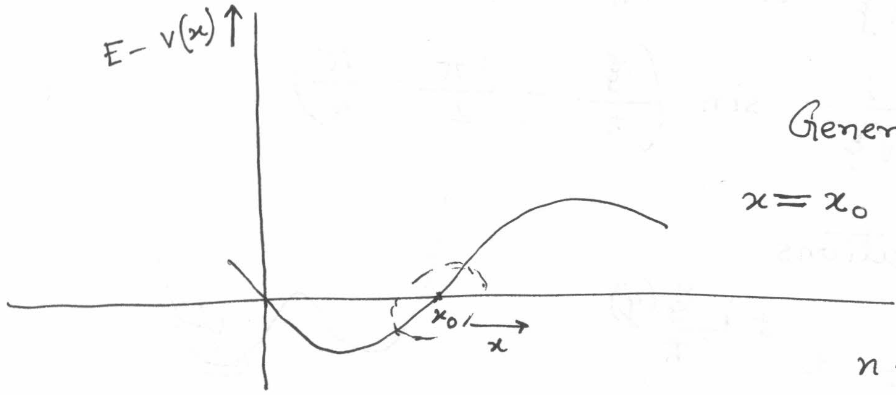
$E > V(x)$:— (Connection formulae)



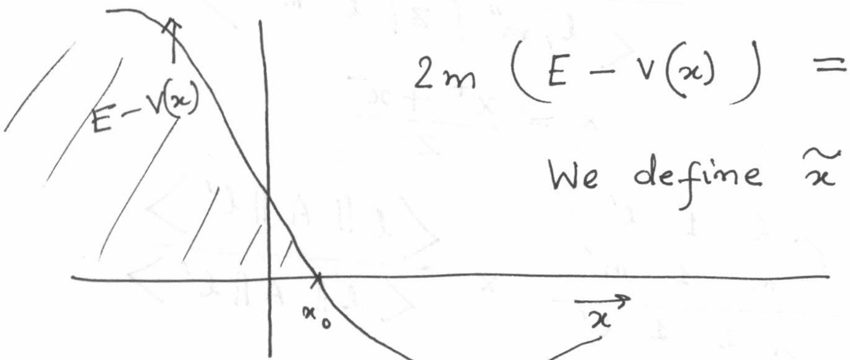
General form near $x = x_0$ is $2m\left(E - V(x)\right) = C(x-x_0)^n$

$C > 0$

$n \longrightarrow$ some number

In a generic situation, $n = 1$. (First term in Taylor expansion)

Take $\tilde{x} = x - x_0 \Rightarrow -\frac{\hbar^2}{\cancel{2m}} \frac{d^2\psi}{d\tilde{x}^2} = C\tilde{x}^n \psi$



$$2m\left(E - V(x)\right) = C(x_0 - x)^n, \quad C > 0.$$

We define $\tilde{x} = x_0 - x$.

The equation takes the form

$$-\hbar^2 \frac{d^2\psi}{d\tilde{x}^2} = C\tilde{x}^n \psi.$$

$$\Rightarrow \frac{d^2\psi}{d\tilde{x}^2} + \frac{C}{\hbar^2}\tilde{x}^n \psi = 0.$$

$\left.\begin{array}{l} \tilde{x} \longrightarrow \rho \\ \psi \longrightarrow \phi \end{array}\right\}$ Change of variables such that $\phi(\rho)$ satisfies Bessel's equation. (Goal!)

Let $\tilde{x} = \alpha \rho^\beta$, $\psi = \rho^\gamma \phi$.

α, β, γ are constants.

$$\frac{d\tilde{x}}{d\rho} = \alpha\beta\rho^{\beta-1}$$

$$\frac{d}{d\tilde{x}} = \frac{d\rho}{d\tilde{x}}\frac{d}{d\rho} = (\alpha\beta)^{-1}\rho^{1-\beta}\frac{d}{d\rho}$$

$$\underbrace{(\alpha\beta)^{-1}\,\rho^{1-\beta}\,\frac{d}{d\rho}\left\{(\alpha\beta)^{-1}\,\rho^{1-\beta}\,\frac{d}{d\rho}\left(\rho^{\gamma}\phi\right)\right\}} +$$

$$\frac{C}{\hbar^2}\,\alpha^{n}\,\rho^{n\beta}\,\rho^{\gamma}\,\phi = 0.$$

$$(\alpha\beta)^{-2}\,\rho^{1-\beta}\,\frac{d}{d\rho}\left\{\rho^{-1-\beta+\gamma}\,\frac{d\phi}{d\rho} + \gamma\,\rho^{\gamma-\cancel{1}+\cancel{1}-\beta}\,\phi\right\}$$

$$\Rightarrow \Big[(\alpha\beta)^{-2}\,\rho^{2-2\beta+\gamma}\,\frac{d^2\phi}{d\rho^2} + (\alpha\beta)^{-2}\,\rho^{1-2\beta+\gamma}\,\frac{d\phi}{d\rho}\times(1-\beta+\gamma+\gamma)$$

$$+\,(\alpha\beta)^{-2}\,\rho^{-2\beta+\gamma}\,\phi\,\gamma(\gamma-\beta)\Big] + \frac{C}{\hbar^2}\,\alpha^{n}\,\rho^{n\beta+\gamma}\,\phi = 0$$

Multiply both sides by $\boxed{(\alpha\beta)^{2}\,\rho^{-2+2\beta-\gamma}}$

$$\cancel{\frac{d^2\phi}{d\rho^2} + \frac{1}{\rho}(1+2\gamma-\beta)\frac{d\phi}{d\rho} + \phi\left\{\gamma(\gamma-\beta)\frac{1}{\rho^2} + \frac{C}{\hbar^2}\alpha^{n+2}\beta^{2}\right.}$$

$$\frac{d^2\phi}{d\rho^2} + \frac{1}{\rho}\,(1+2\gamma-\beta)\,\frac{d\phi}{d\rho} + \phi\left\{\gamma(\gamma-\beta)\frac{1}{\rho^2} + \frac{C}{\hbar^2}\,\alpha^{n+2}\,\beta^{2}\,\rho^{(n+2)\beta-2}\right\} = 0$$

<u>Bessel's equation</u> (for $J_l(\rho)$.)

$$\frac{d^2 J_l}{d\rho^2} + \frac{1}{\rho}\,\frac{dJ_l}{d\rho} + \left(1-\frac{l^2}{\rho^2}\right)J_l(\rho) = 0.$$

Comparing, we have, $\beta - 2\gamma = 0 \Rightarrow \beta = 2\gamma$.

Also, $(n+2)\beta - 2 = 0$

$$\Rightarrow \beta = \frac{2}{n+2} \quad \therefore \gamma = \frac{1}{n+2}.$$

$$\frac{C}{\hbar^2}\,\alpha^{n+2}\,\beta^{2} = 1 \longrightarrow \text{Determines } \alpha.$$

$$\alpha = \left\{\frac{\hbar^2}{\beta^2}\,\frac{1}{C}\right\}^{\frac{1}{n+2}}$$

$$l^2 = \gamma(\beta-\gamma) = \frac{1}{(n+2)^2}$$

$$l = \frac{1}{n+2}.$$

$$\psi(x) = \cancel{\rho^{\frac{1}{n+2}}}\ \rho^{\ell}\left(\underbrace{A_+ J_\ell(\rho)}_{\rho^\ell} + \underbrace{A_- J_{-\ell}(\rho)}_{\rho^{-\ell}}\right)$$

(Using the fact that $\gamma = \ell$)

we choose

[ℓ is never an integer here.]

$$\xrightarrow[\rho \to 0]{}$$

$$\psi = \rho^\gamma J_{\pm\ell}(\rho)$$

$$\tilde{x} = \alpha \rho^\beta$$

$$\psi = \cancel{\rho^\gamma \phi}\ \rho^\gamma \phi$$

$$\cancel{\psi = \left\{\frac{\hbar^2}{C}\left(\frac{(n+2)}{(2)}\right)^2\right\}^{\frac{1}{n+2}}}$$

$$\rho = \left(\frac{1}{\alpha}\tilde{x}\right)^{1/\beta}$$

$$= \left(\frac{\beta^2 C}{\hbar^2 \cancel{4}}\right)^{\frac{1}{n+2} \times \frac{n+2}{2}} \tilde{x}^{\frac{n+2}{2}}$$

$$= \left(\frac{\beta^2 C}{\hbar^2 \cancel{4}}\right)^{\frac{1}{2}} \tilde{x}^{\frac{n+2}{2}}$$

$$\therefore \boxed{\psi = \left(\frac{\beta^2 C}{\hbar^2}\right)^{\frac{1}{2(n+2)}} \tilde{x}^{1/2}\, J_{\pm\ell} \times \left(\left(\frac{\beta^2 C}{\hbar^2}\right)^{1/2} \tilde{x}^{\frac{n+2}{2}}\right)}$$

WKB for $E - V(x) > 0$

$$\psi(x) = \frac{1}{\sqrt{K_1(x)}}\, e^{\left(\pm i \int_{x_0}^{x} K_1(x')\, dx'\right)}$$

x_0 chosen to be x_0

$$K_1(x) = \sqrt{2m\left(E - V(x)\right)} = \sqrt{C\tilde{x}^n} = C^{1/2}\,\tilde{x}^{n/2}$$

$$\xi(x) = \int_{x_0}^{x} K_1(x')\, dx' = C^{1/2}\frac{1}{\left(\frac{n}{2}+1\right)}\tilde{x}^{\frac{n}{2}+1}$$

Match aith argument of $J_{\pm\ell}$.

$$\psi = \frac{\{\xi(x)\}^{1/2}}{\{K_1(x)\}^{1/2}}\, C J_{\pm\ell}\left(\pm \cancel{i}\ \xi/\hbar\right)$$

$$\psi(x) = \frac{1 \cdot B_\pm}{\sqrt{K_1(x)}}\, e^{\left(\pm i\, \xi(x)\right)}$$

$$\frac{\xi(x)}{K_1(x)} \propto \tilde{x}$$

Clearly,

$$\left[\begin{array}{l} \overline{\text{TURNING POINT}} \\ \psi = A_{\pm} \left\{\dfrac{\xi(x)}{K_1(x)}\right\}^{1/2} J_{\pm \ell}\left(\xi/\hbar\right). \\ \overline{\text{WKB}} \\ \psi = \dfrac{1 \cdot B_{\pm}}{\sqrt{K_1(x)}} e^{\pm i \xi(x)} . \end{array}\right]$$

There's some region where $\tilde{x} < 1$ and as $\hbar \to 0$, both expressions remain valid.

Region of overlap

$(\xi << 1 \quad , \quad \xi >> \hbar)$.

(* Characteristic classical parameters are of order 1. $\hbar$ is very small compared to 1.)

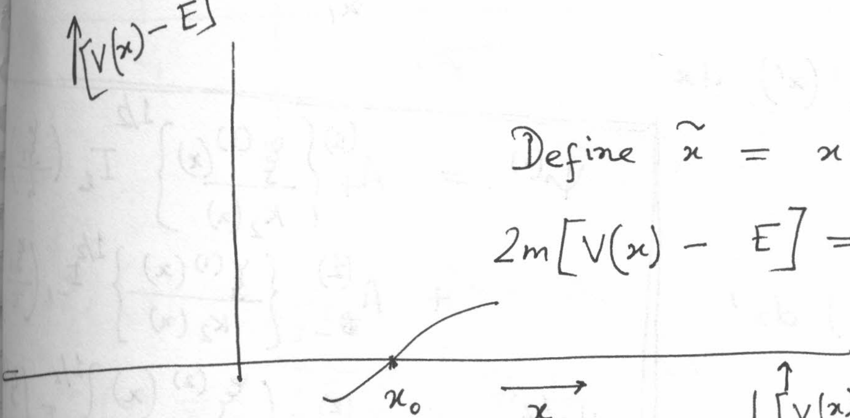
$$J_\ell(\rho) \longrightarrow \sqrt{\frac{\cancel{4}\,2}{\pi \rho}} \cos\left(\rho - \frac{\ell\pi}{2} - \frac{\pi}{4}\right)$$

$$\psi = A_{\pm} \sqrt{\frac{\cancel{\xi}}{K_1}} \times \sqrt{\frac{2\hbar}{\pi \cancel{\xi}}} \cos\left(\frac{\xi}{\hbar} \mp \frac{\ell\pi}{2} - \frac{\pi}{4}\right)$$

$$\psi_{WKB} = \frac{B_{\pm}}{\sqrt{K_1(x)}} \exp\left(\pm i \frac{\xi(x)}{\hbar} + \cdots\right)$$

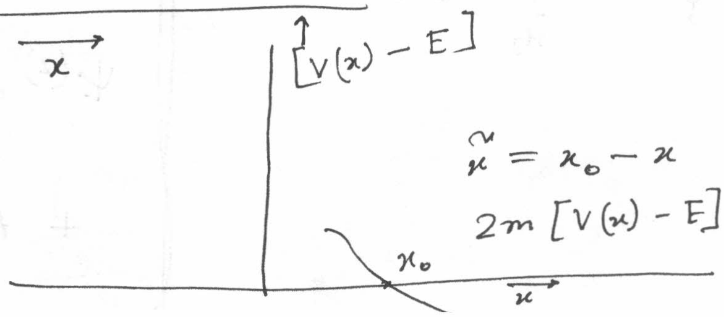
$\Rightarrow$ They look the same !

Consider $E < V(x)$.



Define $\tilde{x} = x - x_0$

$2m[V(x) - E] = C(\tilde{x})^n$; $C > 0$



$\tilde{x} = x_0 - x$

$2m[V(x) - E] = C\tilde{x}^n$;

$C > 0$

$$-\hbar^2 \frac{d^2\psi}{d\tilde{x}^2} = -C\tilde{x}^n \psi .$$

$$K_2(x) = \sqrt{2m(V(x)-E)}$$

$$\xi(x) = \int_{x_0}^{x} K_2(x')\,dx' \quad \text{for } x > x_0$$

$$= \int_{x}^{x_0} K_2(x')\,dx' \quad \text{for } x < x_0$$

Exercise

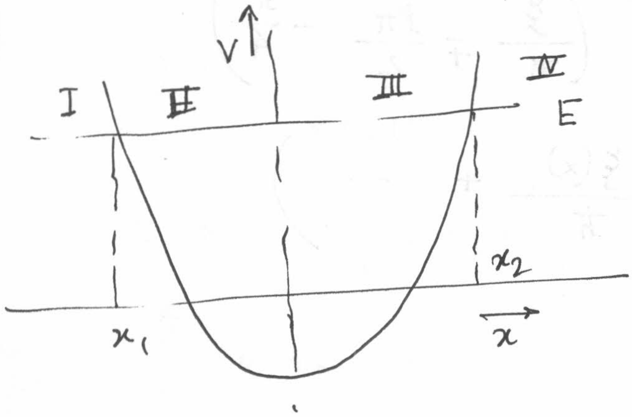
Show that the independent solutions are

$$\psi = A_\pm \frac{\{\xi(x)\}^{1/2}}{\{K_2(x)\}^{1/2}} J_{\pm l}\left(i\,\xi/\hbar\right)$$

$$= \text{- - - -} \quad I_{\pm l}\left(\xi/\hbar\right)$$

$$\boxed{I_l(\rho) = e^{-i\pi/2} J_l(i\rho) .}$$

(overall phase)



Region I

$$K_2^{(1)} = \sqrt{2m(V(x)-E)}$$

$$\xi^{(1)} = \int_{x}^{x_1} K_2^{(1)}(x')\,dx'$$

Region II

$$K_1^{(2)} = \sqrt{2m(E-V(x))}$$

$$\xi^{(2)} = \int_{x_1}^{x} K_1^{(2)}(x')\,dx'$$

Region III

$$\xi^{(3)} = \int_{x}^{x_2} K_1(x')\,dx'$$

Region IV

$$\xi^{(4)} = \int_{x_2}^{x} K_2(x')\,dx'$$

$$\boxed{\begin{aligned}
\psi^{(1)} &= A_+^{(1)}\left\{\frac{\xi^{(1)}(x)}{K_2(x)}\right\}^{1/2} I_l\left(\frac{\xi_1}{\hbar}\right) + A_-^{(1)}\left\{\frac{\xi^{(1)}(x)}{K_2(x)}\right\}^{1/2} I_{-l}\left(\frac{\xi_1}{\hbar}\right)\\
\psi^{(2)} &= A_+^{(2)}\left\{\frac{\xi^{(2)}(x)}{K_1(x)}\right\}^{1/2} J_l\left(\frac{\xi^{(2)}}{\hbar}\right) + A_-^{(2)}\left\{\frac{\xi^{(2)}(x)}{K_1(x)}\right\}^{1/2} J_{-l}\left(\frac{\xi^{(2)}}{\hbar}\right)
\end{aligned}}$$

$$\psi^{(3)} = A_+^{(3)} \left\{ \frac{\xi^{(3)}(x)}{K_1(x)} \right\}^{1/2} J_\ell \left(\frac{\xi^{(3)}}{\hbar} \right) + A_-^{(3)} \left\{ \frac{\xi^{(3)}(x)}{K_1(x)} \right\}^{1/2} \times J_{-\ell} \left(\frac{\xi^{(3)}}{\hbar} \right)$$

$$\psi^{(4)} = A_+^{(4)} \left\{ \frac{\xi^{(4)}(x)}{K_2(x)} \right\}^{1/2} I_\ell \left(\frac{\xi^{(4)}}{\hbar} \right) + A_-^{4} \left\{ \frac{\xi^{(4)}(x)}{K_2(x)} \right\}^{1/2} I_{-\ell} \left(\frac{\xi^{(4)}}{\hbar} \right) = y]$$

Observe that $\xi_{\otimes}^{(2)} + \xi_{\otimes}^{(3)} = \int_{x_1}^{x_2} (\quad) \ldots$

(independent of x)

Exercise

Show that the bound states are the solutions of the following equation —

$$\int_{x_1}^{x_2} \sqrt{2m\left(E - V(x')\right)}\, dx' = \left(n + \frac{1}{2}\right)\pi\hbar \quad \Big\}\ n = \text{integer}$$

(Take $n = 1$ for $C(x - x_0)^n$ near turning pt.)

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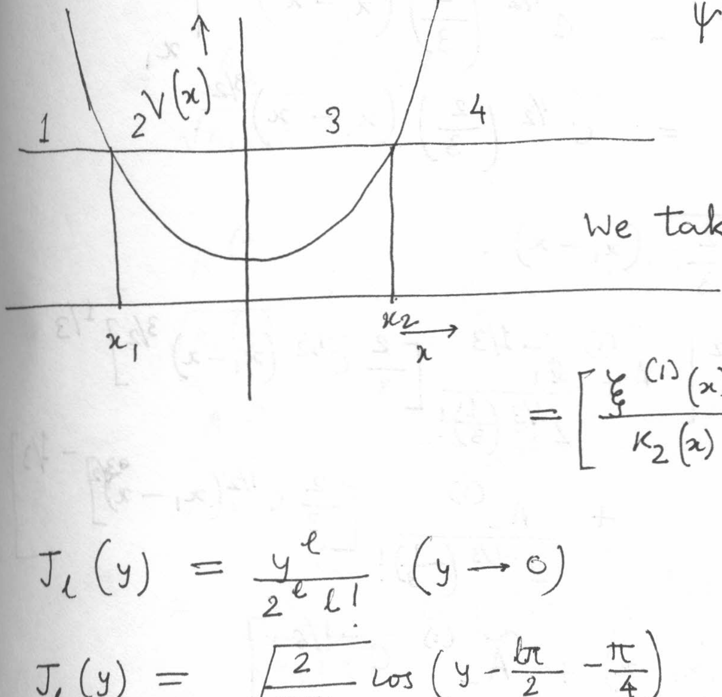

$$\psi^{(1)}(x) = A_+^{(1)} \left[\frac{\xi^{(1)}(x)}{K_2(x)} \right]^{1/2} I_\ell \left(\frac{\xi^{(1)}}{\hbar} \right) + A_-^{(1)} \left[\frac{\xi^{(1)}(x)}{K_2(x)} \right]^{1/2} I_{-\ell} \left(\frac{\xi^{(1)}}{\hbar} \right)$$

We take the asymptotic form and claim a decaying solution.

$$= \left[\frac{\xi^{(1)}(x)}{K_2(x)} \right]^{1/2} \left[A_+^{(1)} i^{-\ell} J_\ell \left(\frac{i\xi^{(1)}}{\hbar} \right) + A_-^{(1)} i^{\ell} J_{-\ell} \left(\frac{i\xi^{(1)}}{\hbar} \right) \right]$$

$$J_\ell(y) = \frac{y^\ell}{2^\ell \ell!} \quad (y \to 0)$$

$$J_\ell(y) = \sqrt{\frac{2}{\pi y}} \cos\left(y - \frac{\ell\pi}{2} - \frac{\pi}{4} \right)$$

$$= \left[\frac{\cancel{\xi^{(1)}(x)}}{K_2(x)} \right]^{1/2} \times \sqrt{\frac{2\hbar}{\pi \cancel{\xi_1}}} \left[A_+^{(1)} i^{-l} \cos\left(\frac{i\xi^{(1)}}{\hbar} - \frac{l\pi}{2} - \frac{\pi}{4} \right) + A_-^{(1)} i^{l} \cos\left(\frac{i\xi^{(1)}}{\hbar} - \frac{l\pi}{2} - \frac{\pi}{4} \right) \right]$$

$$= \sqrt{\frac{\hbar}{2\pi K_2(x)}} \left[A_+^{(1)} i^{-l} \left\{ e^{i\left(\frac{i\xi^{(1)}}{\hbar} - \frac{l\pi}{2} - \frac{\pi}{4}\right)} + e^{-i\left(\frac{i\xi^{(1)}}{\hbar} - \frac{l\pi}{2} - \frac{\pi}{4}\right)} \right\} + A_-^{(1)} i^{l} \left\{ e^{i\left(\frac{i\xi^{(1)}}{\hbar} + \frac{l\pi}{2} - \frac{\pi}{4}\right)} + e^{-i\left(\frac{i\xi^{(1)}}{\hbar} + \frac{l\pi}{2} - \frac{\pi}{4}\right)} \right\} \right]$$

$$A_+^{(1)} \cancel{i^{-l}} \cancel{e^{\frac{il\pi}{2}}} e^{i\frac{\pi}{4}} + A_-^{(1)} \cancel{i^{l}} \cancel{e^{-\frac{il\pi}{2}}} e^{i\frac{\pi}{4}} = 0$$

$$\Rightarrow \boxed{\frac{A_+^{(1)}}{A_-^{(1)}} = -1}$$

$$K_2(x) = \sqrt{2m(V(x) - E)} \qquad \xi^{(1)} = \int_x^{x_1} K_2(x')\, dx'$$

$$K_1(x) = \sqrt{2m(E - V(x))} \qquad = \int_x^{x_1} \sqrt{2m(V(x) - E)}\, dx'$$

Near $x = x_1$,

$$K_2(x) = \sqrt{C(x_1 - x)} \qquad = \cancel{\int_x^{x_1} \sqrt{2m}}$$

$$K_1(x) = \sqrt{C(x - x_1)}$$

$$= \int_x^{x_1} \sqrt{2m(V(x) - E)}\, dx'$$

$$= \sqrt{C} \int_x^{x_1} (x_1 - x')^{1/2}\, dx' = C^{1/2} \left(\frac{2}{3}\right) (x_1 - x')^{3/2} \Big|_{x_1}^{x}$$

$$= C^{1/2} \left(\frac{2}{3}\right) (x_1 - x)^{3/2}.$$

$$\therefore \left[\frac{\xi^{(1)}}{K_2}\right]^{1/2} = \sqrt{\frac{2}{3}}\, (x_1 - x).$$

$$\psi^{(1)}(x) = \sqrt{\frac{2}{3}}\, (x_1 - x)^{1/2} \left[A_+^{(1)} \frac{i^{-1/3}}{2^{1/3} \left(\frac{1}{3}\right)!} \left[\frac{2}{3} C^{1/2} (x_1 - x)^{3/2}\right]^{1/3} + \frac{A_-^{(1)}}{2^{-1/3} \left(-\frac{1}{3}\right)!} \left[\frac{2}{3} C^{1/2} (x_1 - x)^{3/2}\right]^{-1/3} \right]$$

$$\psi^{(1)}(x) = \left[\tilde{A}_+^{(1)} C^{1/6} (x_1 - x) + \tilde{A}_-^{(1)} C^{-1/6} \right]$$

$$\psi^{(2)}(x) = \left[\frac{\xi^{(2)}(x)}{K_1(x)}\right]^{1/2} \left\{ A_+^{(2)} J_l\left(\frac{\xi^{(2)}}{\hbar}\right) + A_-^{(2)} J_{-l}\left(\frac{\xi^{(2)}}{\hbar}\right) \right\}$$

$$\psi^{(2)}(x) = \left[\tilde{A}_+^{(2)}\, c^{1/6}\,(x-x_1) + \tilde{A}_-^{(2)}\, c^{-1/6}\right]$$

$$\cancel{\frac{\tilde{A}_+^{(1)}}{A_2}} \qquad \left\{ \begin{aligned} \tilde{A}_-^{(1)} &= \tilde{A}_-^{(2)} \\ \tilde{A}_+^{(1)} &= -A_+^{(2)} \end{aligned} \right\}$$

[Continuity & derivative matching.]

Now,
$$\boxed{\frac{\tilde{A}_-^{(1)}}{A_-^{(1)}} = -\frac{\tilde{A}_-^{(2)}}{A_-^{(2)}}}$$

$$\boxed{\frac{\tilde{A}_+^{(1)}}{A_+^{(1)}} = \frac{\tilde{A}_+^{(2)}}{A_+^{(2)}}}$$

So,
$$\boxed{\frac{A_+^{(2)}}{A_-^{(2)}} = -\frac{A_+^{(1)}}{A_-^{(1)}} = 1}$$

Similarly,
$$\boxed{\frac{A_+^{(4)}}{A_-^{(4)}} = -1} \qquad \boxed{\frac{A_+^{(3)}}{A_-^{(3)}} = 1}$$

$$\psi^{(2)} = A_2^{(+)} \left(\frac{\xi^{(2)}(q)}{k_1(q)}\right)^{1/2} \left[J_l\left(\frac{\xi^{(2)}}{\hbar}\right) + J_{-l}\left(\frac{\xi^{(2)}}{\hbar}\right)\right]$$

$$\boxed{J_l(\rho) \longrightarrow \frac{1}{\sqrt{\rho}} \cos\left(\rho - \frac{l\pi}{2} - \frac{\pi}{4}\right)} \quad \rho \to \infty$$

$$= \frac{A_2^{(+)}}{\sqrt{k_1(q)}} \left[\cos\left(\rho_2' - \frac{l\pi}{2}\right) + \cos\left(\rho_2' + \frac{l\pi}{2}\right)\right]$$

$$\rho_2' \longrightarrow \frac{\xi^{(2)}}{\hbar} - \frac{\pi}{4}$$

$$= \frac{A_2^{(+)}}{\sqrt{k_1(q)}} \left[2\cos\rho_2' \cos\frac{l\pi}{2}\right]$$

$$= \frac{A_2^{(+)}}{\sqrt{k_1(q)}} \cos\left(\frac{l\pi}{2}\right) \left[e^{i\rho_2'} + e^{-i\rho_2'}\right]$$

$$\psi^{(3)} = \frac{A_3^{(+)}}{\sqrt{k_1(q)}} \cos\left(\frac{l\pi}{2}\right) \left[e^{i\rho_3'} + e^{-i\rho_3'}\right]$$

Now, $\rho_2' + \rho_3' = K$ (constant) $= \left(\dfrac{\xi^{(2)} + \xi^{(3)}}{\hbar} - \dfrac{\pi}{2}\right)$

Because $\xi^{(2)} + \xi^{(3)}$ is const.

$$\psi^{(3)} = \frac{A_3^{(+)}}{\sqrt{K_1(q)}} \cos\left(\frac{l\pi}{2}\right)\left[e^{ik} e^{-i\rho_2'} + e^{-ik} e^{i\rho_2'}\right]$$

$$e^{ik} = e^{-ik} \qquad \therefore \quad \frac{\xi^{(2)} + \xi^{(3)}}{\hbar} = n\pi + \frac{\pi}{2}$$

$$e^{2ik} = 1 \qquad \Rightarrow \int_{x_1}^{x_2} K_1(x')\,dx' = \left(n+\frac{1}{2}\right)\pi\hbar$$

$$\Rightarrow 2k = 2n\pi$$

$$\Rightarrow \underline{\underline{k = n\pi}}. \qquad \Rightarrow \underline{\int_{x_1}^{x_2} \sqrt{2m\left(E - V(x)\right)}\, dx = \left(n+\frac{1}{2}\right)\pi\hbar}$$

$$S(m_1, m_2, m_3, m_4) = \left\langle m_1, j=\frac{3}{2}, m_1 \middle| A^{(1/2)}_{m_2} B^{(1/2)}_{m_3} \middle| n_4, j=\frac{3}{2}, n_4 \right\rangle$$

$$S\left(\frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) = \left\langle \frac{3}{2}, \frac{3}{2} \middle| A^{(\frac{1}{2})}_{\frac{1}{2}} B^{(1/2)}_{1/2} \middle| \frac{3}{2}, \frac{1}{2} \right\rangle = \alpha$$

$$= \left\langle \frac{3}{2}, \frac{3}{2} \middle| R^{(1)}_{1} \middle| \frac{3}{2}, \frac{1}{2} \right\rangle C^{1\,\frac{1}{2}\,\frac{1}{2}}_{1\,\frac{1}{2}\,\frac{1}{2}}$$

$$= C^{\frac{3}{2}\,1\,\frac{1}{2}}_{\frac{3}{2}\,1\,\frac{1}{2}} \left\langle \frac{3}{2} \| R^{(1)} \| \frac{3}{2} \right\rangle = \alpha$$

$$\| R^{(1)} \| = \frac{\alpha}{C^{\frac{3}{2}\,1\,\frac{3}{2}}_{\frac{3}{2}\,1\,\frac{1}{2}}}$$

$$S\left(\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{3}{2}\right) = \left\langle \frac{3}{2}, \frac{3}{2} \middle| A^{(1/2)}_{\frac{1}{2}} B^{(1/2)}_{-1/2} \middle| \frac{3}{2}, \frac{3}{2} \right\rangle$$

$$= \left\langle \frac{3}{2} \middle| R^{(1)}_{0}\, C^{1\,\frac{1}{2}\,\frac{1}{2}}_{0\,\frac{1}{2}\,-\frac{1}{2}} + C^{0\,\frac{1}{2}\,\frac{1}{2}}_{0\,\frac{1}{2}\,-\frac{1}{2}}\, S^{(0)}_{0} \middle| \frac{3}{2} \right\rangle$$

$$= C^{1\,\frac{1}{2}\,\frac{1}{2}}_{0\,\frac{1}{2}\,-\frac{1}{2}}\, C^{\frac{3}{2}\,1\,\frac{3}{2}}_{\frac{3}{2}\,0\,\frac{3}{2}} \| R^{(1)} \|$$

$$+ C^{0\,\frac{1}{2}\,\frac{1}{2}}_{0\,\frac{1}{2}\,-\frac{1}{2}}\, C^{\frac{3}{2}\,0\,\frac{3}{2}}_{\frac{3}{2}\,0\,\frac{3}{2}} \| S^{(0)} \| = \beta.$$

$$\therefore \quad \| S^{(0)} \| \cong \frac{\beta - C^{1\ \frac{1}{2}\ \frac{1}{2}}_{0\ \frac{1}{2}\ -\frac{1}{2}}\, C^{\frac{3}{2}\ 1\ \frac{3}{2}}_{\frac{3}{2}\ 0\ \frac{3}{2}}\, \alpha'}{C^{0\ \frac{1}{2}\ \frac{1}{2}}_{0\ \frac{1}{2}\ -\frac{1}{2}}\, C^{\frac{3}{2}\ 0\ \frac{3}{2}}_{\frac{3}{2}\ 0\ \frac{3}{2}}} = \beta'$$

$$S(m_1, m_2, m_3, m_4) = \langle m_1 | \, C^{1\ \frac{1}{2}\ \frac{1}{2}}_{m\ m_2\ m_3} R^{(1)}_m + C^{0\ \frac{1}{2}\ \frac{1}{2}}_{m\ m_2\ m_3} S^{(0)}_m \, | m_4 \rangle$$

$$= C^{1\ \frac{1}{2}\ \frac{1}{2}}_{m\ m_2\ m_3}\, C^{\frac{3}{2}\ 1\ \frac{3}{2}}_{m_1\ m\ m_4}\, \alpha' + C^{0\ \frac{1}{2}\ \frac{1}{2}}_{m\ m_2\ m_3}\, C^{\frac{3}{2}\ 0\ \frac{3}{2}}_{m_1\ m\ m_4}\, \beta'.$$

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17. 11. 2011

Time-dependent perturbation theory :-

$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$. Let's assume that H has explicit time-dependence.

(*) Initial value problem

small parameter

Let's assume $H = H_0 + \lambda H_1(t)$

time-~~dependent~~ independent

time dependent

(*) It's meaningless to hunt for eigenfunctions as they depend on time.

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

$$\left(H_0 + \lambda H_1(t) \right) \left(\Psi^{(0)} + \lambda \Psi^{(1)} + \lambda^2 \Psi^{(2)} + \cdots \right)$$
$$= i\hbar \left(\frac{\partial \Psi^{(0)}}{\partial t} + \lambda \frac{\partial \Psi^{(1)}}{\partial t} + \cdots \right)$$

Comparing, we get,

$$i\hbar \frac{\partial \Psi^{(0)}}{\partial t} = H_0 \Psi^{(0)}$$

$$i\hbar \frac{\partial \Psi^{(1)}}{\partial t} = H_0 \Psi^{(1)} + H_1 \Psi^{(0)}$$

In general, $\quad i\hbar \dfrac{\partial \psi^{(k)}}{\partial t} = H_0 \psi^{(k)}(t) + H_1(t)\psi^{(k-1)}(t)$

Suppose, $\{u_n\}$ are eigenstates of H_0.

$$H_0 u_n = E_n^{(0)} u_n$$

$$\psi^{(k)}(t) = \sum_n a_n^{(k)}(t)\, u_n .$$

[u_n's form a complete basis]

$$= \sum_n b_n^{(k)} e^{-iE_n^{(0)}t/\hbar} u_n$$

Definition of $b_n^{(k)} = e^{iE_n^{(0)}t/\hbar} a_n^{(k)}$

$$\therefore\ i\hbar \frac{\partial}{\partial t} \sum_n b_n^{(0)}(t)\, e^{-iE_n^{(0)}t/\hbar} u_n$$

$$= \sum_n b_n^{(0)}(t)\, e^{-iE_n^{(0)}t/\hbar} \underbrace{H_0 u_n}_{E_n^{(0)} u_n}$$

or, $\quad i\hbar \left(\dfrac{d b_n^{(0)}}{dt} - \dfrac{iE_n^{(0)}}{\hbar} b_n^{(0)} \right) \cancel{e^{-iE_n^{(0)}t/\hbar}} = E_n^{(0)} b_n^{(0)} \cancel{e^{-iE_n^{(0)}t/\hbar}}$.

(Comparing coefficients of u_n)

$$\therefore\ i\hbar \frac{d b_n^{(0)}}{dt} + \cancel{E_n^{(0)} b_n^{(0)}} = \cancel{E_n^{(0)} b_n^{(0)}}$$

$$\Rightarrow \quad \boxed{b_n^{(0)} = \text{constant.}} \quad \text{(time-independent)}$$

$$i\hbar \frac{\partial}{\partial t} \left\{ \sum_n b_n^{(k)}(t)\, e^{-iE_n^{(0)}t/\hbar} u_n \right\}$$

$$= \sum_n b_n^{(k)}(t)\, e^{-iE_n^{(0)}t/\hbar} E_n^{(0)} u_n$$

$$+ \sum_n b_n^{(k-1)}(t)\, e^{-iE_n^{(0)}t/\hbar} H_1(t)\, u_n$$

(Time-dependence of $H_1(t)$ only means it has a $f(t)$ inside it, no $\dfrac{\partial}{\partial t} \ldots$)

$$\left(\text{Ex.} \longrightarrow \quad V(\vec{r}, t) = (\sin t)\, e^{-r^2}. \right)$$

Perform $\langle m |$ or $\int dq \; u_m^*(q)$

$$i\hbar \frac{\partial}{\partial t} \left\{ b_m^{(k)}(t)\, e^{-iE_m^{(0)} t/\hbar} \right\}$$

$$= b_m^{(k)}(t)\, e^{-iE_m^{(0)} t/\hbar}\, E_m^{(0)} + \sum_n b_n^{(k-1)}(t)\, e^{-iE_n^{(0)} t/\hbar} \langle m | H_1(t) | n \rangle$$

or, $$i\hbar \frac{d b_m^{(k)}}{dt} e^{-iE_m^{(0)} t/\hbar} + \cancel{E_m^{(0)} b_m^{(k)} e^{-iE_m^{(0)} t/\hbar}}$$

$$= \cancel{E_m^{(0)} b_m^{(k)} e^{-iE_m^{(0)} t/\hbar}} + \sum_n b_{\cancel{m}n}^{(k-1)}(t)\, e^{-iE_n^{(0)} t/\hbar} \langle m | H_1(t) | n \rangle$$

$$\Rightarrow \quad i\hbar \frac{d b_m^{(k)}}{dt} = \sum_n b_{\cancel{m}n}^{(k-1)}\, e^{i(E_m^{(0)} - E_n^{(0)})} \langle m | H_1(t) | n \rangle$$

Let $\boxed{\omega_{mn} = \frac{E_m^{(0)} - E_n^{(0)}}{\hbar}}$

$$= \sum_n b_n^{(k-1)}(t)\, e^{i\omega_{mn} t} \langle m | H_1(t) | n \rangle$$

$$\int_{t_1}^{t_2} (\ldots) \; ✓$$

(No problems with degeneracy)

Focus on 1st order perturbation theory

$$i\hbar \frac{d b_m^{(1)}}{dt} = \sum_n b_n^{(0)} \cancel{(t)}\, e^{i\omega_{mn} t} \langle m | H_1(t) | n \rangle$$

Consider $\psi = f(q)$ at $t = 0$

(CHOICE) $= \sum c_n u_n(q)$ at $t = 0$

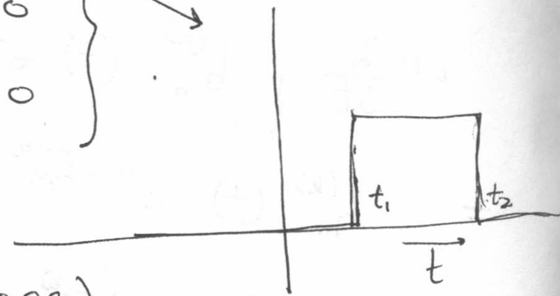
Say $b_n^{(0)} = c_n$, $b_n^{(k)} = 0$ at $t = 0$

(*) How to decompose ψ into $\psi^{(0)}$ & $\psi^{(1)}$ is entirely subjective.

Special case

$$H_1(t) = \underbrace{\Theta(t-t_1)\,\Theta(t_2-t)}\,V(q)$$

$$\Theta(x) = 1 \quad \text{for } x \geq 0$$
$$\quad\;\; = 0 \quad \text{for } x < 0$$



$$t_1 = 0, \qquad t_2 = T$$

$\underline{\underline{t=0}}$ $\quad b^{(0)}_{\cancel{k}n} = \delta_{nk}$ (Choose)

Initially, we have an eigenstate of H_0 with eigenvalue $E_k^{(0)}$.

$$i\hbar \frac{d b_m^{(1)}}{dt} = e^{i\omega_{mk} t} \langle m | H_1(t) | k \rangle$$

$$b_m^{(1)}(T) = -\frac{i}{\hbar}\int_0^T dt\; e^{i\omega_{mk} t} \underbrace{\langle m | H_1(t) | k \rangle}_{V(q)}$$

$$= -\frac{i}{\hbar}\langle m|V|k\rangle \frac{1}{i\omega_{mk}}\left(e^{i\omega_{mk}T} - 1\right)$$

$$= -\frac{1}{\hbar\omega_{mk}} \langle m|V|k\rangle \left(e^{i\omega_{mk}T} - 1\right)$$

$$\omega_{mk} = \frac{E_m^{(0)} - E_k^{(0)}}{\hbar}$$

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

$$= e^{-iE_k^{(0)}t/\hbar}|k\rangle + \lambda\sum_m b_m^{(1)}|m\rangle e^{-iE_m^{(0)}t/\hbar} + \cdots$$

$$\Psi^{(k)} = \sum b_m^{(k)} e^{-iE_m^{(0)}t/\hbar} |m\rangle$$

Probability of finding the particle in state $|m\rangle$

$$= \lambda^2 |b_m^{(1)}|^2 \quad \text{for } m \neq k$$

$$= \frac{\lambda^2}{\hbar^2 \omega_{mk}^2} \left| \langle m | V | k \rangle \right|^2 \underbrace{\left| e^{i\omega_{mk} T} - 1 \right|^2}_{4 \sin^2 \left(\frac{\omega_{mk} T}{2} \right)}$$

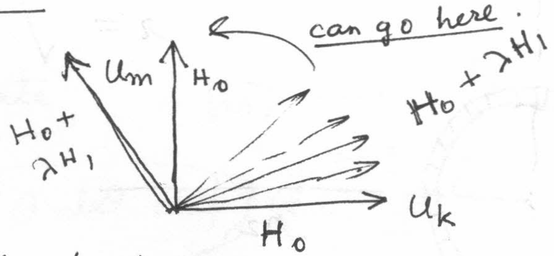
$\Rightarrow$ for $\omega_{mk} \to 0$ $\quad \dfrac{\sin \frac{\omega_{mk}}{2} T}{\omega_{mk}} \to \dfrac{T}{2}$

$T^2/4$

As long as ω_{mk} is finite, λ is small, this probability is small.

If $\omega_{mk} \to 0$, the ~~ratio~~ $\lambda\, b^{(1)}$ becomes of order 1

Closely spaced levels $\longrightarrow$?



⊛ Again degeneracy creates a problem

$\longrightarrow$ Diagonalize $\langle m | V | k \rangle$

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Transition probability to a state $|m\rangle$ starting with state $|k\rangle$

$$\lambda^2 \frac{\left| \langle m | H_1 | k \rangle \right|^2}{\left(E_m^{(0)} - E_k^{(0)} \right)^2} 4 \sin^2 \left(\frac{E_m^{(0)} - E_k^{(0)}}{2\hbar} T \right)$$

Density of states

$\rho(E)\, \Delta E$ = Total no. of states between E & $(E + \Delta E)$.

small

$\longrightarrow$ defines $\rho(E)$.

Example : Free particle

Put it in a box. (periodic box)

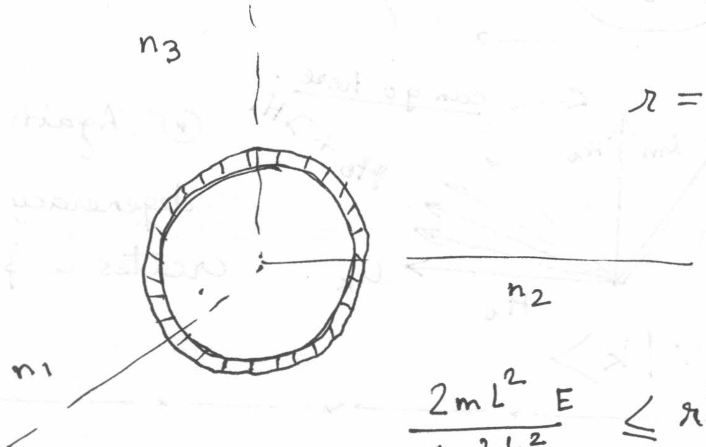
$\psi(x+L, y, z) = \psi(x, y, z), \ldots$

$$\psi = \frac{1}{L^{3/2}} e^{i\left(\frac{2\pi n_1 x}{L} + \frac{2\pi n_2 y}{L} + \frac{2\pi n_3 z}{L}\right)}$$

$$E = \frac{\hbar^2}{2m} 4\pi^2 \left(\frac{n_1^2}{L^2} + \frac{n_2^2}{L^2} + \frac{n_3^2}{L^2} \right)$$

\# of states between E and $E + \Delta E$

$$\underbrace{\frac{2mL^2}{4\pi^2\hbar^2} E < n_1^2 + n_2^2 + n_3^2 < \frac{2mL^2}{4\pi^2\hbar^2} (E + \Delta E)}$$



$$r = \sqrt{n_1^2 + n_2^2 + n_3^2}$$

$$\frac{2mL^2 E}{4\pi^2\hbar^2} \leq r^2 \leq \frac{2mL^2}{4\pi^2\hbar^2} (E + \Delta E)$$

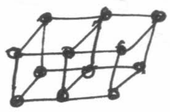
$$\Rightarrow \quad \frac{\sqrt{2m}\, L}{2\pi\hbar} \sqrt{E} \leq r \leq \frac{\sqrt{2m}\, L}{2\pi\hbar} (E + \Delta E)^{1/2}$$

$$\Rightarrow \quad \frac{\sqrt{2m}\, L}{2\pi\hbar} \sqrt{E} \leq r \leq \frac{\sqrt{2mE}\, L}{2\pi\hbar} \left(1 + \frac{\Delta E}{2E}\right)$$

approximately

$$\underbrace{4\pi r_{min.}^2 \Delta r} \longrightarrow \text{volume}$$

$$= L^3 \times (\cdots) \times \Delta E$$

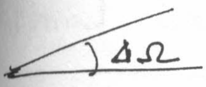


$$\rho(E) = L^3 \times (\cdots)$$

$$8 \times \frac{1}{8} = 1.$$

(Large L limit).

⊙ A similar procedure follows for interacting systems.



One can calculate the density of states in p- space specifying direction of momentum.

H_0 : free particle Hamiltonian

At $t = 0$, switch on $\lambda H_1 = \lambda V(q)$.
at $t = T$, switch it off.

Total transition probability into final state

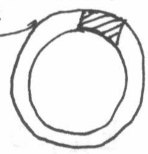
$$\lambda^2 \frac{|\langle m | H_1 | k \rangle|^2}{(E_m - E_k)^2} \, 4 \sin^2 \frac{(E_m^{(0)} - E_k^{(0)})T}{2\hbar}$$

$m \rightarrow$ final state $\qquad |m\rangle \longrightarrow |E, \theta, \phi\rangle$

$$d\Omega \Rightarrow \sin\theta \, d\theta \, d\phi \quad dE \, \rho_\Omega(E)$$

$$\int \lambda^2 \frac{|\langle E, \theta, \phi | H_1 | k \rangle|^2}{(E_m^{(0)} - E_k^{(0)})^2} \, 4 \sin^2 \frac{(E_m^{(0)} - E_k^{(0)})T}{2\hbar} \, d\Omega \, \rho_\Omega(E) dE$$

$E \longrightarrow E_k^{(0)} \longrightarrow$ Large prob.



(Continuum final states).

(*) Study for large T

$$u = \frac{(E - E_k^{(0)})T}{2\hbar}, \qquad du = \frac{T}{2\hbar} dE.$$

(Change of variables)

$$\lambda^2 \int d\Omega \, \frac{2\hbar}{T} du \, \frac{T^2 u^2}{4\hbar^2 u^2}$$

$$\left|\langle E_k^{(0)} + \frac{2\hbar}{T} u, \theta, \phi \,|\, H_1 \,|\, k \rangle\right|^2$$

$$4 \sin^2 u \; \rho_\Omega \left(E_k^{(0)} + \frac{2\hbar}{T} u, \theta, \phi\right)$$

As $T \rightarrow \infty$, $\quad E_k^{(0)} + \frac{2\hbar}{T} u \longrightarrow E_k^{(0)}$.

$$\Longrightarrow \int du \, \frac{\sin^2 u}{u^2} = \pi .$$

$$\lambda^2 T \, \frac{1\cdot 2}{2\hbar} \, \pi \, \left| \langle E_k^{(0)}, \theta, \phi | \, H_1 \, | k \rangle \right|^2 \rho_\Omega (E_k^{(0)}, \theta, \phi) \, d\Omega$$

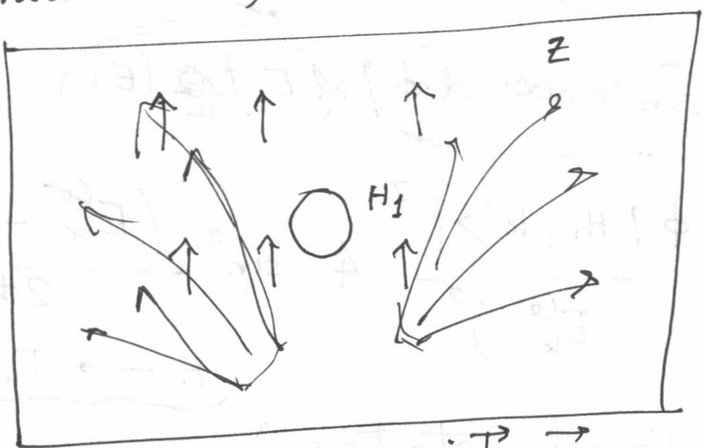
$\rho_\Omega \left(E_k^{(0)} \right)$ only. (Spherical symmetry)

Transition prob. / time

$$= 2\pi / \hbar \; \lambda^2 \left| \langle E_k^{(0)}, \theta, \phi \, | \, H_1 \, | \, k \rangle \right|^2 \rho_\Omega \, d\Omega$$

$|k\rangle \Rightarrow e^{ikz}$ $\qquad \langle k | k \rangle = L^3$

(Initial state)



$$| E_k, \theta, \phi \rangle = \frac{1}{L^{3/2}} e^{i \vec{k} \cdot \vec{r}}$$

$$\vec{k} = k \left(\sin\theta \cos\phi, \ \sin\theta \sin\phi, \ \cos\theta \right)$$

Calculate no. of scattered particles / time / solid angle (Scattering amplitude)

Exercise

$\sigma(\theta, \phi) \longrightarrow$ CALCULATE (!)

Show that this is the same as Born approximation.

Final Exercise :- Suppose $H_1(t) = \Theta(t-t_1)\,\Theta(t_2-t) \times V(q)\left(e^{i\omega t} + e^{-i\omega t}\right)$

Repeat take $T \longrightarrow \infty$.

Final state has energy $\boxed{E_k^{(0)} \pm \hbar\omega.}$

→ Calculate transition amplitudes
(Fermi Golden rule)

END OF QM 1 Course

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