Assignment 7

1) $\Psi(x) = \frac{1}{3}\psi_1(x) + \frac{i}{3}\psi_3(x) - \left(\frac{7}{9}\right)^{1/2}\psi_5(x)$

$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \rightarrow \psi_n^*(x) = \psi_n(x)$

$$\int_0^a \Psi^*(x)\Psi(x)\,dx = \int_0^a \left[\frac{1}{3}\psi_1^*(x) - \frac{i}{3}\psi_3^*(x) - \left(\frac{7}{9}\right)^{1/2}\psi_5^*(x)\right]\left[\frac{1}{3}\psi_1(x) + \frac{i}{3}\psi_3(x) - \left(\frac{7}{9}\right)^{1/2}\psi_5(x)\right]dx$$

$$= \int_0^a \Big[\frac{1}{9}\psi_1(x)\psi_1(x) + \frac{i}{9}\psi_1(x)\psi_3(x) - \frac{\sqrt{7}}{9}\psi_1(x)\psi_5(x) - \frac{i}{9}\psi_3(x)\psi_1(x) + \frac{1}{9}\psi_3(x)\psi_3(x) + \frac{i\sqrt{7}}{9}\psi_3(x)\psi_5(x) - \frac{\sqrt{7}}{9}\psi_5(x)\psi_1(x) - \frac{i\sqrt{7}}{9}\psi_5(x)\psi_3(x) + \frac{7}{9}\psi_5(x)\psi_5(x)\Big]dx$$

$$\int_0^a \psi_n(x)\psi_m(x)\,dx = \frac{2}{a}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi x}{a}\right)dx = \frac{2}{a}\int_0^a \frac{1}{2}\left[\cos\left(\frac{(n-m)\pi x}{a}\right) - \cos\left(\frac{(n+m)\pi x}{a}\right)\right]dx$$

$$= \frac{1}{a}\left[\frac{a}{\pi(n-m)}\sin\left(\frac{(n-m)\pi x}{a}\right) - \frac{a}{\pi(n+m)}\sin\left(\frac{(n+m)\pi x}{a}\right)\right]_0^a$$

$$= \frac{1}{a}\left[\frac{a}{\pi}\right]\left[\left(\frac{1}{n-m}\right)\sin\left(\frac{(n-m)\pi a}{a}\right) - \left(\frac{1}{n+m}\right)\sin\left(\frac{(n+m)\pi a}{a}\right)\right]$$

$$= \frac{1}{\pi}\left[\left(\frac{1}{n-m}\right)\sin((n-m)\pi) - \left(\frac{1}{n+m}\right)\sin((n+m)\pi)\right] = \delta_{mn}$$

only 3 terms for m=n

a)

$$= \frac{1}{9}\int_0^a \psi_1(x)\psi_1(x)\,dx + \frac{1}{9}\int_0^a \psi_3(x)\psi_3(x)\,dx + \int_0^a \frac{7}{9}\psi_5(x)\psi_5(x)\,dx = \frac{1}{9} + \frac{1}{9} + \frac{7}{9} = \frac{9}{9} = 1$$

normalized

b) Possible energy values: E_1, E_3, E_5

$E_1 = \frac{h^2}{8ma^2}$; $E_3 = \frac{9h^2}{8ma^2}$; $E_5 = \frac{25h^2}{8ma^2}$

c) $P(E=E_1) = \left|\int_0^a \psi_1^*(x)\Psi(x)\,dx\right|^2 = \left|\int_0^a \psi_1(x)\left[\frac{1}{3}\psi_1(x) + \frac{i}{3}\psi_3(x) + \left(\frac{7}{9}\right)^{1/2}\psi_5(x)\right]dx\right|^2 = \left|\frac{1}{3}\int_0^a \psi_1(x)\psi_1(x)\,dx\right|^2 = \left(\frac{1}{3}\right)^2 = \frac{1}{9}$

$P(E=E_3) = \left|\int_0^a \psi_3^*(x)\Psi(x)\,dx\right|^2 = \left|\frac{i}{3}\right|^2 = \frac{1}{9}$

$P(E=E_5) = \left|\int_0^a \psi_5^*(x)\Psi(x)\,dx\right|^2 = \left(\frac{7}{9}\right)^2 = \frac{7}{9}$

d) $\langle E\rangle = \int_0^a \Psi(x)\hat{H}\Psi(x)\,dx \rightarrow$ "long way".

$\langle E\rangle = P(E=E_1)\times E_1 + P(E=E_2)\times E_2 + P(E=E_3)\times E_3 = \frac{1}{9}\left(\frac{h^2}{8ma^2}\right) + \frac{1}{9}\left(\frac{9h^2}{8ma^2}\right) + \frac{7}{9}\left(\frac{25h^2}{8ma^2}\right)$

$= \frac{1+9+7(25)}{9}\left(\frac{h^2}{8ma^2}\right) = \frac{185h^2}{72ma^2}$

2) a) $\hat{H}_T = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2$

b) $E_T = E_x + E_y = \hbar\sqrt{\frac{k_x}{m}}\left(n_x + \frac{1}{2}\right) + \hbar\sqrt{\frac{k_y}{m}}\left(n_y + \frac{1}{2}\right)$

$\Psi_T(x,y) = \psi_{n_x}(x)\psi_{n_y}(y) = \left[\left(\frac{\sqrt{k_x m}}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{\sqrt{k_x m}}{2\hbar}x^2\right)\right]\left[\left(\frac{\sqrt{k_y m}}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{\sqrt{k_y m}}{2\hbar}y^2\right)\right]$

c) $n_x = n_y = 0 \rightarrow E_{ZPE} = \hbar\sqrt{\frac{k_x}{m}}\left(\frac{1}{2}\right) + \hbar\sqrt{\frac{k_y}{m}}\left(\frac{1}{2}\right) = \left(\frac{\sqrt{k_x} + \sqrt{k_y}}{\sqrt{m}}\right)\left(\frac{\hbar}{2}\right)$

d) $k_x = k_y \rightarrow E_T = \hbar\sqrt{\frac{k_x}{m}}\left(n_x + n_y + \frac{1}{2} + \frac{1}{2}\right) = \hbar\sqrt{\frac{k_x}{m}}(n_x + n_y + 1) = 10E_{ZPE} = 10\sqrt{\frac{k_x}{m}}(\hbar)$

$\hbar\sqrt{\frac{k_x}{m}}(n_x + n_y + 1) = 10\sqrt{\frac{k_x}{m}}\,\cancel{\hbar}$

$10 = n_x + n_y + 1$

$n_x + n_y = 9$

n_x	n_y
1	8
2	7
3	6
4	5

n_x	n_y
5	4
6	3
7	2
8	1

8 degenerate states

3) a) $E_n^{(1)} = \int_{a/4}^{3a/4}\left(\frac{2}{a}\right)\sin^2\left(\frac{n\pi x}{a}\right)V_0\,dx = \frac{2}{a}V_0\int_{a/4}^{3a/4}\left(\frac{1}{2} - \frac{1}{2}\cos\left(\frac{2n\pi x}{a}\right)\right)dx$

$= \frac{V_0}{a}\left[x - \frac{a}{2n\pi}\sin\left(\frac{2n\pi x}{a}\right)\right]_{a/4}^{3a/4}$

$= \frac{V_0}{a}\left[\frac{3a}{4} - \frac{a}{4} - \frac{a}{2n\pi}\sin\left(\frac{2n\pi(3a/4)}{a}\right) + \frac{a}{2n\pi}\sin\left(\frac{2n\pi(a/4)}{a}\right)\right]$

$= \frac{V_0}{a}\left[\frac{a}{2} - \frac{a}{2n\pi}\sin\left(\frac{3n\pi}{2}\right) + \frac{a}{2n\pi}\sin\left(\frac{n\pi}{2}\right)\right]$

$E_1^{(1)} = \frac{V_0}{2} - \frac{V_0}{2\pi}\sin\left(\frac{3\pi}{2}\right) + \frac{V_0}{2\pi}\sin\left(\frac{\pi}{2}\right)$

$= \frac{V_0}{2} + \frac{V_0}{\pi}$

b) $\Psi_n^{(1)}(x) = \sum_{m\neq n}^{\infty}\frac{\int\Psi_m^*(0,x)V(x)\Psi_n(0,x)\,dx}{E_n(0) - E_m(0)}\Psi_m(0,x)$

$= \sum_{m\neq n}^{\infty}\frac{\int_{a/4}^{3a/4}\left(\frac{2}{a}\right)\sin\left(\frac{m\pi x}{a}\right)V_0\sin\left(\frac{n\pi x}{a}\right)dx}{(n^2-m^2)h^2/(8Ma^2)}\left(\sqrt{\frac{2}{a}}\right)\sin\left(\frac{m\pi x}{a}\right)$

$= \left(\frac{2}{a}\right)^{3/2}(V_0)\left(\frac{8Ma^2}{h^2}\right)\sum_{m\neq n}^{\infty}\frac{\sin\left(\frac{m\pi x}{a}\right)}{n^2-m^2}\int_{a/4}^{3a/4}\frac{1}{2}\cos\left(\frac{[m-n]\pi x}{a}\right) - \frac{1}{2}\cos\left(\frac{[m+n]\pi x}{a}\right)dx$

$= \frac{2^{7/2}V_0 Ma^{1/2}}{h^2}\sum_{m\neq n}^{\infty}\frac{\sin\left(\frac{m\pi x}{a}\right)}{n^2-m^2}\left[\left(\frac{a}{[m-n]\pi}\right)\sin\left(\frac{[m-n]\pi x}{a}\right) - \left(\frac{a}{[m+n]\pi}\right)\sin\left(\frac{[m+n]\pi x}{a}\right)\right]_{a/4}^{3a/4}$

$= \frac{2^{7/2}V_0 Ma^{1/2}}{h^2}\left(\frac{a}{\pi}\right)\sum_{m\neq n}^{\infty}\frac{\sin\left(\frac{m\pi x}{a}\right)}{n^2-m^2}\left[\left(\frac{1}{m-n}\right)\sin\left(\frac{3\pi(m-n)}{4}\right) - \left(\frac{1}{m-n}\right)\sin\left(\frac{\pi(m-n)}{4}\right) - \left(\frac{1}{m+n}\right)\sin\left(\frac{3\pi(m+n)}{4}\right) + \left(\frac{1}{m+n}\right)\sin\left(\frac{\pi(m+n)}{4}\right)\right]$

$\Psi_1^{(1)}(x) = \frac{2^{7/2}V_0 Ma^{3/2}}{\pi h^2}\sum_{m=2}^{\infty}\left[\frac{\sin\left(\frac{m\pi x}{a}\right)}{1-m^2}\right]\left\{\left(\frac{1}{m-1}\right)\left[\sin\left(\frac{3\pi(m-1)}{4}\right) - \sin\left(\frac{\pi(m-1)}{4}\right)\right] - \left(\frac{1}{m+1}\right)\left[\sin\left(\frac{3\pi(m+1)}{4}\right) - \sin\left(\frac{\pi(m+1)}{4}\right)\right]\right\}$

c) $E_n^{(2)} = 2\sum_{m\neq n}^{\infty}\frac{\left[\int_{a/4}^{3a/4}\Psi_m^*(0,x)V(x)\Psi_n(0,x)\,dx\right]^2}{E_n(0) - E_m(0)} = 2\sum_{m\neq n}^{\infty}\frac{\left[\frac{2V_0}{a}\left(\frac{1}{2}\right)\int_{a/4}^{3a/4}\cos\left(\frac{[m-n]\pi x}{a}\right) - \cos\left(\frac{[m+n]\pi x}{a}\right)dx\right]^2}{\frac{(n^2-m^2)h^2}{8Ma^2}}$

$= \frac{16Ma^2}{h^2}\left(\frac{V_0^2}{a^2}\right)\sum_{m\neq n}^{\infty}\frac{1}{(n^2-m^2)}\left[\frac{a}{\pi}\right]^2\left[\left(\frac{1}{m-n}\right)\sin\left(\frac{[m-n]3\pi}{4}\right) - \left(\frac{1}{m-n}\right)\sin\left(\frac{\pi(m-n)}{4}\right) - \left(\frac{1}{m+n}\right)\sin\left(\frac{3\pi(m+n)}{4}\right) + \left(\frac{1}{m+n}\right)\sin\left(\frac{\pi(m+n)}{4}\right)\right]^2$

$E_1^{(2)} = \frac{16MV_0^2a^2}{h^2\pi^2}\sum_{m=2}^{\infty}\left(\frac{1}{1-m^2}\right)\left[\left(\frac{1}{m-1}\right)\left\{\sin\left(\frac{3\pi(m-1)}{4}\right) - \sin\left(\frac{\pi(m-1)}{4}\right)\right\} - \left(\frac{1}{m+1}\right)\left\{\sin\left(\frac{3\pi(m+1)}{4}\right) - \sin\left(\frac{\pi(m+1)}{4}\right)\right\}\right]^2$

d) This problem is missing the value of V_0

If $V_0 = \hbar^2/Ma^2$, then: $E_1^{(1)} = \left(\frac{1}{2} + \frac{1}{\pi}\right)\left(\frac{\hbar^2}{Ma^2}\right) \approx 0.8183\left(\frac{\hbar^2}{ma^2}\right)$

$E_1^{(2)} = \frac{16Ma^2}{h^2\pi^2}\left(\frac{\hbar^2}{Ma^2}\right)^2\left[\left(\frac{1}{1-4}\right)\left(\frac{\sqrt{2}}{2} - \frac{\sqrt{2}}{2} - \frac{1}{3}\left[\frac{\sqrt{2}}{2} - \frac{\sqrt{2}}{2}\right]\right)^2 + \left(\frac{1}{1-9}\right)\left(\frac{-1-1}{2} - \frac{0-0}{4}\right)^2 + \left(\frac{1}{1-16}\right)\left(\frac{\frac{\sqrt{2}}{2} - \frac{\sqrt{2}}{2}}{3} - \frac{-\sqrt{2}/2 - (-\sqrt{2}/2)}{5}\right)^2 + \dots\right]$

$\approx \left(\frac{\hbar^2}{Ma^2}\right)\left(\frac{4}{\pi^4}\right)\left[-\frac{1}{8}\right][-1]^2 \approx -0.005133\frac{\hbar^2}{Ma^2}$

$E_1^{(0)} = \frac{h^2}{8ma^2} = (2\pi)^2\left(\frac{\hbar^2}{8ma^2}\right) = 4.9348\frac{\hbar^2}{ma^2}$

$E_1^{(0)} + E_1^{(1)} = \frac{h^2}{8ma^2} + 0.8183\frac{\hbar^2}{Ma^2} = \frac{(2\pi)^2}{8}\frac{\hbar^2}{Ma^2} + 0.8183\frac{\hbar^2}{Ma^2} = 5.7531\frac{\hbar^2}{Ma^2}$

$E_1^{(0)} + E_1^{(1)} + E_{\frac{1}{2}}^{(2)} = 5.7531\frac{\hbar^2}{Ma^2} + \frac{1}{2}\left(-0.005133\frac{\hbar^2}{Ma^2}\right) = 5.7505\frac{\hbar^2}{Ma^2}$

$\hbar = \frac{h}{2\pi}$

$h = 2\pi\hbar$