Density of states 1

To compute transition rates to final states of nearly degenerate energies $\longrightarrow$ density of final states.

Consider, for example, the emisson of a particle $\longrightarrow$
$\longrightarrow$ free particle

$$\langle x | p \rangle = A e^{\frac{i}{\hbar} \vec{p} \cdot \vec{x}}$$

In a box of side L $\Rightarrow A = \frac{1}{L^{3/2}}$

And the we impose periodic boundary c.

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

$$e^{i p_x L/\hbar} = e^{i p_y L/\hbar} = e^{i p_z L/\hbar} = 1$$

which means

$$p_x = \frac{2\pi\hbar}{L} n_1 \qquad p_y = \frac{2\pi\hbar}{L} n_2 \qquad p_z = \frac{2\pi\hbar}{L} n_3$$

In a transition rate $\Gamma = \sum_{n_1} \sum_{n_2} \sum_{n_1} \Gamma_{i \to f(n_1, n_2, n_3)} \longrightarrow \int d^3n \, \Gamma$

continuum limit

$$d^3n = dn_1 \, dn_2 \, dn_3 = \frac{V}{(2\pi\hbar)^3} dp_x \, dp_y \, dp_z$$

$$E = \frac{\vec{p}^2}{2m} \Rightarrow \frac{V}{(2\pi\hbar)^3} d^3\vec{p} = \frac{V}{(2\pi\hbar)^3} d\Omega \, p^2 dp = \frac{V}{(2\pi\hbar)^3} p m \, dE \, d\Omega$$

$$d^3n = \frac{V}{(2\pi\hbar)^3} p \cdot m \, dE \, d\Omega \quad \Rightarrow \quad \rho(E) = \frac{d^3n}{dE} = \frac{V}{(2\pi\hbar)^3} p \cdot m \, d\Omega$$

(The density increases with V, correctly more states per energy unit if V increases, see quantisation of p_s).

For a relativistic particle

$$\hbar\omega = E = pc \quad \Rightarrow \quad \frac{V}{(2\pi\hbar)^3} d^3\bar{p} = \frac{V}{(2\pi\hbar)^3} d\Omega \, p^2 dp =$$

$$= \frac{V}{(2\pi\hbar)^3} d\Omega \, \frac{E^2 dE}{c^3} = \frac{V}{(2\pi\hbar)^3} \frac{\hbar^2\omega^2 dE}{c^3}$$

$$dE = \hbar d\omega$$

$$\rho(E) = \frac{V}{(2\pi\hbar)^3} \frac{p^2}{c} d\Omega =$$

$$\Rightarrow \tilde{\rho}(\omega) = \frac{d^3n}{d\omega} = \frac{V}{(2\pi\hbar)^3} \left(\frac{\hbar}{c}\right)^3 \omega^2 d\Omega = \frac{V}{(2\pi c)^3} \omega^2 d\Omega$$

How do we understand this in terms of Fermi-Golden rule?

$$R_{i\to f} \sim |\langle f|V|i\rangle|^2 \, \delta(E_f - E_i - \hbar\omega)$$

$$\frac{P_{i\to f}}{T} \text{ prob. per unit time.}$$

The point is: how many states do we have with $E_f - E_i = \hbar\omega$? $R_{i\to f} = \sum_{\text{states}} \to \int dE \rho(E)$

In case of more than one particle

$$\int \prod_K \frac{V d^3 p_K}{(2\pi\hbar)^3}\, \delta\Big(E_f - E_i + \sum_K E_K\Big)\, \delta\Big(\vec{p}_f - \sum_K \vec{p}_K - \vec{p}_i\Big)\, |\langle f|H|i\rangle|^2$$

$|f\rangle \to$ FINAL STATE SYSTEM

$\{K\} \to$ EMITTED PARTICLES

Example: decay $\quad M \to$ 2 particle of mass m_1, m_2

$$\vec{p}_2, m_2 \longleftarrow \underset{M}{\bullet} \longrightarrow \vec{p}_1, m_1$$

$\vec{p}_i = 0,\ E_i = Mc^2 \Longrightarrow \vec{p}_f, E_f = 0$ (no final state which is not a decay product)

$$E_i = Mc^2 = \sqrt{(\vec{p}_1 c)^2 + m_1^2 c^4} + \sqrt{(\vec{p}_2 c)^2 + m_2^2 c^4}$$

$$\delta(\vec{p}_1 + \vec{p}_2 - \vec{0}) \Rightarrow \vec{p}_1 = -\vec{p}_2 \equiv \vec{p}$$

$$\Rightarrow \frac{V^2}{(2\pi\hbar)^6} \int d^3\vec{p}\ \delta\Big(Mc^2 - \sqrt{(\vec{p}c)^2 + m_1^2 c^4} - \sqrt{(pc)^2 + m_2^2 c^4}\Big)$$

$$Mc^2 = \sqrt{p^2c^2 + m_1^2 c^4} + \sqrt{(p^2c^2) + m_2^2 c^4}$$

$$M^2 c^4 = 2p^2c^2 + (m_1^2 + m_2^2)c^4 + 2\sqrt{(\vec{p}^2c^2 + m_1^2c^4)(p^2c^2 + m_2^2c^4)}$$

$$\left[M^2c^4 - (m_1^2 + m_2^2)c^4\right] - 2p^2c^2 = 2\sqrt{(\quad)(\quad)}$$

Square again, call, $p^2 = x$

$$[\cdots]^2 + 4x^2c^4 - 4xc^2[\cdots] = 4(xc^2 + m_1^2c^4)(xc^2 + m_2^2c^4)$$

Solving for p^2: $\quad p^2 = \underbrace{\frac{c^2}{4M^2}(M - m_1 - m_2)(M + m_1 - m_2)(M - m_1 + m_2)(M + m_1 + m_2)}_{\tilde{p}^2}$

$$p = \frac{c}{2M}\sqrt{M - m_1 - m_2}\,\sqrt{(M + m_1 - m_2)(M - m_1 + m_2)(M + m_1 + m_2)}$$

$\hookrightarrow$ cannot decay in $m_1 + m_2 > M$.

$$\frac{V^2}{(2\pi\hbar)^6}\int d^3\vec{p}\;\delta\left(Mc^2-\sqrt{(\vec{p}c)^2+m_1^2c^4}-\sqrt{(pc)^2+m_2^2c^4}\right) =$$

$$= \frac{V^2}{(2\pi\hbar)^6}\,4\pi\cdot\int_0^{+\infty} dp\,p^2\;\delta(p-\tilde{p})\cdot\frac{1}{\underbrace{\left|\frac{\partial}{\partial p}\left(Mc^2-\sqrt{\ }\ \sqrt{\ }\right)\right|_{p=\tilde{p}}}} =$$

$$-\frac{1}{2}\frac{1}{\sqrt{\quad m_1}}2pc^2-\frac{1}{2}\frac{1}{\sqrt{\cdots m_2\cdots}}2pc^2 = -pc^2\left(\frac{1}{\sqrt{\ m_1}}+\frac{1}{\sqrt{\ m_2}}\right)$$

$$= -pc^2\left(\frac{\sqrt{\ }+\sqrt{\ }}{\sqrt{\ }\ \sqrt{\ }}\right) = \star$$

evaluating in $p=\tilde{p}$: numerator $= Mc^2$ (it must be)

denominator, using ✱ $\left.\frac{\left(M^2c^4-(m_1^2+m_2^2)c^4\right)-2p^2c^2}{2}\right|_{p=\tilde{p}}$

After some algebra:

$$\star = -\frac{c^3\sqrt{(M-m_1-m_2)(M+m_1-m_2)(M-m_1+m_2)(M+m_1+m_2)}\,\left(M^4+(m_1^2-m_2^2)^2\right)}{M\left(M^4-(m_1^2-m_2^2)^2\right)}$$

But then there is still p^2 in numerator, solving last δ

$$\Rightarrow = \frac{V^2}{(2\pi\hbar)^6}4\pi\frac{\left(M^4-(m_1^2-m_2^2)^2\right)}{4cM\left(M^4+(m_1^2-m_2^2)^2\right)}\cdot\sqrt{(M-m_1-m_2)(M+m_1-m_2)(M-m_1+m_2)\cdot(M+m_1+m_2)}$$

2) Hidrogen Atom

At $t=-\infty \longrightarrow$ ground state

An elektric field is turned on at $t=-\infty$ and has the form

$$\vec{E}(t) = \varepsilon\, \hat{n}\, e^{-t^2/\tau^2}$$

what is the probability of finding the atom in a state with $n=2$ at $t=+\infty$?

The time dependent potential is $V(t) = -e\vec{E}\cdot\vec{r}$

choose $\hat{n} = \hat{e}_z \Rightarrow V(t) = -e z \varepsilon e^{-t^2/\tau^2}$

$$C_{fi}^{(1)}(t) = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\, e^{\frac{i}{\hbar}(E_f-E_i)t} \langle f|V(t)|i\rangle =$$

$$= -\frac{i}{\hbar}\int_{t_0}^{t} dt'\, e^{\frac{i}{\hbar}(E_f-E_i)t}\, e^{-t^2/\tau^2}(-e\varepsilon)\langle f|\hat{z}|i\rangle$$

$$P_{i\to f}(t\to\infty, t_0\to-\infty) = \frac{e^2\varepsilon^2}{\hbar^2}\left|\int_{-\infty}^{+\infty} dt\, e^{-(\frac{t^2}{\tau^2}-i\omega_{fi}t)}\right|^2 |\langle f|\hat{z}|i\rangle|^2 \Rightarrow$$

$$\tau\int_{-\infty}^{+\infty} dt\, e^{-(t^2-i\omega_{if}\tau t)^2} = \tau\, e^{-\frac{\omega_{if}^2\tau^2}{4}}\int_{-\infty}^{+\infty} dt\, e^{-(t-\frac{i\omega_{if}\tau}{2})^2} =$$

$$= \tau\sqrt{\pi}\, e^{-\frac{\omega_{if}^2\tau^2}{4}}$$

$$\Rightarrow P_{i\to f}(t\to\infty, t_0\to-\infty) = \frac{e^2\varepsilon^2}{\hbar^2}\tau^2\pi\, e^{-\frac{\omega_{if}^2\tau^2}{2}}$$

We need to compute $\langle f|\hat{z}|i\rangle$ where

$|i\rangle = |1,0,0\rangle \qquad \langle r,\theta,\varphi|1,0,0\rangle = \frac{1}{\sqrt{\pi a_0^3}} \exp\left(-\frac{r}{a_0}\right)$

$$\langle n,\ell,m|\hat{z}|1,0,0\rangle =$$

$$= \int_0^{+\infty} dr\, r^2 d\Omega\, \Psi^*_{n,\ell,m}(r,\theta,\varphi)\, r\cos\theta\, \frac{1}{\sqrt{\pi a_0^3}} \exp\left(-\frac{r}{a_0}\right)$$

$$= \int_0^{+\infty} dr\, r^2 d\Omega\, R^*_{n\ell}(r)\, Y_\ell^{m*}(\theta,\varphi)\, r\cos\theta\, \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}$$

Consider the angular part

$$\int_0^{2\pi} d\phi \int_{-1}^{+1} d\cos\theta\, Y_\ell^{m*}(\theta,\varphi)\cos\theta$$

$\ell=0, m=0 \implies \int d\Omega \cos\theta = 0$

$\ell=1, \pm1 \implies \int_0^{2\pi} d\phi\, e^{\pm i\phi} = 0$

$$\boxed{\begin{aligned} P_{100\to200} &= 0 \\ P_{100\to21\pm1} &= 0 \end{aligned}}$$

$\ell=1, m=0$

$$\langle 2,1,0|\hat{z}|1,0,0\rangle = \frac{1}{\sqrt{\pi}\, a_0^{3/2}} \frac{1}{4} \frac{1}{\sqrt{2\pi a_0^3}} \int_0^{+\infty} dr\, r^2 \int_0^{2\pi} d\varphi \int_{-1}^{+1} d\cos\theta \cos^2\theta\, \frac{r}{a_0} e^{-\frac{r}{2a_0}}\, r\, e^{-\frac{r}{a_0}}$$

$$= \frac{1}{\cancel{\pi}\, a_0^3\, \cancel{4}_{2}\sqrt{2}}\, \cancel{2\pi}\, \frac{1}{3}\, \cancel{2}\, \frac{1}{a_0} \int_0^{+\infty} dr\, r^4\, e^{-\frac{3}{2}\frac{r}{a_0}} =$$

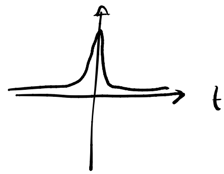
$$= \frac{1}{3\sqrt{2}\, a_0^3}\, a_0^4 \int_0^{+\infty} dz\, z^4 e^{-\frac{3}{2}z} = \frac{a_0}{3\sqrt{2}} \frac{256}{81} = \frac{128}{243}\sqrt{2}\, a_0 = \frac{2^7}{3^5}\sqrt{2}\, a_0$$

$$P_{100\to210} = \left(\frac{e\varepsilon}{\hbar}\right)^2 \tau^2 \pi\, e^{-\frac{w_{if}^2\tau^2}{2}}\, \frac{2^{15}}{3^{10}}\, a_0^2$$

The total probability to jump in any $n=2$ state is then

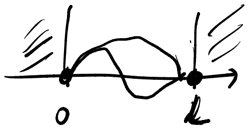
$$P_{gs \to n=2}(t \to \infty) = \left(\frac{e\mathcal{E}}{\hbar}\right)^2 \left(\frac{2^{15}}{3^{10}} a_0^2\right) \pi \tau^2 e^{-\omega^2\tau^2/2}$$

- For $\tau \to 0$ $\quad P_{gs \to n=2} \to 0$



sudden change

3)



$$\psi(x) = N \sin(Kx) \quad K = \frac{n\pi}{L}, n \in \mathbb{Z}$$

$$\int_0^L dx\, N^2 \sin^2(Kx) = N^2 \frac{L}{2} \Rightarrow N = \sqrt{\frac{2}{L}}$$

$$\left\{ \begin{array}{l} \psi_n(x) = \sqrt{\frac{2}{L}} \sin(Kx) \\ K = \frac{n\pi}{L}, n \in \mathbb{Z} \end{array} \right\}$$

$$E_n = \frac{\hbar^2}{2m} \frac{n\pi^2}{L^2} \qquad E_{gs} = \frac{\hbar^2\pi^2}{2mL^2} = \frac{(mv)^2}{2m} = \frac{(m \frac{L}{T})^2}{2m}$$

$$\frac{\hbar^2\pi^2}{L^2} = m^2 \frac{L^2}{T^2} \Rightarrow T^2 = \frac{m^2 L^4}{\hbar^2 \pi^2} \Rightarrow \boxed{T = \frac{mL^2}{\hbar\pi}}$$

The wave function for the ground state of the expanded box is:

$$\psi_1^{2L}(x) = \sqrt{\frac{2}{2L}} \sin\left(\frac{\pi}{2L} x\right)$$

$$\langle gs\,2 | gs\,1 \rangle = \frac{\sqrt{2}}{L} \int_0^L dx \sin\left(\frac{\pi}{L} x\right) \sin\left(\frac{\pi}{2L} x\right)$$

$$P = |\langle \cdots \rangle|^2 = \left| \frac{4}{3} \frac{\cancel{L}}{\pi} \frac{\sqrt{2}}{\cancel{L}} \right|^2 = \frac{16 \cdot 2}{9\pi^2} = \frac{2^5}{(3\pi)^2}$$

4)

H^3 (tritium)

$H^3 \to (He^3)^+ + e^- + \bar{\nu}_e$ Suppose $E_e^{kin} \simeq 16\, KeV$

$\Psi_i = \Psi_{100}(r,\theta,\varphi)$ initial state

$E = \gamma mc^2 = 16\, KeV + 0{,}5\, MeV = 516\, KeV$

$\gamma \sim 1{,}0320 = \dfrac{1}{\sqrt{1 - v^2/c^2}} \Rightarrow v = c \cdot \sqrt{\dfrac{\gamma^2 - 1}{\gamma^2}} = 0{,}244\, c$

The atom has size $\sim a_0$.

$\tau_{escape} \sim \dfrac{a_0}{v} \sim 7 \cdot 10^{-19}\, s$

Energy levels for single electron atoms $\sim (-13{,}6\, eV)\dfrac{Z^2}{n^2}$

$E_0^{Z=1} = -13{,}6\, eV$

$(-13{,}6\, eV)\left(-1 + \dfrac{4}{n^2}\right) = \Delta E = \left(\dfrac{4 - n^2}{n^2}\right)(-13{,}6\, eV)$

$Z=2$

$\tau_{levels} \sim \dfrac{n^2}{-4+n^2} \dfrac{\hbar}{13{,}6\, eV} = \dfrac{n^2}{n^2-4} \, 4{,}84 \cdot 10^{-17} \sim 10^{-17} \gg 10^{-19}$

even for $n \gg 1$

sudden approx. can be used

The probability to fall into the ground state of Helium is

$$P = \left| \int d^3r \, \varphi_0^*(\bar{r}, Z=1)\, \varphi_0(\bar{r}, Z=2) \right|^2 =$$

$$= \left| \frac{\sqrt{8}}{\cancel{\pi} a_0^3} 4\cancel{\pi} \int_0^{+\infty} dr\, r^2 e^{-3r/a_0} \right|^2 =$$

$$= \frac{8 \cdot 16}{\cancel{a_0^6}} \cancel{a_0^6} \frac{4}{27^2} = \frac{512}{729} \sim 70\%$$

$$P \, |n=16, \ell=3, m=0\rangle = ? = 0$$

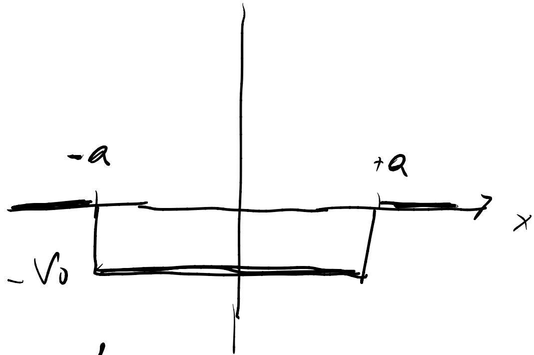
↳ orthogonal

5)

$V(x) = -V_0 \qquad |x|<a$

$p = \hbar K$ incoming

$E \gg V_0$



We quantise on a volume $L \gg a$.

$K = \frac{2\pi n}{L}$ and $n \gg 1$, $E \gg V_0$

$\psi_{in}(x) = \frac{1}{\sqrt{L}} e^{iKx} \qquad \psi_{out}(x) = \frac{1}{\sqrt{L}} e^{-iKx}$

To apply Fermi Golden Rule

$$\langle f|V(x)|i\rangle = \int_{-L/2}^{L/2} dx \, \frac{1}{L} (e^{-iKx})^* V(x)\, e^{iKx} =$$

$$= -V_0 \frac{1}{L} \int_{-a}^{a} dx \, e^{2iKx} = -\frac{V_0}{L} \frac{1}{2iK} (e^{2iKa} - e^{-2iKa})$$

$$= -\frac{V_0}{LK} \sin(2Ka) \Rightarrow R_{i\to f} = \frac{2\pi}{\hbar} V_0^2 \frac{\sin^2(2Ka)}{L^2K^2}\, g(E)$$

Repeat exercise 1 in 1-d

$$dn = \frac{L}{2\pi\hbar} dp = \frac{L}{2\pi\hbar} \frac{m}{p} dE \qquad \left(\frac{p^2}{2m} = E \qquad \frac{dp\, p}{m} = dE \right)$$

$$\Rightarrow \rho(E) = \frac{L}{2\pi\hbar} \frac{m}{p} = \frac{L}{2\pi\hbar} \frac{1}{2} \sqrt{\frac{2m}{E}} = \frac{L}{4\pi\hbar} \sqrt{\frac{2m}{E}}$$

$$R_{i\to f} = \frac{2\pi}{\hbar} V_0^2 \frac{\sin^2(2Ka)}{L^{\cancel{2}} K^2} \frac{\cancel{L}}{4\pi\hbar} \sqrt{\frac{2m}{E}}$$

$$= \frac{V_0^2}{2\hbar^2} \sqrt{\frac{2m}{E}} \frac{\sin^2(2Ka)}{L K^2}$$

$R_{i\to f} \xrightarrow[L\to\infty]{} 0$ because the scattering potential is located in limited area $\ll L$, $L \to \infty$.

The space travelled in a time τ is:

$$v_0 \tau_L = \sqrt{\frac{2}{m} E}\, \tau_L \overset{!}{=} L \Rightarrow \tau_L = \frac{L\sqrt{m}}{\sqrt{2E}}$$

$$\Rightarrow P_{\tau_L} = R_{i\to f} \tau_L = \frac{V_0^2}{2\hbar^2} \frac{\sqrt{2m}}{\sqrt{E}} \frac{\sqrt{m}}{\sqrt{2E}} \frac{\sin^2(2Ka)}{K^2}$$

$$= \frac{V_0^2}{2\hbar^2} \frac{m}{E} \frac{\sin^2(2Ka)}{K^2} = \frac{V_0^2}{4E^2} \sin^2(2Ka)$$

Solving the exact problem (in, out, normalisation, boundaries... OM 1)

$$P_{refl} = \frac{(\mathcal{K}/k - k/\mathcal{K})^2 \sin(2\mathcal{K}a)}{(\mathcal{K}/k + k/\mathcal{K})^2 \sin^2(2\mathcal{K}a) + 4\cos^2(2\mathcal{K}a)}$$

where $\mathcal{K}^2 - k^2 = 2mV_0/\hbar^2 << k^2$ so we can approximate, for $V_0 << E$, $\mathcal{K}a \sim ka$ and $\mathcal{K}/k \approx 1$

$$P_{refl} \simeq \left(\frac{\mathcal{K}^2 - k^2}{2k\mathcal{K}} \right)^2 \sin^2(2\mathcal{K}a) \simeq \frac{V_0^2}{4E^2} \sin^2(2ka)$$

Delta potential

The sudden approximation is based on the assumption that

$$\int_{-\varepsilon}^{+\varepsilon} dt\; H(t)\,|\psi(t)\rangle \xrightarrow[\varepsilon \to 0]{} 0$$

this is true for any "regular" function $H(t)$

But $\delta(t)$ has <u>FINITE</u> area over an <u>INFINITESIMAL</u> interval.

$$\Rightarrow \quad |\psi_{0^+}\rangle \neq |\psi_{0^-}\rangle \quad \text{in general.}$$

Using perturbation theory:

$$c_{if}(t) = -\frac{i}{\hbar}\int_{-\varepsilon}^{+\varepsilon} dt\, \langle f|\underbrace{H(t)}_{V\,\delta(t)}|i\rangle\, e^{i\omega_{fi}(t+\varepsilon)} = -\frac{i}{\hbar}\langle f|V|i\rangle$$