Solutions to PC4130 AY0809 Paper

1(i) Dynamical phase, $\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n[\lambda(t')]dt'$

1(ii) Let $|\psi(t)\rangle = \sum_n c_n(t)|\psi_n(t)\rangle e^{i\theta_n(t)}$, put into Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(\lambda(t))|\psi(t)\rangle$$

$$i\hbar\frac{\partial}{\partial t}\sum_n c_n(t)|\psi_n(\lambda)\rangle e^{i\theta_n(t)} = H(\lambda(t))\sum_n c_n(t)|\psi_n(\lambda)\rangle e^{i\theta_n(t)}$$

$$i\hbar\sum_n\left(\dot{c}_n|\psi_n\rangle + c_n\frac{d|\psi_n\rangle}{dt} + ic_n|\psi_n\rangle\dot{\theta}_n\right)e^{i\theta_n} = \sum_n c_n(t)H(\lambda)|\psi_n\rangle e^{i\theta_n(t)}$$

Since $\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n[\lambda(t')]dt'$, $\dot{\theta}_n = -\frac{E_n(\lambda)}{\hbar}$

$$i\hbar\sum_n\left(\dot{c}_n|\psi_n\rangle + c_n\frac{d|\psi_n\rangle}{dt}\right)e^{i\theta_n} + \sum_n c_nE_n|\psi_n\rangle e^{i\theta_n} = \sum_n c_n(t)E_n|\psi_n\rangle e^{i\theta_n}$$

$$\sum_n \dot{c}_n|\psi_n\rangle e^{i\theta_n} = -\sum_n c_n\frac{d|\psi_n\rangle}{dt}e^{i\theta_n}$$

Taking inner product with $\langle\psi_m|$,

$$\sum_n \dot{c}_n\langle\psi_m|\psi_n\rangle e^{i\theta_n} = -\sum_n c_n\left\langle\psi_m\left|\frac{d\psi_n}{dt}\right.\right\rangle e^{i\theta_n}$$

$$\dot{c}_m e^{i\theta_m} = -\sum_n c_n\left\langle\psi_m\left|\frac{d\psi_n}{dt}\right.\right\rangle e^{i\theta_n} \qquad \Rightarrow \qquad \dot{c}_m = -\sum_n c_n\left\langle\psi_m\left|\frac{d\psi_n}{dt}\right.\right\rangle e^{i(\theta_n-\theta_m)}$$

Reexpress $\left\langle\psi_m\left|\frac{d\psi_n}{dt}\right.\right\rangle$:

From $H(\lambda)|\psi_n(\lambda)\rangle = E_n(\lambda)|\psi_n(\lambda)\rangle$,

$$\frac{dH(\lambda)}{dt}|\psi_n(\lambda)\rangle + H(\lambda)\frac{d}{dt}|\psi_n(\lambda)\rangle = \frac{dE_n(\lambda)}{dt}|\psi_n(\lambda)\rangle + E_n(\lambda)\frac{d}{dt}|\psi_n(\lambda)\rangle$$

$$\langle\psi_m|\frac{dH(\lambda)}{dt}|\psi_n\rangle + E_m(\lambda)\left\langle\psi_m\left|\frac{d\psi_n}{dt}\right.\right\rangle = \dot{E}_n(\lambda)\delta_{mn} + E_n(\lambda)\left\langle\psi_m\left|\frac{d\psi_n}{dt}\right.\right\rangle$$

For $m \neq n$, $\left\langle\psi_m\left|\frac{d\psi_n}{dt}\right.\right\rangle = \frac{\langle\psi_m(\lambda)|\frac{dH(\lambda)}{dt}|\psi_n(\lambda)\rangle}{E_n - E_m}$

$$\dot{c}_m = -c_m\left\langle\psi_m\left|\frac{d\psi_m}{dt}\right.\right\rangle - \sum_{n\neq m} c_n e^{i(\theta_n-\theta_m)}\frac{\langle\psi_m(\lambda)|\frac{dH(\lambda)}{dt}|\psi_n(\lambda)\rangle}{E_n - E_m}$$

For adiabatic approximation, assume $\dot{\lambda}_i \approx 0$

$$\frac{dH(\lambda)}{dt} = \sum_i \frac{dH(\lambda)}{d\lambda_i}\dot{\lambda}_i \approx 0$$

$$\dot{c}_m = -c_m\left\langle \psi_m \left| \frac{d\psi_m}{dt} \right.\right\rangle - \sum_{n\neq m} c_n e^{i(\theta_n-\theta_m)} \frac{\left\langle \psi_m(\lambda) \right| \frac{dH(\lambda)}{dt} \left| \psi_n(\lambda) \right\rangle}{E_n - E_m} \approx -c_m\left\langle \psi_m \left| \frac{d\psi_m}{dt} \right.\right\rangle$$

$$\frac{dc_m}{dt} = --c_m\left\langle \psi_m \left| \frac{d\psi_m}{dt} \right.\right\rangle$$

$$c_m(t) = c_m(0)\exp\left(-\int_0^t \left\langle \psi_m \left| \frac{d\psi_m}{dt'} \right.\right\rangle dt'\right)$$

Express $c_m(t) = c_m(0)e^{i\gamma_m(t)}$, $\gamma_m(t) = i\int_0^t \left\langle \psi_m \left| \frac{d\psi_m}{dt'} \right.\right\rangle dt'$

2 $V(x) = cx^2$ (even)

To get first excited state, let $\psi(x) = Axe^{-bx^2}$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = |A|^2 \int_{-\infty}^{\infty} x^2 e^{-2bx^2} dx = |A|^2 \sqrt{\frac{\pi}{8b}}\frac{1}{8b}\frac{2!}{1!}\times 2 = 1 \qquad \Rightarrow |A|^2 = 4b\sqrt{\frac{2b}{\pi}}$$

$$H = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

$$\frac{d}{dx}\psi(x) = Ae^{-bx^2} - A(2bx^2)e^{-bx^2} \qquad \frac{d^2}{dx^2}\psi(x) = Ae^{-bx^2}(4b^2x^3 - 6bx)$$

$$\left\langle \frac{p^2}{2m} \right\rangle = -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty} (4b^2x^4 - 6bx^2)e^{-2bx^2} dx$$

$$= -\frac{\hbar^2}{2m}|A|^2 \left[4b^2\sqrt{\frac{\pi}{8b}}\left(\frac{1}{8b}\right)^2 \frac{4!}{2!}\times 2 - 6b\sqrt{\frac{\pi}{8b}}\frac{1}{8b}4 \right] = \frac{3\hbar^2 b}{2m}$$

$$\langle V \rangle = c|A|^2 \int_{-\infty}^{\infty} x^4 e^{-2bx^2} dx = c|A|^2 \sqrt{\frac{\pi}{8b}}\left(\frac{1}{8b}\right)^2 \frac{4!}{2!}\times 2 = \frac{3c}{4b}$$

$$\langle H \rangle = \frac{3\hbar^2 b}{2m} + \frac{3c}{4b}$$

$$\frac{d\langle H \rangle}{db} = \frac{3\hbar^2}{2m} - \frac{3c}{4b^2} = 0 \Rightarrow b = \sqrt{\frac{mc}{2\hbar^2}}$$

$$\frac{d^2\langle H \rangle}{db} = \frac{3c}{2b^3} > 0 \text{ (minimum)}$$

$$\langle H \rangle = \frac{3\hbar^2}{2m}\sqrt{\frac{mc}{2\hbar^2}} + \frac{3c}{4}\sqrt{\frac{2\hbar^2}{mc}} = 3\hbar\sqrt{\frac{c}{2m}}$$

3(i) $f(\theta,\phi) = -\frac{2m}{\hbar^2\kappa}\int_0^{\infty} rdr\sin(\kappa r)V(r)$, $\kappa = 2k\sin(\frac{\theta}{2})$

$V(r) = V_0\delta(r-a)$

$$f(\theta,\phi) = -\frac{2m}{\hbar^2\kappa}\int_0^\infty rdr\sin(\kappa r)V(r) = -\frac{2m}{\hbar^2\kappa}\int_0^\infty rdr\sin(\kappa r)V_0\delta(r-a) = -\frac{2mV_0a}{\hbar^2\kappa}\sin(\kappa a)$$

Differential cross-section $= \left|f(\theta,\phi)\right|^2 = \left(\frac{2mV_0a}{\hbar^2\kappa}\right)^2\sin^2(\kappa a)$

3(ii) Total cross-section, $\sigma_{tot} = \int\left|f(\theta,\phi)\right|^2 d\Omega = \int_0^{2\pi}\int_0^\pi\left|f(\theta,\phi)\right|^2\sin\theta d\theta d\phi$

$$\sigma_{tot} = 2\pi\int_0^\pi\left|f(\theta,\phi)\right|^2\sin\theta d\theta$$

For high energy scattering, the total cross section can be estimated as follows:

$$\sigma_{tot} = 2\pi\int_0^\pi\left|f(\theta,\phi)\right|^2\sin\theta d\theta \approx \int_0^{1/ka}\left|f(0)\right|^2\sin\theta d\theta = \left|f(0)\right|^2\left[-\cos\theta\right]_0^{1/ka}$$

$$= \left|f(0)\right|^2\left[1-\cos(1/ka)\right] \approx \frac{\left|f(0)\right|^2}{k^2a^2}$$

Since $f(0)$ is independent of *k*, and $E \propto k^2$, $\sigma_{tot} \propto \frac{1}{E}$

4 $$P_{n\leftarrow 1} = \frac{1}{\hbar^2}\left|\int_0^t\left\langle\psi_n^0\right|V(t_1)\left|\psi_1^0\right\rangle e^{\frac{i}{\hbar}(E_n-E_1)t_1}dt_1\right|^2$$

Let $\omega_{n1} = \frac{E_n - E_1}{\hbar}$, $V(t) = Ae^{-t/\tau}$

$$P_{n\leftarrow 1} = \frac{1}{\hbar^2}\left|\int_0^\infty\left\langle\psi_n^0\right|V(t_1)\left|\psi_1^0\right\rangle e^{\frac{i}{\hbar}(E_n-E_1)t_1}dt_1\right|^2 = \frac{1}{\hbar^2}\left|\int_0^\infty\left\langle\psi_n^0\right|Ae^{-t_1/\tau}\left|\psi_1^0\right\rangle e^{i\omega_{n1}t_1}dt_1\right|^2$$

$$= \frac{\left|\left\langle\psi_n^0\right|A\left|\psi_1^0\right\rangle\right|^2}{\hbar^2}\left|\int_0^\infty e^{-t_1/\tau}e^{i\omega_{n1}t_1}dt_1\right|^2$$

$$= \frac{\left|\left\langle\psi_n^0\right|A\left|\psi_1^0\right\rangle\right|^2}{\hbar^2}\left|\left[\frac{1}{i\omega_{n1}-1/\tau}e^{(i\omega_{n1}-1/\tau)t_1}\right]_0^\infty\right|^2$$

$$= \frac{\left|\left\langle\psi_n^0\right|A\left|\psi_1^0\right\rangle\right|^2}{\hbar^2}\frac{1}{\omega_{n1}^2+1/\tau^2}$$

$$= \frac{\left|\left\langle\psi_n^0\right|A\left|\psi_1^0\right\rangle\right|^2}{(E_n-E_1)^2+\hbar^2/\tau^2}$$

The validity condition of this perturbation result is that the transition probability should be very small.