SOLUTION MANUAL FOR HW # 3

4.5)

Conditions to be satisfied by the wavefunction for particle in 1D box;

$$\Psi(x=0)=\Psi(x=a)=0 \Rightarrow \textit{Boundary conditions}$$

$$\Psi^{'}(x=0)=\Psi^{'}(x=0) \Rightarrow \textit{Derivative}$$

$$\int_0^a \Psi^{'}(x)\Psi(x)dx = 1 \Rightarrow \textit{Normalization}$$

a)

$\Psi(x=0)=A$

$\Psi(x=a)=\pm A$

Not acceptable because of boundary conditions

b)

$\Psi(x=0)=0$

$\Psi(x=a)=B(a+a^2)$

Not acceptable because of boundary conditions

c)

$\Psi(x=0)=\Psi(x=a)=0$

$\Psi^{'}(x=0)=\Psi^{'}(x=a)=0$

Acceptable

d)

$\Psi(x=a)=\Psi(x=0)=\infty$ Not acceptable because of boundary conditions

4.9)

$$\hat{H} = \frac{-h^2}{2m}\frac{d^2}{dx^2}$$

$$\Psi(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$$

Ψ(x) is not an eigenfunction of position operator, x.

$$\hat{x} = \int_0^a \Psi^*(x) x \Psi(x) dx = \int_0^a x \sqrt{\frac{2}{a}} \sin(\frac{n\pi x}{a}) \sqrt{\frac{2}{a}} \sin(\frac{n\pi x}{a}) dx$$

$$= \frac{2}{a} \int_0^a x \sin^2(\frac{n\pi x}{a}) dx$$

$$u = \frac{n\pi x}{a} \Rightarrow x = \frac{au}{n\pi} \qquad \& \qquad dx = \frac{a}{n\pi} du$$

$$= \frac{2}{a} \int_0^a \frac{au}{n\pi} \sin^2(u) \frac{a}{n\pi} du = \frac{2a}{(n\pi)^2} \int_0^{n\pi} u \sin^2(u) du$$

$$\therefore \sin^2(u) = \frac{1}{2}(1 - \cos 2u)$$

$$\therefore \int_0^{n\pi} u \sin^2(u) du = \int_0^{n\pi} u \frac{1}{2}(1 - \cos 2u) du = \frac{1}{2} \int_0^{n\pi} (u - u \cos 2u) du = \frac{1}{2} \int_0^{n\pi} u du - \frac{1}{2} \int_0^{n\pi} u \cos 2u du$$

$$(\therefore \int_0^{n\pi} u \cos 2u du = \frac{1}{2}(u \sin 2u + \cos 2u) \Big|_0^{n\pi})$$

$$\int_0^{n\pi} u \sin^2(u) du = \frac{1}{2}(\frac{u^2}{2}) \Big|_0^{n\pi} - \frac{1}{2}(\frac{1}{2}(u \sin 2u + \cos 2u)) \Big|_0^{n\pi} = \frac{1}{4}(u^2 - u \sin 2u - \cos 2u) \Big|_0^{n\pi} = \frac{(n\pi)^2}{4}$$

$$\hat{x} = \frac{2a}{(n\pi)^2} \cdot \frac{(n\pi)^2}{4} = \frac{a}{2}$$

So average value of x does not depend on n.
$\hat{x}$(n=3)= $\hat{x}$(n=5)=a/2
As predicted by the classical theory.

4.12)

$$\hat{H} = \frac{-h^2}{2m} \frac{d^2}{dx^2}$$

$$\Psi(x) = \sqrt{\frac{2}{a}} \{\sin(\frac{n\pi x}{a}) + \sin(\frac{m\pi x}{a})\}$$

$$\hat{H}\Psi(x) = \frac{h^2}{2m} \sqrt{\frac{2}{a}} \{(\frac{n\pi}{a})^2 \sin(\frac{n\pi x}{a}) + (\frac{m\pi}{a})^2 \sin(\frac{m\pi x}{a})\} \Rightarrow \quad \textit{not} \quad \textit{eigenfunction}$$

$$\textit{only} \quad \textit{if} \quad n = m \quad \Rightarrow \quad \textit{eigenfunction}$$

4.21)

a)

$$E(n_x, n_y) = (n_x^2 + n_y^2)\frac{h^2}{8mL^2} = \frac{5h^2}{8mL^2} \Rightarrow (n_x^2 + n_y^2) = 5$$

$$\Rightarrow n_x = 2 \; \& \; n_y = 1$$

$$or \quad n_x = 1 \; \& \; ny = 2$$

*Degeneracy is "**2**".*

b)

$$E(n_x, n_y, n_z) = (n_x^2 + n_y^2 + n_z^2)\frac{h^2}{8mL^2} = \frac{9h^2}{8mL^2} \Rightarrow (n_x^2 + n_y^2 + n_z^2) = 9$$

$$\Rightarrow n_x = 2 \; \& \; n_y = 2 \; \& \; n_z = 1 \Rightarrow (n_x^2 + n_y^2 + n_z^2) = 9$$

$$\Rightarrow n_x = 2 \; \& \; n_y = 1 \; \& \; n_z = 2 \Rightarrow (n_x^2 + n_y^2 + n_z^2) = 9$$

$$\Rightarrow n_x = 1 \; \& \; n_y = 2 \; \& \; n_z = 2 \Rightarrow (n_x^2 + n_y^2 + n_z^2) = 9$$

*Degeneracy is "**3**".*

5.4)

H_2C=CH-HC=CH-HC=CH-HC=CH_2

$$L = 4*135 + 3*154 = 1002\,pm = 1.002*10^{-9}\,m$$

$$E = \frac{h^2}{8mL^2}n^2$$

$$m = 9.1*10^{-31}\,kg(mass \quad of \quad an \quad e^-)$$

$$E = 6.01*10^{-20}\,n^2 J$$

4 pair of π e^-s therefore first excited state is n=5 (n=4 → n=5)

$$\Delta E = 6.01*10^{-20}(5^2 - 4^2) = 5.40*10^{-19}\,J = \frac{hc}{\lambda}$$

$$\Rightarrow \lambda = \frac{hc}{\Delta E} = 368nm$$

5.5)

$$\frac{n_{conductance}}{n_{valence}} = \frac{g_{conductance}}{g_{valence}} e^{-\Delta E/kT}$$

$$\frac{g_{conductance}}{g_{valence}} = 1$$

$$\frac{n_{conductance}}{n_{valence}} = 5.5 * 10^{-7}$$

$$\Delta E_{Si} = 1.12eV = 1.79 * 10^{-19} J$$

$$\Delta E_{Diamond} = 5.5eV = 8.79 * 10^{-19} J$$

$$\ln(\frac{n_{conductance}}{n_{valence}}) = \ln e^{-\Delta E/kT}$$

$$-14.41 = \frac{-\Delta E}{kT} \Rightarrow T = \frac{\Delta E}{14.41k}$$

$$T_{Si} = 902K \; \& \; T_{Diamond} = 4429K$$

No, diamond will sublimate at that temperature.