Assignment (6)

False
(1) a) Only pairs of observables that don't commute is subject to the uncertainty principle
b) False, time dependent Schrödinger equation depends on time
c) True

$E_{box} = \frac{h^2 n^2}{8ma^2}$ $\quad E_{HO} = \hbar\sqrt{\frac{k}{m}}\left(n + \frac{1}{2}\right)$

(2) $^{75}Br^{19}F \rightarrow 380\ cm^{-1} = \tilde{\nu} = \frac{1}{\lambda}$

$\Delta E = \frac{hc}{\lambda} = \hbar\sqrt{\frac{k}{m}} \rightarrow \lambda = \frac{hc\sqrt{m}}{\hbar\sqrt{k}} = 2\pi c\sqrt{\frac{m}{k}}$

$2\pi c\sqrt{\frac{m}{k}} = \frac{1}{\tilde{\nu}}$

$\tilde{\nu}(2\pi c) = \sqrt{\frac{k}{m}}$

$k = (2\pi c\tilde{\nu})^2 m = (2\pi[2.998\times10^8\ m/s][380\ cm^{-1}][100\ cm/m])^2(2.52\times10^{-26}\ kg)$

$k = 129\ N\cdot m^{-1}$

$m = \frac{(75\ amu)(19\ amu)}{(75+19)\ amu} \cdot 1.661\times10^{-27}\ kg/amu$

$m = 2.52\times10^{-26}\ kg$

(4) $\langle\nabla^2\rangle = \int \Psi^* \nabla^2 \Psi\, d\vec{r}$

$\frac{dE_n}{dm_e} = \int \Psi^* \frac{\partial \hat{H}}{\partial m_e} \Psi\, d\vec{r}$

$\frac{z^2 e^4}{8\varepsilon_0^2 h^2 n^2} = \int \Psi^* \left(-\frac{\hbar^2}{2m_e^2}[-1]\nabla^2\right)\Psi\, d\vec{r}$

$\frac{z^2 e^4}{4\, 8\varepsilon_0^2 h^2 n^2}\left[\frac{2m_e^2}{\hbar^2}\right] = \int \Psi^* \nabla^2 \Psi\, d\vec{r}$

$\frac{z^2 e^4 m_e^2 (4\pi^2)}{4\varepsilon_0^2 h^4 n^2} = \frac{z^2 e^4 m_e^2 \pi^2}{\varepsilon_0^2 h^4 n^2} = \langle\nabla^2\rangle$

(5) $E^{(0)} = \frac{h^2 n^2}{8ma^2}$

a) $E^{(1)} = \int_0^{a/2} \frac{2\varepsilon}{a}\sin^2\left\{\frac{n\pi x}{a}\right\}dx = \frac{2\varepsilon}{a}\left[\frac{a}{4}\right] = \frac{\varepsilon}{2}$ $\quad E_{TOTAL} = E^{(0)} + E^{(1)} = \frac{h^2 n^2}{8ma^2} + \varepsilon/2$

if $\varepsilon > 0 \rightarrow E^{(1)} > 0$ {Makes sense because the perturbation is positive and it is $\frac{\varepsilon}{2}$ because it only extends over half the box}

n	E_{TOTAL}
1	$\frac{h^2}{8ma^2} + \frac{\varepsilon}{2}$
2	$\frac{4h^2}{8ma^2} + \frac{\varepsilon}{2}$
3	$\frac{9h^2}{8ma^2} + \frac{\varepsilon}{2}$

b) $\Delta E = E_{n=2} - E_{n=1} = \frac{4h^2}{8ma^2} + \frac{\varepsilon}{2} - \left[\frac{h^2}{8ma^2} + \frac{\varepsilon}{2}\right] = \frac{3h^2}{8ma^2} = h\nu$

$\nu = \frac{3h}{8ma^2}$

only consider the first transition {most likely to occur}

c) $\Psi^{(1)} = \sum_{m=1}^{\infty} \frac{\int_0^{a/2} \Psi_m^*\{x\}\,\varepsilon\,\Psi_0\{x\}\,dx}{E_m - E_0}\Psi_m\{x\} = \frac{2\varepsilon}{a}\int_0^{a/2} \sin\left\{\frac{2\pi x}{a}\right\}\sin\left\{\frac{\pi x}{a}\right\}dx \left[\frac{1}{3h/8ma^2}\right]\Psi_2\{x\}$

$= \frac{2\varepsilon}{a}\int_0^{a/2}\frac{1}{2}\left[\cos\left\{\frac{\pi x}{a}\right\} - \cos\left\{\frac{3\pi x}{a}\right\}\right]dx\left[\frac{8ma^2}{3h}\right]\Psi_2\{x\}$

$= \frac{\varepsilon}{a}\left[\frac{a}{\pi}\sin\left\{\frac{\pi x}{a}\right\} - \frac{a}{3\pi}\sin\left\{\frac{3\pi x}{a}\right\}\right]_0^{a/2}\left[\frac{8ma^2}{3h}\right]\Psi_2\{x\}$

$= \frac{\varepsilon}{a}\left[\frac{a}{\pi}(1) - 0 - \frac{a}{3\pi}(-1) - 0\right]\left[\frac{8ma^2}{3h}\right]\Psi_2\{x\}$

$= \frac{\varepsilon}{a}\left[\frac{4a}{3\pi}\right]\left[\frac{8ma^2}{3h}\right]\Psi_2\{x\}$

$= \frac{8ma^2\varepsilon}{9\pi h}\left[\sqrt{\frac{2}{a}}\right]\sin\left\{\frac{2\pi x}{a}\right\}$