HW#9 —Phys374—Fall 2013 Prof. Alessandra Buonanno
Due before class, Tuesday, Dec. 10, 2013 Room 4212, (301)405-1440
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1. Consider a mass m suspended by a spring with spring constant k from another mass m which is suspended from a fixed support by another spring with spring constant k. (This is the system demonstrated and discussed in class.) Let y_1 and y_2 denote the displacements from their equilibrium positions of the top and bottom masses respectively, with the downward direction taken as positive.

   (a) Write out Newton's second law governing the displacement of each of the two masses from their equilibrium positions. (Note the equilibrium spring forces balance the gravitational forces, which therefore drop out of the problem.)

   (b) Combine the two Newton's law equations into a single 2×2 matrix equation $\ddot{\mathbf{y}} = A\mathbf{y}$, and specify the components of the matrix A in units with $k = m = 1$.

   (c) Determine the normal mode frequencies and displacement ratios y_2/y_1 by finding the eigenvectors and eigenvalues of A *by hand*. (*To check your result*: The squared frequencies are $(3 \pm \sqrt{5})/2$ and the displacement ratios are $y_2/y_1 = (1 \mp \sqrt{5})/2$.)

   (d) Describe and indicate with arrows the nature of the two normal mode motions, showing both direction and approximate relative displacement of each mass. Label with the frequency of each mode. Which is the higher one?

Solution:

(a) The gravitational force is balanced by spring forces in the equilbrium configuration. Since the spring force is linear in the displacement the residual force is just that due to the extra displacement from equilibrium. Hence we have

$$m\ddot{y}_1 = -ky_1 - k(y_1 - y_2) \quad (1)$$

$$m\ddot{y}_2 = -k(y_2 - y_1). \quad (2)$$

(b) The column vector $\mathbf{y}$ has components (y_1, y_2), and

$$A = \begin{pmatrix} -2 & 1 \\ 1 & -1 \end{pmatrix}.$$

(c) A solution with harmonic time dependence takes the form $\mathbf{y} = \cos(\omega t + \varphi)\mathbf{y}_0$, for which $\ddot{\mathbf{y}} = -\omega^2 \mathbf{y} = A\mathbf{y}$, so the eigenvalues of A are $-\omega^2$. To find the eigenvalues λ compute the characteristic polynomial:

$$\begin{vmatrix} -2-\lambda & 1 \\ 1 & -1-\lambda \end{vmatrix} = \lambda^2 + 3\lambda + 1,$$

whose roots are $\lambda_\pm = (-3 \pm \sqrt{5})/2$. The corresponding frequencies are $\omega_\pm = \sqrt{(3 \mp \sqrt{5})/2}\sqrt{k/m} = 0.382,\ 2.618\sqrt{k/m}$. The eigenvectors satisfy $(A - \lambda I)\mathbf{v} = 0$, i.e.

$$\begin{pmatrix} -2-\lambda & 1 \\ 1 & -1-\lambda \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} (-2-\lambda)y_1 + y_2 \\ y_1 - (1+\lambda)y_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Both components must vanish, but if λ is an eigenvalue, then if one vanishes, the other does as well. The lower component implies $y_2/y_1 = 1/(\lambda+1) = 2/(-1 \pm \sqrt{5})$. Numerically, these ratios are 1.618 for λ_+, and -0.618 for λ_-.

(d) $|\lambda_+| < |\lambda_-|$, so $\omega_+ < \omega_-$. For the lower frequency, the two masses move in the same direction, with the displacement of the lower mass always 1.618 times that of the upper mass. For the higher frequency, the two masses move in opposite directions, with the displacement of the lower mass always -0.618 times that of the upper mass. The frequency of the opposing mode is higher, since the spring connecting the masses is compressed, hence adds to the upper spring producing an effective spring constant that is *greater* than k.

2. Re-do all parts of the previous problem in the case that there are *three* equal masses hanging in a chain from three springs. In this case the characteristic equation is a cubic and the frequencies and amplitudes cannot be found in a simple closed form, so instead use a computer to get them.[1]

Solution:

(a)

$$\begin{aligned} m\ddot{y}_1 &= -ky_1 + k(y_2 - y_1) && (3) \\ m\ddot{y}_2 &= -k(y_2 - y_1) + k(y_3 - y_2) && (4) \\ m\ddot{y}_2 &= -k(y_3 - y_2) && (5) \end{aligned}$$

(b) The column vector $\mathbf{y}$ has components (y_1, y_2, y_3), and

$$A = \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{pmatrix}.$$

(c) The characteristic polynomial is

$$\begin{vmatrix} -2-\lambda & 1 & 0 \\ 1 & -2-\lambda & 1 \\ 0 & 1 & -1-\lambda \end{vmatrix} = -(\lambda^3 + 5\lambda^2 + 6\lambda + 1),$$

[1] Use the help function to learn the right command. In Mathematica, the command would be, for example, "Eigensystem[{{1., 2, 3},{0, 1, 0},{1, 0, 1}}]". Note the period after the first entry 1. That tells Mathematica to treat the entries as real numbers rather than integers. This is necessary, when the result has no nice closed form, to obtain a numerical result rather than an abstract "root" expression. Try it—you'll see what I mean.

which has no nice factorization. Instead I put the matrix into Mathematica with the command "Eigensystem[{{-2, 1, 0},{1, -2, 1},{0, 1, -1.}}]". Note the period after the last entry -1. I put that in to tell Mathematica to treat the entries as real numbers rather than integers, to make it give a numerically computed result rather than an abstract "root" expression. The result is
{{-3.24698, -1.55496, -0.198062},
{{-0.591009, 0.736976, -0.327985},
{0.736976, 0.327985, -0.591009},
{0.327985, 0.591009, 0.736976}}}.
The first row is the three eigenvalues, which are equal to $-\omega^2$. These correspond to the frequencies $\omega = 1.80, 1.25, 0.45\sqrt{k/m}$, respectively. The next three rows are the components of the corresponding eigenvectors.

(d) The greatest frequency is the first one. The first eigenvector shows the center mass moves opposite to the first and last masses, with the greatest amplitude. The bottom mass has the smallest amplitude. The lowest frequency is the last one, and the corresponding eigenvector has all positive components, so all masses move in the same direction, with increasing amplitude going down. The middle frequency eigenvector has first two components positive and the last one negative, so the top two masses move together, opposite to the bottom mass. The top mass moves the most, the middle mass the least.

By the way, it is easy to see why, for the middle frequency mode, the top two masses must move in the same direction. In a normal mode, each mass must have the same "effective spring constant" k_{eff}, i.e. the same force for a given displacement, since otherwise (given that the masses are equal) the masses would not oscillate with the same frequency. Suppose the bottom two masses moved together, opposite to the top mass. Then k_{eff} for the bottom mass would be less than k, but k_{eff} for the top mass would be *greater* than k, since the top spring contributes k and the middle spring contributes as well. This rules out such a normal mode motion, so it must be that the top two move together.

3. Find the ratio of the two nonzero normal mode frequencies for longitudinal vibrations of the model of the carbon dioxide molecule discussed in class: two oxygen mass points with mass m_O each connected by a spring of spring constant k to a carbon atom in the center with mass $m_C = (3/4)m_O$. (The equilibrium length of the springs is nonzero.) Section 13.6 of the texbook shows that if all masses were equal the frequencies would be $\omega_1 = \sqrt{k/m}$ and $\omega_2 = \sqrt{3k/m}$, so $\omega_2/\omega_1 = \sqrt{3}$. The point of this problem is to find the ratio taking into account that $m_O/m_C = 4/3 \neq 1$. Use units with $k = 1$ and $m_O = 1$, and write your equations using the parameter $a = m_O/m_C$. Put $a = 4/3$ only at the end of your calculation to evaluate the result.

(a) Use the characteristic polynomial to show *by hand* (no computer or calculator) that the frequencies are given by 0, 1, and $\sqrt{1+2a}$. For each mode find the displacement ratios x_2/x_1 and x_3/x_1, where $x_{1,3}$ are the displacements of the oxygen atoms and x_2 is the displacement of the carbon atom. Describe and indicate with arrows the nature of the three normal mode motions, showing both direction and approximate relative replacements. Label with the frequency of each mode. Which is the highest one?

(b) Look at www.phy.davidson.edu/StuHome/jimn/CO2/Pages/CO2Theory.htm for information on carbon dioxide vibrations. Compare the ratio $\sqrt{11/3}$ of the frequencies in our simple model[2] to the measured value[3] of the ratio for the corresponding modes of carbon dioxide. Show that the measured ratio is smaller, and determine by what fraction it differs from the simple model.

(c) Try to give a physical reason (or reasons) why the observed ratio is smaller than that in our simple model. I'm not sure, but I don't think the difference between quantum and classical mechanics is really the important issue in this case. *Hint*: Think about the physical nature of the "springs" in the molecule and how they differ from those in our model. I think one can explain along these lines the dominant reason why the measured ratio is smaller.

Solution:

(a) $A\mathbf{x}_0 = -\omega^2\mathbf{x}_0$, with

$$\begin{pmatrix} -1 & 1 & 0 \\ a & -2a & a \\ 0 & 1 & -1 \end{pmatrix}$$

in units with $k = 1$ and $m_O = 1$, and with $a = m_O/m_C = 4/3$.

The eigenvalues are determined by the characteristic polynomial,

$$\begin{vmatrix} -1-\lambda & 1 & 0 \\ a & -2a-\lambda & a \\ 0 & 1 & -1-\lambda \end{vmatrix} = \lambda(\lambda+1)(\lambda+2a+1),$$

so the eigenvalues are $-\omega^2 = 0, -1, -1-2a$, hence the frequencies are $\omega = 0, 1, \sqrt{1+2a} = \sqrt{11/3} \approx 1.92$, in units with $k/m_O = 1$.

The eigenvectors satisfy $(A - \lambda I)\mathbf{v} = 0$, i.e.

$$\begin{pmatrix} -1-\lambda & 1 & 0 \\ a & -2a-\lambda & a \\ 0 & 1 & -1-\lambda \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -(1+\lambda)x_1 + x_2 \\ ax_1 - (2+\lambda)x_2 + ax_3 \\ x_2 - (1+\lambda)x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

For $\lambda = 0$ we have $x_1 = x_2 = x_3$. This is the translational mode. For $\lambda = -1$ we have $x_2 = 0$ and $x_3 = -x_1$. This is the asymmetric mode. Note the center of mass remains at rest. For $\lambda = -1-2a$ we have $x_1 = x_3$ and $x_2 = 2ax_1$. Again, the center of mass remains at rest.

[2]Note you don't need to know the spring constant or the magnitude of each mass to determine this ratio! This is because it is dimensionless, so can depend only on the mass ratio.

[3]The frequencies are given on the above web page in units of cm^{-1}. This refers to the inverse wavelength λ^{-1} of the radiation that is in resonance with the transitions between the vibrational levels, which is proportional to the frequency ω since $\omega = ck = 2\pi c/\lambda$, where c is the speed of light.

(b) The measured frequency of the asymmetric mode (oxygens move opposite) is listed as 2349 in units of cm^{-1}, while that of the symmetric mode (oxygens move in same direction) is 1388. The ratio is 1.69, which is smaller than the above result 1.92, though only by 12%, which ain't bad!

(c) The actual frequency ratio is lower than in the model, so the ratio of effective spring constants in the asymmetric and symmetric modes in the actual molecule is lower than in the model. Maybe this is because the model treats the individual springs as fixed and independent, whereas in the CO_2 molecule the springs arise from electronic interactions, with the same electrons providing for both springs. In the symmetric mode the electrons on the carbon are, so to speak, pushed towards the center from both sides. Since the electrons repel each other this makes the spring "stiffer" than in the asymmetric mode. That would raise the frequency of the symmetric mode relative to the asymmetric one, which would decrease the ratio, which is consistent with the observed values. I don't know whether or not this is really the dominant effect, but it seems plausible.