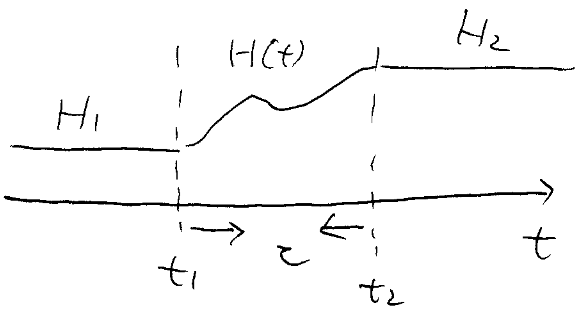
Sudden and Adiabatic Approximations



Sudden : τ is small ($<< \frac{\hbar}{\Delta E}$)

Slow : τ is large ($>> \frac{\hbar}{\Delta E}$)

ΔE : the typical energy diff among the energy levels

☆ Sudden change, the states cannot catch up with the change

Sudden approximation : $H_1|i_1\rangle = E_i|i_1\rangle$ at $t=t_1$

is used unchanged at $t=t_2$, $|\psi(t_2)\rangle = |i_1\rangle$

After t_2, it evolves according to H_2.

$$|\psi(t)\rangle = e^{\frac{-iH_2(t-t_2)}{\hbar}}|i_1\rangle = \sum_f e^{\frac{-iE_f(t-t_2)}{\hbar}}|f\rangle\langle f|i_1\rangle$$

$$e^{\frac{-iH_2t}{\hbar}}\sum_n c_n|n\rangle = e^{\frac{-iE_it}{\hbar}}\sum_n c_n|n\rangle e^{\frac{-i(E_n-E_i)t}{\hbar}}$$

$\Rightarrow$ $t \gtrsim \frac{\hbar}{E_n-E_i}$ then diff states accquire substantially diff phases.

$$\Delta t \sim \frac{\hbar}{\Delta E}, \quad \& \quad \tau << \Delta t$$

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e.g. β-decay of the tritium $^3H \longrightarrow {}^3He + e^- + \bar{\nu}_e$

^3H (pnn) $Z=1$; ^3He (ppn) $Z=2$

$$\langle T_\beta\rangle = \langle \tfrac{1}{2}m_e v_e^2\rangle \simeq 5.7\,keV \Rightarrow \langle v_\beta\rangle \sim 0.15c$$

$$\tau \simeq \frac{a_0}{0.15c} = \frac{0.5\,\mathring{A}}{0.15c} = 1.2\times10^{-18}\,sec$$

$$\Delta E \simeq E_{n=2}-E_{n=1} \simeq 10\,eV, \Rightarrow \frac{\hbar}{\Delta E} \sim 6.4\times10^{-17}\,sec >> \tau$$

For heavier N, the better the sudden approximation

☆ Adiabatic Approximation

Slow change, the states can adjust themselves to adopt the instant $H(t)$, solve the Schrödinger Eq for any t.

$\Rightarrow$ $H(t)|i\rangle_t = E_i(t)|i\rangle_t$ for each t

Instaneous eigenstates $|i\rangle_t$, and

$$|i(t)\rangle = \exp\left[-i\int_{t_1}^{t} dt' \, E_i(t')\right] \underbrace{e^{i\phi(t)}} |i\rangle_t$$

This additional phase is called geometrical phase (Berry's phase)

For this approximation to work, it is crucial that $\tau << \Delta t \sim \frac{\hbar}{\Delta E}$

A good example is the t-dep B field.

Consider $\vec{B} = (B_x, B_y, B_z) = B(\sin\theta\cos\omega t, \sin\theta\sin\omega t, \cos\theta)$

$\vec{B}$ rotates about $\hat{z}$ with angular velocity ω.

For spin-$\frac{1}{2}$ particle,

$$H = -\vec{\mu}\cdot\vec{B} = -\mu B\begin{pmatrix} c\theta & s\theta e^{-i\omega t} \\ s\theta e^{+i\omega t} & -c\theta \end{pmatrix}$$

the $e^{\pm i\omega t}$ ($\cos\omega t$) has no eff

$$= \mu B_{\parallel}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, -\mu B_{\perp}\begin{pmatrix} 0 & e^{-i\omega t} \\ e^{i\omega t} & 0 \end{pmatrix}, \quad B_{\parallel} \equiv B\cos\theta, \quad B_{\perp} = B\sin\theta$$

Comparing to the previous 2-state system, we can identify

$$E_1 \Leftrightarrow -\mu B_{\parallel} \qquad \gamma \Leftrightarrow -\mu B_{\perp}$$
$$E_2 \Leftrightarrow +\mu B_{\parallel} \qquad \omega \Leftrightarrow -\omega \qquad \Rightarrow \omega_{21} = \frac{2}{\hbar}\mu B_{\parallel}$$

So, immediatly, we know

$$\beta_{\pm} = \frac{1}{2}\left[+\omega + \frac{2\mu B_{\parallel}}{\hbar} \pm \sqrt{\frac{1}{\hbar^2}(2\mu B_{\parallel} + \omega\hbar)^2 + \frac{4\mu^2 B_{\perp}^2}{\hbar^2}}\right]$$

$$= \frac{1}{2\hbar}\left[(2\mu B_{\parallel} + \omega\hbar) \pm \sqrt{(2\mu B_{\parallel} + \omega\hbar)^2 + 4\mu^2 B_{\perp}^2}\right]$$

$$\alpha_{\pm} = \frac{1}{2\hbar}\left[-(2\mu B_{\parallel} + \omega\hbar) \pm \sqrt{\quad\cdots\quad}\right]$$

Consider a solution

$$C_2(t) = b e^{i\beta_+ t}$$

from $i\hbar \dot{c}_2 e^{-\frac{iE_2 t}{\hbar}} = \gamma c_1 e^{\frac{-i}{\hbar}(E_1+\hbar\omega)t}$

$$\Rightarrow c_1 = b\frac{\hbar\beta_+}{\mu B_\perp} e^{-\frac{i}{\hbar}(2\mu B_\parallel+\hbar\omega)t} e^{i\beta_+ t}$$

$$\Rightarrow \psi(t) = b\begin{pmatrix} \frac{\hbar\beta_+}{\mu B_\perp} e^{+\frac{i}{\hbar}\mu B_\parallel t} e^{-\frac{i}{\hbar}(2\mu B_\parallel+\hbar\omega)t} e^{i\beta_+ t} \\ e^{i\beta_+ t} e^{-\frac{i}{\hbar}\mu B_\parallel t} \end{pmatrix}$$

$$= b\begin{pmatrix} \frac{\hbar\beta_+}{\mu B_\perp} e^{-i\omega t} \\ 1 \end{pmatrix} e^{\frac{i}{\hbar}(\beta_+\hbar - \mu B_\parallel)t}$$

The normalization const $\quad b = \dfrac{1}{\sqrt{1+\left(\frac{\hbar\beta_+}{\mu B_\perp}\right)^2}}$

First, we consider the fast change of the Hamiltonian, $\omega \gg \omega_{21} = \frac{2\mu B_\parallel}{\hbar}$

In this case, $\tau \sim \frac{1}{\omega}$ and

$\beta_+ \simeq \frac{1}{2\hbar}[\omega\hbar + \omega\hbar] = \omega$, $\sqrt{\ ''} \sim \omega$, $b \sim \frac{\mu B_\perp}{\hbar\omega} \ll 1$

$\Rightarrow \psi(t) \simeq \begin{pmatrix} e^{-i\omega t} \\ 0 \end{pmatrix} e^{i\omega t} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. namely, the state doesn't move over the time interval $\tau \sim \frac{1}{\omega}$!

On the other hand, the case of slowly change, $\omega \ll \omega_{21}$

$$\sqrt{\ ''} = \frac{1}{\hbar}\sqrt{4\mu^2 B^2\cos^2\theta + 4\mu B\cos\theta\,\omega\hbar + \omega^2\hbar + 4\mu^2 B^2\sin^2\theta}$$

$$= \frac{1}{\hbar}\sqrt{4\left(\mu B + \frac{\omega\hbar}{2}\cos\theta\right)^2 + \omega^2\hbar^2(1-\cos^2\theta)} \sim \frac{2\mu B}{\hbar} + \omega\cos\theta$$

$$\Rightarrow \beta_+ \simeq \frac{1}{2\hbar}[2\mu B(1+\cos\theta) + \omega\hbar(1+\cos\theta)] = \frac{1}{\hbar}(2\mu B + \omega\hbar)\cos^2\frac{\theta}{2}$$

$$\frac{1}{\hbar}(\beta_+\hbar - \mu B_\parallel) = \frac{1}{\hbar}(\mu B) + \frac{\omega\hbar}{2\hbar}(1+c\theta)$$

$$b \simeq \frac{1}{\sqrt{1+\left[\left[1+\frac{\omega\hbar}{2\mu B}\right]\frac{\cos\frac{\theta}{2}}{\sin\frac{\theta}{2}}\right]^2}} \simeq \sin\frac{\theta}{2}, \quad \frac{\hbar\beta_+}{\mu B_\perp} \simeq \frac{(2\mu B+\omega\hbar)\cos^2\frac{\theta}{2}}{2\mu B\sin\frac{\theta}{2}\cos\frac{\theta}{2}} \simeq \frac{\cos\frac{\theta}{2}}{\sin\frac{\theta}{2}}$$

$$\Rightarrow \psi(t) \simeq \sin\frac{\theta}{2}\begin{pmatrix}\frac{\cos\frac{\theta}{2}}{\sin\frac{\theta}{2}} e^{-i\omega t} \\ 1\end{pmatrix} e^{\frac{i\mu B t}{\hbar}} e^{i\frac{\omega}{2}(1+\cos\theta)t}$$

$$= \begin{pmatrix}\cos\frac{\theta}{2} e^{-i\omega t} \\ \sin\frac{\theta}{2}\end{pmatrix} \underbrace{e^{\frac{i\mu B t}{\hbar}}}_{\Rightarrow \text{ eigenvalue } E=-\mu B} e^{\frac{i\omega}{2}(1+\cos\theta)t}$$

$$\vec{\sigma}\cdot\vec{n}\begin{pmatrix}a\\b\end{pmatrix} = +\begin{pmatrix}a\\b\end{pmatrix} \Rightarrow \frac{b}{a} = \frac{s\frac{\theta}{2}}{c\frac{\theta}{2}}e^{i\phi} \Rightarrow \begin{array}{l}\phi = \omega t\\ \theta=\theta\end{array}$$

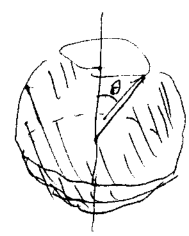
* The state is always the instaneous eigenstate of the H with $E=-\mu B$
* The last phase factor is the Berry's phase.
* When the $\vec{B}$ rotates about the $\hat{z}$ once, $\omega t = 2\pi$

  the phase is $e^{i\pi(1+\cos\theta)} = e^{im\Omega}$

  $m=\frac{1}{2}$ is the magnetic quantum number $S_z = m\hbar$

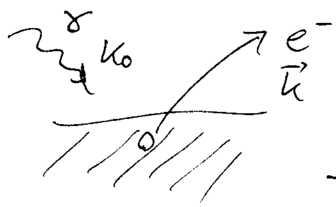
  Ω is the area swept by the $\vec{B}$ field.

  $$\Omega = \int_{-1}^{\cos\theta} d(\cos\theta')\int_0^{2\pi} d\phi = 2\pi(1+\cos\theta)$$



See Supplement I in Sakurai for more detail.

Photoelectric Effect & EM field



E_g: ground state energy (<0)

$\hbar\omega_0 > |E_g|$

In order to treat the outgoing e^- as free particle, namely ignoring the long range Coulomb int, we take $\hbar\omega_0 \gg |E_g|$

$\hbar\omega_0 + E_g = E$, $\underbrace{|E_g| \ll E}_{\text{plane wave}} \underbrace{\ll mc^2}_{\text{such that N.R. QM}}$, or $(Z\alpha)^2 \ll \frac{E}{mc^2} \ll 1$

Then the photon energy lies in $\sim$ far UV $\longrightarrow$ X-ray
100 eV 100 keV

Incident photon (classically)

$$\vec{A}(\vec{r},t) = A_0 \underbrace{\vec{\epsilon}}_{\text{polarization vector}} e^{i(\vec{k}_0\cdot\vec{r} - \omega_0 t)} + c.c. \quad = 2A_0\vec{\epsilon}\cos(\vec{k}_0\cdot\vec{r} - \omega_0 t)$$

Coulomb gauge , $\nabla\cdot\vec{A} = 0$, and $\vec{\epsilon}\cdot\vec{k}_0 = 0$

$$\vec{E} = -\frac{1}{c}\frac{\partial}{\partial t}\vec{A} = -\frac{2\omega_0}{c}A_0\vec{\epsilon}\sin(\vec{k}_0\cdot\vec{r} - \omega_0 t)$$

$\vec{B} = \nabla\times\vec{A}$

start from an example $\vec{k}_0 = k_0\hat{z}$, then $\vec{\epsilon} = (\epsilon_x, \epsilon_y, 0)$, $\epsilon_x^2 + \epsilon_y^2 = 1$

$$\vec{B} = \nabla\times\vec{A} = 2A_0\begin{vmatrix} i & j & k \\ \partial_x & \partial_y & \partial_z \\ \epsilon_x\cos(k_0 z - \omega_0 t), & \epsilon_y\cos(k_0 z - \omega_0 t), & 0 \end{vmatrix} = -2A_0 k_0 \sin(k_0 z - \omega_0 t)(-\epsilon_y, \epsilon_x, 0)$$

or a general expression $\vec{B} = (\vec{\epsilon}\times\vec{k}_0)A_0\sin(\vec{k}_0\cdot\vec{r} - \omega_0 t)$

★ For 1-electron atom

$$H_0 = \frac{p^2}{2m} + V(r), \quad \left(\text{in latter calculation, we take } V(r) = -\frac{Ze^2}{r} \right)$$

and $\quad H_0|g\rangle = E_g|g\rangle$

And the unbounded e^- in the final state is plane wane (box normalization)

$$\psi_{\vec{k}}(r) = \langle \vec{r}|\vec{k}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}, \qquad E = \frac{\hbar^2 k^2}{2m}$$

★ The perturbing Hamiltonian is

$$H' = \frac{e}{mc}\vec{p}\cdot\vec{A}$$

which comes from

$$\frac{1}{2m}\left(\vec{p} + \frac{e\vec{A}}{c}\right)^2 \longrightarrow \frac{\vec{p}^{\,2}}{2m} + \frac{e}{2mc}\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right) + \cancel{\frac{e^2}{2mc}\vec{A}^2} \quad \text{ignored}$$

$\vec{p}\cdot\vec{A} = \vec{A}\cdot\vec{p}$ in the Coulomb gauge.

★ $$H' = \frac{e}{mc}A_0\,\hat{\epsilon}\cdot\hat{p}\; e^{i(\vec{k}_0\cdot\vec{r} - \omega_0 t)} + c.c.$$

$$= \underbrace{\frac{eA_0}{mc}\vec{\epsilon}\cdot\vec{p}\, e^{i\vec{k}_0\cdot\vec{r}}}_{\hat{O}\ \Downarrow\ \text{for absorption}} \underbrace{e^{-i\omega_0 t}}_{t\text{-depend}} + \underbrace{c.c.}_{\Downarrow\ \text{for emission}} = \hat{O}^+$$

★ Transition rate (O^+ has no contribution)

$$W = \frac{2\pi}{\hbar}\sum_{\underbrace{k}_{\text{box points}}} |\langle \vec{k}|\hat{O}|g\rangle|^2\, \delta\!\left(\frac{\hbar^2 k^2}{2m} - \hbar\omega_0 - E_g\right)$$

Again, we are interested in the diffentiral cross section,

$\Rightarrow$ need to calculate $\frac{dw}{d\Omega}$ and the flux of incident photon.

The δ-function can be replaced by

$$\frac{\delta(k - k_f)}{\left|\frac{2\hbar^2 k}{2m}\right|}, \quad \text{with } k_f = \sqrt{\frac{2m}{\hbar}(\hbar\omega_0 + E_g)}$$

$\vec{k} = \frac{2\pi}{L}\vec{n}, \quad dn^3 = \frac{V}{(2\pi)^3}dk^3$

So,

$$\frac{dw}{d\Omega}\Delta\Omega = \sum_{k\in\Delta\Omega} \frac{2\pi}{\hbar}\left(\delta(k-k_f)\times\frac{m}{\hbar^2 k}\right)|\langle\vec{k}|\hat{O}|g\rangle|^2$$

$$= \frac{2\pi m}{\hbar^3}\Delta\Omega\int_0^\infty \frac{V}{(2\pi)^3}\frac{k^2 dk}{k}\,\delta(k-k_f)\,|\langle\vec{k}|\hat{O}|g\rangle|^2$$

$$= \frac{mV}{\hbar^3(2\pi)^2}\Delta\Omega\; k_f\;|\langle k_f|\hat{O}|g\rangle|^2$$

The matrix element

$$\langle\vec{k}|\hat{O}|g\rangle = \frac{eA_0}{mc}\vec{\epsilon}\cdot\int dr^3\,\frac{1}{\sqrt{V}}\left(e^{i\vec{k}\cdot\vec{r}}\right)^*\hat{\vec{p}}\,e^{i\vec{k}_0\cdot\vec{r}}\,\psi_g(r)$$

$$= \frac{eA_0\hbar(\vec{\epsilon}\cdot\vec{k})}{mc\sqrt{V}}\int dr^3\,e^{-i(\vec{k}-\vec{k}_0)\cdot\vec{r}}\,\psi_g(r)$$

$$= \frac{e\hbar A_0}{mc}(\vec{\epsilon}\cdot\vec{k})\frac{(2\pi)^{\frac{3}{2}}}{\sqrt{V}}\underbrace{\tilde{\psi}_g(\vec{q})}_{\text{Fourier transformation of }\psi_g(\vec{r})}, \quad \vec{q}\equiv\vec{k}-\vec{k}_0$$

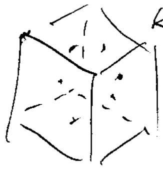
$$\Rightarrow \frac{dw}{d\Omega} = \frac{mV}{\hbar^3(2\pi)^2}k_f\left(\frac{e\hbar A_0}{mc}\right)^2(\vec{\epsilon}\cdot\vec{k})^2\frac{(2\pi)^3}{V}\left|\tilde{\psi}_g(\vec{q})\right|^2$$

$$= \frac{2\pi}{\hbar}\frac{e^2A_0^2}{mc^2}k_f(\vec{\epsilon}\cdot\vec{k}_f)^2\left|\tilde{\psi}_g(\vec{q}_f)\right|^2, \quad \vec{q}_f\equiv\vec{k}_f-\vec{k}_0$$

b) flux of incident photon

$$\vec{j}_\gamma = n_\gamma\vec{v}, \quad \vec{v} = c\hat{k}_0$$

To compute n_γ, we must mix classical and quantum concepts.



← unit volume, n_γ monochrom photons.

U (energy per unit volume) $= n_\gamma\hbar\omega_0$

On the other hand, by classical E&M,

$$U = \frac{1}{8\pi}(\vec{E}^2+\vec{B}^2) = \frac{\omega_0^2A_0^2}{2\pi c^2} \longrightarrow n_\gamma = \frac{\omega_0A_0^2}{2\pi\hbar c^2}$$

$$\Rightarrow \boxed{j_\gamma = \frac{\omega_0A_0^2}{2\pi\hbar c}}$$

Therefore $\frac{d\sigma}{d\Omega} = \left(\frac{2\pi\hbar c}{\omega_0 A_0^2}\right) \frac{2\pi}{\hbar} \frac{e^2 A_0^2}{mc^2} k_f (\vec{\epsilon}\cdot\vec{k}_f)^2 \left|\tilde{\psi}_g(\vec{q}_f)\right|^2$

$$= \frac{(2\pi)^2 e^2}{mc\omega_0} k_f (\vec{\epsilon}\cdot\vec{k}_f)^2 \left|\tilde{\psi}_g(\vec{q}_f)\right|^2$$

(note A_0^2 dissapear as it should.)

$c = \frac{\omega_0}{k_0}$, Take hydrogen atom w.f. $\psi_g(r) = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}$ as a model,

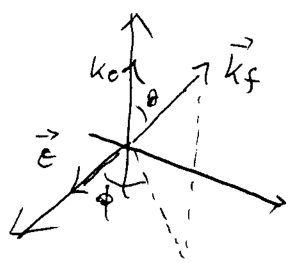
$$\Rightarrow \tilde{\psi}_g(\vec{q}_f) = \frac{1}{\pi} \frac{(2a)^{\frac{3}{2}}}{(1+a^2 q_f^2)^2}$$

$$\Rightarrow \boxed{\frac{d\sigma}{d\Omega} = 32 \frac{e^2}{mc^2} \frac{k_f}{k_0} \left|\vec{\epsilon}\cdot\vec{k}_f\right|^2 \frac{a^3}{(1+a^2 q_f^2)^4}}$$

* since $\hbar\omega_0 >> |E_g| \Rightarrow \hbar k_0 c = \hbar\omega_0 \simeq \frac{\hbar^2 k_f^2}{2m}$

or $k_0 \simeq \frac{\hbar k_f^2}{2mc}$, $\frac{k_f}{k_0} \simeq \frac{2mc}{\hbar k_f} = \frac{2mc}{p_f} = \frac{2c}{v} >> 1$

* $\vec{\epsilon} = (1, 0, 0)$



$$q_f^2 = (\vec{k}_f^{\,2} - \vec{k}_0^{\,2}) = k_f^2 + k_0^2 - 2k_f k_0 \cos\theta$$
$$\simeq k_f\left(1 - \frac{2k_0}{k_f}\cos\theta\right) = k_f\left(1 - \frac{v_f}{c}\cos\theta\right)$$

& $\vec{\epsilon}\cdot\vec{k}_f = k_f \sin\theta\cos\phi$

* $a^2 q_f^2 \simeq a^2 k_f^2 \left(1 - \frac{v_f}{c}\cos\theta\right)$

$a^2 k_f^2 = \left(\frac{2ma^2}{\hbar^2}\right)\left(\frac{\hbar^2 k_f^2}{2m}\right) \sim \frac{E}{|E_g|} >> 1$, $\because p_e \sim \frac{\hbar}{a}$, $|E_g| \sim \frac{p_e^2}{2m}$

$\Rightarrow 1 + a^2 q_f^2 \simeq a^2 q_f^2$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{32 e^2}{mc^2 k_0} \frac{\sin^2\theta\cos^2\phi}{(ak_f)^5 \left(1 - \frac{v}{c}\cos\theta\right)^4}$$

for $e = (0, 1, 0)$, $\cos\phi \longrightarrow \sin\phi$

Unpolarized diff cross section

$$\left(\frac{d\sigma}{d\Omega}\right)_{unpol} = \frac{1}{2}\sum_{\vec{\epsilon}} \frac{d\sigma}{d\Omega} \simeq \frac{16e^2}{mc^2 k_0} \frac{\sin^2\theta}{(a k_f)^5} \left(1 + \frac{4V}{c}\cos\theta\right)$$

and total cross section

$$\sigma_{total} = \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \left(\frac{d\sigma}{d\Omega}\right)_{unpol} \quad , \quad \text{let } x = \cos\theta$$

$$= (2\pi)\frac{16e^2}{mc^2 k_0}\frac{1}{(ak_f)^5}\int_{-1}^{1} dx \left[\underbrace{(1-x^2)}_{\frac{4}{3}} + \underbrace{\cancel{\frac{4V}{c}(1-x^2)\,x}}_{=0,\ \text{odd in } x} \right]$$

$$\boxed{\sigma_{total} = \frac{128}{3}\frac{e^2}{mc^2 k_0}\frac{1}{(ak_f)^5}}$$

Expressed in terms of the incident photon energy $E_0 = \hbar\omega_0$ and the Bohr radius a_0 of hydrogen like atom:

$$\boxed{\sigma_{total} = \frac{16\pi\sqrt{2}}{3}\alpha^8 Z^5 a_0^2 \left(\frac{mc^2}{E_0}\right)^{\frac{7}{2}}}$$

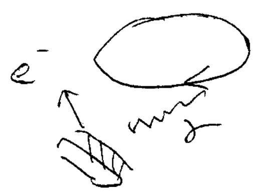
It is clear now it is an area.

Pretty good for discriping the k-shell e^- ejection by x-ray ~

Strong Z dependence $\Rightarrow$ heavier atoms are more effective in stopping x-rays.

strong inverse E_0-dependence $\Rightarrow$ hard x-rays are more penetrating than soft ones,

Q: ① Sychrotron radiation exp ~



② angular distribution. why?

③ X-ray emmition?