Graduate QM
HW #7 – Solution
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① $V(x) = \frac{1}{2} m w_0^2 x^2$; $H'(t) = 2\alpha x \cos wt$ Periodic Perturbation

transition probability is $|a_{i\to f}(t)|^2$

$$|a_{i\to f}(t)|^2 = \frac{2\pi}{\hbar^2} |H'_{fi}|^2 \delta(w_{fi} - w) t \rightarrow \text{Fermi's Golden Rule}$$

$$= \frac{2\pi}{\hbar^2} |H'_{fi}|^2 \delta(n w_0 - w) t$$

$$w_{fi} = \frac{E_f - E_i}{\hbar} = \frac{(n+\frac{1}{2})\hbar w_0 - \frac{1}{2}\hbar w_0}{\hbar} = n w_0$$

Now $H'(t) = 2\alpha x \cos wt = H'_{fi} \cos wt$

where $H'_{fi} = 2\alpha x$

$\langle n | H'_{fi} | 0 \rangle = 2\alpha \langle n | x | 0 \rangle$; where $x = \sqrt{\frac{\hbar}{2m w_0}} (a + a^+)$

$$\Rightarrow x|0\rangle = \sqrt{\frac{\hbar}{2m w_0}} (\overset{0}{a} + a^+)|0\rangle = \sqrt{\frac{\hbar}{2m w_0}} a^+|0\rangle = \sqrt{\frac{\hbar}{2m w_0}} |1\rangle$$

$$\langle n | x | 0 \rangle = \sqrt{\frac{\hbar}{2m w_0}} \langle n | 1 \rangle = \sqrt{\frac{\hbar}{2m w_0}} \delta_{n,1}$$; the particle can be excited only to the first excited state (one choice)

$$\therefore |\langle n | H'_{fi} | 0 \rangle|^2 = 4\alpha^2 \frac{\hbar}{2m w_0} \delta_{n,1}$$

$$\Rightarrow |a_{i\to f}(t)|^2 = \frac{2\pi}{\hbar^2} \frac{4\alpha^2 \hbar}{2m w_0} \delta_{n,1} \delta(n w_0 - w) t = \frac{4\pi\alpha^2}{\hbar m w_0} \delta(w_0 - w) t$$

Now using the identity $\lim \frac{\sin^2(yt)}{\pi y^2 t} = \delta(y)$

$$\Rightarrow |a_{i\to f}(t)|^2 = \frac{4\pi\alpha^2}{\hbar m w_0} \frac{\sin^2(w_0 - w)t}{\pi (w_0 - w)t} t$$

$$= \frac{4\alpha^2}{\hbar m w_0} \frac{\sin^2(w_0 - w)t}{(w_0 - w)^2}$$

this is the transition probability from the G.S ($n=0$) to the first excited state ($n=1$)

② $V(x) = \frac{1}{2} m w_0^2 x^2$; $H'(t) = \frac{\alpha x}{\sqrt{\pi}\tau} e^{-t^2/\tau^2}$

$$a_{i\to f}^{(t)} = \frac{1}{i\hbar}\int_{-\infty}^{\infty} \frac{\alpha x}{\sqrt{\pi}\tau} e^{i w_{fi} t} e^{-t^2/\tau^2} dt = \frac{\alpha \langle n|x|0\rangle}{i\hbar\sqrt{\pi}\tau}\int_{-\infty}^{\infty} e^{i w_{fi} t - \frac{t^2}{\tau^2}} dt$$

$$= \frac{\alpha}{i\hbar\sqrt{\pi}\tau}\langle n|x|0\rangle \int_{-\infty}^{\infty} e^{i n w_0 t - \frac{t^2}{\tau^2}} dt \quad ; \text{ where } w_{fi} = \frac{E_f - E_i}{\hbar} = n w_0$$

$$= \frac{\alpha}{i\hbar\sqrt{\pi}\tau}\langle n|x|0\rangle \int_{-\infty}^{\infty} e^{-\frac{1}{\tau^2}(t^2 - i n w_0 \tau^2 t)} dt$$

completing the square $-\frac{1}{\tau^2}(t^2 - i n w_0 \tau^2 t) = -\frac{1}{\tau^2}\left(t - \frac{i n w_0 \tau^2}{2}\right)^2 - \frac{n^2 w_0^2 \tau^2}{4}$

$$\Rightarrow a_{i\to f} = \frac{\alpha}{i\hbar\sqrt{\pi}\tau}\langle n|x|0\rangle e^{-\frac{n^2 w_0^2 \tau^2}{4}} \int_{-\infty}^{\infty} e^{-\frac{1}{\tau^2}\left(t - \frac{i n w_0 \tau^2}{2}\right)^2} dt$$

let $u = t - \frac{i n w_0 \tau^2}{2} \Rightarrow du = dt$

$$\Rightarrow a_{i\to f} = \frac{\alpha}{i\hbar\sqrt{\pi}\tau}\langle n|x|0\rangle e^{-\frac{n^2 w_0^2 \tau^2}{4}} \underbrace{\int_{-\infty}^{\infty} e^{-\frac{1}{\tau^2}u^2} du}_{\sqrt{\frac{\pi}{1/\tau^2}} = \sqrt{\pi}\tau}$$

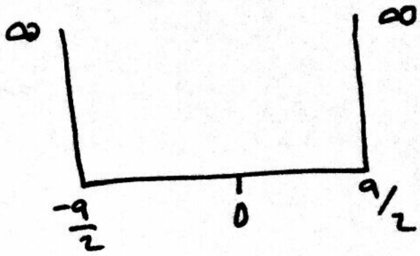
$$= \frac{\alpha}{i\hbar} e^{-\frac{n^2 w_0^2 \tau^2}{4}} \langle n|x|0\rangle = \frac{\alpha}{i\hbar} e^{-\frac{n^2 w_0^2 \tau^2}{4}} \sqrt{\frac{\hbar}{2 m w_0}}\, \delta_{n,1}$$

$\Rightarrow$ transition probability

$$|a_{i\to f}^{(t)}|^2 = \frac{\alpha^2}{\hbar^2} e^{-\frac{n^2 w_0^2 \tau^2}{2}} \frac{\hbar}{2 m w_0}\delta_{n,1} = \frac{\alpha^2}{2 m \hbar w_0} e^{-\frac{1}{2} w_0^2 \tau^2}$$

Again the only allowed transition is only from the ground state to the first excited state $(n=1)$ due to the selection rule governed by $\delta_{n,1}$.

③ $V(x) = \begin{cases} 0 & ; \ |x| \lesssim a/2 \\ \infty & ; \ \text{elsewhere} \end{cases}$



symmetric potential ⇒ we have even and odd solutions

$$u_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}\left(x - \frac{a}{2}\right)\right) \ ; \quad n = 1, 2, 3, 4, \ldots \ ; \ E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

using $\sin(A-B) = \sin A \cos B - \cos A \sin B$, we find the first three eigenstates

$$u_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}\left(x - \frac{a}{2}\right)\right) = -\sqrt{\frac{2}{a}} \cos\left(\frac{\pi x}{a}\right) ; \quad E_1 = \frac{\pi^2\hbar^2}{2ma^2} \quad \text{even}$$

$$u_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}\left(x - \frac{a}{2}\right)\right) = -\sqrt{\frac{2}{a}} \sin\frac{2\pi x}{a} ; \quad E_2 = \frac{4\pi^2\hbar^2}{2ma^2} \quad \text{odd}$$

$$u_3(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi}{a}\left(x - \frac{a}{2}\right)\right) = \sqrt{\frac{2}{a}} \cos\left(\frac{3\pi x}{a}\right) ; \quad E_3 = \frac{9\pi^2\hbar^2}{2ma^2} \quad \text{even}$$

and so on. Now $H'(t) = x^2 e^{-t/\tau}$

transition probability

$$|a_{i\to f}(t)|^2 = \frac{1}{\hbar^2} \left| \int_0^\infty \langle \psi_f | H(t) | \psi_i \rangle e^{i\omega_{fi} t} \, dt \right|^2$$

$$= \frac{1}{\hbar^2} |\langle \psi_f | H(t) | \psi_i \rangle|^2 \ \underbrace{\left| \int_0^\infty e^{-\left(\frac{1}{\tau} - i\omega_{fi}\right) t} \, dt \right|^2}$$

let $u = \left(\frac{1}{\tau} - i\omega_{fi}\right) t \Rightarrow du = \left(\frac{1}{\tau} - i\omega_{fi}\right) dt = \frac{1 - i\omega_{fi}\tau}{\tau} dt$

$$\Rightarrow dt = \frac{\tau}{1 - i\omega_{fi}\tau} du$$

$$\therefore \int_0^\infty e^{-\left(\frac{1}{\tau} - i\omega_{fi}\right)t} dt = \frac{\tau}{1 - i\omega_{fi}\tau} \underbrace{\int_0^\infty du\, e^{-u}}_{\frac{(1)!}{(1)^{1+1}} = 1}$$

$$= \frac{\tau}{1 - i\omega_{fi}\tau} \times \frac{1 + i\omega_f\tau}{1 + i\omega_{fi}\tau} = \frac{\tau + i\omega_{fi}\tau^2}{1 + \omega_{fi}^2\tau^2}$$

$$\therefore \left| \int_0^\infty e^{-\left(\frac{1}{\tau} - i\omega_{fi}\right)t} dt \right|^2 = \frac{\tau + i\omega_{fi}\tau^2}{1 + \omega_{fi}^2\tau^2} \times \frac{\tau - i\omega_{fi}\tau^2}{1 + \omega_{fi}^2\tau^2} = \frac{\tau^2 + \omega_{fi}^2\tau^4}{(1 + \omega_{fi}^2\tau^2)^2}$$

$$\therefore \left| a_{i\to f}^{(1)} \right|^2 = \frac{1}{\hbar^2} \langle \psi_f | x^2 | \psi_i \rangle \frac{\tau^2 + \omega_{fi}^2\tau^4}{(1 + \omega_{fi}^2\tau^2)^2}$$

i) $P_{1\to 2} = \left| a_{1\to 2}^{(1)} \right|^2 = \frac{1}{\hbar^2} \left| \langle u_2(x) | x^2 | u_1(x) \rangle \right|^2 \frac{\tau^2 + \omega_{fi}^2\tau^4}{(1 + i\omega_{fi}^2\tau^2)^2}$; $\omega_{fi} = \omega_{21}$

where $\langle u_2 | x^2 | u_1 \rangle = \int_{-a/2}^{a/2} dx\, x^2 \left(-\sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)\right)\left(-\sqrt{\frac{2}{a}} \cos\left(\frac{\pi x}{a}\right)\right)$

$$= \frac{2}{a} \int_{-a/2}^{a/2} dx\, x^2 \sin\left(\frac{2\pi x}{a}\right) \cos\left(\frac{\pi x}{a}\right)$$

$$= \int_{-a/2}^{a/2} \text{odd function} = 0$$

integral of odd function over symmetric interval vanishes

$\therefore P_{1\to 2} = 0$ No allowed transition from the ground state to the first excited state $(n=2)$

now $P_{1\to3} = \left| a^{(1)}_{1\to3} \right|^2 = \frac{1}{\hbar^2} \left|\langle u_3 | x^2 | u_1 \rangle\right|^2 \frac{\tau^2 + \omega_{31}^2 \tau^4}{(1+\omega_{31}^2\tau^2)^2}$

where $\omega_{31} = \frac{E_3 - E_1}{\hbar} = \frac{1}{\hbar}\left(\frac{\pi \hbar^2}{2ma^2}\right)(9-1) = \frac{4\pi^2 \hbar}{ma^2}$

and $\langle u_3 | x^2 | u_1 \rangle = -\frac{2}{a} \int_{-a/2}^{a/2} dx\, x^2 \cos\left(\frac{3\pi x}{a}\right) \cos\left(\frac{\pi x}{a}\right)$

now using $\cos A \cos B = \frac{1}{2}\left[\cos(A-B) + \cos(A+B)\right]$, we have

$$\langle u_3 | x^2 | u_1 \rangle = -\frac{1}{a} \int_{-a/2}^{a/2} dx\, x^2 \left[\cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{4\pi x}{a}\right)\right]$$

$$= -\frac{1}{a}\left[\int_{-a/2}^{a/2} x^2 \cos\left(\frac{2\pi x}{a}\right) dx + \int_{-a/2}^{a/2} x^2 \cos\left(\frac{4\pi x}{a}\right) dx\right]$$

use integral calculator on internet

$$= -\frac{1}{a}\left[\frac{-a^3}{2\pi^2} + \frac{a^3}{8\pi^2}\right]$$

$$= \frac{3a^2}{8\pi^2}$$

$$\Rightarrow \left|\langle u_3 | x^2 | u_1 \rangle\right|^2 = \frac{9a^4}{64\pi^4}$$

$$\Rightarrow P_{1\to3} = \frac{1}{\hbar^2}\left(\frac{9a^4}{64\pi^4}\right) \frac{\tau^2 + \omega_{31}^2\tau^4}{(1+\omega_{31}^2\tau^2)^2} = \frac{1}{\hbar^2} \frac{9}{64} \frac{a^4}{\pi^4} \frac{\tau^2(1+\omega_{31}^2\tau^2)}{(1+\omega_{31}^2\tau^2)^2}$$

$$= \frac{9}{64} \frac{a^4}{\hbar^2\pi^4} \frac{\tau^2}{1+\omega_{31}^2\tau^2} = \frac{9a^4}{64\hbar^2\pi^4} \frac{1}{\omega_{31}^2 + \frac{1}{\tau^2}}$$

$$= \frac{9a^4}{64\hbar^2\pi^4} \frac{1}{\frac{16\pi^4\hbar^2}{m^2a^4} + \frac{1}{\tau^2}} = \left(\frac{3a^2}{8\hbar\pi^2}\right)^2 \left[\frac{16\pi^4\hbar^2}{m^2a^4} + \frac{1}{\tau^2}\right]^{-1}$$

Q.E.D

(4) H atom

initial state $\psi_i = \psi_{100} = \psi_{1s} = R_{10}(r)\, Y_{00}(\theta,\phi) = \frac{1}{\sqrt{\pi a_0^3}}\, e^{-r/a_0}$

find state $\psi_f = \psi_{210} = \psi_{2p} = R_{21}(r)\, Y_{10}(\theta,\phi) = \frac{1}{\sqrt{8\pi a_0^3}}\, \frac{r}{2a_0}\, e^{-\frac{r}{2a_0}} \cos\theta$

here we take $\psi_f = \psi_{2p} =$ as all p states degenerate

$\psi_{210}, \psi_{211}, \psi_{21-1}$

$$\vec{E} = E_0 e^{-t/\tau}$$

$$H'(t) = -e\vec{r}\cdot\vec{E} = -ezE_0 e^{-t/\tau}$$

$$\therefore P_{1s\to 2p} = \frac{1}{\hbar^2}\left| \int |\langle \psi_f | H'(t) | \psi_i \rangle|^2 e^{i\omega_{fi} t}\, dt \right|^2$$

$$= \frac{1}{\hbar^2} |\langle \psi_f | -ezE_0 | \psi_i \rangle|^2 \left| \underbrace{\int_0^\infty dt\, e^{-t/\tau} e^{i\omega_{fi} t}} \right|^2$$

as done in problem 3 $\int_0^\infty dt\, e^{-(\frac{1}{\tau} - i\omega_{fi})t} = \frac{\tau + i\omega_{fi}\tau^2}{1+\omega_{fi}^2\tau^2}$

and $\langle \psi_f | -ezE_0 | \psi_i \rangle = -eE_0 \langle \psi_f | z | \psi_i \rangle$

$$= -eE_0 \int_{-\infty}^{\infty} \frac{1}{\sqrt{8\pi a_0^3}} \frac{r}{2a_0} e^{-r/2a_0} \cos\theta\, z\, \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}\, d^3r$$

using $z = r\cos\theta$ and $d^3r = r^2 \sin\theta\, d\theta\, d\phi\, dr$

$$-eE_0 \langle \psi_f | z | \psi_i \rangle = \frac{-eE_0}{4\pi\sqrt{2}\, a_0^4} \underbrace{\int_0^{2\pi} d\phi}_{2\pi} \underbrace{\int_0^\infty r^4 e^{-\frac{3r}{2a_0}} dr}_{\frac{4!}{(3/2a_0)^5}} \underbrace{\int_0^\pi \cos^2\theta \sin\theta\, d\theta}_{-\frac{\cos^3\theta}{3}\Big|_0^\pi = \frac{2}{3}}$$

$$= \frac{-eE_0 a_0 2^8}{3^5\sqrt{2}}$$

$$\therefore \langle \psi_f | -ez\mathcal{E}_0 | \psi_i \rangle = \frac{-e\mathcal{E}_0 a_0 2^8}{3^5 \sqrt{2}}$$

$$\Rightarrow |\langle \psi_f | -ez\mathcal{E}_0 | \psi_i \rangle|^2 = \frac{e^2 \mathcal{E}_0^2 a_0^2 2^{16}}{3^{10} \times 2} = \frac{e^2 \mathcal{E}_0^2 a_0^2 2^{15}}{3^{10}}$$

$$\therefore P_{1s\to 2p} = \frac{1}{\hbar^2} \frac{e^2 \mathcal{E}_0^2 a_0^2 2^{15}}{3^{10}} \frac{\tau^2}{1 + \omega_{fi}^2 \tau^2}$$

; when $\omega_{fi} = \frac{E_{2p} - E_{1s}}{\hbar}$

$$= \frac{1}{\hbar}\left(\frac{E_{1s}}{4} - E_{1s}\right)$$

$$= \frac{-3}{4\hbar} E_{1s}$$

$$= \frac{-3}{4\hbar}(\underbrace{-13.6\,eV}_{R_y})$$

$$= \frac{3R_y}{4\hbar}$$

$R_y = 13.6$ eV
Rydberg const

$$= \frac{2^{15} e^2 \mathcal{E}_0^2 a_0^2}{3^{10} \hbar^2} \left[\frac{1}{\omega_{fi}^2 + \frac{1}{\tau^2}}\right]$$

$$= \frac{2^{15} e^2 \mathcal{E}_0^2 a_0^2}{3^{10} \hbar^2} \left[\omega_{fi}^2 + \frac{1}{\tau^2}\right]^{-1}$$

$$= \frac{2^{15} e^2 \mathcal{E}_0^2 a_0^2}{3^{10} \hbar^2} \left\{\frac{9R_y^2}{16\hbar^2} + \frac{1}{\tau^2}\right\}^{-1}$$

Q.E.D