Assignment (9)

(1) $\Psi_{trial} = \sum_n c_n \Psi_n$ where $\hat{H}\Psi_n = E_n \Psi_n$; $E_0 < E_1 < E_2 < \ldots$

$$E_{trial} = \frac{\int \Psi_{trial}^* \hat{H} \Psi_{trial}\, dx}{\int \Psi_{trial}^* \Psi_{trial}\, dx} = \frac{\sum_{n,m} c_n^* c_m \int \Psi_n^* \hat{H} \Psi_m\, dx}{\sum_{n,m} c_n^* c_m \int \Psi_n^* \Psi_m\, dx} = \frac{\sum_{n,m} c_n^* c_m \int \Psi_n^* E_m \Psi_m\, dx}{\sum_{n,m} c_n^* c_m \int \Psi_n^* \Psi_m\, dx}$$

orthogonal $\{\Psi_i\}$

$$= \frac{\sum_{n,m} c_n^* c_m E_m \delta_{nm}}{\sum_{n,m} c_n^* c_m \delta_{nm}} = \frac{\sum_n |c_n|^2 E_n}{\sum_n |c_n|^2} = \sum_n |c_n|^2 E_n \geq \sum_n |c_n|^2 E_0 = E_0 \sum_n |c_n|^2 = E_0$$

normalized

$\therefore E_{trial} \geq E_0$

(2) $\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{V}$

~~Braket Notation for~~

$$\frac{\partial E}{\partial \lambda} = E'(\lambda) = \langle \Psi(\lambda) | \hat{V} | \Psi(\lambda) \rangle = \int_\tau \Psi^*(\lambda) \hat{V} \Psi(\lambda)\, d\tau$$

Variational Principle in Braket Notation: $E_{trial} = \langle \Psi_{trial} | \hat{H} | \Psi_{trial} \rangle \geq E_0$, if $\{\Psi_n\}$ is orthonormal $\rightarrow \langle \Psi_{trial} | \Psi_{trial} \rangle = 1$

"trial"

a) $E_{\Psi(\lambda_2)} = \langle \Psi(\lambda_2) | \hat{H} | \Psi(\lambda_2) \rangle = \langle \Psi(\lambda_2) | \hat{H}_0 + \lambda_1 \hat{V} | \Psi(\lambda_2) \rangle$

"E_0" $= \int \Psi^*(\lambda_2)(\hat{H}_0 + \lambda_1 \hat{V}) \Psi(\lambda_2)\, d\tau = \int \Psi^*(\lambda_2) \hat{H}_0 \Psi(\lambda_2)\, d\tau + \lambda_1 \int \Psi^*(\lambda_2) \hat{V} \Psi(\lambda_2)\, d\tau$

$E(\lambda_1) = \langle \Psi(\lambda_1) | \hat{H} | \Psi(\lambda_1) \rangle = \int \Psi^*(\lambda_1) \hat{H}_0 \Psi(\lambda_1)\, d\tau + \lambda_1 \int \Psi^*(\lambda_1) \hat{V} \Psi(\lambda_1)\, d\tau$.

$\int \Psi^*(\lambda_1) \hat{H}_0 \Psi(\lambda_1)\, d\tau + \lambda_1 \int \Psi^*(\lambda_1) \hat{V} \Psi(\lambda_1)\, d\tau < \int \Psi^*(\lambda_2) \hat{H}_0 \Psi(\lambda_2)\, d\tau + \lambda_1 \int \Psi^*(\lambda_2) \hat{V} \Psi(\lambda_2)\, d\tau$

b) $E_{\Psi(\lambda_1)} = \langle \Psi(\lambda_1) | \hat{H} | \Psi(\lambda_1) \rangle = \int \Psi^*(\lambda_1) \hat{H}_0 \Psi(\lambda_1)\, d\tau + \lambda_2 \int \Psi^*(\lambda_1) \hat{V} \Psi(\lambda_1)\, d\tau$

"E_0" $\rightarrow E(\lambda_2) = \langle \Psi(\lambda_2) | \hat{H} | \Psi(\lambda_2) \rangle = \int \Psi^*(\lambda_2) \hat{H}_0 \Psi(\lambda_2)\, d\tau + \lambda_2 \int \Psi^*(\lambda_2) \hat{V} \Psi(\lambda_2)\, d\tau$

$\int \Psi^*(\lambda_2) \hat{H}_0 \Psi(\lambda_2)\, d\tau + \lambda_2 \int \Psi^*(\lambda_2) \hat{V} \Psi(\lambda_2)\, d\tau < \int \Psi^*(\lambda_1) \hat{H}_0 \Psi(\lambda_1)\, d\tau + \lambda_2 \int \Psi^*(\lambda_1) \hat{V} \Psi(\lambda_1)\, d\tau$

c) $\cancel{\int \Psi^*(\lambda_1) \hat{H}_0 \Psi(\lambda_1)\, d\tau} + \lambda_1 \int \Psi^*(\lambda_1) \hat{V} \Psi(\lambda_1)\, d\tau + \cancel{\int \Psi^*(\lambda_2) \hat{H}_0 \Psi(\lambda_2)\, d\tau} + \lambda_2 \int \Psi^*(\lambda_2) \hat{V} \Psi(\lambda_2)\, d\tau < \cancel{\int \Psi^*(\lambda_2) \hat{H}_0 \Psi(\lambda_2)\, d\tau} + \lambda_1 \int \Psi^*(\lambda_2) \hat{V} \Psi(\lambda_2)\, d\tau + \cancel{\int \Psi^*(\lambda_1) \hat{H}_0 \Psi(\lambda_1)\, d\tau} + \lambda_2 \int \Psi^*(\lambda_1) \hat{V} \Psi(\lambda_1)\, d\tau$

$\lambda_1 \int \Psi^*(\lambda_1) \hat{V} \Psi(\lambda_1)\, d\tau + \lambda_2 \int \Psi^*(\lambda_2) \hat{V} \Psi(\lambda_2)\, d\tau < \lambda_1 \int \Psi^*(\lambda_2) \hat{V} \Psi(\lambda_2)\, d\tau + \lambda_2 \int \Psi^*(\lambda_1) \hat{V} \Psi(\lambda_1)\, d\tau$

$\lambda_1 E'(\lambda_1) + \lambda_2 E'(\lambda_2) < \lambda_1 E'(\lambda_2) + \lambda_2 E'(\lambda_1)$

$\lambda_1 (E'(\lambda_1) - E'(\lambda_2)) + \lambda_2 (E'(\lambda_2) - E'(\lambda_1)) < 0$

$(\lambda_1 - \lambda_2)(E'(\lambda_1) - E'(\lambda_2)) < 0$

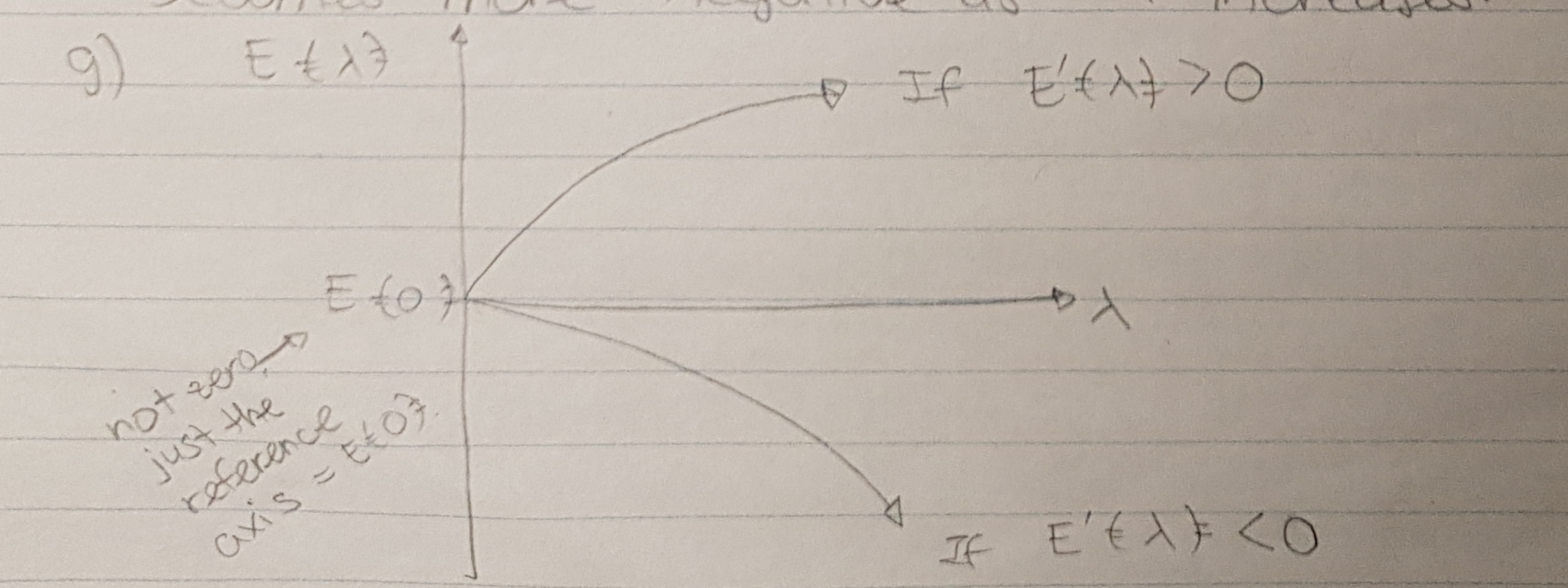
d) $(\lambda_1 - \lambda_2)$ or $(E'(\lambda_1) - E'(\lambda_2))$ has to be <0, so that $(\lambda_1 - \lambda_2)(E'(\lambda_1) - E'(\lambda_2)) < 0$

If $\lambda_1 > \lambda_2$ then $(\lambda_1 - \lambda_2)$ is >0 and $(E'(\lambda_1) - E'(\lambda_2)) < 0$, meaning $E'(\lambda_1) < E'(\lambda_2)$. In other words, as λ increases, $E'(\lambda)$ decreases.

e) $E''(\lambda) < 0$.

f) $E'(\lambda) > 0$ doesn't mean stabilizing. If $E'(\lambda) < 0$, then the slope of E becomes more negative as λ increases.

g)



$E''(\lambda) < 0$ for both

(3) $\Psi(x) = \frac{1}{\sqrt{2}}(\psi_1(x) + \psi_2(x))$

a) $\int_0^a \psi^*(x) \hat{p} \psi(x)\, dx = \frac{1}{2} \int_0^a (\psi_1(x) + \psi_2(x))^* \hat{p} (\psi_1(x) + \psi_2(x))\, dx$

$= \frac{1}{2} \int_0^a \psi_1^*(x) \hat{p} \psi_1(x)\, dx + \frac{1}{2} \int_0^a \psi_2^*(x) \hat{p} \psi_2(x)\, dx$

$+ \frac{1}{2} \int_0^a \psi_1^*(x) \hat{p} \psi_2(x)\, dx + \frac{1}{2} \int_0^a \psi_2^*(x) \hat{p} \psi_1(x)\, dx$

$\int_0^a \psi_1^*(x) \hat{p} \psi_1(x)\, dx = \int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)(-i\hbar)\frac{d}{dx}\left(\sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)\right) dx = \left(-\frac{2i\hbar}{a}\right)\left(\frac{\pi}{a}\right)\int_0^a \sin\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi x}{a}\right) dx$

$u = \sin(\pi x/a)$

$du = \frac{\pi}{a} \cos(\pi x/a)\, dx$

$= \left(-\frac{2i\hbar}{a}\right) \int_0^a u\, du = \left(-\frac{2i\hbar}{a}\right) \frac{u^2}{2}\Big|_0^a$

$= \left(-\frac{i\hbar}{a}\right) \sin^2\left(\frac{\pi x}{a}\right)\Big|_0^a = 0$

$\int_0^a \psi_2^*(x) \hat{p} \psi_2(x)\, dx = \left(-\frac{2i\hbar}{a}\right) \int_0^a \sin\left(\frac{2\pi x}{a}\right) \frac{d}{dx}\left(\sin\left(\frac{2\pi x}{a}\right)\right) dx = \left(-\frac{2i\hbar}{a}\right)\left(\frac{1}{2}\right) \sin^2\left(\frac{2\pi x}{a}\right)\Big|_0^a = 0$

$= \frac{1}{2} \int_0^a \psi_1^*(x) \hat{p} \psi_2(x)\, dx + \frac{1}{2} \int_0^a \psi_2^*(x) \hat{p} \psi_1(x)\, dx = \frac{1}{2} \int_0^a \hat{p}^* \psi_1^*(x) \psi_2(x)\, dx + \frac{1}{2} \int_0^a \psi_2^*(x) \hat{p} \psi_1(x)\, dx$

$\psi_1(x), \psi_2(x)$ real

$= \frac{1}{2} \int_0^a \left(-i\hbar \frac{d}{dx}\right)^* \psi_1^*(x) \psi_2(x)\, dx + \frac{1}{2} \int_0^a \psi_2^*(x) \left(-i\hbar \frac{d}{dx}\right) \psi_1(x)\, dx$

$= \frac{1}{2}\left[i\hbar \int_0^a \frac{d}{dx} \psi_1(x) \psi_2(x)\, dx - i\hbar \int_0^a \psi_2(x) \frac{d}{dx} \psi_1(x)\, dx \right] = 0$

b) $E = E_1 = \frac{h^2 1^2}{8ma^2} = \frac{h^2}{8ma^2}$ or $E = E_2 = \frac{h^2 (2)^2}{8ma^2} = \frac{4h^2}{8ma^2} = \frac{h^2}{2ma^2} = 4E_1$

c) $\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_1(x) e^{-iE_1 t/\hbar} + \psi_2(x) e^{-iE_2 t/\hbar}\right) = \frac{1}{\sqrt{2}}\left(\psi_1(x) e^{-iE_1 t/\hbar} + \psi_2(x) e^{-4iE_1 t/\hbar}\right)$

d) $\exp(-iE_1 t/\hbar)$ and $\exp(-iE_2 t/\hbar)$ are periodic, and for $\Psi(x,t)$ to be in the "original state" $\Psi(x,t) = \Psi(x)$, $e^{-iE_1 t/\hbar}$ and $e^{-iE_2 t/\hbar}$ must be 1.

$n_1 = 1, 2, \ldots$ $\quad n_2 = 1, 2, \ldots$

$e^{-iE_1 t/\hbar} = 1 = e^{-iE_1 t/\hbar} \rightarrow E_1 t/\hbar = 2\pi n_1$ and $E_2 t/\hbar = 2\pi n_2$

$t = \frac{2\pi n_1 \hbar}{E_1} = \frac{2\pi n_2 \hbar}{4E_1}$

$n_2 = 4n_1$

if $n_1 = 1$, $n_2 = 4$

$t = \frac{2\pi (1) \hbar}{E_1} = 2\pi\left(\frac{h}{2\pi}\right)\left(\frac{8ma^2}{h^2}\right) = \frac{8ma^2 h}{h^2}$

$t = \frac{4.136 \times 10^{-15}\ \text{eV·s}}{1.00\ \text{eV}} = 4.136$ ps