frac{1}{r\sin(\theta)} \frac{\partial}{\partial \varphi}$$

this term dominates when $r$ is large.

$$\hat{\theta} \cdot \vec{j}_{sc} = \frac{\hbar}{2im} \left( \psi_{\vec{k}}^{sc*} \frac{1}{r} \frac{\partial}{\partial \theta} \psi_{\vec{k}}^{sc} - \frac{1}{r} \left( \frac{\partial}{\partial \theta} \psi_{\vec{k}}^{sc*} \right) \psi_{\vec{k}}^{sc} \right) \sim \frac{1}{r^3}$$

$$(\hat{\theta} \cdot \vec{j}_{sc}) r^2 d\Omega \sim \frac{1}{r} \qquad (\hat{\varphi} \cdot \vec{j}_{sc}) r^2 d\Omega \sim \frac{1}{r}$$

$$\hat{r} \cdot \vec{j}_{sc} = \frac{\hbar}{2im} \left( \psi_{\vec{k}}^{sc*} \frac{\partial}{\partial r} \psi_{\vec{k}}^{sc} - \left( \frac{\partial}{\partial r} \psi_{\vec{k}}^{sc*} \right) \psi_{\vec{k}}^{sc} \right)$$

$$= \frac{\hbar}{2im} \left( \psi_{\vec{k}}^{sc*} \left( f_+ \frac{\partial}{\partial r} \left( \frac{e^{ikr}}{r} \right) \right) - \left( f_+^* \frac{\partial}{\partial r} \frac{e^{-ikr}}{r} \right) \psi_{\vec{k}}^{sc} \right)$$

$$\frac{\partial}{\partial r}\left(\frac{e^{ikr}}{r}\right) = ik\,\frac{e^{ikr}}{r} - \cancel{\frac{e^{ikr}}{r^2}}$$ →0 when r large

$$\boxed{\hat{r}\cdot\vec{j}_{sc} = \frac{\hbar k}{mr^2}\left|f_+(\vec{k}',\vec{k})\right|^2}$$ (r large)

$$(\hat{r}\cdot\vec{j}_{sc})\,r^2\,d\Omega = \frac{\hbar k}{m}\underbrace{\left|f_+(\vec{k}',\vec{k})\right|^2}_{|f(\theta,\varphi)|^2}d\Omega$$

Differential Cross Section

$$d\sigma = \left(\frac{d\sigma}{d\Omega}\right)d\Omega = \frac{\#\text{ particles scattered into } d\Omega \text{ per unit time}}{\#\text{ incident particles crossing unit area per unit time}}$$

$$= \frac{(\hat{r}\cdot\vec{j}_{sc})\,r^2 d\Omega}{|\vec{j}_{inc}|}$$

$$= \frac{\frac{\hbar k}{m}|f(\theta,\varphi)|^2 d\Omega}{\frac{\hbar k}{m}}$$

$$\boxed{d\sigma = |f(\theta,\varphi)|^2\,d\Omega}$$

$$f_+(\vec{k}',\vec{k}) = \frac{-4\pi^2 m}{\hbar^2}\int d^3x'\,\langle\vec{k}'|V|\vec{x}'\rangle\langle\vec{x}'|\psi^+\rangle$$

$$\uparrow \int d^3x''\,|\vec{x}''\rangle\langle\vec{x}''| \qquad\qquad \langle\vec{x}''|V|\vec{x}'\rangle = V(\vec{x}')\,\delta^3(\vec{x}'-\vec{x}'')$$

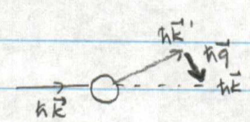
$$= \frac{-4\pi^2 m}{\hbar^2}\int d^3x'\,\underbrace{\langle\vec{k}'|\vec{x}'\rangle}_{\frac{e^{-i\vec{k}'\cdot\vec{x}'}}{(2\pi)^{3/2}}}\,V(\vec{x}')\,\langle\vec{x}'|\psi^+\rangle$$

* First Order Born Approximation $\Rightarrow$ $\langle\vec{x}'|\psi^+\rangle \to \langle\vec{x}'|\phi\rangle = \langle\vec{x}'|\vec{k}\rangle = \frac{e^{i\vec{k}\cdot\vec{x}'}}{(2\pi)^{3/2}}$

$$\boxed{f_+^{(1)}(\vec{k}',\vec{k}) = \frac{-m}{2\pi\hbar^2}\int d^3x'\,e^{i(\vec{k}-\vec{k}')\cdot\vec{x}'}\,V(\vec{x}')}$$

Fourier transform of the local potential

$\hbar(\vec{k}-\vec{k}') = \hbar\vec{q}$
↑
momentum transfer



$$\vec{q}^{\,2} = (\vec{k} - \vec{k}')^2 = 2k^2(1-\cos(\theta)) = 4k^2 \sin^2(\theta/2)$$

$$\boxed{q = |\vec{q}| = 2k\sin\left(\frac{\theta}{2}\right)}$$

Differential Cross Section for Spherically Symmetric Potential $(V(\vec{x}') = V(r'))$

$$f^{(1)}(\vec{k}', \vec{k}) = f^{(1)}(\theta) = \frac{-m}{2\pi\hbar^2} \int r'^2 dr' d\varphi' d\cos(\theta') \, e^{iqr'\cos(\theta')} \, V(r')$$

$$= \frac{-m}{2\pi\hbar^2} (2\pi) \int r'^2 dr' \, V(r') \left( \frac{e^{iqr'} - e^{-iqr'}}{iqr'} \right)$$

$$= \frac{-m}{\hbar^2} \int r'^2 dr' \, V(r') \left( \frac{2\sin(qr')}{qr'} \right)$$

$$\boxed{f^{(1)}(\theta) = \frac{-2m}{\hbar^2} \frac{1}{q} \int_0^\infty dr' \, r' \sin(qr') \, V(r')}$$

Example: Coulomb Potential

$$V(r) = \frac{ZZ'e^2}{r}$$

$$f^{(1)}(\theta) = \frac{-2m}{\hbar^2 q} \int_0^\infty dr' \, \cancel{r'} \sin(qr') \left( \frac{ZZ'e^2}{\cancel{r'}} \right)$$

03/11/2010

$$\int_0^\infty e^{-\mu r} \sin(qr) dr = \frac{q}{\mu^2 + q^2}$$

$$\lim_{\mu \to 0} \int_0^\infty e^{-\mu r} \sin(qr) dr$$

$$= \int_0^\infty \sin(qr) dr = \frac{1}{q}$$

$$= \frac{-2m}{\hbar^2 q} ZZ'e^2 \int_0^\infty dr' \sin(qr')$$

$$= \frac{+2m}{\hbar^2 q} ZZ'e^2 \frac{1}{q} \cos(qr') \Big|_0^\infty \qquad (\cos(\infty) = 0)$$

$$\boxed{f^{(1)}(\theta) = \frac{-2m ZZ'e^2}{\hbar^2 q^2}}$$

$$\frac{d\sigma}{d\Omega} = |f^{(1)}(\theta)|^2 = \frac{(2m)^2 (ZZ'e^2)^2}{\hbar^4} \frac{1}{16 k^4 \sin^4(\theta/2)}$$

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

$$\boxed{\frac{d\sigma}{d\Omega} = \left( \frac{ZZ'e^2}{4E} \right)^2 \frac{1}{\sin^4(\theta/2)}}$$

Rutherford Scattering Cross Section

Higher Order Born Approximation

$$f_+(\vec{k}',\vec{k}) = \frac{-4\pi^2 m}{\hbar^2} \underbrace{\langle \vec{k}'|V|\psi^{(+)}\rangle}_{T|\phi\rangle} \qquad T - \text{transition operator}$$

$$|\psi^{(+)}\rangle = |\phi\rangle + \frac{1}{E-H_0+i\epsilon} V|\psi^{(+)}\rangle$$

$$V|\psi^{(+)}\rangle = V|\phi\rangle + V\frac{1}{E-H_0+i\epsilon} V(V|\psi^{(+)}\rangle)$$

$$T|\phi\rangle = V|\phi\rangle + V\frac{1}{E-H_0+i\epsilon} T|\phi\rangle$$

$$T = V + V\frac{1}{E-H_0+i\epsilon}T = V + V\frac{1}{E-H_0+i\epsilon}V + V\frac{1}{E-H_0+i\epsilon}V\frac{1}{E-H_0+i\epsilon}V + \dots$$

$$T = V \rightarrow \text{First order Born approx}$$

$$T = V + V\frac{1}{E-H_0+i\epsilon}V \rightarrow \text{Second order Born approx.}$$

etc.

$$f_+(\vec{k}',\vec{k}) = -\frac{4\pi^2 m}{\hbar^2}\langle \vec{k}'|T|\vec{k}\rangle$$

$$= \sum_{n=1}^{\infty} f^{(n)}(\vec{k}',\vec{k})$$

$$f^{(1)}(\vec{k}',\vec{k}) = \frac{-4\pi^2 m}{\hbar^2}\langle \vec{k}'|V|\vec{k}\rangle = \frac{-m}{2\pi\hbar^2}\int d^3x'\, e^{i(\vec{k}-\vec{k}')\cdot\vec{x}'} V(\vec{x}')$$

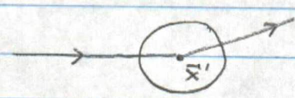
$$f^{(2)}(\vec{k}',\vec{k}) = \frac{-4\pi^2 m}{\hbar^2}\langle \vec{k}'|V\frac{1}{E-H_0+i\epsilon}V|\vec{k}\rangle$$

$$= \frac{-m}{2\pi\hbar^2}\int d^3x' \int d^3x''\, e^{-i\vec{k}'\cdot\vec{x}'} V(\vec{x}')\left(\frac{2m}{\hbar^2}G_+(\vec{x}',\vec{x}'')\right)V(\vec{x}'')\, e^{i\vec{k}\cdot\vec{x}''}$$

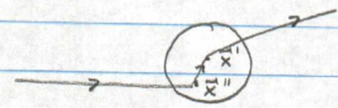
$$\boxed{f^{(2)}(\vec{k}',\vec{k}) = \frac{-m^2}{4\pi^2\hbar^4}\int d^3x'\, d^3x''\, e^{-i\vec{k}'\cdot\vec{x}'} V(\vec{x}')\frac{e^{ik|\vec{x}'-\vec{x}''|}}{|\vec{x}'-\vec{x}''|} V(\vec{x}'')\, e^{i\vec{k}\cdot\vec{x}''}}$$

Physical Meaning →

First order




Second order




etc.

03/11/2010

## Optical Theorem and Eikonal Approximation

$$f(\vec{k}', \vec{k}) = \frac{-4\pi^2 m}{\hbar^2} \langle \vec{k}' | T | \vec{k} \rangle$$

$$T = V + V \frac{1}{E-H_0+i\epsilon} V + V \frac{1}{E-H_0+i\epsilon} V \frac{1}{E-H_0+i\epsilon} V + \dots$$

Optical theorem →

$$\text{Im}(f(\vec{k}, \vec{k})) = \frac{k}{4\pi} \int d\Omega \underbrace{|f(\vec{k}', \vec{k})|^2}_{\frac{d\sigma}{d\Omega}} = \frac{k}{4\pi} \sigma_{tot}$$

$$\text{Im}(f(\theta=0)) = \frac{k}{4\pi} \sigma_{tot}$$ (forward scattering amplitude $f(\theta=0)$)

Proof:

$$\langle \vec{k} | T | \vec{k} \rangle = \langle \vec{k} | V | \psi^{(+)} \rangle$$

$$= \langle \psi^{(+)} | V | \psi^{(+)} \rangle - \langle \psi^{(+)} | V \frac{1}{E-H_0-i\epsilon} V | \psi^{(+)} \rangle$$

$$|\psi^{(+)}\rangle = |\vec{k}\rangle + \frac{1}{E-H_0+i\epsilon} V |\psi^{(+)}\rangle$$

$$\rightarrow |\vec{k}\rangle = |\psi^{(+)}\rangle - \frac{1}{E-H_0+i\epsilon} V |\psi^{(+)}\rangle$$

$$\Rightarrow \langle \vec{k} | = \langle \psi^{(+)} | - \langle \psi^{(+)} | V \frac{1}{E-H_0-i\epsilon}$$

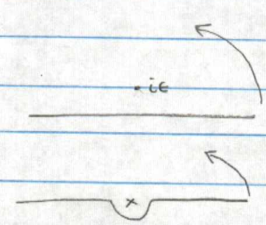
$$\Rightarrow \langle \vec{k} | T | \vec{k} \rangle = \langle \psi^{(+)} | V | \psi^{(+)} \rangle - \langle \psi^{(+)} | V \frac{1}{E-H_0-i\epsilon} V | \psi^{(+)} \rangle$$

$$\frac{1}{E-H_0-i\epsilon} = P \frac{1}{E-H_0} + i\pi \delta(E-H_0)$$

↑ principle value

$$\frac{1}{x-i\epsilon} = P \frac{1}{x} + i\pi \delta(x)$$

pole at $x = +i\epsilon$




$$\boxed{P \int \frac{f(x)}{x} dx = \int \frac{f(x) - f(0)}{x} dx}$$

$$x = \epsilon e^{i\theta} \qquad dx = \epsilon i d\theta\, e^{i\theta} = i x\, d\theta$$

$$i\int_{\pi}^{2\pi} d\theta = \pi \qquad \text{gives} \quad i\pi\,\delta(x)$$

$$\text{Im}(\langle \vec{k}|T|\vec{k}\rangle) = -\pi \langle \psi^{(+)}|V\,\delta(E-H_0)\,V|\psi^{(+)}\rangle$$

$$= -\pi \langle \vec{k}|T^{\dagger}\,\delta(E-H_0)\,T|\vec{k}\rangle$$

$$= -\pi \int d^3\vec{k}' \langle \vec{k}|T^{\dagger}\delta(E-H_0)|\vec{k}'\rangle\langle \vec{k}'|T|\vec{k}\rangle$$

$$= -\pi \int d^3k' \langle \vec{k}|T^{\dagger}|\vec{k}'\rangle\langle \vec{k}'|T|\vec{k}\rangle\, \delta\left(E - \frac{\hbar^2 k'^2}{2m}\right)$$

$$d^3k' = k'^2\, dk'\, d\Omega$$

$$E = \frac{\hbar^2 k'^2}{2m} \qquad dE = \frac{\hbar^2 k'}{m}\, dk'$$

$$d^3k' = \frac{m}{\hbar^2} k'\, dE\, d\Omega$$

$$\text{Im}(\langle \vec{k}|T|\vec{k}\rangle) = \frac{-m\pi}{\hbar^2}\int d\Omega\; k'|\langle \vec{k}'|T|\vec{k}\rangle|^2$$

$$\text{Im}(f(\vec{k},\vec{k})) = \frac{-4\pi^2 m}{\hbar^2}\,\text{Im}(\langle \vec{k}|T|\vec{k}\rangle)$$

$$= \frac{-4\pi^2 m}{\hbar^2}\left(\frac{-m\pi}{\hbar^2}k\right)\int d\Omega\, \underbrace{|\langle \vec{k}'|T|\vec{k}\rangle|^2}_{\left|\frac{-\hbar^2}{4\pi^2 m}\right|^2 \frac{d\sigma}{d\Omega}}$$

$$\boxed{\text{Im}(f(\vec{k},\vec{k})) = \frac{k}{4\pi}\int d\Omega\, \frac{d\sigma}{d\Omega} = \frac{k}{4\pi}\,\sigma_{tot}}$$

Example : Partial Wave Expansion

Eq. 7.6.17 $\quad f(\theta) = \frac{1}{k} \sum_\ell (2\ell+1) e^{i\delta_\ell} \sin(\delta_\ell) P_\ell(\cos(\theta))$

$$\mathrm{Im}(f(\theta=0)) = \mathrm{Im}\left(\frac{1}{k} \sum_\ell (2\ell+1) e^{i\delta_\ell} \sin(\delta_\ell)\right) \qquad (e^{i\delta_\ell} = \cos(\delta_\ell) + i\sin(\delta_\ell))$$

$$= \frac{1}{k} \sum (2\ell+1) \sin^2(\delta_\ell)$$

$$\sigma_{tot} = \int d\Omega \, |f(\theta)|^2$$

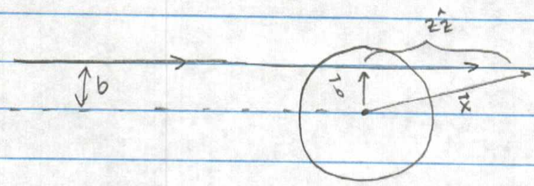
$$= \frac{1}{k^2} \int d\phi \, d\cos(\theta) \sum_\ell \sum_{\ell'} (2\ell+1)(2\ell'+1) e^{i\delta_\ell} \sin(\delta_\ell) e^{-i\delta_{\ell'}} \sin(\delta_{\ell'}) P_\ell(\cos(\theta)) P_{\ell'}(\cos(\theta))$$

$$\int_0^1 d\cos(\theta) \, P_\ell(\cos(\theta)) P_{\ell'}(\cos(\theta)) = \frac{1}{2\ell+1} \delta_{\ell\ell'}$$

$$\sigma_{tot} = \frac{1}{k^2} 2\pi \sum \left(\frac{2}{2\ell+1}\right) (2\ell+1)^2 \sin^2(\delta_\ell)$$

$$\frac{k}{4\pi} \sigma_{tot} = \frac{1}{k} \sum (2\ell+1) \sin^2(\delta_\ell) = \mathrm{Im}(f(\theta=0)) \quad \checkmark$$

Eikonal Approximation




(high energy, just goes straight through)

→ phase shift caused by potential

Semi-classical approximation, $\vec{L} = \vec{r} \times \vec{p}$

$$\ell \sim kb$$

$$\sum_{\ell=0}^{\infty} \rightarrow \int_0^\infty d(kb)$$

$$P_\ell(\cos(\theta)) \approx (\cos(\theta))^\ell J_0((\ell + \tfrac{1}{2})\sin(\theta)) \quad \text{(for large } \ell)$$

$$\theta \approx 0 \rightarrow \quad P_\ell(\cos(\theta)) \rightarrow J_0(kb\theta)$$

$$f(\theta) = \frac{1}{ik} \sum_{l} (l+\tfrac{1}{2})(e^{2i\delta_l} - 1) P_l(\cos(\theta))$$ (from Eq 7.6.17)

$$\approx \frac{1}{ik} \int_0^\infty d(kb) \left( kb \, (e^{2i\Delta(b)} - 1) J_0(kb\theta) \right)$$

$$f(\theta) = -ik \int_0^\infty db \left( b J_0(kb\theta)(e^{2i\Delta(b)} - 1) \right)$$ (Eikonal approximation)

Derivation in Sakurai

$$\psi = \sqrt{\rho} \, e^{iS/\hbar} \qquad \left( \rho = \psi^* \psi \, , \; \vec{j} = \rho \left( \frac{\vec{\nabla} S}{m} \right) \right)$$

Hamilton-Jacobi Equation → $\frac{(\vec{\nabla} S)^2}{2m} + V(r) = E = \frac{\hbar^2 k^2}{2m}$ (Chapter 2)

$$|\vec{\nabla} S| = \hbar \sqrt{k^2 - \frac{2m}{\hbar^2} V(r)}$$

$$\vec{x} = \vec{b} + z\hat{z} \quad \rightarrow \quad V(r) = V(\sqrt{b^2 + z^2})$$

$$\frac{S}{\hbar} = \int_{-\infty}^{z} dz' \sqrt{k^2 - \frac{2m}{\hbar^2} V(\sqrt{b^2 + z'^2})} + \text{const}$$

As $V \rightarrow 0$ , $\psi^{(+)} \sim e^{ikz}$ $\left( \frac{S}{\hbar} \rightarrow kz \right)$

$$\frac{S}{\hbar} = kz + \int_{-\infty}^{z} dz' \left( \sqrt{k^2 - \frac{2m}{\hbar^2} V(\sqrt{b^2 + z'^2})} - k \right)$$

$E \gg V \rightarrow$

$$\sqrt{k^2 - \frac{2m}{\hbar^2} V} \approx k - \frac{mV}{\hbar^2 k}$$

$$\frac{S}{\hbar} \approx kz - \frac{m}{\hbar^2 k} \int_{-\infty}^{z} dz' \, V(\sqrt{b^2 + z'^2})$$

$$f(\vec{k}', \vec{k}) = -\frac{m}{2\pi\hbar^2} (2\pi)^3 \int d^3x' \, \frac{e^{-i\vec{k}' \cdot \vec{x}'}}{(2\pi)^{3/2}} V(\vec{x}') \langle \vec{x}' | \psi^{(+)} \rangle$$

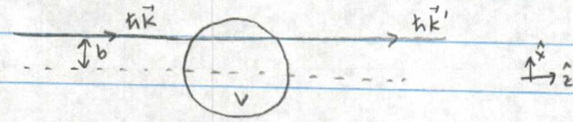
$$= \frac{-m}{2\pi\hbar^2} (2\pi)^3 \int d^3x' \, \frac{e^{-i\vec{k}' \cdot \vec{x}'}}{(2\pi)^{3/2}} V(\vec{x}') \underbrace{\left( \sqrt{\rho} \, e^{iS/\hbar} \right)}_{\approx \frac{1}{(2\pi)^{3/2}} e^{ikz} e^{-\frac{im}{\hbar^2 k} \int_{-\infty}^{z} dz' V(\sqrt{b^2 + z'^2})}}$$

$$f(\vec{k}', \vec{k}) = \frac{-m}{2\pi\hbar^2} \int d^3x' \, e^{-i\vec{k}'\cdot\vec{x}'} \, V\left(\sqrt{b^2 + z'^2}\right) e^{ikz'} \exp\left[\frac{-im}{\hbar^2 k} \int_{-\infty}^{z'} dz'' \, V\left(\sqrt{b^2 + z''^2}\right)\right]$$

$$e^{ikz'} = e^{i\vec{k}\cdot\vec{x}'} \qquad (\vec{x}' = \vec{b} + z'\hat{z}) \quad (\vec{k} \perp \vec{b})$$

03/23/2010 <u>Plane Waves and Spherical Waves</u>

Starting with Eikonal Approximation (finish from last class)




$(E \gg V)$

$$f(\vec{k}', \vec{k}) = \frac{-m}{2\pi\hbar^2} \int d^3x' \, e^{-i\vec{k}'\cdot\vec{x}'} \, V\left(\sqrt{b^2+z'^2}\right) e^{ikz'} \exp\left[\frac{-im}{\hbar^2 k}\int_{-\infty}^{z'} dz'' \, V\left(\sqrt{b^2+z''^2}\right)\right]$$

$$e^{ikz'} = e^{i\vec{k}\cdot\vec{x}'} \qquad (\vec{k} = k\hat{z} \ , \ \vec{x}' = \vec{b} + z'\hat{z})$$

$$f(\vec{k}', \vec{k}) = \frac{-m}{2\pi\hbar^2} \int d^3x' \, e^{i(\vec{k}-\vec{k}')\cdot\vec{x}'} \, V\left(\sqrt{b^2+z'^2}\right) \exp\left[\frac{-im}{\hbar^2 k}\int_{-\infty}^{z'} dz'' \, V\left(\sqrt{b^2+z''^2}\right)\right]$$

$$d^3x' = b\,db\,d\phi_b\,dz'$$

$$(\vec{k}-\vec{k}')\cdot\vec{x}' = (\vec{k}-\vec{k}')\cdot(\vec{b} + z'\hat{z})$$

$$= -\vec{k}'\cdot\vec{b} + z'(\vec{k}-\vec{k}')\cdot\hat{z}$$

$$= -(k\sin(\theta)\,\hat{x} + k\cos(\theta)\,\hat{z})\cdot(b\cos(\phi_b)\,\hat{x} + b\sin(\phi_b)\,\hat{y}) + z'(\vec{k}-\vec{k}')\cdot\hat{z}$$

(small angle approximation) $\qquad \simeq -kb\theta\cos(\phi_b) + z'k(1-\cos(\theta))$

$$= -kb\theta\cos(\phi_b) + \underbrace{z'k\sin^2\left(\tfrac{\theta}{2}\right)}_{O(\theta^2)}$$

$$(\vec{k}-\vec{k}')\cdot\vec{x}' \simeq -kb\theta\cos(\phi_b)$$

$$f(\vec{k}', \vec{k}) = \frac{-m}{2\pi\hbar^2} \int_0^{\infty}\int_0^{2\pi}\int_{-\infty}^{\infty} dz'\,d\phi_b\,db\; b\, e^{-ikb\theta\cos(\phi_b)} \, V \exp\left[\frac{-im}{\hbar^2 k}\int_{-\infty}^{z'} dz'' \, V\right]$$

1. $\int_0^{2\pi} d\phi_b \, e^{-ikb\theta\cos(\phi_b)} = 2\pi J_0(kb\theta)$ (Bessel function)

2. $\int_{-\infty}^{\infty} dz \, V \exp\left[\frac{-im}{\hbar^2 k}\int_{-\infty}^{z} V \, dz'\right]$

$$= \int_{-\infty}^{\infty} dz \, \frac{d}{dz}\left(\exp\left[\frac{-im}{\hbar^2 k}\int_{-\infty}^{z} V \, dz'\right]\right)\left(\frac{i\hbar^2 k}{m}\right)$$

$$= \frac{i\hbar^2 k}{m} \exp\left[\frac{-im}{\hbar^2 k}\int_{-\infty}^{z} V \, dz'\right]\Bigg|_{-\infty}^{\infty}$$

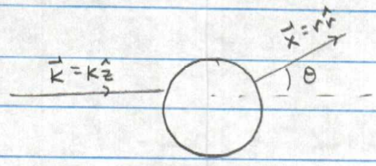
$$= \frac{i\hbar^2 k}{m}\left(\exp\left[\frac{-im}{\hbar^2 k}\int_{-\infty}^{\infty} V \, dz'\right] - 1\right)$$

$$\boxed{\begin{gathered} f(\vec{k}', \vec{k}) = -ik \int_0^{\infty} db \, b \, J_0(kb\theta)\left(e^{2i\Delta(b)} - 1\right) \\ \Delta(b) = \frac{-m}{2\hbar^2 k}\int_{-\infty}^{\infty} dz \, V(\sqrt{b^2+z^2}) \end{gathered}}$$

$$\Delta(b) = \frac{-k}{2E}\int_0^{\infty} dz \, V(\sqrt{b^2+z^2})$$

$$f(\theta) = \frac{1}{k}\sum (2l+1) e^{i\delta_l} \sin(\delta_l) P_l(\cos(\theta))$$

This gives a consistent result with Eikonal approximation.




$$\psi_{\vec{k}}(\vec{x}) \xrightarrow[r\to\infty]{} e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$$

$$\langle \vec{x} | \psi^{(+)} \rangle = \frac{1}{(2\pi)^{3/2}} \psi_{\vec{k}}(\vec{x})$$

Plane Wave

$$e^{ikz} = e^{ikr\cos(\theta)} = \sum i^{\ell}(2\ell+1)\underbrace{j_\ell}_{\text{Spherical Bessel function}}(kr)\, P_\ell(\cos(\theta))$$

As $r \to \infty$, $\quad j_\ell(kr) \to \dfrac{\sin(kr - \frac{\ell\pi}{2})}{kr}$

$$e^{ikr\cos(\theta)} \xrightarrow[r\to\infty]{} \frac{1}{2ik}\sum i^{\ell}(2\ell+1)\Bigg(\underbrace{\frac{e^{i(kr-\ell\pi/2)}}{r}}_{\text{outgoing}} - \underbrace{\frac{e^{-i(kr-\ell\pi/2)}}{r}}_{\text{infalling}}\Bigg)P_\ell(\cos(\theta))$$

$$i^{\ell} = e^{i\ell\pi/2}$$

$$e^{ikr(\cos(\theta))} \xrightarrow[r\to\infty]{} \frac{1}{2ik}\sum(2\ell+1)\left(\frac{e^{ikr}}{r} - \frac{e^{-i(kr-\ell\pi)}}{r}\right)P_\ell(\cos(\theta))$$

Scattered Wave

$$\psi_{\vec{k}}(\vec{x}) \xrightarrow[r\to\infty]{} \frac{1}{2ikr}\sum(2\ell+1)\left(e^{ikr}e^{2i\delta_\ell} - e^{-i(kr-\ell\pi)}\right)P_\ell(\cos(\theta))$$

$$f(\theta)\frac{e^{ikr}}{r} = \psi_{\vec{k}}(\vec{x}) - e^{ikz}$$

$$f(\theta)\frac{e^{ikr}}{r} = \frac{e^{ikr}}{r}\sum(2\ell+1)\frac{e^{2i\delta_\ell}-1}{2ik}P_\ell(\cos(\theta))$$

$$\Rightarrow \boxed{\begin{aligned} f(\theta) &= \frac{1}{k}\sum(2\ell+1)\frac{e^{2i\delta_\ell}-1}{2i}P_\ell(\cos(\theta)) \\ &= \frac{1}{k}\sum(2\ell+1)e^{i\delta_\ell}\sin(\delta_\ell)P_\ell(\cos(\theta)) \end{aligned}}$$

Spherically Symmetric Potential

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

Separation of variables $\rightarrow$ $\psi_E(r,\theta,\phi) = R_{E\ell}(r)\,Y_{\ell m}(\theta,\phi)$

$$\vec{L}^2\,Y_{\ell m}(\theta,\phi) = \ell(\ell+1)\hbar^2\,Y_{\ell m}(\theta,\phi)$$

$$L_z\,Y_{\ell m}(\theta,\phi) = m\hbar\,Y_{\ell m}(\theta,\phi) \quad \rightarrow \quad L_z = \frac{\hbar}{i}\partial_\phi$$

Radial equation $\quad u_{E\ell}(r) \equiv r\,R_{E\ell}(r) \qquad (u_{E\ell}(0)=0)$

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

03/25/2010 Partial-Wave Expansion

Radial equation

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

Look at $V(r) = 0$ (Free equation)

$$E = \frac{\hbar^2 k}{2m} \rightarrow \text{cancel factors of } \frac{\hbar^2}{2m}$$

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right)u_{E\ell}(r) = 0 \qquad \text{(Free Schrödinger Equation)}$$

$$\left(\frac{d^2}{d(kr)^2} + 1 - \frac{\ell(\ell+1)}{(kr)^2}\right)u_{E\ell}(r) = 0$$

Let $\rho = kr \rightarrow u_{E\ell}(r) = u_\ell(\rho)$

$$\left(\frac{d^2}{d\rho^2} + 1 - \frac{\ell(\ell+1)}{\rho^2}\right)u_\ell(\rho) = 0$$

1. $\ell = 0 \Rightarrow \quad \frac{d^2u_0}{d\rho^2} + u_0 = 0$

$u_0 = \sin(\rho)$ (to satisfy boundary condition $u_0(0) = 0$)

$$R_0(\rho) = \frac{1}{\rho}u_0(\rho) = \frac{\sin(\rho)}{\rho} = j_0(\rho)$$

2. $\ell \neq 0 \Rightarrow \quad \underbrace{\left(-\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2}\right)}\, u_\ell(\rho) = u_\ell(\rho)$

$$\left(\frac{d}{d\rho} + \frac{(\ell+1)}{\rho}\right)\left(-\frac{d}{d\rho} + \frac{\ell+1}{\rho}\right)$$

$$= -\frac{d^2}{d\rho^2} - \frac{\ell+1}{\rho^2} + \frac{\ell+1}{\rho}\frac{d}{d\rho} - \frac{\ell+1}{\rho}\frac{d}{d\rho} + \frac{(\ell+1)^2}{\rho^2}$$

$$= -\frac{d^2}{d\rho^2} + \frac{1}{\rho^2}(\ell+1)(\ell+1-1)$$

$$= -\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} \checkmark$$

$$\left(\frac{-d}{d\rho} + \frac{\ell+1}{\rho}\right) u_\ell = u_{\ell+1} \quad \text{(will show later)}$$

$$\Rightarrow \left(\frac{d}{d\rho} + \frac{\ell+1}{\rho}\right) u_{\ell+1} = u_\ell$$

$$\left(\frac{-d}{d\rho} + \frac{\ell+1}{\rho}\right)\left(\frac{d}{d\rho} + \frac{\ell+1}{\rho}\right) = \frac{-d^2}{d\rho^2} + \frac{\ell+1}{\rho^2} - \frac{\ell+1}{\rho}\frac{d}{d\rho} + \frac{\ell+1}{\rho}\frac{d}{d\rho} + \frac{(\ell+1)^2}{\rho^2}$$

$$= \frac{-d^2}{d\rho^2} + \frac{1}{\rho^2}(\ell+1)(\ell+1+1)$$

$$= -\frac{d^2}{d\rho^2} + \frac{(\ell+1)(\ell+2)}{\rho^2}$$

$$= \left(\frac{d}{d\rho} + \frac{\ell+2}{\rho}\right)\left(\frac{-d}{d\rho} + \frac{\ell+2}{\rho}\right)$$

$$\left(\frac{-d}{d\rho} + \frac{\ell+1}{\rho}\right)\left(\frac{d}{d\rho} + \frac{\ell+1}{\rho}\right)\left[\left(\frac{-d}{d\rho} + \frac{\ell+1}{\rho}\right) u_\ell\right] = \left[\left(\frac{-d}{d\rho} + \frac{\ell+1}{\rho}\right) u_\ell\right]$$

$$\left(\frac{d}{d\rho} + \frac{\ell+2}{\rho}\right)\left(\frac{-d}{d\rho} + \frac{\ell+2}{\rho}\right) u_{\ell+1} = u_{\ell+1} \quad \text{(all } \ell \to \ell+1 \text{ from original equation)}$$

$$\Rightarrow \left(\frac{-d}{d\rho} + \frac{\ell+1}{\rho}\right) u_\ell = u_{\ell+1}$$

So . . .

$\left(\frac{-d}{d\rho} + \frac{\ell+1}{\rho}\right)$ serves as a "raising operator" in $\ell$

$\left(\frac{d}{d\rho} + \frac{\ell+1}{\rho}\right)$ serves as a "lowering operator" in $\ell$

Let's find $u_1(\rho)$

$$u_1(\rho) = \left(\frac{-d}{d\rho} + \frac{1}{\rho}\right) u_0 = \left(\frac{-d}{d\rho} + \frac{1}{\rho}\right)\sin(\rho)$$

$$u_1(\rho) = -\cos(\rho) + \frac{\sin(\rho)}{\rho}$$

$$R_1(\rho) = \frac{1}{\rho} u_1(\rho) = \frac{-\cos(\rho)}{\rho} + \frac{\sin(\rho)}{\rho^2} = j_1(\rho)$$

$$u_2(\rho) = \left(\frac{-d}{d\rho} + \frac{2}{\rho}\right)\left(-\cos(\rho) + \frac{\sin(\rho)}{\rho}\right)$$

$$= -\sin(\rho) - \frac{\cos(\rho)}{\rho} + \frac{\sin(\rho)}{\rho^2} - \frac{2\cos(\rho)}{\rho} + \frac{2\sin(\rho)}{\rho^2}$$

$$u_2(\rho) = -\sin(\rho) - \frac{3\cos(\rho)}{\rho} + \frac{3\sin(\rho)}{\rho^2} = \left(\frac{3}{\rho^2} - 1\right)\sin(\rho) - \frac{3\cos(\rho)}{\rho}$$

$$R_2(\rho) = \frac{-\sin(\rho)}{\rho} - \frac{3\cos(\rho)}{\rho^2} + \frac{3\sin(\rho)}{\rho^3} = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin(\rho) - \frac{3\cos(\rho)}{\rho^2} = j_2(\rho)$$

$$\Rightarrow \quad \boxed{R_\ell(\rho) = j_\ell(\rho)}$$

$$\frac{R_\ell}{\rho^\ell} = \frac{-1}{\rho}\frac{d}{d\rho}\left(\frac{R_{\ell-1}}{\rho^{\ell-1}}\right)$$

$$= \left(\frac{-1}{\rho}\frac{d}{d\rho}\right)^2\left(\frac{R_{\ell-2}}{\rho^{\ell-2}}\right)$$

$$= \left(\frac{-1}{\rho}\frac{d}{d\rho}\right)^\ell\left(\frac{R_0}{\rho^0}\right)$$

$$\boxed{R_\ell = (-\rho)^\ell \left(\frac{+1}{\rho}\frac{d}{d\rho}\right)^\ell \left(\frac{\sin(\rho)}{\rho}\right) = j_\ell(\rho)}$$

Integral representation of $j_\ell(\rho)$

$$j_\ell(\rho) = \frac{1}{2i^\ell}\int_{-1}^{+1} e^{i\rho z} P_\ell(z)\, dz \qquad \text{(Eq. 7.5.19)}$$

$\ell = 0 \rightarrow$

$$j_0(\rho) = \frac{1}{2}\int_{-1}^{1} e^{i\rho z}\, dz = \frac{1}{2i\rho}\left(e^{i\rho} - e^{-i\rho}\right) = \frac{\sin(\rho)}{\rho}$$

$$R_{El}(r) = j_l(kr)$$

$$\boxed{\psi_{Elm}(r,\theta,\phi) = j_l(kr)\, Y_{lm}(\theta,\phi)} \qquad (V(r)=0)$$

Plane-wave

$$e^{ikz} = e^{ikr\cos(\theta)} = \sum_{l,m} C_{lm}\, j_l(kr)\, Y_{lm}(\theta,\phi)$$

No $\phi$ dependence $\rightarrow$ $m=0$ $\qquad \left(Y_{l0} = \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos(\theta))\right)$

$$= \sum_l C_l\, j_l(kr)\, P_l(\cos(\theta))$$

$$j_l(kr) = \frac{1}{2i^l} \int_{-1}^{1} \left(\sum_{l'} C_{l'}\, j_{l'}(kr)\, P_{l'}(\cos(\theta))\right) P_l(\cos(\theta))\, d\cos(\theta)$$

$$= \frac{1}{2i^l} \sum_{l'} C_{l'}\, j_{l'}(kr) \underbrace{\int_{-1}^{1} P_{l'}(\cos(\theta))\, P_l(\cos(\theta))\, d\cos(\theta)}_{\frac{2}{2l+1}\delta_{ll'}}$$

$$j_l(kr) = \frac{C_l}{i^l}\, j_l(kr)\, \frac{1}{2l+1}$$

$$\Rightarrow \; C_l = i^l (2l+1)$$

$$\Rightarrow \boxed{e^{ikz} = \sum_l i^l (2l+1)\, j_l(kr)\, P_l(\cos(\theta))}$$

$$r\to\infty: \quad j_l(kr) \to \frac{\sin(kr - l\pi/2)}{kr}$$

$$e^{ikz} \xrightarrow[r\to\infty]{} \frac{1}{2ik} \sum_l (2l+1) \left(\frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r}\right) P_l(\cos(\theta))$$

$$\psi_{\vec{k}}(\vec{r}) \xrightarrow[r\to\infty]{} \frac{1}{2ikr} \sum_l (2l+1) \left(e^{ikr} \underbrace{e^{2i\delta_l}}_{\text{phase shift}} - e^{-i(kr-l\pi)}\right) P_l(\cos(\theta))$$

$$f(\theta)\frac{e^{ikr}}{r} = \psi_{\vec{k}}(\vec{r}) - e^{ikz} = \frac{e^{ikr}}{r} \sum (2l+1) \frac{e^{2i\delta_l} - 1}{2ik} P_l(\cos(\theta))$$

$$\boxed{f(\theta) = \frac{1}{k} \sum (2l+1)\, e^{i\delta_l} \sin(\delta_l)\, P_l(\cos(\theta))}$$

$$u_2(\rho) = \left(\frac{-d}{d\rho} + \frac{2}{\rho}\right)\left(-\cos(\rho) + \frac{\sin(\rho)}{\rho}\right)$$

$$= -\sin(\rho) - \frac{\cos(\rho)}{\rho} + \frac{\sin(\rho)}{\rho^2} - \frac{2\cos(\rho)}{\rho} + \frac{2\sin(\rho)}{\rho^2}$$

$$u_2(\rho) = -\sin(\rho) - \frac{3\cos(\rho)}{\rho} + \frac{3\sin(\rho)}{\rho^2} = \left(\frac{3}{\rho^2} - 1\right)\sin(\rho) - \frac{3\cos(\rho)}{\rho}$$

$$R_2(\rho) = \frac{-\sin(\rho)}{\rho} - \frac{3\cos(\rho)}{\rho^2} + \frac{3\sin(\rho)}{\rho^3} = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin(\rho) - \frac{3\cos(\rho)}{\rho^2} = j_2(\rho)$$

$$\Rightarrow \quad \boxed{R_\ell(\rho) = j_\ell(\rho)}$$

$$\frac{R_\ell}{\rho^\ell} = \frac{-1}{\rho}\frac{d}{d\rho}\left(\frac{R_{\ell-1}}{\rho^{\ell-1}}\right)$$

$$= \left(\frac{-1}{\rho}\frac{d}{d\rho}\right)^2\left(\frac{R_{\ell-2}}{\rho^{\ell-2}}\right)$$

$$= \left(\frac{-1}{\rho}\frac{d}{d\rho}\right)^\ell\left(\frac{R_0}{\rho^0}\right)$$

$$\boxed{R_\ell = (-\rho)^\ell\left(\frac{+1}{\rho}\frac{d}{d\rho}\right)^\ell\left(\frac{\sin(\rho)}{\rho}\right) = j_\ell(\rho)}$$

Integral representation of $j_\ell(\rho)$

$$j_\ell(\rho) = \frac{1}{2i^\ell}\int_{-1}^{+1} e^{i\rho z} P_\ell(z)\, dz \qquad \text{(Eq. 7.5.19)}$$

$\ell = 0 \rightarrow$

$$j_0(\rho) = \frac{1}{2}\int_{-1}^{1} e^{i\rho z}\, dz = \frac{1}{2i\rho}\left(e^{i\rho} - e^{-i\rho}\right) = \frac{\sin(\rho)}{\rho}$$

$$R_{E\ell}(r) = j_\ell(kr)$$

$$\boxed{\psi_{E\ell m}(r,\theta,\phi) = j_\ell(kr)\, Y_{\ell m}(\theta,\phi)} \qquad (V(r)=0)$$

Plane-wave

$$e^{ikz} = e^{ikr\cos(\theta)} = \sum_{\ell,m} C_{\ell m}\, j_\ell(kr)\, Y_{\ell m}(\theta,\phi)$$

No $\phi$ dependence $\rightarrow$ $m=0$ $\qquad \left(Y_{\ell 0} = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos(\theta))\right)$

$$= \sum_\ell C_\ell\, j_\ell(kr)\, P_\ell(\cos(\theta))$$

$$j_\ell(kr) = \frac{1}{2i^\ell}\int_{-1}^{1}\left(\sum_{\ell'} C_{\ell'}\, j_{\ell'}(kr)\, P_{\ell'}(\cos(\theta))\right) P_\ell(\cos(\theta))\, d\cos(\theta)$$

$$= \frac{1}{2i^\ell}\sum_{\ell'} C_{\ell'}\, j_{\ell'}(kr)\underbrace{\int_{-1}^{1} P_{\ell'}(\cos(\theta))\, P_\ell(\cos(\theta))\, d\cos(\theta)}_{\frac{2}{2\ell+1}\delta_{\ell\ell'}}$$

$$j_\ell(kr) = \frac{C_\ell}{i^\ell}\, j_\ell(kr)\, \frac{1}{2\ell+1}$$

$$\Rightarrow C_\ell = i^\ell(2\ell+1)$$

$$\Rightarrow \boxed{e^{ikz} = \sum_\ell i^\ell(2\ell+1)\, j_\ell(kr)\, P_\ell(\cos(\theta))}$$

$$r\to\infty: \quad j_\ell(kr) \to \frac{\sin(kr - \ell\pi/2)}{kr}$$

$$e^{ikz} \xrightarrow[r\to\infty]{} \frac{1}{2ik}\sum_\ell (2\ell+1)\left(\frac{e^{ikr}}{r} - \frac{e^{-i(kr-\ell\pi)}}{r}\right) P_\ell(\cos(\theta))$$

$$\psi_{\vec{k}}(\vec{r}) \xrightarrow[r\to\infty]{} \frac{1}{2ikr}\sum_\ell (2\ell+1)\left(e^{ikr}\underbrace{e^{2i\delta_\ell}}_{\text{phase shift}} - e^{-i(kr-\ell\pi)}\right) P_\ell(\cos(\theta))$$

$$f(\theta)\frac{e^{ikr}}{r} = \psi_{\vec{k}}(\vec{r}) - e^{ikz} = \frac{e^{ikr}}{r}\sum (2\ell+1)\frac{e^{2i\delta_\ell}-1}{2ik} P_\ell(\cos(\theta))$$

$$\boxed{f(\theta) = \frac{1}{k}\sum(2\ell+1)\, e^{i\delta_\ell}\sin(\delta_\ell)\, P_\ell(\cos(\theta))}$$

04/08/2010 Phase Shift Analysis

Example: Hard Sphere Scattering

$$\psi_k(\vec{x}) = e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$$

$$f(\theta) = \frac{1}{k}\sum(2l+1)e^{i\delta_l}\sin(\delta_l)P_l(\cos(\theta))$$

$$e^{ikz} = \sum i^l(2l+1)j_l(kr)P_l(\cos(\theta))$$

$$\psi_k(\vec{x}) = \sum i^l(2l+1)A_l(kr)P_l(\cos(\theta))$$

$$V(r) = \begin{cases} V_0 > 0 & r < R \\ 0 & r > R \end{cases}$$

Schrödinger Equation

$$\psi_{El}(r,\theta,\phi) = R_{El}(r)Y_{lm}(\theta,\phi) \qquad u_{El}(r) = r R_{El}(r)$$

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

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

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

$$r > R \rightarrow \left(\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right)u_{El}^{ext} = 0$$

$$r < R \rightarrow \left(\frac{d^2}{dr^2} + K^2 - \frac{l(l+1)}{r^2}\right)u_{El}^{int} = 0$$

Consider $\ell = 0$

$$\left(\frac{d^2}{dr^2} + k^2\right) u_{E0}^{ext} = 0$$

$$\left(\frac{d^2}{dr^2} + K^2\right) u_{E0}^{int} = 0$$

$$u_{E0}^{int}(r) = A\sin(Kr) \qquad \left(\text{satisfies } u_{E0}^{int}(0) = 0\right)$$

$$u_{E0}^{ext}(r) = B\sin(kr) + C\cos(kr) = D\sin(kr + \delta_0)$$

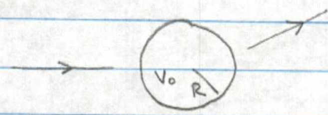
$$\psi_{\vec{k}}^{\ell=0}(r) = j_0(kr) + \frac{1}{k} e^{i\delta_0} \sin(\delta_0) \frac{e^{ikr}}{r}$$

$$= \frac{\sin(kr)}{kr} + \frac{1}{k} e^{i\delta_0} \sin(\delta_0) \frac{e^{ikr}}{r}$$

$$= \frac{e^{i\delta_0}}{kr} \sin(kr + \delta_0)$$

04/13/2010 Low Energy Scattering : Bound States and Resonances

Hard Sphere Scattering




$$V(r) = \begin{cases} V_0 & r < R \\ 0 & r > R \end{cases}$$

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

$l = 0$ case

$$r < R \quad : \quad u_{E0}^{int}(r) = A\sin(Kr)$$

$$r > R \quad : \quad u_{E0}^{ext}(r) = B\sin(kr) + C\cos(kr) = D\sin(kr + \delta_0)$$

To find $\delta_0$, we use boundary condition at $r = R$

$$u_{E0}^{int}(R) = u_{E0}^{ext}(R)$$

$$\left.\frac{du_{E0}^{int}}{dr}\right|_{r=R} = \left.\frac{du_{E0}^{ext}}{dr}\right|_{r=R}$$

$$\Rightarrow \quad A\sin(KR) = D\sin(kR + \delta_0)$$

$$KA\cos(KR) = kD\cos(kR + \delta_0)$$

Logarithmic derivative : $\left.\frac{r}{A_l}\frac{dA_l}{dr}\right|_{r=R}$

$$\frac{1}{K}\tan(Kr) = \frac{1}{k}\tan(kR + \delta_0)$$

$$\tan(kR + \delta_0) = \frac{k}{K}\tan(KR)$$

$$\boxed{\delta_0 = \arctan\left(\frac{k}{K}\tan(KR)\right) - kR}$$

As $V_0 \to \infty$, then $E < V_0$

$$\Rightarrow \quad K^2 = \frac{2m}{\hbar^2}(E - V_0) = -q^2 < 0$$

$$K \to iq$$

$$\tan(KR) \to \tan(iqR) = i\tanh(qR)$$

$$\tan(KR) = \frac{e^{iKR} - e^{-iKR}}{i(e^{iKR} + e^{-iKR})} = \frac{1}{i}\,\frac{e^{-qR} - e^{qR}}{e^{-qR} + e^{qR}}$$

$$\Rightarrow \quad \boxed{\delta_0 = \arctan\left(\frac{k}{q}\tanh(qR)\right) - kR}$$

If $V_0 \to \infty$, then $qR = \frac{\sqrt{2m(V_0 - E)}}{\hbar} R \to \infty$

$$\frac{\tanh(qR)}{qR} \to 0$$

$$\Rightarrow \quad \delta_0 \to -kR$$

$$f(\theta) = \frac{1}{k}\sum (2\ell+1)\, e^{i\delta_\ell}\sin(\delta_\ell)\, P_\ell(\cos(\theta))$$

$$\frac{4\pi}{k}\,\mathrm{Im}(f_0(\theta)) = \sigma_{\ell=0}$$

$$\frac{4\pi}{k^2}\sin^2(\delta_0) = \sigma_{\ell=0} \approx \frac{4\pi}{k^2}\sin^2(kR) \approx 4\pi R^2 \ \checkmark$$

What about $\ell \neq 0$? (Take $V_0 \to \infty$)

$$\psi_{\vec{k}}(\vec{x}) = e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$$

$$= \sum i^\ell (2\ell+1) A_\ell(kr) P_\ell(\cos(\theta))$$

$$\text{where } A_\ell(kr) = e^{i\delta_\ell}\left(\cos(\delta_\ell) j_\ell(kr) - \sin(\delta_\ell) n_\ell(kr)\right)$$

$j_\ell$ - spherical Bessel

$n_\ell$ - spherical Neumann

$$A_0(kr) = e^{i\delta_0}\left(\cos(\delta_0)\frac{\sin(kr)}{kr} + \sin(\delta_0)\frac{\cos(kr)}{kr}\right)$$

$$= \frac{e^{i\delta_0}}{kr}\left(\cos(\delta_0)\sin(kr) + \sin(\delta_0)\cos(kr)\right)$$

$$= \frac{e^{i\delta_0}}{kr}\sin(kr + \delta_0) \quad \checkmark$$

As $V_0 \to \infty$, $A_\ell(kR) = 0$

$$\cos(\delta_\ell) j_\ell(kR) = \sin(\delta_\ell) n_\ell(kR)$$

$$\Rightarrow \boxed{\tan(\delta_\ell) = \frac{j_\ell(kR)}{n_\ell(kR)}}$$

For low energy ($kR \ll 1$)

$$j_\ell(kR) \approx \frac{(kR)^\ell}{(2\ell+1)!!}$$

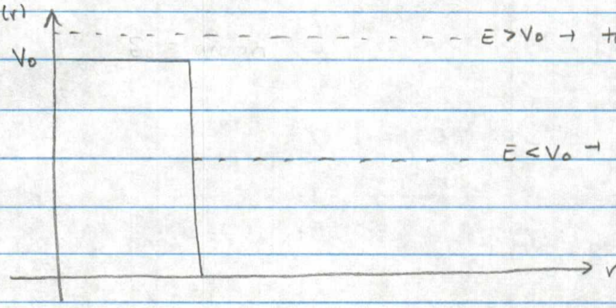
$$\left((2\ell+1)!! = (2\ell+1)(2\ell-1)\cdots 5\cdot 3\cdot 1\right)$$
$$= (2\ell+1)(2\ell-1)!!$$

$$n_\ell(kR) \approx \frac{-(2\ell-1)!!}{(kR)^{\ell+1}}$$

$$\Rightarrow \tan(\delta_\ell) = \frac{-(kR)^{2\ell+1}}{(2\ell+1)\left((2\ell-1)!!\right)^2}$$

Phase shifts for large $\ell$ values are suppressed.

Going back to $l = 0$, we have an exact solution for $\delta_0$




$E > V_0 \rightarrow \tan(\delta_0 + kR) = \frac{k}{K}\tan(KR) \quad \left(K = \frac{\sqrt{2m(E-V_0)}}{\hbar}\right)$

$E < V_0 \rightarrow \tan(\delta_0 + kR) = \frac{kR}{qR}\tanh(qR) \quad \left(q = \frac{\sqrt{2m(V_0-E)}}{\hbar}\right)$

$$\tan(\delta_0 + kR) = \frac{\tan(\delta_0) + \tan(kR)}{1 + \tan(\delta_0)\tan(kR)}$$

$$\tan(\delta_0) = \frac{kR\left(\frac{\tan(KR)}{KR} - \frac{\tan(kR)}{kR}\right)}{1 + \frac{kR}{KR}\tan(KR)\tan(kR)} \qquad (E > V_0)$$

$$\tan(\delta_0) = \frac{kR\left(\frac{\tanh(qR)}{qR} - \frac{\tan(kR)}{kR}\right)}{1 + \frac{kR}{qR}\tanh(qR)\tan(kR)} \qquad (E < V_0)$$

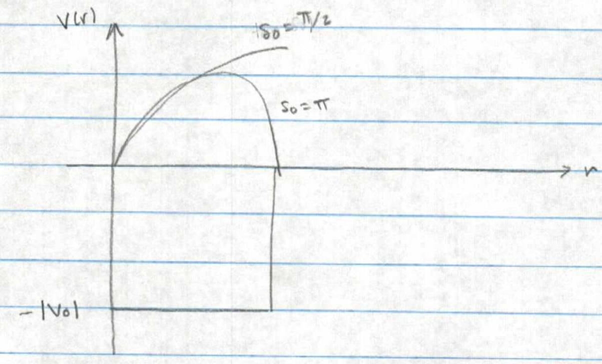
$$\tan(x) \simeq x + \frac{1}{3}x^3 + \cdots \qquad (x \ll 1)$$

$$\tanh(x) \simeq x - \frac{1}{3}x^3 + \cdots$$

Both expand to

$$\tan(\delta_0) \sim \frac{-2m}{\hbar^2} V_0 < 0$$

Attractive Potential $(V_0 < 0)$




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

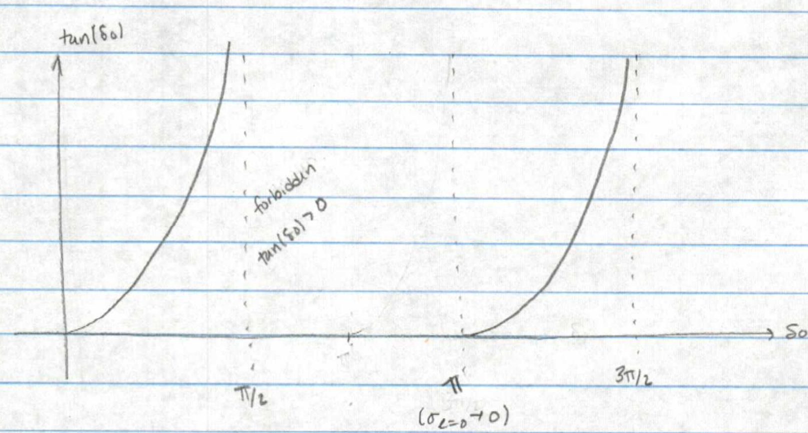
$$\tan(\delta_0) \sim \frac{2m}{\hbar^2}|V_0| > 0$$

$$KR \to \frac{\pi}{2} : \quad \tan(\delta_0) \to \frac{1}{\tan(KR)}$$

Low energy, $kR \ll 1 \Rightarrow \tan(\delta_0) \to \infty$ or $\delta_0 \approx \frac{\pi}{2}$

$$\sigma_{\ell=0} = \frac{4\pi}{k^2}\sin^2(\delta_0) = \frac{4\pi}{k^2} \to \infty \quad \text{(maximum value)}$$

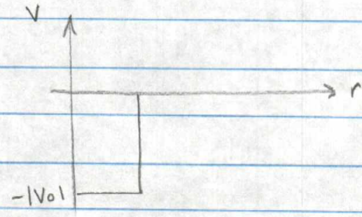
→ Formation of bound states as depth of well grows




Almost perfect transmission → 1923 Ramsauer - Townsend Effect
$^{18}Ar$, $^{36}Kr$, $^{54}Xe$, ...

04/15/2010

Bound States and Resonances




Zero-Energy Scattering and Bound States

$$r > R \qquad \left(\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right) u_{E\ell}(r) = 0$$

For $\ell = 0$ and $k \to 0$ (zero-energy)

$$\frac{d^2}{dr^2} u_0(r) = 0$$

$$u_0(r) = \alpha(r - a) \qquad a\text{- scattering length}$$

Solution from before

$$u_{E0}^{ext}(r) = D\sin(kr + \delta_0) \xrightarrow[k\to 0]{} u_0(r) = \alpha(r-a)$$

Logarithmic derivative

$$\frac{u_{E0}^{ext\,\prime}}{u_{E0}^{ext}} = k\cot(kr + \delta_0) \xrightarrow[k\to 0]{} \frac{u_0'}{u_0} = \frac{1}{r-a}$$

$$r - a \approx \frac{\tan(kr + \delta_0)}{k} \qquad (k \to 0)$$

$$= \frac{\tan(kr) + \tan(\delta_0)}{k(1 - \tan(kr)\tan(\delta_0))}$$

$$= \frac{kr + \frac{1}{3}(kr)^3 + \ldots + \tan(\delta_0)}{k - k(kr + \frac{1}{3}(kr)^3 + \ldots)\tan(\delta_0)}$$

$$\approx \frac{kr + \tan(\delta_0)}{k} \approx r + \frac{1}{k}\tan(\delta_0) + \frac{1}{3}k^2 r^3 + \ldots$$

$$\tan(\delta_0) = -ka \rightarrow k\cot(\delta_0) = \frac{-1}{a} \qquad (a<0)$$

With a correction term (Eq 7.7.22)

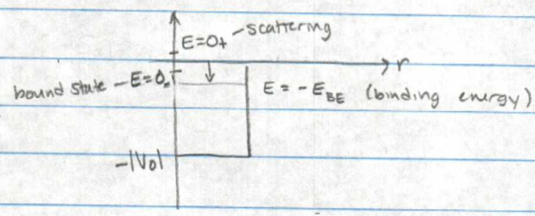
$$k\cot(\delta_0) \approx \frac{-1}{a} + \frac{1}{2} r_0 k^2 \qquad r_0 \text{ - effective range}$$

$$\sigma_{tot} \approx \sigma_{\ell=0} = \frac{4\pi}{k^2}\sin^2(\delta_0)$$

$$\sin^2(\delta_0) = \frac{\tan^2(\delta_0)}{1+\tan^2(\delta_0)} = \frac{k^2a^2}{1+k^2a^2} \approx k^2a^2$$

$$\Rightarrow \quad \sigma_{tot} \approx 4\pi a^2$$

Formation of Bound States $(E<0)$




$$-\frac{\hbar^2}{2m}\frac{d^2u_0}{dr^2} + V(r)\,u_0 = E u_0$$

For $r > R$

$$-\frac{\hbar^2}{2m}\frac{d^2u_0}{dr^2} = -E_{BE}\,u_0$$

$$\frac{d^2u_0}{dr^2} = \frac{2mE_{BE}}{\hbar^2}u_0 = K^2 u_0$$

$$u_0 = \overset{0}{\cancel{A}}e^{Kr} + Be^{-Kr}$$

$r < R$

$$\left(\frac{d^2}{dr^2} + K'^2\right)u_0^{int} = 0 \qquad K'^2 = \frac{2m(E+|V_0|)}{\hbar^2} \approx \frac{2m|V_0|}{\hbar^2}$$

No difference between scattering and bound state for the internal solutions.

$E = 0_+$ $\qquad\qquad\qquad\qquad$ $E = 0_-$

$$\frac{u_0'}{u_0}\bigg|_{r=R} = \frac{1}{r-a}\bigg|_{r=R} = \frac{1}{R-a} \qquad\qquad \frac{u_0'}{u_0}\bigg|_{r=R} = -K$$

these must be equal since internal solutions are identical

$$\frac{1}{R-a} \approx -K$$

$$R \ll a \rightarrow \quad \frac{-1}{a} \approx -K$$

$$E_{BE} = \frac{\hbar^2}{2ma^2}$$ Use scattering to determine binding energy

Example: np scattering/ Deuteron binding energy

$$E_{BE} = 2.22 \text{ MeV}$$

$$^{2S+1}L_j = {}^3S_1 \quad \text{(triplet state)}$$

$$a_{triplet} = 5.4 \times 10^{-13} \text{ cm}$$

$$\frac{\hbar^2}{2\mu a^2} = \frac{\hbar^2}{m_N a^2} = (m_N c^2)\left(\frac{\hbar}{m_N c\, a}\right)^2 = (938 \text{ MeV})\left(\frac{2.1\times10^{-14}\text{cm}}{5.4\times10^{-13}\text{cm}}\right)^2$$

$$\frac{\hbar}{m_N c} = \lambda_c = 2.1 \times 10^{-14} \text{ cm}$$

$$E_{BE} \approx 1.4 \text{ MeV}$$

Scattering Amplitude and Bound State

$$f(\theta) = \frac{1}{k} \sum (2l+1)\, e^{i\delta_l} \sin(\delta_l)\, P_l(\cos(\theta))$$

$$= \sum (2l+1)\, f_l(k)\, P_l(\cos(\theta))$$

Partial wave amplitude $\rightarrow$ $f_l(k) = \frac{1}{k} e^{i\delta_l} \sin(\delta_l)$

$$= \frac{1}{2ik}\left(e^{2i\delta_l} - 1\right)$$

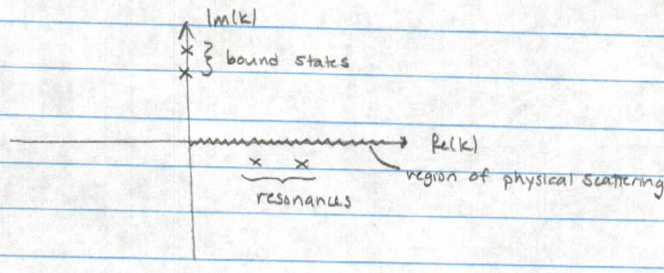
$e^{2i\delta_l} = S_l(k)$ ($l^{th}$ diagonal element of $S$ operator)

$$f_l(k) = \frac{1}{k\cot(\delta_l) - ik}$$

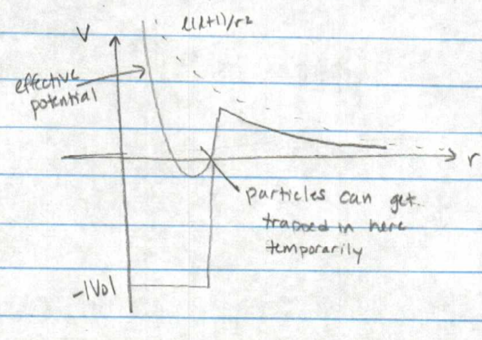
$l=0 \rightarrow \quad k\cot(\delta_0) \xrightarrow[k\to 0]{} \frac{-1}{a} = \frac{-1}{K}$

$$f_{l=0}(k) = \frac{1}{-K - ik}$$

If $k = iK$, $f_{l=0}$ has a pole



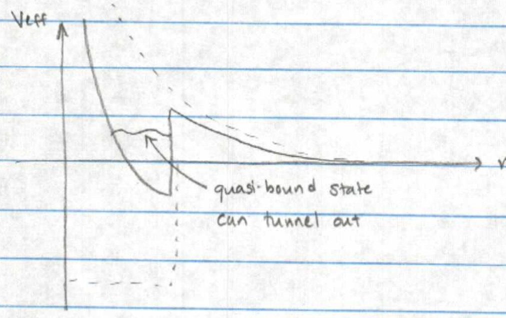

Resonances appear when $l \neq 0$



04/20/2010

## Resonances and Breit-Wigner Formula

$$-\frac{\hbar^2}{2m}\frac{d^2u_\ell}{dr^2} + \underbrace{\left(V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right)}_{V_{eff}} u_\ell = E u_\ell$$




$$k = k_r - i\frac{\eta}{2}$$

$$E = \frac{\hbar^2 k^2}{2m} \approx \frac{\hbar^2 k_r^2}{2m} - i\frac{\hbar^2 k_r \eta}{2m} - \cancel{\frac{\hbar^2\eta^2}{8m}}^{\to 0\ (\eta \ll 1)}$$

$$E \approx E_r - i\frac{\Gamma}{2} \qquad \left(E_r \equiv \frac{\hbar^2 k_r^2}{2m},\ \Gamma = \frac{\hbar^2 k_r \eta}{m}\right)$$

$$\delta_\ell(E_r) = \frac{\pi}{2}$$

$$\tan(\delta_\ell(E)) = \frac{-1}{c(E-E_r)} \qquad (\tan(\delta_\ell(E)) > 0 \text{ when } E < E_r;\ \tan(\delta_\ell(E)) < 0 \text{ when } E > E_r)$$

$$\cot(\delta_\ell(E)) = \cot(\delta_\ell(E_r)) - c(E-E_r) + \Theta((E-E_r)^2)$$

$$(\cot(\tfrac{\pi}{2}) = 0)$$

$$\cot(\delta_\ell(E)) = -c(E-E_r)$$

$$\left.\frac{d}{dE}\left(\cot(\delta_\ell(E))\right)\right|_{E\approx E_r} = -c \equiv \frac{-2}{\Gamma} \qquad \text{(Eq. 7.8.8)}$$

$$\Gamma = {}^{-2}\Big/ \left.\frac{d}{dE}(\cot(\delta_\ell))\right|_{E\approx E_r}$$

$$\tan(\delta_\ell(E)) = \frac{-\Gamma/2}{(E-E_r)}$$

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\sin^2(\delta_\ell)$$

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\frac{\tan^2(\delta_\ell)}{1+\tan^2(\delta_\ell)}$$

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\left(\frac{-\Gamma/2}{(E-E_r)}\right)^2\left(1+\left(\frac{-\Gamma/2}{E-E_r}\right)^2\right)^{-1}$$

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\frac{\Gamma^2/4}{(E-E_r)^2+\Gamma^2/4}$$

Breit-Wigner Formula : $\dfrac{\Gamma^2/4}{(E-E_r)^2+\Gamma^2/4}$

<u>Time Dependent Formulation of Scattering Theory</u>

Lippmann-Schwinger Equation

$$(H_0+V)|\psi\rangle = E|\psi\rangle \qquad (H_0|\phi\rangle = E|\phi\rangle)$$

$$|\psi^{(+)}\rangle = |\phi\rangle + \frac{1}{E-H_0+i\epsilon}V|\psi^{(+)}\rangle$$

Time Dependent Schrödinger Equation

$$(i\hbar\partial_t - H_0)|\psi(t)\rangle = V(t)|\psi(t)\rangle \qquad \big((i\hbar\partial_t - H_0)|\phi(t)\rangle = 0\big)$$

Use "slow turn on" method from Chapter 5.

$$t\to-\infty,\quad V(t)\to 0 \quad\Rightarrow\quad V(t) = V\,e^{\eta t} \qquad (0<\eta<1)$$

$$|\psi^{(+)}(t)\rangle = |\phi(t)\rangle + \int_{-\infty}^{\infty}dt'\; G_+(t,t')\,V(t')\,|\psi^{(+)}(t')\rangle$$

$$(i\hbar\partial_t - H_0)\,G(t,t') = \delta(t-t')$$

$$t<t' \qquad G_+(t,t') = 0 \qquad \text{(causality requirement)}$$

$$G_+(t,t') = \frac{-i}{\hbar}\,\Theta(t-t')\,e^{-iH_0(t-t')/\hbar}$$

$\uparrow$ Heaviside theta

$$\begin{cases} t<t' \to \Theta(t-t')=0 \\ t>t' \to \Theta(t-t')=1 \end{cases}$$

$$(i\hbar\partial_t - H_0)\,G_+(t,t') = i\hbar\,\partial_t\left(\frac{-i}{\hbar}\,\Theta(t-t')\,e^{-iH_0(t-t')/\hbar}\right) - H_0\left(\frac{-i}{\hbar}\,\Theta(t-t')\,e^{-iH_0(t-t')/\hbar}\right)$$

$$= \delta(t-t')\,e^{-iH_0(t-t')/\hbar} - \frac{iH_0}{\hbar}\,e^{-iH_0(t-t')/\hbar}\,\Theta(t-t')$$

$$+ \frac{iH_0}{\hbar}\,\Theta(t-t')\,e^{-iH_0(t-t')/\hbar}$$

$$= \delta(t-t')\,e^{-iH_0(t-t')/\hbar}$$

$$= \delta(t-t') \qquad \text{(let } t\to t' \text{ in exponential)}$$

$$|\psi^{(+)}(t)\rangle = |\psi^{(+)}(0)\rangle\,e^{-iEt/\hbar}, \qquad |\phi(t)\rangle = |\phi(0)\rangle\,e^{-iEt/\hbar}$$

$$|\psi^{(+)}(0)\rangle = |\phi(0)\rangle + \int_{-\infty}^{\infty} dt'\,G_+(0,t')\,V(t')\,|\psi^{(+)}(t')\rangle$$

$$= |\phi(0)\rangle + \int_{-\infty}^{\infty} dt'\left(\frac{-i}{\hbar}\,\Theta(-t')\,e^{+iH_0t'/\hbar}\right)\left(V e^{\eta t'}\right)\left(|\psi^{(+)}(0)\rangle\,e^{-iEt'/\hbar}\right)$$

$$= |\phi(0)\rangle + \int_{-\infty}^{0} dt'\left(\frac{-i}{\hbar}\,V\,\exp\left[\frac{i}{\hbar}(H_0-E-i\eta\hbar)t'\right]\right)|\psi^{(+)}(0)\rangle$$

$$= |\phi(0)\rangle - \frac{1}{H_0-E-i\eta\hbar}\,\underbrace{\exp\left[\frac{i}{\hbar}(H_0-E-i\eta\hbar)t'\right]\Big|_{-\infty}^{0}}_{1-\lim_{t'\to-\infty}\exp\left[\frac{i}{\hbar}(H_0-E)t'\right]\exp[\eta t']\to 1}\,V\,|\psi^{(+)}(0)\rangle$$

$$\boxed{|\psi^{(+)}(0)\rangle = |\phi(0)\rangle - \frac{1}{H_0-E-i\eta\hbar}\,V\,|\psi^{(+)}(0)\rangle}$$

04/22/2010 Symmetries and Conservation Laws

1917 - Emmy Noether - Dynamic implication of symmetry

Noether's Theorem :

| | Symmetry | Conservation Law |
|---|---|---|
| continuous | Translation in time | Energy |
| | Translation in space | Linear Momentum |
| | Rotation | Angular Momentum |
| | Gauge transformation | Charge |
| discrete | Inversion of space | Parity |
| | Lattice translation | Periodicity |

Special Relativity $ISL(2, C)$ (Inhomogeneous Special Linear Group (2D, complex))

Continuous transformation → 10 generators (translations, rotations, boosts)

Discrete transformation → 3 generators (C, P, T)

Example : 1D Space Translation

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

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

$$\psi(x-a) = \psi(x) - a \frac{d}{dx} \psi(x) + \frac{1}{2!} a^2 \frac{d^2}{dx^2} \psi(x) + \ldots$$

$$= \left(1 - a \frac{d}{dx} + \frac{1}{2!} a^2 \frac{d^2}{dx^2} + \ldots \right) \psi(x)$$

$$= e^{-a\, d/dx} \psi(x) \longrightarrow e^{-ipa/\hbar} \psi(x) \qquad \left(p = -i\hbar \frac{d}{dx}\right)$$

p is a generator of space translation.

$[x, p] = i\hbar$

$$e^{ipa/\hbar}\, x\, e^{-ipa/\hbar} = x + \frac{ia}{\hbar}[p, x] + \underbrace{\frac{1}{2!}\left(\frac{ia}{\hbar}\right)^2 [p, [p, x]] + \ldots}_{=0}$$

$$= x + \frac{ia}{\hbar}(-i\hbar) = x + a$$

In 3D, $e^{-ipa/\hbar} \longrightarrow e^{-i\vec{p}\cdot\vec{a}/\hbar}$

$e^{+i\vec{p}\cdot\vec{a}/\hbar}\, H\, e^{-i\vec{p}\cdot\vec{a}/\hbar} = H$ if invariant under translation

$$e^{i\vec{p}\cdot\vec{a}/\hbar}\, H = H\, e^{i\vec{p}\cdot\vec{a}/\hbar} \rightarrow [e^{i\vec{p}\cdot\vec{a}/\hbar}, H] = 0$$

$$\Rightarrow [\vec{p}, H] = 0$$

Heisenberg equation of motion

$$\frac{d\vec{p}}{dt} = \frac{1}{i\hbar}[\vec{p}, H] = 0 \Rightarrow \vec{p} \text{ is conserved}$$

In classical mechanics

$$\frac{d\vec{p}}{dt} = \{\vec{p}, H\}_{PB} \rightarrow \frac{dp_i}{dt} = \frac{-dH}{dq_i} = 0$$

(Poisson Bracket)

If $q_i$ is cyclic, H is invariant under $q_i$ translation $\rightarrow$ $p_i$ is conserved.

Symmetry in Quantum Mechanics and Degeneracy

$$H|n\rangle = E_n|n\rangle$$

$[H, G] = 0$ ($G$ is some generator)

$$H(G|n\rangle) = G(H|n\rangle) = G(E_n|n\rangle) = E_n(G|n\rangle)$$

If $|n\rangle \neq G|n\rangle$, these states are degenerate

Example: Rotation

$[H, \vec{L}] = 0$ $\quad$ $[H, \vec{L}^2] = 0$

States $|n, l, m\rangle$ are degenerate for different values of $m$
$\rightarrow 2l+1$ degeneracy.

In hydrogen atom, for given $n$

$$\sum_{l=0}^{n-1} (2l+1) = 2\sum_{l=0}^{n-1} l + n = 2\frac{n(n-1)}{2} + n = n^2 \text{ degeneracy}$$

From dynamical symmetry

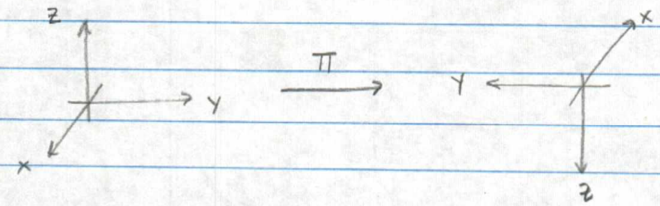
$\frac{1}{r}$ potential has more symmetry than expected

Laplace-Runge-Lenz Vector $\vec{A} = \vec{p} \times \vec{L} - mk\frac{\vec{r}}{r}$

$\vec{A}$ is conserved

Parity ($\Pi$)

Definition: Operation of space inversion.




$$\Pi|\vec{x}\rangle = e^{i\delta}|-\vec{x}\rangle \qquad (\text{Convention: } \delta=0)$$

Properties of $\Pi$

1. $\Pi$ is unitary

$$\langle\vec{x}|\vec{x}\rangle = \langle-\vec{x}|-\vec{x}\rangle = (\langle\vec{x}|\Pi^\dagger)(\Pi|\vec{x}\rangle) = \langle\vec{x}|\vec{x}\rangle$$

$$\Rightarrow \Pi^\dagger\Pi = 1$$

2. Group $\{1, \Pi\}$

$$\Pi^2 = I \quad \text{or} \quad \Pi = \Pi^{-1}$$

3. $\Pi$ is Hermitian

$$\Pi^\dagger\Pi = 1 \rightarrow \Pi^\dagger = \Pi^{-1} = \Pi$$

4. $\{\Pi, \vec{x}\} = 0 \rightarrow \Pi^\dagger\vec{x}\,\Pi = -\vec{x}$

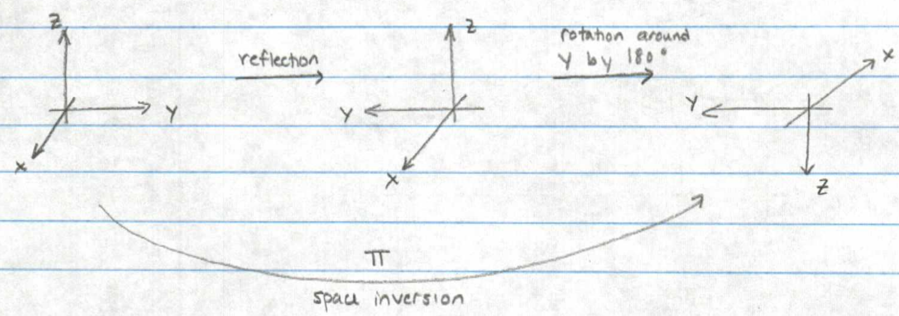
$$|\psi'\rangle = \Pi|\psi\rangle \rightarrow \langle\psi'|\vec{x}|\psi'\rangle = -\langle\psi|\vec{x}|\psi\rangle$$

5. Similarly $\{\Pi, \vec{p}\} = 0$

However, $\vec{L} = \vec{x} \times \vec{p}$

$$[\Pi, \vec{L}] = 0$$

$\Pi$ is <u>not</u> mirror symmetry!




Example:

$$\langle \theta, \varphi | lm \rangle = Y_{lm}(\theta, \varphi)$$

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

$$\Rightarrow \Pi | lm \rangle = (-1)^l | lm \rangle$$

$\Pi$ and $\vec{L}$ have simultaneous eigenvalues since $[\Pi, \vec{L}] = 0$

Other operators:

$[\Pi, \vec{S}] = 0$ (spin up, spin down have same parity)

$[\Pi, \vec{J}] = 0$

04/27/2010

## Parity Violation and Lattice Translation

Parity $(\Pi)$

$$\Pi^{+} = \Pi \qquad \Pi^{+}\Pi = 1 \qquad \text{(Hermitian and unitary)}$$
$$\Pi = \Pi^{-1}$$

$$\{\Pi, \vec{x}\} = 0 \qquad \{\Pi, \vec{p}\} = 0 \quad \longrightarrow \text{Polar vectors}$$

$$[\Pi, \vec{L}] = 0 \qquad [\Pi, \vec{S}] = 0 \qquad [\Pi, \vec{J}] = 0 \quad \longrightarrow \text{Axial vectors}$$

Example: Parity Violation in Weak Interaction

V - A theory (vectors and axial vectors together)

$$\mathcal{L}_W = g_W (V_\mu - A_\mu) \cdot W^\mu$$

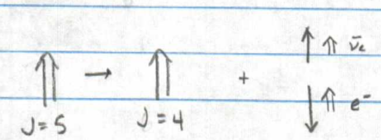
where
$$V_\mu = \bar{\psi} \gamma_\mu \psi$$
$$A_\mu = \bar{\psi} \gamma_\mu \gamma_5 \psi$$

Experiment: $\beta$ - decay

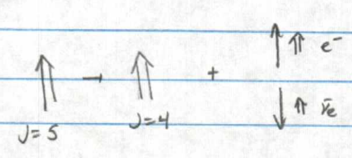
$$n \rightarrow p + e^- + \bar{\nu}_e$$

$^{60}Co$ decay $\quad J = 5 \quad$ cooled + polarized

$$^{60}Co \rightarrow {}^{60}Ni^{*} + e^- + \bar{\nu}_e$$




Never saw




(electron always detected in same direction)

Antineutrino is right handed always.

Neutrino is left handed always.

$\rightarrow$ Clear parity violation.

Example: Parity Conservation in Electromagnetic Interaction

V theory

$$\mathcal{L}_{EM} = e\, J_\mu \cdot A^\mu$$

Parity Selection Rule (in Parity Conservation)

Vector operator selection rule $\langle l'm' | ez | lm \rangle \sim \delta_{l', l\pm 1}\, \delta_{m', m}$

$|lm\rangle$ has parity $(-1)^l$

$z$ has parity $-1$

$|l'm'\rangle$ must have parity $(-1)^{l\pm 1}$

Neutron electron dipole moment

$\langle n | e\vec{x} | n \rangle = 0$ if $|n\rangle$ is non degenerate

Theorem: If $[H, \Pi] = 0$ and $|n\rangle$ is nondegenerate eigenket of $H$ with eigenvalue $E_n$, then $|n\rangle$ is also parity eigenket.

Proof:

$$\Pi\left(\tfrac{1}{2}(1 \pm \Pi)|n\rangle\right) = \tfrac{1}{2}(\Pi \pm 1)|n\rangle = \pm\left(\tfrac{1}{2}(1 \pm \Pi)|n\rangle\right)$$

$\frac{1}{2}(1 \pm \Pi)|n\rangle$ has parity eigenvalue $\pm 1$

$$H\left(\tfrac{1}{2}(1 \pm \Pi)|n\rangle\right) = E_n\left(\tfrac{1}{2}(1 \pm \Pi)|n\rangle\right)$$

$|n\rangle$ must have either even or odd parity, not both or it would be degenerate.

Example: Simple Harmonic Oscillator

$|0\rangle$ - even parity

$|1\rangle = a^{+}|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)|0\rangle$ - odd parity

$|2\rangle = a^{+}|1\rangle$ - even parity

$\vdots$

$|n\rangle$ - $(-1)^n$ parity

Example: Stark Effect

Saw mixing of 2p (odd) and 2s (even) states.
→ No definite parity.

2p and 2s are degenerate, so the theorem does not apply.

04/29/2010 Lattice Translation

Translation operator $\tau(l) = e^{-ipl/\hbar}$

$$\tau(l)\,|x\rangle = |x+l\rangle$$

$$\tau^{\dagger}(l)\, x\, \tau(l) = x + l$$

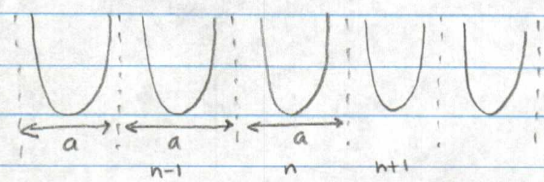
$$H = \frac{p^2}{2m} + V(x)$$

$\tau^{\dagger}(l) H \tau(l)$ not invariant in general

If $V(x)$ is periodic $(V(x \pm a) = V(x))$, $\tau^{\dagger}(a) H \tau(a) = H$

$$H\tau(a) = \tau(a) H \qquad ([H, \tau(a)] = 0)$$

Start with an infinite barrier potential




no leakage/tunneling

$H|n\rangle = E_0|n\rangle$ $\qquad \langle x|n\rangle$ exists only in $n^{th}$ site

$\tau(a)|n\rangle = |n+1\rangle$ (not an eigenstate)

What is the simultaneous eigenstate?

$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle$ where $\theta$ is a real parameter $-\pi \le \theta \le \pi$

$$H|\theta\rangle = E_0 \sum e^{in\theta}|n\rangle = E_0|\theta\rangle$$

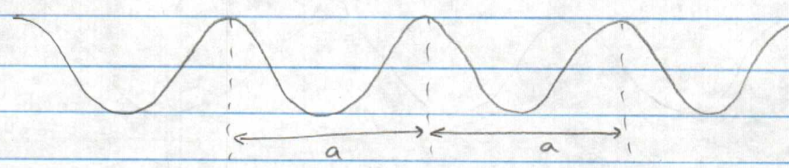
$$\tau(a)|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle = e^{-i\theta}\sum e^{i(n+1)\theta}|n+1\rangle$$

$$= e^{-i\theta}\sum e^{in\theta}|n\rangle = e^{-i\theta}|\theta\rangle$$

So $|\theta\rangle$ is in fact a simultaneous eigenstate.

$$H|\theta\rangle = E_0|\theta\rangle$$
$$\tau(a)|\theta\rangle = e^{-i\theta}|\theta\rangle$$

Now consider a periodic potential with finite barrier




Leakage is possible (only into nearest neighbor cell)

$\rightarrow$ $|n\rangle$ not an eigenstate for $H$ anymore

$$H|n\rangle = E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle \quad \text{(Tight-binding approximation)}$$

$$\langle n|H|n\rangle = E_0 \qquad \langle n\pm 1|H|n\rangle = -\Delta \neq 0$$

Is $|\theta\rangle$ an eigenket of $H$?

$$H|\theta\rangle = \sum e^{in\theta} H|n\rangle$$

$$= \sum e^{in\theta}\left(E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle\right)$$

$$= E_0\sum e^{in\theta}|n\rangle - \Delta e^{-i\theta}\sum e^{i(n+1)\theta}|n+1\rangle - \Delta e^{i\theta}\sum e^{i(n-1)\theta}|n-1\rangle$$

$$= (E_0 - 2\Delta\cos(\theta))|\theta\rangle$$

Energy eigenvalue has changed. In fact, it depends on value of $\theta$. (See Figure 4.7)

Energy spectrum now has a band structure.

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

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

$= e^{-i\theta}\langle x|\theta\rangle = e^{-i\theta}\psi(x)$

$\Rightarrow \psi(x-a) = e^{-i\theta}\psi(x)$

Bloch Theorem: The wavefunction of $|\theta\rangle$ can be written as a plane wave ($e^{ikx}$) times a periodic function with periodicity $a$.

Proof:

Let $\psi(x) = e^{ikx} u_k(x)$

where $u_k(x) = u_k(x \pm a)$

Then $\psi(x-a) = e^{ik(x-a)} u_k(x-a) = e^{-i\theta} e^{ikx} u_k(x)$

$e^{ik(x-a)} u_k(x) = e^{i(kx-\theta)} u_k(x)$

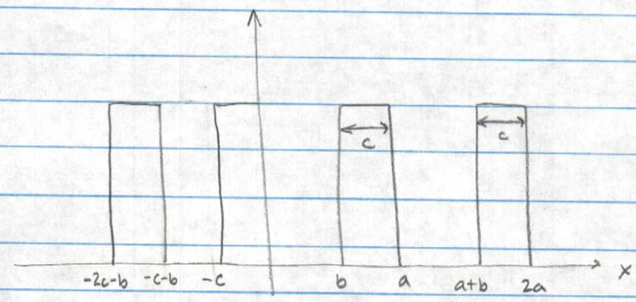
$\Rightarrow e^{i(kx-ka)} u_k(x) = e^{i(kx-\theta)} u_k(x)$

$\Rightarrow$ If $\theta = ka$, then Bloch theorem works

$\theta = ka \quad (-\pi < \theta < \pi) \rightarrow -\frac{\pi}{a} < k < \frac{\pi}{a}$

$E(k) = E_0 - 2\Delta \cos(ka)$ (Energy-Momentum Dispersion Relation)

In solid state physics, use the Kronig-Penny Model.




$a = b + c$

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

Apply Bloch theorem $\rightarrow \psi(x) = e^{ikx}u_k(x)$

Use Schrödinger equation to find

$$\frac{d^2u}{dx^2} + 2ik\frac{du}{dx} + \frac{2m}{\hbar^2}\left(E - V(x) - \frac{\hbar^2k^2}{2m}\right)u(x) = 0$$

$E < V_0 \rightarrow \quad k_w = \sqrt{\frac{2mE}{\hbar^2}} \qquad k_h = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

(in well) (in hill)

$$u_w(x) = Ae^{i(k_w-k)x} + Be^{-i(k_w+k)x}$$

$$u_h(x) = Ce^{(k_h-ik)x} + De^{-(k_h+ik)x}$$

Apply boundary condition

$u_w(x=0) = u_h(x=a) \qquad u_w(x=b) = u_h(x=b)$

$u_w'(x=0) = u_h'(x=a) \qquad u_w'(x=b) = u_h'(x=b)$

Band structure emerges