SOLUTIONS

PROBLEM SET 2 Due Friday October 7

Physics 115B– FALL 2011

Points assigned

Analytic:

10 [1.] Griffiths Problem 4.2

10 [2.] Griffiths Problem 4.3

10 [3.] A piano manufacturing company is accidentally sent piano wire whose thickness gradually tapers off, so that its mass per unit length is $\mu - \mu' x/L$. (Here L is the length of the wire.) Fortunately for the piano company, μ' is small. This is also fortunate for you, because you can use perturbation theory to compute the frequency shifts of the different modes. Do so. Look up typical values for the tension T, length L, and mass per unit length μ of piano wires, and select values that give middle C for the fundamental mode $n = 1$. How much is the frequency shifted if $\mu' = 10^{-3}\mu$? Could your ear tell the difference?

20 [4.] Compute the first and second order shifts of the energy levels of the 3D harmonic oscillator for a perturbation $H' = Bxz$. Assume the levels are nondegenerate, that is, ω_x, ω_y, and ω_z are all non-equal. Then compute the first order shifts for the isotropic case $\omega_x = \omega_y = \omega_z$. In what way do the two cases fundamentally differ?

10 [5.] Show that, if you use the Euler method in Molecular Dynamics, then the energy of a simple harmonic oscillator increases by the factor $1 + k\,dt^2/m$ in each iteration. Suppose $t = N dt$, how is $E(t)$ related to $E(0)$? Show that this growth is exponential (terrible!) but that even so the argument of the exponential can be driven to zero by making dt small. Note: Leapfrog, as you will see below, completely avoids this instability.

Numeric:

Comment: For the first part of the course, as you develop skill in programming, the computational problems will not necessarily have anything to do with quantum mechanics.

10 [6.] Write a C or C++ program to solve the classical harmonic oscillator $F = -kx$ using the leapfrog Molecular Dynamics method. Make a plot of your results for $k = 3, m = 0.8, x_0 = 1.4, v_0 = 0$. Plot $x(t)$ for 4 or 5 periods. Using your plot, and what you know about the analytic result for the period T, argue why you think your code is working properly.

10 [7.] Then make a plot of your results for $k = 3, m = 0.8, x_0 = 1.4, v_0 = 2$. Again plot $x(t)$ for 4 or 5 periods. Using your plot, and what you know about using energy conservation to compute the amplitude, argue why you think your code is working properly.

80 Total

Physics 115B, HW2

#1 Griffiths 4.2

3D cubic infinite well: $V(x,y,z) = \begin{cases} 0 & |x|,|y|,|z| < a \\ \infty & \text{otherwise} \end{cases}$

TISE: $-\frac{\hbar^2}{2m}\nabla^2\psi + \underbrace{V(x,y,z)}_{=0 \text{ inside box!}}\psi = E\psi$

Let $\psi(x,y,z) = X(x)Y(y)Z(z)$ — Separation of variables method

$$\Rightarrow -\frac{\hbar^2}{2m}\left(YZ\frac{\partial^2 X}{\partial x^2} + XZ\frac{\partial^2 Y}{\partial y^2} + XY\frac{\partial^2 Z}{\partial z^2}\right)$$

Divide by XYZ:
$$-\frac{\hbar^2}{2m}\left(\underbrace{\frac{1}{X}\frac{d^2X}{dx^2}}_{-k_x^2} + \underbrace{\frac{1}{Y}\frac{d^2Y}{dy^2}}_{-k_y^2} + \underbrace{\frac{1}{Z}\frac{d^2Z}{dz^2}}_{-k_z^2}\right) = \underbrace{E_x}_{\frac{\hbar^2}{2m}k_x^2} + \underbrace{E_y}_{\frac{\hbar^2}{2m}k_y^2} + \underbrace{E_z}_{\frac{\hbar^2}{2m}k_z^2}$$

So equations separate into: — Solution

$\frac{d^2X}{dx^2} = -k_x^2 X$ — $X(x) = \sqrt{\frac{2}{a}}\sin(k_x x)$, $k_x = \frac{n_x\pi}{a}$

$\frac{d^2Y}{dx^2} = -k_y^2 Y$ — $Y(y) = \sqrt{\frac{2}{a}}\sin(k_y y)$, $k_y = \frac{n_y\pi}{a}$

$\frac{d^2Z}{dz^2} = -k_z Z$ — $Z(z) = \sqrt{\frac{2}{a}}\sin(k_z z)$, $k_z = \frac{n_z\pi}{a}$

$$\Rightarrow \boxed{\begin{aligned}\psi(x,y,z) &= XYZ = \left(\frac{2}{a}\right)^{3/2}\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{a}y\right)\sin\left(\frac{n_z\pi}{a}z\right)\\ E_{n_x,n_y,n_z} &= \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2+n_y^2+n_z^2\right)\end{aligned}}$$

#1 b) Energy levels:

	n_x	n_y	n_z	Total energy	# of Degeneracies
E_1	1	1	1	$3\ \dfrac{\pi^2\hbar^2}{2ma^2}$	1X
E_2	2 1 1	1 2 1	1 1 1	6 "	3X
E_3	2 2 1	2 1 2	1 2 2	9 "	3X
E_4	3 1 1	1 3 1	1 1 3	11 "	3X
E_5	2	2	2	12 "	1X
E_6	3 + permutations	2	1	14 "	6X
E_7	3 + perm	2	2	17 "	3X
E_8	4	1	1 + perm	18	3X
E_9	3	3	1 + perm	19	3X
E_{10}	4	2	1 + perm	21	6X
E_{11}	3	3	2 + perm	22	3X
E_{12}	4	$\overset{4}{2}$	$\overset{4}{2}$ + perm	24	3X
E_{13}	4	3	1	26	6X
E_{14}	3 5	3 1	3 1	27	1X + 3X = 4X

E_{14} has permutations from two different groups of states

#2 Griffiths problem 4.3

Use
$$\begin{cases} P_\ell^m(x) = (1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|} P_\ell(x) \\ P_\ell(x) = \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell \\ Y_\ell^m(\theta,\phi) = (-1)^m\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\, e^{im\phi} P_\ell^m(\cos\theta) \end{cases}$$

$$\boxed{Y_0^0 = \sqrt{\frac{1}{4\pi}(1)}\, P_0^0(\cos\theta) = \sqrt{\frac{1}{4\pi}}\,(1) = \sqrt{\frac{1}{4\pi}}}$$

$$Y_2^1 = -\sqrt{\frac{5}{4\pi}\frac{1!}{3!}}\, e^{i\phi} P_2^1(\cos\theta) \qquad P_2^1(x) = (1-x^2)^{1/2}\frac{d}{dx}P_2(x)$$

$$P_2(x) = \frac{1}{8}\left(\frac{d}{dx}\right)^2 (x^2-1)^2 = \frac{1}{2}(3x^2-1)$$

$$\Rightarrow P_2^1(x) = (1-x^2)^{1/2}\left(\frac{d}{dx}\right)\left(\frac{3}{2}x^2-\frac{1}{2}\right) = (1-x^2)^{1/2}\,3x$$

$$\Rightarrow Y_2^1 = -\sqrt{\frac{5}{24\pi}}\, e^{i\phi}(1-\cos^2\theta)^{1/2}\,3\cos\theta$$

$$\boxed{Y_2^1 = -\sqrt{\frac{5}{24\pi}}\, e^{i\phi}\, 3\sin\theta\cos\theta}$$

Normalizing functions:

① $\iint \sin\theta\, d\theta\, d\phi\, |Y_0^0|^2 = \frac{1}{4\pi}\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi = \frac{4\pi}{4\pi} = \boxed{1}$

② $\iint \sin\theta\, d\theta\, d\phi\, |Y_2^1|^2 = \frac{5}{24\pi}(9)\left[\int_0^\pi \sin^3\theta\cos^2\theta\, d\theta\right]\left[\int_0^{2\pi} d\phi\right]$

$$= \underbrace{\frac{45}{24\pi}(2\pi)}\left[\int_0^\pi \cos^2\theta\sin\theta\, d\theta - \cos^4\theta\sin\theta\, d\theta \quad d\theta\right]$$

$$= \frac{15}{4}\left[-\frac{1}{3}\cos^3\theta\Big|_0^\pi + \frac{1}{5}\cos^5\theta\Big|_0^\pi\right] = \frac{15}{4}\left(\frac{2}{3}-\frac{2}{5}\right) = \boxed{1}$$

Are Y_0^0 & Y_1^2 orthogonal?

$$\langle Y_0^0 | Y_1^2\rangle = \frac{1}{\sqrt{4\pi}}\sqrt{\frac{5}{24\pi}}(3)\left[\int_0^{2\pi} e^{i\phi} d\phi\right]\left[\int_0^{2\pi} \sin\theta\cos\theta\, d\theta\right] = 0!$$

$$\cos^2\theta\Big|_0^{2\pi} = 0$$

#3 Piano manufacturer!

Mass per unit length perturbed $= \mu - \mu'\left(\frac{x}{L}\right)$ $\quad \mu' << \mu$

Let $y(x,t)$ represent vertical displacement of string. Wave eqn is:
$$\frac{\partial^2 y}{\partial x^2} = \frac{\mu}{T}\frac{\partial^2 y}{\partial t^2} \quad \text{where } \frac{\mu}{T} = \frac{1}{v^2} \quad v = \text{wave velocity}$$

Separate variables & solve for "x" equation: $Y = f(x)\, g(t)$

$$v^2 \frac{1}{f}\frac{\partial^2 f}{\partial x^2} = \frac{1}{g}\frac{\partial^2 g}{\partial t^2} = -\omega^2$$

$$\frac{T}{\mu}\frac{d^2 f}{dx^2} = -\omega_n^2 f_n \Rightarrow \frac{d^2 f(x)}{dx^2} = -\frac{\omega^2}{v^2} f(x)$$

$H_0 \qquad E_n^0$

Sol'n $\quad f(x) = A \sin\left(\frac{\omega}{v} x\right)$ $\quad$ where $\frac{\omega}{v} L = n\pi$

or $f_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right)$ $\quad \boxed{\text{eigenstates for } H_0}$

Following class notes; perturbation is in $\mu_0 \Rightarrow$

$$\frac{T}{\mu_0} \rightarrow \frac{T}{\mu_0 - \mu'\frac{x}{L}} = \frac{T}{\mu_0}\left(\frac{1}{1 - \frac{\mu'}{\mu_0}\frac{x}{L}}\right) \approx \frac{T}{\mu_0}\left(1 + \frac{\mu'}{\mu_0}\frac{x}{L}\right)$$

$$H = H_0 + H'$$

$$\boxed{\frac{T}{\mu_0}\frac{d^2 f}{dx^2}} + \boxed{\frac{T}{\mu_0}\frac{\mu'}{\mu_0}\frac{x}{L}\frac{d^2 f}{dx^2}} = -\omega_{new}^2 f$$

$$\delta(-\omega^2) = \langle f_n | H' | f_n \rangle = \frac{2}{L}\int_0^L dx \sin\left(\frac{n\pi}{L}x\right)\left(\frac{T\mu'}{\mu_0^2}\frac{x}{L}\frac{d^2}{dx^2}\right)\sin\left(\frac{n\pi}{L}x\right)$$

For $n = 1$ (continued)

#3 (Continued)

$$\delta(-\omega^2) = \frac{2}{L}\int_0^L dx\ \sin\left(\frac{\pi}{L}x\right) x\left(\frac{-T\mu'}{\mu_0^2 L}\ \frac{\pi^2}{L^2}\right) \sin\left(\frac{\pi}{L}x\right)$$

$$= -\frac{2T\mu'\pi^2}{\mu_0^2 L^4}\int_0^L dx\ x \sin^2\left(\frac{\pi}{L}x\right) dx$$

$$= \quad '' \quad \int_0^L dx\ \frac{x}{2}\left(1 - \cos\left(\frac{2\pi}{L}x\right)\right)$$

$$= \frac{-2T\mu'\pi^2}{\mu_0^2 L^4}\left[\frac{x^2}{4} - \frac{L^2}{8\pi^2}\cancel{\cos\left(\frac{2\pi}{L}x\right)}^{0} - \frac{xL^2}{8\pi^2}\cancel{\sin\left(\frac{2\pi}{L}x\right)}^{0}\right]\Bigg|_0^L$$

$$= \frac{-2T\mu'\pi^2}{\mu_0^2 L^4}\left(\frac{L^2}{4}\right) = \frac{-T\mu'\pi^2}{2\mu_0^2 L^2} = -\frac{1}{2}\frac{\mu'}{\mu_0}\underbrace{\left(\frac{T\pi^2}{\mu_0 L^2}\right)}_{\omega_0^2} = -\frac{1}{2}\frac{\mu'}{\mu_0}\omega_0^2$$

$$\boxed{\delta(-\omega_0^2) = \frac{1}{2}\frac{\mu'}{\mu_0}(-\omega_0^2) \Rightarrow \delta(\omega_0) = \left(\frac{\mu'}{2\mu_0}\right)^{1/2}\omega_0}$$

Since $\delta f = \frac{\delta\omega_0}{2\pi}$ (frequency: $f = \omega/2\pi$)

Frequency shift is: $\delta f = \left(\frac{\mu'}{2\mu_0}\right)^{1/2}\left(\frac{\omega_0}{2\pi}\right) = \left(\frac{\mu'}{2\mu_0}\right)^{1/2} f_0$ ← unperturbed freq.

Middle C is 256 - 264 Hz (based on which web site you select)

So $\boxed{\delta f = \left(\frac{10^{-3}\mu_0}{2\mu_0}\right)^{1/2} 256 \cong 6\ Hz}$ Not audible for most non-musicians?

Other values: $T \approx 1750\ N$ $L \approx .6m$ $\mu_0 \approx .01\ kg/m$

(4) 3D Harm Osc. with $H' = Bxz$

(a) $\omega_x \neq \omega_y \neq \omega_z$ Non-degenerate (b) $\omega_x = \omega_y = \omega_z$

$$\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z \quad \left(\hat{H}_x = \frac{1}{2m}\hat{p}_x^2 + \frac{1}{2}m\omega_x^2\hat{x}^2\right)$$

$$E = E_x + E_y + E_z = \hbar\omega_x(n_x + \tfrac{1}{2}) + \hbar\omega_y(n_y + \tfrac{1}{2}) + \hbar\omega_z(n_z + \tfrac{1}{2})$$

Eigenstates are $|n_x n_y n_z\rangle$ - where $n_x, n_y, n_z = 0, 1, \ldots \infty$

<u>Non-degenerate Case</u>: $\omega_x \neq \omega_y \neq \omega_z$

$$E_n^1 = \langle n_x n_y n_z | Bxz | n_x n_y n_z \rangle \qquad \begin{cases} x = \sqrt{\frac{\hbar}{2m\omega_x}}(\hat{a}_x^+ + \hat{a}_x) \\ z = \sqrt{\frac{\hbar}{2m\omega_z}}(\hat{a}_z^+ + \hat{a}_z) \end{cases}$$

x, z operators act independently on states:

$$E_n^1 = B\frac{\hbar}{2m\sqrt{\omega_x\omega_y}} \underbrace{\langle n_x | x | n_x \rangle}_{0} \underbrace{\langle n_z | z | n_z \rangle}_{0} \langle n_y | n_y \rangle$$

$$\boxed{E_n^1 = 0} \qquad 1^{ST} \text{ order energy perturbation}$$

<u>2^{ND} Order</u>: $$E_n^2 = \sum_{m \neq n} \frac{|\langle m | H' | n \rangle|^2}{E_n^0 - E_m^0}$$

<u>Here</u>: $|m\rangle = |m_x m_y m_z\rangle$ and $|n\rangle = |n_x n_y n_z\rangle$

So:
$$\langle m | H' | n \rangle = \langle m_x m_y m_z | Bxz | n_x n_y n_z \rangle$$
$$= B \langle m_x | \sqrt{\frac{\hbar}{2m\omega_x}}(\hat{a}_x^+ + a_x)|n_x\rangle \langle m_z | \sqrt{\frac{\hbar}{2m\omega_z}}(\hat{a}_z^+ + \hat{a}_z)|n_z\rangle \underbrace{\langle n_y | n_y \rangle}_{1}$$
$$= \frac{B\hbar}{2m\sqrt{\omega_x\omega_z}} \underbrace{\langle m_x | \hat{a}_x^+ + \hat{a}_x | n_x \rangle}_{(1)} \underbrace{\langle m_z | \hat{a}_z + \hat{a}_z | n_z \rangle}_{(2)} \quad (A)$$

Now, $E^0_{n_x n_z} - E^0_{m_x m_z} = \hbar\omega_x(n_x - m_x) + \hbar\omega_z(n_z - m_z)$

Note that for $\langle m | H' | n \rangle \neq 0$ requires that <u>both</u> term (1) and (2) in (A) above must be positive so only a limit number of states are <u>non-zero</u>.

(4) (continued)
Let's create a table of non-zero values for:

$\langle m_x\, m_y\, m_z |\, xz\, | n_x\, n_y\, n_z \rangle$, Fix $|n_x\, n_y\, n_z\rangle$

Non-zero states are

	m_x	m_z	xz	$E^0_{n_x n_z} - E^0_{m_x m_z}$
(1)	n_x+1	n_z+1	$\sqrt{n_x+1}\sqrt{n_z+1}$	$-\hbar(\omega_x+\omega_z)$
(2)	n_x+1	n_z-1	$\sqrt{n_x+1}\sqrt{n_z}$	$-\hbar(\omega_x-\omega_z)$
(3)	n_x-1	n_z+1	$\sqrt{n_x}\sqrt{n_z+1}$	$\hbar(\omega_x-\omega_z)$
(4)	n_x-1	n_z-1	$\sqrt{n_x}\sqrt{n_z}$	$\hbar(\omega_x+\omega_z)$

(4) states

$$E_n^2 = \frac{B^2\hbar^2}{4m^2\omega_x\omega_z}\left[\frac{(n_x+1)(n_z+1)}{-\hbar(\omega_x+\omega_z)} + \frac{(n_x+1)n_z}{-\hbar(\omega_x-\omega_z)} + \frac{n_x(n_z+1)}{\hbar(\omega_x-\omega_z)} + \frac{n_x n_z}{\hbar(\omega_x+\omega_z)}\right]$$

$$= \;''\; \left(\frac{1}{\hbar}\right)\left[\frac{-n_x-n_z-1}{\omega_x+\omega_z} + \frac{n_x-n_z}{\omega_x-\omega_z}\right]$$

$$\boxed{E_n^2 = \frac{B^2\hbar}{2m^2\omega_x\omega_z}\left[\frac{(2n_x+1)\omega_z-(2n_z+1)\omega_x}{\omega_x^2-\omega_z^2}\right]}$$

(b) Degenerate (isotropic) model $\quad \omega_x=\omega_y=\omega_z=\underline{\underline{\omega}}$

First excited state $\quad n_x, n_y, n_z = (1,0,0) = (0,1,0) = (0,0,1)$

Energies are degenerate $= \frac{5}{2}\hbar\omega \Rightarrow$ Must use degenerate perturb. theory

We want to find eigenvalues of matrix $\overline{W}$ where

$W_{ij} = \langle i | H' | j \rangle$ where $i,j = |100\rangle, |010\rangle, |001\rangle$

Diagonal elements are easy:

$\langle 100 | Bxz | 100\rangle = \langle 010 | Bxz | 010\rangle = \langle 001 | Bxz | 001\rangle = \underline{0}$

since $\hat{x}, \hat{z}$ operators raise/lower states

④ ⓑ <u>Continued</u>

As in 2^{ND} order perturb calculation in part a, the states with non-zero terms are ones where $n_x \neq m_x$, $n_z \neq m_z$:

$$\langle 1\,0\,0 \,|\, Bxz \,|\, 0\,0\,1 \rangle = B\frac{\hbar}{2m\omega}(\sqrt{1}\sqrt{1}) \quad \frac{B\hbar}{2m\omega}$$

$$\langle 0\,0\,1 \,|\, Bxz \,|\, 1\,0\,0 \rangle = B\frac{\hbar}{2m\omega}(\sqrt{1}\sqrt{1}) = \frac{B\hbar}{2m\omega}$$

Let $\alpha = \frac{B\hbar}{2m\omega}$. Then the perturbation matrix $\overline{W}$ is:

$$\overline{W} = \begin{array}{c} \begin{matrix} |100\rangle & |010\rangle & |001\rangle \end{matrix} \\ \begin{pmatrix} 0 & 0 & \alpha \\ 0 & 0 & 0 \\ \alpha & 0 & 0 \end{pmatrix} \end{array} \qquad \det(\overline{W} - \lambda I) = -\lambda^3 + \lambda\alpha^2 = 0$$

Eigenvalues are $\lambda = 0 \qquad \lambda = \pm\alpha = \pm\frac{B\hbar}{2m\omega}$

$$\boxed{\text{So, } 1^{ST} \text{ order shifts for isotropic case are: } E_1' = 0 \text{ (no shift)} \qquad E_{2,3}^1 = \pm\frac{B\hbar}{2m\omega} \text{ (split)}}$$

<u>Major difference</u> between <u>Non-degenerate</u> & <u>Isotropic</u> Case is in 1^{ST} order perturbation:

1) No 1^{ST} order shifts for <u>non-degenerate</u> case, but 2^{ND} order non-zero.

2) For isotropic, 1^{ST} order <u>shifts</u> occur.

#5 Euler method:

For Euler method, equations are:

① $x_n = x_{n-1} + v_{n-1}\,dt$

② $v_n = v_{n-1} + \frac{F(x_{n-1})}{m}\,dt = v_{n-1} - \frac{k}{m} x_{n-1}\,dt$

$F = -kx$ for harm. osc.

Energies for SHO expressed as:

$$E_n = \underbrace{\tfrac{1}{2} k x_n^2}_{V} + \underbrace{\tfrac{1}{2} m v_n^2}_{T}$$

Now substitute in ① and ② above

$$E_n = \tfrac{1}{2} k (x_{n-1} + v_{n-1}\,dt)^2 + \tfrac{1}{2} m \left(v_{n-1} - \tfrac{k}{m} x_{n-1}\,dt\right)^2$$

$$= \tfrac{1}{2} k x_{n-1}^2 + \cancel{k x_{n-1} v_{n-1}\,dt} + \tfrac{1}{2} k v_{n-1}^2\,dt^2$$
$$+ \tfrac{1}{2} m v_{n-1}^2 - \cancel{m v_{n-1} \tfrac{k}{m} x_{n-1}\,dt} + \tfrac{1}{2} m \tfrac{k^2}{m^2} x_{n-1}^2\,dt^2$$

$$E_n = \underbrace{\tfrac{1}{2} k x_{n-1}^2 + \tfrac{1}{2} m v_{n-1}^2}_{E_{n-1}} + \tfrac{1}{2} k v_{n-1}^2\,dt^2 + \tfrac{1}{2} \tfrac{k^2}{m} x_{n-1}^2\,dt^2$$

$$= E_{n-1} + \tfrac{1}{2} m v_{n-1}^2 \left(\tfrac{k}{m} dt^2\right) + \tfrac{1}{2} k x_{n-1}^2 \left(\tfrac{k}{m} dt^2\right)$$

$$\boxed{E_n = E_{n-1}\left(1 + \tfrac{k}{m} dt^2\right)}$$

Let $t = N\,dt$ (N "time slices")

$E_1 = E(0)\left(1 + \frac{k}{m} dt^2\right)$

$E_2 = E_1\left(1 + \frac{k}{m} dt^2\right) = E(0)\left(1 + \frac{k}{m} dt^2\right)^2$ and so on...

$$\boxed{E(t) = E_N = E(0)\left(1 + \tfrac{k}{m} dt^2\right)^N}$$

$\lim_{N \to \infty} \left(1 + \frac{k}{m} dt \left(\frac{t}{N}\right)\right)^N = e^{\frac{k}{m}(dt)\,t}$ so $E(t)$ experiences <u>exponential growth</u>. However, if <u>**dt**</u> is <u>small enough</u> so $t\,dt \ll 1$ then $e^{\frac{k}{m}(dt)t} \approx \underline{\underline{1}}$

(#6) For SHO, $T = 2\pi\sqrt{\frac{m}{k}} = 2\pi\sqrt{\frac{.8}{.3}} \approx 3.25$

Period on graph should be approx. this value

(#7) Energy for SHO, $E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2$

$E = \frac{1}{2}(.8)(2)^2 + \frac{1}{2}(3)(1.4)^2 \approx 4.55$

Largest x displacement (and amplitude) occurs where $KE = 0$ or

$$E = \frac{1}{2}k x_{max}^2 \Rightarrow x_{max} = \pm\sqrt{\frac{2E}{k}}$$

In this case, $x_{max} = \sqrt{\frac{2(4.55)}{3}} \approx 1.75$

Maximum $x(t)$ value on graph should be approx. this.

Example for #6 & #7

```
//
//  P115B  HW2  #6
//
//  Program to implement Molecular Dynamics
//    with Leapfrog method
#include <iostream>
#include <fstream>
#include <math.h>
using namespace std;
double k,m, xn, xn_m1, vn, vn_m1,x0, v0,  dt ;
int num_periods;
int main()
{
   k  = 3.0;
   m =   .8;
   x0 = 1.4;
   v0 = 0.0;
   dt = .2;
   num_periods = 20;
// Set up disk file for output
   ofstream fout("MD_out1.dat");
   fout << " t     x(t)    "  << endl;
// Generate data with leapfrog
   xn_m1 = x0;
   vn_m1 = v0;
   for ( int i= 0; i< num_periods; i++)
   {
      xn = xn_m1 + vn_m1 * dt;
      vn = vn_m1 - (k/m)*xn * dt;
      fout << "  "<<i + 1 << "   "<< xn << endl;
      xn_m1 = xn;
      vn_m1 = vn;
   }
   cout << " Finished writing data to file" << endl;
   return 0;
}
```