

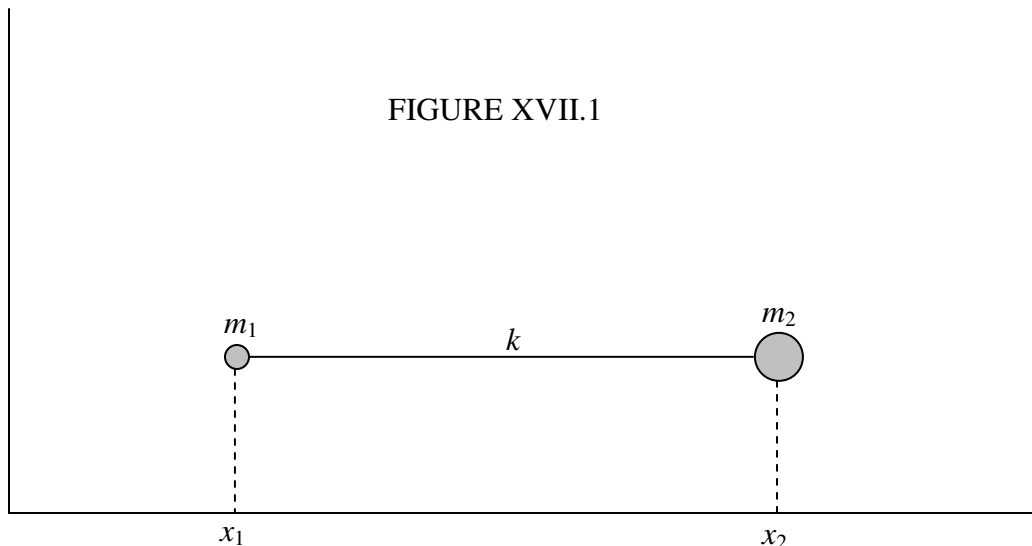
## CHAPTER 17 VIBRATING SYSTEMS

### 17.1 Introduction

A mass  $m$  is attached to an elastic spring of force constant  $k$ , the other end of which is attached to a fixed point. The spring is supposed to obey Hooke's law, namely that, when it is extended (or compressed) by a distance  $x$  from its natural length, the tension (or thrust) in the spring is  $kx$ , and the equation of motion is  $m\ddot{x} = -kx$ . This is simple harmonic motion of period  $2\pi/\omega$ , where  $\omega^2 = k/m$ . Most readers will have no difficulty with that problem. But now suppose that, instead of one end of the spring being attached to a fixed point, we have two masses,  $m_1$  and  $m_2$ , one at either end of the spring. A diatomic molecule is much the same thing. Can you calculate the period of simple harmonic oscillations? It looks like an easy problem, but it somehow seems difficult to get a hand on it by conventional newtonian methods. In fact it can be done quite readily by newtonian methods, but this problem, as well as more complicated problems where you have several masses connected by several springs and several possible modes of vibration, is particularly suitable by lagrangian methods, and this chapter will give several examples of vibrating systems tackled by lagrangian methods.

### 17.2 The Diatomic Molecule

Two particles, of masses  $m_1$  and  $m_2$  are connected by an elastic spring of force constant  $k$ . What is the period of oscillation?



Let's suppose that the equilibrium separation of the masses – i.e. the natural, unstretched, uncompressed length of the spring – is  $a$ . At some time suppose that the  $x$ -coordinates of the two masses are  $x_1$  and  $x_2$ . The extension  $q$  of the spring from its natural length at that

moment is  $q = x_2 - x_1 - a$ . We'll also suppose that the velocities of the two masses at that instant are  $\dot{x}_1$  and  $\dot{x}_2$ . We know from chapter 13 how to start any calculation in lagrangian mechanics. We don't have to think about it. We always start with  $T = \dots$  and  $V = \dots$ :

$$T = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2, \quad 17.2.1$$

$$V = \frac{1}{2}kq^2. \quad 17.2.2$$

We want to be able to express the equations in terms of the internal coordinate  $q$ .  $V$  is already expressed in terms of  $q$ . Now we need to express  $T$  (and therefore  $\dot{x}_1$  and  $\dot{x}_2$ ) in terms of  $q$ . Since  $q = x_2 - x_1 - a$ , we have, by differentiation with respect to time,

$$\dot{q} = \dot{x}_2 - \dot{x}_1. \quad 17.2.3$$

We need one more equation. The linear momentum is constant and there is no loss in generality in choosing a coordinate system such that the linear momentum is zero:

$$0 = m_1\dot{x}_1 + m_2\dot{x}_2. \quad 17.2.4$$

From these two equations, we find that

$$\dot{x}_1 = \frac{m_2}{m_1 + m_2}\dot{q} \quad \text{and} \quad \dot{x}_2 = \frac{m_1}{m_1 + m_2}\dot{q}. \quad 17.2.5a,b$$

Thus we obtain

$$T = \frac{1}{2}m\dot{q}^2 \quad 17.2.6$$

and

$$V = \frac{1}{2}kq^2, \quad 17.2.2$$

where

$$m = \frac{m_1m_2}{m_1 + m_2}. \quad 17.2.7$$

Now apply Lagrange's equation

$$\frac{d}{dt} \frac{\partial T}{\partial \dot{q}_j} - \frac{\partial T}{\partial q_j} = - \frac{\partial V}{\partial q_j}. \quad 13.4.13$$

to the single coordinate  $q$  in the fashion to which we became accustomed in Chapter 13, and the equation of motion becomes

$$m\ddot{q} = -kq, \quad 17.2.8$$

which is simple harmonic motion of period  $2\pi\sqrt{m/k}$ , where  $m$  is given by equation 17.2.7. The frequency is the reciprocal of this, and the “angular frequency”  $\omega$ , also sometimes called the “pulsatance”, is  $2\pi$  times the frequency, or  $\sqrt{k/m}$ .

The quantity  $m_1 m_2 / (m_1 + m_2)$  is usually called the “reduced mass” and one may wonder in what sense it is “reduced”. I believe the origin of this term may come from an elementary treatment of the Bohr atom of hydrogen, in which one at first assumes that there is an electron moving around an immovable nucleus – i.e. a nucleus of “infinite mass”. One develops formulas for various properties of the atom, such as, for example, the Rydberg constant, which is the energy required to ionize the atom from its ground state. This and similar formulas include the mass  $m$  of the electron. Later, in a more sophisticated model, one takes account of the finite mass of the nucleus, with nucleus and electron moving around their mutual centre of mass. One arrives at the same formula, except that  $m$  is replaced by  $mM/(m + M)$ , where  $M$  is the mass of the nucleus. This is slightly less (by about 0.05%) than the mass of the electron, and the idea is that you can do the calculation with a fixed nucleus provided that you use this “reduced mass of the electron” rather than its true mass. Whether this is the appropriate term to use in our present context is debatable, but in practice it is the term almost universally used.

It may also be remarked upon by readers with some familiarity with quantum mechanics that I have named this section “The Diatomic Molecule” – yet I have ignored the quantum mechanical aspects of molecular vibration. This is true – in this series of notes on *Classical Mechanics* I have adopted an entirely classical treatment. It would be wrong, however, to assume that classical mechanics does not apply to a molecule, or that quantum mechanics would not apply to a system consisting of a cricket ball and a baseball connected by a metal spring. In fact both classical mechanics and quantum mechanics apply to both. The formula derived for the frequency of vibration in terms of the reduced mass and the force constant (“bond strength”) applies as accurately for the molecule as for the cricket ball and baseball. Quantum mechanics, however, predicts that the total *energy* (the eigenvalue of the hamiltonian operator) can take only certain discrete values, and also that the lowest possible value is not zero. It predicts this not only for the molecule, but also for the cricket ball and baseball – although in the latter case the energy levels are so closely spaced together as to form a quasi continuum, and the zero point vibrational energy is so close to zero as to be unmeasurable. Quantum mechanics makes its effects *evident* at the molecular level, but this does not mean that it does not *apply* at macroscopic levels. One might also take note that one is not likely to understand why wave mechanics predicts only discrete energy levels unless one has had a good background in the classical mechanics of waves. In other words, one must not assume that classical mechanics does not apply to microscopic systems, or that quantum mechanics does not apply to macroscopic systems.

Below leaving this section, in case you tried solving this problem by newtonian methods and ran into difficulties, here’s a hint. Keep the centre of mass fixed. When the length of the spring is  $x$ , the lengths of the portions on either side of the centre of mass are

$\frac{m_2 x}{m_1 + m_2}$  and  $\frac{m_1 x}{m_1 + m_2}$ . The force constants of the two portions of the spring are

inversely proportional to their lengths. Take it from there.

### 17.3 Two Masses, Two Springs and a Brick Wall

The system is illustrated in figure XVII.2, first in its equilibrium (unstretched) position, and then at some instant when it is not in equilibrium and the springs are stretched. You

can imagine that the masses are resting upon and can slide upon a smooth, horizontal table. I could also have them hanging under gravity, but this would introduce a distracting complication without illustrating any further principles. I also want to assume that all the motion is linear, so we could have them sliding on a smooth horizontal rail, or have them confined in the inside of a smooth, fixed drinking-straw. For the present, I don't want the system to bend.

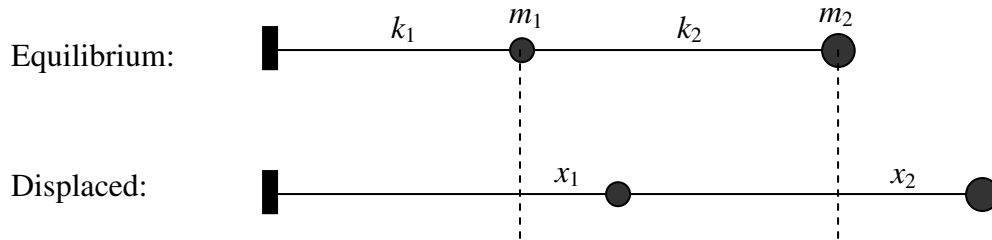


FIGURE XVII.2

The displacements from the equilibrium positions are  $x_1$  and  $x_2$ , so that the two springs are stretched by  $x_1$  and  $x_2 - x_1$  respectively. The velocities of the two masses are  $\dot{x}_1$  and  $\dot{x}_2$ . We now start the lagrangian calculation in the usual manner:

$$T = \frac{1}{2} m_1 \dot{x}_1^2 + \frac{1}{2} m_2 \dot{x}_2^2, \quad 17.3.1$$

$$V = \frac{1}{2} k_1 x_1^2 + \frac{1}{2} k_2 (x_2 - x_1)^2. \quad 17.3.2$$

Apply Lagrange's equation to each coordinate in turn, to obtain the following equations of motion:

$$m_1 \ddot{x}_1 = -(k_1 + k_2)x_1 + k_2 x_2 \quad 17.3.3$$

and 
$$m_2 \ddot{x}_2 = k_2 x_1 - k_2 x_2. \quad 17.3.4$$

Now we seek solutions in which the system is vibrating in simple harmonic motion at angular frequency  $\omega$ ; that is, we seek solutions of the form  $\ddot{x}_1 = -\omega^2 x_1$  and  $\ddot{x}_2 = -\omega^2 x_2$ . When we substitute these in equations 17.3.3 and 4, we obtain

$$(k_1 + k_2 - m_1 \omega^2)x_1 - k_2 x_2 = 0 \quad 17.3.5$$

and 
$$k_2 x_1 - (k_2 - m_2 \omega^2)x_2 = 0. \quad 17.3.6$$

Either of these gives us the displacement ratio  $x_2/x_1$  (and hence amplitude ratio). The first gives us

$$\frac{x_2}{x_1} = \frac{-m_1\omega^2 + k_1 + k_2}{k_2} \quad 17.3.7$$

and the second gives us

$$\frac{x_2}{x_1} = \frac{k_2}{k_2 - m_2\omega^2}. \quad 17.3.8$$

These are equal, and, by equating the right hand sides, we obtain the following equation for the *angular frequencies of the normal modes*:

$$m_1m_2\omega^4 - (m_1k_2 + m_2k_1 + m_2k_2)\omega^2 + k_1k_2 = 0. \quad 17.3.9$$

This equation can also be derived by noting, from the theory of equations, that equations 17.3.5 and 6 are consistent only if the determinant of the coefficients is zero.

The meaning of these equations and of the expression “normal modes” can perhaps be best illustrated with a numerical example. Let us suppose, for example, that  $k_1 = k_2 = 1$  and  $m_1 = 3$  and  $m_2 = 2$ . In that case equation 17.3.9 is  $6\omega^4 - 7\omega^2 + 1 = 0$ . This is a quartic equation in  $\omega$ , but it is also a quadratic equation in  $\omega^2$ , and there are just two positive solutions for  $\omega$ . These are  $1/\sqrt{6} = 0.4082$  (slow, low frequency) and 1 (fast, high frequency). If you put the low frequency  $\omega$  into either of equations 17.3.7 or 8 (or in both, to check for arithmetic or algebraic mistakes) you find a displacement ratio of +1.5; but if you put the high frequency  $\omega$  into either equation, you find a displacement ratio of -1.0. The first of these *normal modes* is a low-frequency slow oscillation in which the two masses oscillate in phase, with  $m_2$  having an amplitude 50% larger than  $m_1$ . The second normal mode is a high-frequency fast oscillation in which the two masses oscillate out of phase but with equal amplitudes.

So, how does the system actually oscillate? This depends on the *initial conditions*. For example, if you displace the first mass by one inch to the right and the second mass by 1.5 inches to the right (this implies stretching the first spring by 1 inch and the second by 0.5 inches), and then let go, the system will oscillate in the slow, in-phase mode. But if you start by displacing the first mass by one inch to the right and the second mass by one inch to the left (this implies stretching the first spring by 1 inch and compressing the second by 2 inches), the system will oscillate in the fast, out-of-phase mode. For other initial conditions, the system will oscillate in a *linear combination of the normal modes*.

Thus,  $m_1$  might oscillate with an amplitude  $A$  in the slow mode, and an amplitude  $B$  in the fast mode:

$$x_1 = A\cos(\omega_1t + \alpha_1) + B\cos(\omega_2t + \alpha_2), \quad 17.3.10$$

in which case the oscillation of  $m_2$  is given by

$$x_2 = 1.5A \cos(\omega_1 t + \alpha_1) - B \cos(\omega_2 t + \alpha_2). \quad 17.3.11$$

In our example,  $\omega_1$  and  $\omega_2$  are  $1/\sqrt{6}$  and 1 respectively.

Let's suppose that the initial conditions are that, at  $t = 0$ ,  $\dot{x}_1$  and  $\dot{x}_2$  are both zero. This means that  $\alpha_1$  and  $\alpha_2$  are both zero or  $\pi$  (I'll take them to be zero), so that

$$x_1 = A \cos \omega_1 t + B \cos \omega_2 t \quad 17.3.12$$

and 
$$x_2 = 1.5A \cos \omega_1 t - B \cos \omega_2 t. \quad 17.3.13$$

Suppose further that at  $t = 0$ ,  $x_1$  and  $x_2$  are both +1, which means that we start by stretching both springs equally. Equations 17.3.12 and 13 then become  $1 = A + B$  and  $1 = 1.5A - B$ . That is,  $A = 0.8$  and  $B = 0.2$ . I'll leave you to draw graphs of  $x_1$  and  $x_2$  versus time.

Here's an exercise that might be useful if, perhaps, you wanted to construct a real system with two equal masses  $m$  and two equal springs, each of constant  $k$ , to demonstrate the vibrations. Show that in that case, the angular frequency (which is, of course,  $2\pi$  times the actual frequency) of the slow, in phase, mode is

$$\omega_1 = \frac{1}{2}(\sqrt{5} - 1) \sqrt{\frac{k}{m}} = 0.6180 \sqrt{\frac{k}{m}}$$

with a displacement ratio  $x_2 / x_1 = \frac{1}{2}(\sqrt{5} + 1) = 1.6180$ ;

and the angular frequency of the fast, out of phase, mode is

$$\omega_2 = \frac{1}{2}(\sqrt{5} + 1) \sqrt{\frac{k}{m}} = 1.6180 \sqrt{\frac{k}{m}}$$

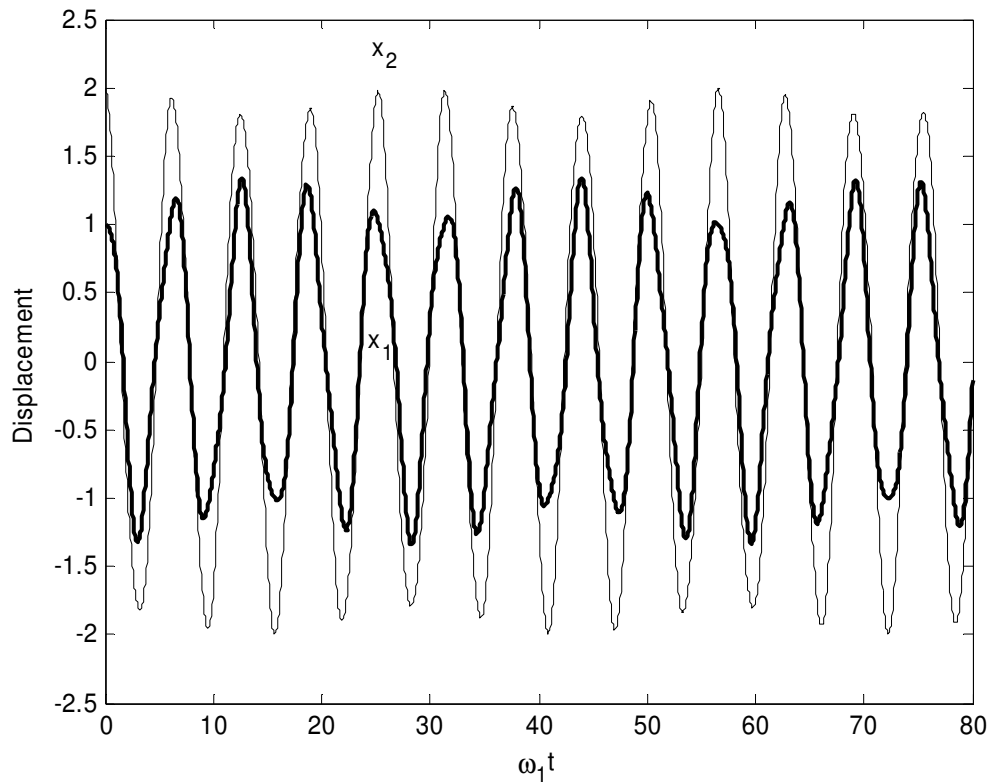
with a displacement ratio,  $x_2 / x_1 = -\frac{1}{2}(\sqrt{5} - 1) = -0.6180$ .

*Knowing these displacements ratios will enable you to start with the appropriate initial conditions for each normal mode.*

If you were to start at  $t = 0$  with a displacements  $x_1 = 1$  and  $x_2 = 2$  which isn't right for either normal mode, you can show that the subsequent displacements would be

$$\begin{aligned} x_1 &= 1.170820 \cos \omega_1 t - 0.170820 \cos \omega_2 t \\ x_2 &= 1.894427 \cos \omega_1 t + 0.105572 \cos \omega_2 t. \end{aligned}$$

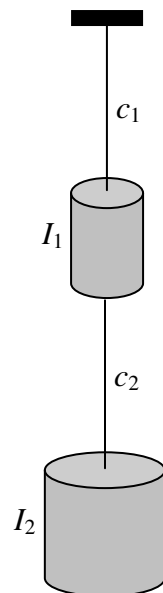
That looks like this:



Although at first it looks like fast in-phase mode for both of them, you can see the influence of the slow mode, which has about 2.6 times the period of the last mode, in the slow amplitude modulation. If you look carefully at the modulation amplitudes of both displacements, you will see that the amplitude of the  $x_1$  displacement is out of phase with the amplitude of the  $x_2$  displacement.

#### 17.4 Double Torsion Pendulum

FIGURE XVII.3



Here we have two cylinders of rotational inertias  $I_1$  and  $I_2$  hanging from two wires of torsion constants  $c_1$  and  $c_2$ . At any instant, the top cylinder is turned through an angle  $\theta_1$  from the equilibrium position and the lower cylinder by an angle  $\theta_2$  from the equilibrium position (so that, relative to the upper cylinder, it is turned by  $(\theta_2 - \theta_1)$ ). The equations and the description of the motion are just the same as in the previous example, except that  $x_1, x_2, m_1, m_2, k_1, k_2$  are replaced by  $\theta_1, \theta_2, I_1, I_2, c_1, c_2$ . The kinetic and potential energies are

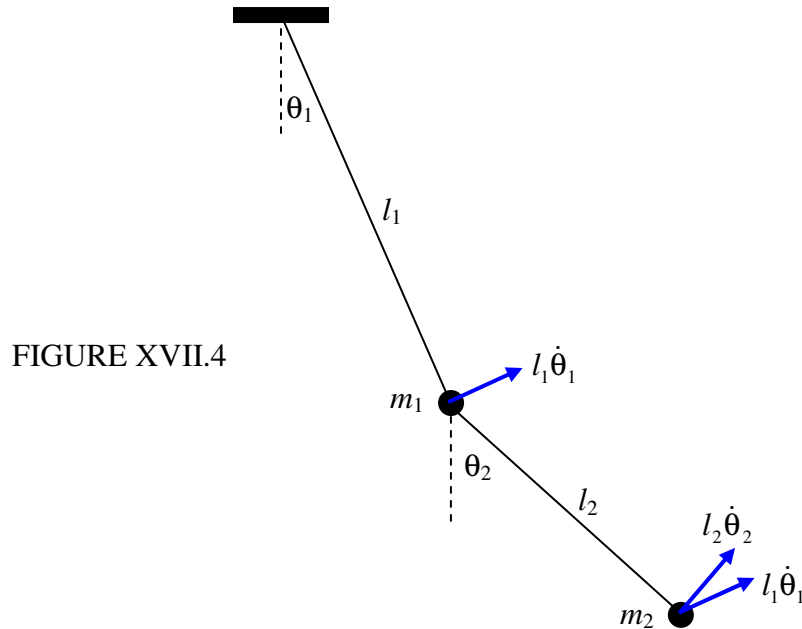
$$T = \frac{1}{2} I_1 \dot{\theta}_1^2 + \frac{1}{2} I_2 \dot{\theta}_2^2, \quad 17.4.1$$

$$V = \frac{1}{2} c_1 \theta_1^2 + \frac{1}{2} c_2 (\theta_2 - \theta_1)^2. \quad 17.4.2$$

The equations for  $\omega$  and the displacement ratios are just the same, and there is an in-phase and an out-of-phase mode.

### 17.5 Double Pendulum

This is another similar problem, though, instead of assuming Hooke's law, we shall assume that angles are small ( $\sin \theta \approx \theta$ ,  $\cos \theta \approx 1 - \frac{1}{2} \theta^2$ ). For clarity of drawing, however, I have drawn large angles in figure XVIII.4.



Because I am going to use the lagrangian equations of motion, I have not marked in the forces and accelerations; rather, I have marked in the velocities. I hope that the two components of the velocity of  $m_2$  that I have marked are self-explanatory; the speed of  $m_2$



is given by  $v_2^2 = l_1^2 \dot{\theta}_1^2 + l_2^2 \dot{\theta}_2^2 + 2l_1 l_2 \dot{\theta}_1 \dot{\theta}_2 \cos(\theta_2 - \theta_1)$ . The kinetic and potential energies are

$$T = \frac{1}{2} m_1 l_1^2 \dot{\theta}_1^2 + \frac{1}{2} m_2 [l_1^2 \dot{\theta}_1^2 + l_2^2 \dot{\theta}_2^2 + 2l_1 l_2 \dot{\theta}_1 \dot{\theta}_2 \cos(\theta_2 - \theta_1)], \quad 17.5.1$$

$$V = \text{constant} - m_1 g l_1 \cos \theta_1 - m_2 g (l_1 \cos \theta_1 + l_2 \cos \theta_2). \quad 17.5.2$$

If we now make the small angle approximation, these become

$$T = \frac{1}{2} m_1 l_1^2 \dot{\theta}_1^2 + \frac{1}{2} m_2 (l_1 \dot{\theta}_1 + l_2 \dot{\theta}_2)^2 \quad 17.5.3$$

$$\text{and } V = \text{constant} + \frac{1}{2} m_1 g l_1 \theta_1^2 + \frac{1}{2} m_2 g (l_1 \theta_1^2 + l_2 \theta_2^2) - m_1 g l_1 - m_2 g l_1 - m_2 g l_2. \quad 17.5.4$$

Apply the lagrangian equation in turn to  $\theta_1$  and  $\theta_2$ :

$$(m_1 + m_2) l_1^2 \ddot{\theta}_1 + m_2 l_1 l_2 \ddot{\theta}_2 = -(m_1 + m_2) g l_1 \theta_1 \quad 17.5.5$$

$$\text{and } m_2 l_1 l_2 \ddot{\theta}_1 + m_2 l_2^2 \ddot{\theta}_2 = -m_2 g l_2 \theta_2. \quad 17.5.6$$

Seek solutions of the form  $\ddot{\theta}_1 = -\omega^2 \theta_1$  and  $\ddot{\theta}_2 = -\omega^2 \theta_2$ .

$$\text{Then } (m_1 + m_2)(l_2 \omega^2 - g) \theta_1 + m_2 l_2 \omega^2 \theta_2 = 0 \quad 17.5.7$$

$$\text{and } l_1 \omega^2 \theta_1 + (l_2 \omega^2 - g) \theta_2 = 0. \quad 17.5.8$$

Either of these gives the displacement ratio  $\theta_2/\theta_1$ . Equating the two expressions for the ratio  $\theta_2/\theta_1$ , or putting the determinant of the coefficients to zero, gives the following equation for the frequencies of the normal modes:

$$m_1 l_1 l_2 \omega^4 - (m_1 + m_2) g (l_1 + l_2) \omega^2 + (m_1 + m_2) g^2 = 0. \quad 17.5.9$$

As in the previous examples, there is a slow in-phase mode, and fast out-of-phase mode.

For example, suppose  $m_1 = 0.01$  kg,  $m_2 = 0.02$  kg,  $l_1 = 0.3$  m,  $l_2 = 0.6$  m,  $g = 9.8$  m s<sup>-2</sup>.

Then  $0.0018\omega^4 - 0.2646\omega^2 + 2.8812 = 0$ . The slow solution is  $\omega = 3.441$  rad s<sup>-1</sup> ( $P = 1.826$  s), and the fast solution is  $\omega = 11.626$  rad s<sup>-1</sup> ( $P = 0.540$  s). If we put the first of these (the slow solution) in either of equations 17.5.7 or 8 (or both, as a check against mistakes) we obtain the displacement ratio  $\theta_2/\theta_1 = 1.319$ , which is an in-phase mode. If we put the second (the fast solution) in either equation, we obtain  $\theta_2/\theta_1 = -0.5689$ , which is an out-of-phase mode. If you were to start with  $\theta_2/\theta_1 = 1.319$  and let go, the

pendulum would swing in the slow in-phase mode. . If you were to start with  $\theta_2/\theta_1 = -0.5689$  and let go, the pendulum would swing in the fast out-of-phase mode. Otherwise the motion would be a linear combination of the normal modes, with the fraction of each determined by the initial conditions, as in the example in section 17.3.

### 17.6 Linear Triatomic Molecule

In Chapter 2, Section 2.9, we discussed a *rigid* triatomic molecule. Now we are going to discuss three masses held together by springs, of force constants  $k_1$  and  $k_2$ . We are going to allow it to vibrate, but not to rotate. Also, for the time being, I don't want the molecule to bend, so we'll put it inside a drinking straw to that all the vibrations are linear. By the way, for real triatomic molecules, the force constants and rotational inertias are such that molecules vibrate much faster than they rotate. To see their vibrations you look in the near infra-red spectrum; to see their rotation, you have to go to the far infrared or the microwave spectrum.

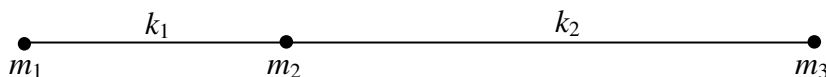


FIGURE XVII.5

Suppose that the equilibrium separations of the atoms are  $a_1$  and  $a_2$ . Suppose that at some instant of time, the  $x$ -coordinates (distances from the left hand edge of the page) of the three atoms are  $x_1, x_2, x_3$ . The extensions from the equilibrium distances are then  $q_1 = x_2 - x_1 - a_1$ ,  $q_2 = x_3 - x_2 - a_2$ . We are now ready to start:

$$T = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2, \quad 17.6.1$$

$$V = \frac{1}{2}k_1q_1^2 + \frac{1}{2}k_2q_2^2. \quad 17.6.2$$

We need to express the kinetic energy in terms of the internal coordinates, and, just as for the diatomic molecule (Section 17.2), the relevant equations are

$$\dot{q}_1 = \dot{x}_2 - \dot{x}_1, \quad 17.6.3$$

$$\dot{q}_2 = \dot{x}_3 - \dot{x}_2 \quad 17.6.4$$

and 
$$0 = m_1\dot{x}_1 + m_2\dot{x}_2 + m_3\dot{x}_3. \quad 17.6.5$$

These can conveniently be written

$$\begin{pmatrix} \dot{q}_1 \\ \dot{q}_2 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix}. \quad 17.6.6$$

By one dexterous flick of the fingers (!) we invert the matrix to obtain

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix} = \begin{pmatrix} -\frac{m_2+m_3}{M} & -\frac{m_3}{M} & \frac{1}{M} \\ \frac{m_1}{M} & -\frac{m_3}{M} & \frac{1}{M} \\ \frac{m_1}{M} & \frac{m_1+m_2}{M} & \frac{1}{M} \end{pmatrix} \begin{pmatrix} \dot{q}_1 \\ \dot{q}_2 \\ 0 \end{pmatrix}, \quad 17.6.7$$

where  $M = m_1 + m_2 + m_3$ . On putting these into equation 17.6.1, we now have

$$T = \frac{1}{2}(a\dot{q}_1^2 + 2h\dot{q}_1\dot{q}_2 + b\dot{q}_2^2) \quad 17.6.8$$

and 
$$V = \frac{1}{2}k_1q_1^2 + \frac{1}{2}k_2q_2^2, \quad 17.6.2$$

where 
$$a = m_1(m_2 + m_3) / M, \quad 17.6.9$$

$$h = m_3m_1 / M, \quad 17.6.10$$

$$b = m_3(m_1 + m_2) / M \quad 17.6.11$$

and, for future reference,

$$ab - h^2 = m_1m_2m_3 / M = m_2h. \quad 17.6.12$$

On application of Lagrange's equation in turn to the two internal coordinates we obtain

$$a\ddot{q}_1 + h\ddot{q}_2 + k_1q_1 = 0 \quad 17.6.13$$

and 
$$b\ddot{q}_2 + h\ddot{q}_1 + k_2q_2 = 0. \quad 17.6.14$$

Seek solutions of the form  $\ddot{q}_1 = -\omega^2q_1$  and  $\ddot{q}_2 = -\omega^2q_2$  and we obtain the following two expressions for the extension ratios:

$$\frac{q_1}{q_2} = \frac{h\omega^2}{k_1 - a\omega^2} = \frac{k_2 - b\omega^2}{h\omega^2}. \quad 17.6.15$$

Equating them gives the equation for the normal mode frequencies:

$$(ab - h^2)\omega^4 - (ak_2 + bk_1)\omega^2 + k_1k_2 = 0. \quad 17.6.16$$

For example, if  $k_1 = k_2 = k$  and  $m_1 = m_2 = m_3 = m$ , we obtain, for the slow symmetric (“breathing”) mode,  $q_1/q_2 = +1$  and  $\omega^2 = k/m$ . For the fast asymmetric mode,  $q_1/q_2 = -1$  and  $\omega^2 = 3k/m$ .

*Example.*

Consider the linear OCS molecule whose atoms have masses 16, 12 and 32. Suppose that the angular frequencies of the normal modes, as determined from infrared spectroscopy, are 0.905 and 0.413. (I just made these numbers up, in unstated units, just for the purpose of illustrating the calculation. Without searching the literature, I can’t say what they are in the real OCS molecule.) Determine the force constants.

In Chapter 2 we considered a rigid triatomic molecule. We were given the moment of inertia, and we were asked to find the two internuclear distances. We couldn’t do this with just one moment of inertia, so we made an isotopic substitution ( $^{18}\text{O}$  instead of  $^{16}\text{O}$ ) to get a second equation, and so we could then solve for the two internuclear distances. This time, we are dealing with vibration, and we are going to use equation 17.6.16 to find the two force constants. This time, however, we are given two frequencies (of the normal modes), and so we have no need to make an isotopic substitution – we already have two equations.

Here are the necessary data.

$^{16}\text{OCS}$					
Fast $\omega$	0.905				
Slow $\omega$	0.413				
$m_1$	$m_2$	$m_3$	16	12	32
$M$	60				
$a$	11.73				
$h$	8.53				
$b$	14.93				
$ab - h^2$	102.4				

Use equation 17.6.16 for each of the frequencies, and you’ll get two equations, in  $k_1$  and  $k_2$ . As in the rotational case, they are quadratic equations, but they are a bit easier to solve than in the rotational case. You’ll get two equations, each of the form

$A - Bk_1 - Ck_2 + k_1k_2 = 0$ , where the coefficients are functions of  $a, b, h, \omega$ . You’ll have to work out the values of these coefficients, but, before you substitute the numbers

in, you might want to give a bit of thought to how you would go about solving two simultaneous equations of the form  $A - Bk_1 - Ck_2 + k_1k_2 = 0$ .

You will find that there are two possible solutions:

$$k_1 = 2.8715 \quad k_2 = 4.9818$$

and

$$k_1 = 3.9143 \quad k_2 = 3.6547$$

Both of these will result in the same frequencies. You would need some additional information to determine which obtains for the actual molecule, perhaps with measurements on an isotopomer, such as  $^{18}\text{OCS}$ .

Note that in this section we considered a linear triatomic molecule that was not allowed either to rotate or to bend, whereas in Chapter 2 we considered a rigid triatomic molecule that was not allowed either to vibrate or to bend. If all of these restrictions are removed, the situation becomes rather more complicated. If a rotating molecule vibrates, the moving atoms, in a co-rotating reference frame, are subject to the Coriolis force, and hence they do not move in a straight line. Further, as it vibrates, the rotational inertia changes periodically, so the rotation is not uniform. If we allow the molecule to bend, the middle atom can oscillate up and down in the plane of the paper (so to speak) or back and forth at right angles to the plane of the paper. These two motions will not necessarily have either the same amplitude or the same phase. Consequently the middle atom will whirl around in a Lissajous ellipse, giving rise to what has been called “vibrational angular momentum”. In a real triatomic molecule, the vibrations are usually much faster than the relatively slow, ponderous rotation, so that vibration-rotation interaction is small – but is by no means negligible and is readily observed in the spectrum of the molecule.

### 17.7 Two Masses, Three Springs, Two Brick Walls

The three masses are equal, and the two outer springs are identical. Figure XVII.6 shows the equilibrium position.

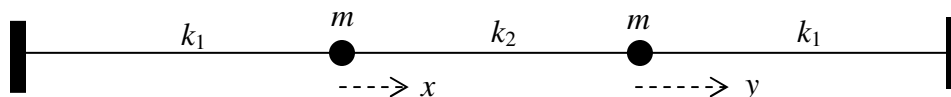


FIGURE XVII.6

Suppose that at some instant the first mass is displaced a distance  $x$  to the right and the second mass is displaced a distance  $y$  to the right. The extensions of the first two springs are  $x$  and  $y - x$  respectively, and the compression of the third spring is  $y$ . If the speeds of the masses are  $\dot{x}$  and  $\dot{y}$ , we have for the kinetic and potential energies:

$$T = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\dot{y}^2 \quad 17.7.1$$

and 
$$V = \frac{1}{2}k_1x^2 + \frac{1}{2}k_2(y-x)^2 + \frac{1}{2}k_1y^2. \quad 17.7.2$$

Apply Lagrange's equation in turn to  $x$  and to  $y$ .

$$m\ddot{x} + (k_1 + k_2)x - k_2y = 0 \quad 17.7.3$$

and 
$$m\ddot{y} + (k_1 + k_2)y - k_2x = 0. \quad 17.7.4$$

Seek solutions of the form  $\ddot{x} = -\omega^2x$  and  $\ddot{y} = -\omega^2y$ .

$$(-m\omega^2 + k_1 + k_2)x - k_2y = 0 \quad 17.7.5$$

and 
$$-k_2x + (-m\omega^2 + k_1 + k_2)y = 0. \quad 17.7.6$$

On putting the determinant of the coefficients to zero, we find for the frequencies of the normal modes

$$\omega^2 = \frac{k_1}{m} \quad \text{and} \quad \omega^2 = \frac{k_1 + 2k_2}{m}, \quad 17.7.7a,b$$

corresponding to displacement ratios

$$\frac{x}{y} = 1 \quad \text{and} \quad \frac{x}{y} = -1. \quad 17.7.8a,b$$

In the first, slow, mode, the masses move in phase and there is no extension or compression of the connecting spring. In the second, fast, mode, the masses move in antiphase and the compression or extension of the coupling spring is twice the extension or compression of the outer springs.

The general motion is a linear combination of the normal modes:

$$x = A\cos(\omega_1t + \alpha_1) + B\cos(\omega_2t + \alpha_2), \quad 17.7.9$$

$$y = A\cos(\omega_1t + \alpha_1) - B\cos(\omega_2t + \alpha_2), \quad 17.7.10$$

$$\dot{x} = -A\omega_1 \sin(\omega_1 t + \alpha_1) - B\omega_2 \sin(\omega_2 t + \alpha_2), \quad 17.7.11$$

$$\dot{y} = -A\omega_1 \sin(\omega_1 t + \alpha_1) + B\omega_2 \sin(\omega_2 t + \alpha_2). \quad 17.7.12$$

Suppose that the initial condition is at  $t = 0$ ,  $y = \dot{y} = 0$ ,  $x = x_0$ ,  $\dot{x} = 0$ . That is, we pull the first mass a little to the right (keeping the second mass fixed) and then we let go. The second two equations establish that  $\alpha_1 = \alpha_2 = 0$ , and the first two equations tell us that  $A = B = x_0/2$ . The displacements are then given by

$$x = \frac{1}{2}x_0(\cos \omega_1 t + \cos \omega_2 t) = x_0 \cos \frac{1}{2}(\omega_1 - \omega_2)t \cos \frac{1}{2}(\omega_1 + \omega_2)t \quad 17.7.13$$

$$\text{and } y = \frac{1}{2}x_0(\cos \omega_1 t - \cos \omega_2 t) = -x_0 \sin \frac{1}{2}(\omega_1 - \omega_2)t \sin \frac{1}{2}(\omega_1 + \omega_2)t. \quad 17.7.14$$

Let us imagine, for example, that  $k_2$  is much less than  $k_1$  (but not negligible), so that we have two *weakly-coupled oscillators*. In that case equations 17.7.7 tell us that the frequencies of the two normal modes are nearly equal. What equation 17.7.13 describes, then, is a rapid oscillation of the first mass with angular frequency  $\frac{1}{2}(\omega_1 + \omega_2)$  whose amplitude is modulated with a slow angular frequency  $\frac{1}{2}(\omega_1 - \omega_2)$ . Equation 17.7.14 describes the same sort of motion for the second mass, except that the modulation is out of phase by  $90^\circ$  with the modulation of the motion of the first mass. For a while the first mass will oscillate with a large amplitude. This will gradually decrease, while the amplitude of the motion of the second mass increases until the motion of the first mass momentarily ceases. After that, the amplitude of the motion of the second mass starts to decrease, while the first mass starts up again. And so the motion continues, with the first mass and the second mass alternately taking up the motion.

### 17.8 Transverse Oscillations of Masses on a Taut String

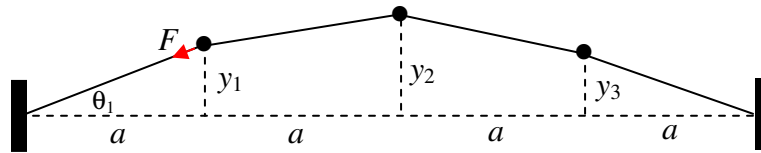


FIGURE XVII.7

A light string of length  $4a$  is held taut, under tension  $F$  between two fixed points. Three equal masses  $m$  are attached at equidistant points along the string. They are set into transverse oscillation of small amplitudes, the transverse displacements of the three masses at some time being  $y_1$ ,  $y_2$  and  $y_3$ .

The kinetic energy is easy. It is just

$$T = \frac{1}{2}m(\dot{y}_1^2 + \dot{y}_2^2 + \dot{y}_3^2). \quad 17.8.1$$

The potential energy is slightly more difficult.

In the undisplaced position, the length of each portion of the string is  $a$ .

In the displaced position, the lengths of the four portions of the string are, respectively,

$$\sqrt{y_1^2 + a^2} \quad \sqrt{(y_2 - y_1)^2 + a^2} \quad \sqrt{(y_2 - y_3)^2 + a^2} \quad \sqrt{y_3^2 + a^2}$$

For small displacements (i.e. the  $y$ s much smaller than  $a$ ), these are, approximately (by binomial expansion),

$$a + \frac{y_1^2}{2a} \quad a + \frac{(y_2 - y_1)^2}{2a} \quad a + \frac{(y_2 - y_3)^2}{2a} \quad a + \frac{y_3^2}{2a}$$

so the extensions are

$$\frac{y_1^2}{2a} \quad \frac{(y_2 - y_1)^2}{2a} \quad \frac{(y_2 - y_3)^2}{2a} \quad \frac{y_3^2}{2a}$$

It is also supposed that the tension in the string is  $F$  and that the displacements are sufficiently small that this is constant. The work done in displacing the masses, which is the elastic energy stored in the string as a result of the displacements, is therefore

$$V = \frac{F}{2a} [y_1^2 + (y_2 - y_1)^2 + (y_2 - y_3)^2 + y_3^2] = \frac{F}{a} (y_1^2 + y_2^2 + y_3^2 - y_1 y_2 - y_2 y_3).$$

We note with mild irritation the presence of the cross-terms  $y_1 y_2$ ,  $y_2 y_3$ .

Apply Lagrange's equation in turn to the three coordinates:

$$am\ddot{y}_1 + F(2y_1 - y_2) = 0, \quad 17.8.3$$

$$am\ddot{y}_2 + F(-y_1 + 2y_2 - y_3) = 0, \quad 17.8.4$$

$$am\ddot{y}_3 + F(-y_2 + 2y_3) = 0. \quad 17.8.5$$

Seek solutions of the form  $\ddot{y}_1 = -\omega^2 y_1$ ,  $\ddot{y}_2 = -\omega^2 y_2$ ,  $\ddot{y}_3 = -\omega^2 y_3$ .

$$\text{Then} \quad (2F - am\omega^2)y_1 - Fy_2 = 0, \quad 17.8.6$$

$$-Fy_1 + (2F - am\omega^2)y_2 - Fy_3 = 0, \quad 17.8.7$$



$$-Fy_2 + (2F - am\omega^2)y_3 = 0. \quad 17.8.8$$

Putting the determinant of the coefficients to zero gives an equation for the frequencies of the normal modes. The solutions are:

$$\begin{array}{ccc} \text{Slow} & \text{Medium} & \text{Fast} \\ \omega_1^2 = \frac{(2 - \sqrt{2})F}{am} & \omega_2^2 = \frac{2F}{am} & \omega_3^2 = \frac{(2 + \sqrt{2})F}{am} \end{array}$$

Substitution of these into equations 17.8.6 to 8 gives the following displacement ratios for these three modes:

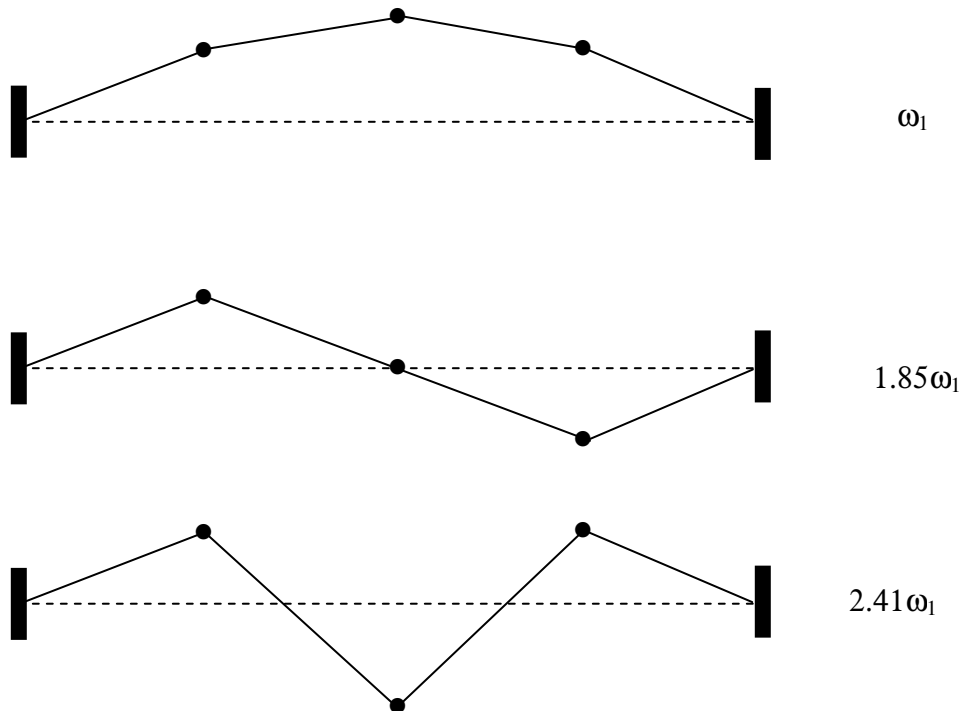
$$y_1 : y_2 : y_3 = 1 : \sqrt{2} : 1 \qquad 1 : 0 : -1 \qquad 1 : -\sqrt{2} : 1$$

These are illustrated in figure XVII.8.

As usual, the general motion is a linear combination of the normal modes, the relative amplitudes and phases of the modes depending upon the initial conditions.

If the motion of the first mass is a combination of the three modes with relative amplitudes in the proportion  $\hat{q}_1 : \hat{q}_2 : \hat{q}_3$ , and with initial phases  $\alpha_1, \alpha_2, \alpha_3$ , its motion is described by

$$y_1 = \hat{q}_1 \sin(\omega_1 t + \alpha_1) + \hat{q}_2 \sin(\omega_2 t + \alpha_2) + \hat{q}_3 \sin(\omega_3 t + \alpha_3). \quad 17.8.9$$



The motions of the second and third masses are then described by

FIGURE XVII.8

$$y_2 = \sqrt{2}\hat{q}_1 \sin(\omega_1 t + \alpha_1) - \sqrt{2}\hat{q}_3 \sin(\omega_3 t + \alpha_3) \quad 17.8.10$$

and 
$$y_3 = \hat{q}_1 \sin(\omega_1 t + \alpha_1) - \hat{q}_2 \sin(\omega_2 t + \alpha_2) + \hat{q}_3 \sin(\omega_3 t + \alpha_3). \quad 17.8.11$$

These can be written

$$y_1 = q_1 + q_2 + q_3, \quad 17.8.12$$

$$y_2 = \sqrt{2}q_1 - \sqrt{2}q_3 \quad 17.8.13$$

and 
$$y_1 = q_1 - q_2 + q_3, \quad 17.8.14$$

where the  $q_i$ , like the  $y_i$ , are time-dependent coordinates.

We could, if we wish, express the  $q_i$  in terms of the  $y_i$ , by solving these equations:

$$q_1 = \frac{1}{4}(y_1 + \sqrt{2}y_2 + y_3), \quad 17.8.15$$

$$q_2 = \frac{1}{2}(y_1 - y_3) \quad 17.8.16$$

and 
$$q_3 = \frac{1}{4}(y_1 - \sqrt{2}y_2 + y_3). \quad 17.8.17$$

We have hitherto described the state of the system as a function of time by giving the values of the coordinates  $y_1$ ,  $y_2$  and  $y_3$ . We could equally well, if we wished, describe the state of the system by giving, instead, the values of the coordinates  $q_1$ ,  $q_2$  and  $q_3$ . Indeed it turns out that it is very useful to do so, and these coordinates are called the *normal coordinates*, and we shall see that they have some special properties. Thus, if you express the kinetic and potential energies in terms of the normal coordinates, you get

$$T = \frac{1}{2}m(4\dot{q}_1^2 + 2\dot{q}_2^2 + 4\dot{q}_3^2) \quad 17.8.18$$

and 
$$V = \frac{2F}{a} \left[ (2 - \sqrt{2})q_1^2 + q_2^2 + (2 + \sqrt{2})q_3^2 \right]. \quad 17.8.19$$

Note that there are *no cross terms*. When you apply Lagrange's equation in turn to the three normal coordinates, you obtain

$$am\ddot{q}_1 = -(2 - \sqrt{2})Fq_1, \quad 17.8.20$$

$$am\ddot{q}_2 = -2Fq_2 \quad 17.8.21$$

and 
$$am\ddot{q}_3 = -(2 + \sqrt{2})Fq_3. \quad 17.8.22$$

Notice that the normal coordinates have become completely separated into three independent equations and that each is of the form  $\ddot{q} = -\omega^2 q$  and that each of the normal coordinates oscillates with one of the frequencies of the normal modes. Much of the art of solving problems involving vibrating systems concerns identifying the normal coordinates.

### 17.9 Vibrating String

It is possible that the three modes of vibration of the three masses in section 17.8 reminded you of the fundamental and first two harmonic vibrations of a stretched string – and it is quite proper that it did. If you were to imagine ten masses attached to a stretched string and to carry out the same sort of analysis, you would find ten normal modes, of which one would be quite like the fundamental mode of a stretched string, and the remainder would remind you of the first nine harmonics. You could continue with the same analysis but with a very large number of masses, and eventually you would be analysing the vibrations of a continuous heavy string. We do that now, and we assume that we have a heavy, taut string of mass  $\mu$  per unit length, and under a tension  $F$ .

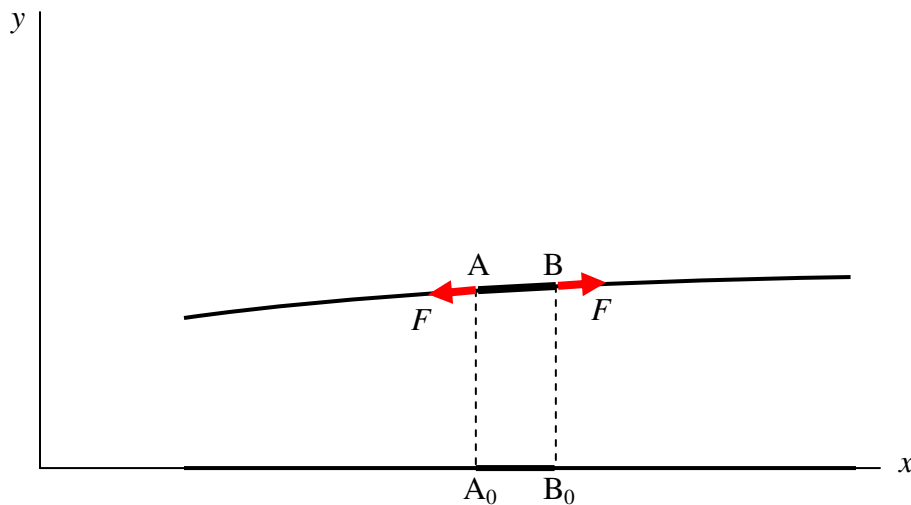


FIGURE XVII.9

I show in figure XVII.9 a portion of length  $\delta x$  of a vibrating rope, represented by  $A_0B_0$  in its equilibrium position and by  $AB$  in a displaced position. The rope makes an angle  $\psi_A$

with the horizontal at A and an angle  $\psi_B$  with the horizontal at B. The tension in the rope is  $F$ . The vertical equation of motion is

$$F(\sin \psi_B - \sin \psi_A) = \mu \delta x \frac{\partial^2 y}{\partial t^2}. \quad 17.9.1$$

If the angles are small, then  $\sin \psi \cong \frac{\partial y}{\partial x}$ , so the expression in parenthesis is  $\frac{\partial^2 y}{\partial x^2} \delta x$ . The equation of motion is therefore

$$c^2 \frac{\partial^2 y}{\partial x^2} = \frac{\partial^2 y}{\partial t^2}, \text{ where } c = \sqrt{\frac{T}{\mu}}. \quad 17.9.2, a, b$$

As can be verified by substitution, the general solution to this is of the form

$$y = f(x - ct) + g(x + ct). \quad 17.9.3$$

This represents a function that can travel in either direction along the rope at a speed  $c$  given by equation 17.9.2b. Should the disturbance be a periodic disturbance, then a wave will travel along the rope at that speed. Further analysis of waves in ropes and strings is generally done in chapters concerned with wave motion. This section, however, at least establishes the speed at which a disturbance (periodic or otherwise) travels along a stretched strong or rope.

### 17.10 Water

Water consists of a mass  $M$  ("oxygen") connected to two smaller equal masses  $m$  ("hydrogen") by two equal springs of force constants  $k$ , the angle between the springs being  $2\theta$ . The equilibrium length of each spring is  $r$ . The torque needed to increase the angle between the springs by  $2\delta\theta$  is  $2c\delta\theta$ . See figure XVII.10. ( $\theta$  is about  $52^\circ$ .)

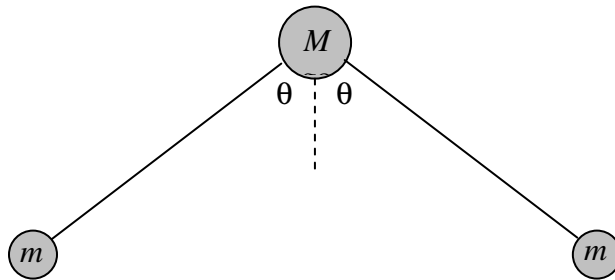


FIGURE XVII.10

At any time, let the coordinates of the three masses (from left to right) be

$$(x_1, y_1), (x_2, y_2), (x_3, y_3)$$

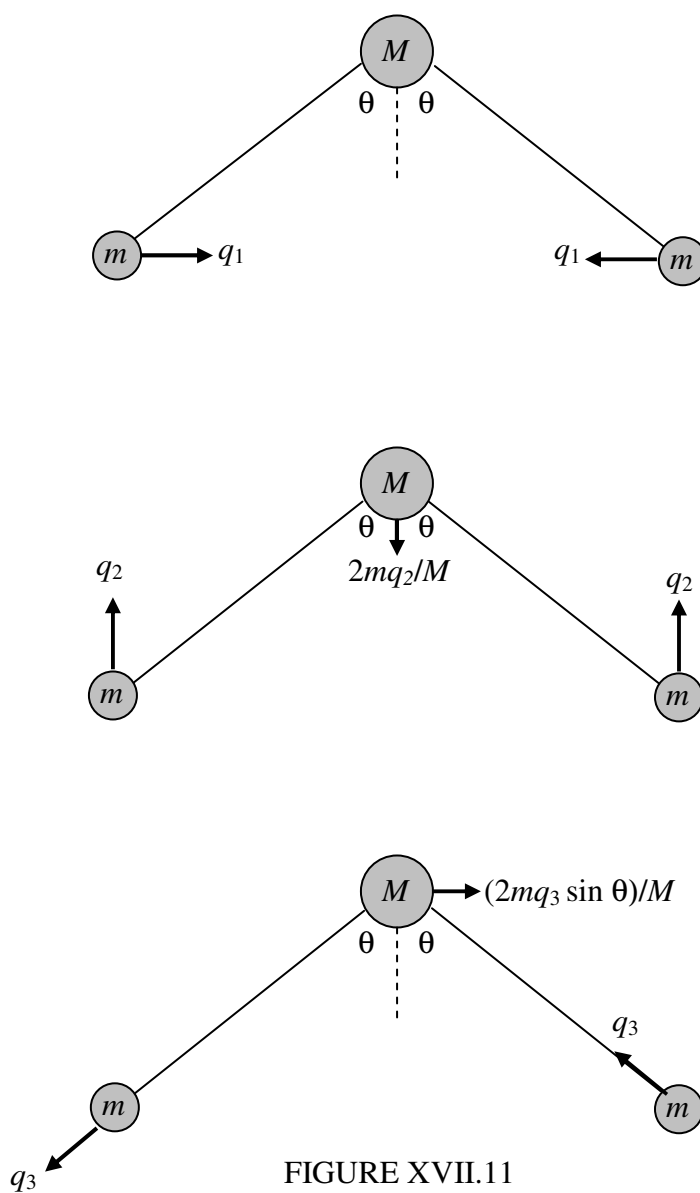
and let the equilibrium positions be

$$(x_{10}, y_{10}), (x_{20}, y_{20}), (x_{30}, y_{30}), \text{ where } y_{30} = y_{10}.$$

We suppose that these coordinates are referred to a frame in which the centre of mass of the system is stationary.

Let us try and imagine, in figure XVII.11, the vibrational modes. We can easily imagine a mode in which the angle opens and closes symmetrically. Let us resolve this mode into an  $x$ -component and a  $y$ -component. In the  $x$ -component of this motion, one hydrogen atom moves to the right by a distance  $q_1$  while the other moves to the left by an equal distance  $q_1$ . In the  $y$ -component of this symmetric motion, both hydrogens move upwards by a distance  $q_2$ , while, in order to keep the centre of mass of the system unmoved, the oxygen necessarily moves down by a distance  $2mq_2/M$ . We can also imagine an asymmetric mode in which one spring expands while the other contracts. One hydrogen moves down to the left by a distance  $q_3$ , while the other moves up to the left by the same distance. In the meantime, the oxygen must move to the right by a distance  $(2mq_3 \sin \theta)/M$ , in order to keep the centre of mass unmoved.

We are going to try to write down the kinetic and potential energies in terms of the internal coordinates  $q_1, q_2$  and  $q_3$ .



It is easy to write down the kinetic energy in terms of the  $(x, y)$  coordinates:

$$T = \frac{1}{2}m(\dot{x}_1^2 + \dot{y}_1^2) + \frac{1}{2}M(\dot{x}_2^2 + \dot{y}_2^2) + \frac{1}{2}m(\dot{x}_3^2 + \dot{y}_3^2). \quad 17.10.1$$

From geometry, we have:

$$\dot{x}_1 = \dot{q}_1 - \dot{q}_3 \sin \theta \quad \dot{y}_1 = \dot{q}_2 - \dot{q}_3 \cos \theta \quad 17.10.2a,b$$

$$\dot{x}_2 = \frac{2m\dot{q}_3 \sin \theta}{M} \quad \dot{y}_2 = -\frac{2m\dot{q}_2}{M} \quad 17.10.3a,b$$

$$\dot{x}_3 = -\dot{q}_1 - \dot{q}_3 \sin \theta \quad \dot{y}_3 = \dot{q}_2 + \dot{q}_3 \cos \theta \quad 17.10.4a,b$$

On putting these into equation 17.10.1 we obtain

$$T = m\dot{q}_1^2 + m(1 + 2m/M)\dot{q}_2^2 + m(1 + (2m \sin^2 \theta)/M)\dot{q}_3^2. \quad 17.10.5$$

For short, I am going to write this as

$$T = a_{11}\dot{q}_1^2 + a_{22}\dot{q}_2^2 + a_{33}\dot{q}_3^2. \quad 17.10.6$$

Now for the potential energy.

The extension of the left hand spring is

$$\begin{aligned} \delta r_1 &= -q_1 \sin \theta - q_2 \cos \theta - \frac{2mq_2 \cos \theta}{M} + q_3 + \frac{2mq_3 \sin \theta \cos \theta}{M} \\ &= -q_1 \sin \theta - q_2(1 + 2m/M) \cos \theta + q_3(1 + (2m \sin \theta \cos \theta)/M). \end{aligned} \quad 17.10.7$$

The extension of the right hand spring is

$$\begin{aligned} \delta r_2 &= -q_1 \sin \theta - q_2 \cos \theta - \frac{2mq_2 \cos \theta}{M} - q_3 - \frac{2mq_3 \sin^2 \theta}{M} \\ &= -q_1 \sin \theta - q_2(1 + 2m/M) \cos \theta - q_3(1 + (2m \sin^2 \theta)/M). \end{aligned} \quad 17.10.8$$

The increase in the angle between the springs is

$$2\delta\theta = -\frac{2q_1 \cos \theta}{r} + \frac{2(1 + 2m/M)q_2 \sin \theta}{r}. \quad 17.10.9$$

The potential energy (above the equilibrium position) is

$$V = \frac{1}{2}k(\delta r_1)^2 + \frac{1}{2}k(\delta r_2)^2 + \frac{1}{2}c(2\delta\theta)^2. \quad 17.10.10$$

On substituting equations 17.10,7,8 and 9 into this, we obtain an equation of the form

$$V = b_{11}q_1^2 + 2b_{12}q_1q_2 + b_{22}q_2^2 + b_{33}q_3^2, \quad 17.10.11$$

where I leave it to the reader, if s/he wishes, to work out the detailed expressions for the coefficients. We still have a cross term, so we can't completely separate the coordinates, but we can easily apply Lagrange's equation to equations 17.10.6 and 11, and then seek simple harmonic solutions in the usual way. Setting the determinant of the coefficients to zero leads to the following equation for the angular frequencies of the normal modes:

$$\begin{vmatrix} b_{11} - \omega^2 a_{11} & b_{12} & 0 \\ b_{12} & b_{22} - \omega^2 a_{22} & 0 \\ 0 & 0 & b_{33} - \omega^2 a_{33} \end{vmatrix} = 0. \quad 17.10.12$$

Thus, given the masses and  $r$ ,  $\theta$ ,  $k$  and  $c$ , one can predict the frequencies of the normal modes. Can one calculate  $k$  and  $c$  given the frequencies? I don't know, to tell the truth. Can I leave it to the reader to investigate further?

### 17.11 *A General Vibrating System*

For convenience, I'll refer to a collection of masses connected by springs as a "molecule", and the individual masses as "atoms". In a molecule with  $N$  atoms, the number of degrees of vibrational freedom (the number of normal modes of vibration)  $n = 3N - 6$  for nonlinear molecules, or  $n = 3N - 5$  for linear molecules. Three equations are needed to express zero translational motion, and three (or two) are needed to express zero rotational motion.

[While reading this Section, it might be worthwhile for the reader to follow at the same time the treatment given to the OCS molecule in Section 17.6. Bear in mind, however, that in that section we did not consider the possibility of the molecule bending. Indeed we treated the molecule as if it were constrained inside a drinking straw, and it remained linear at all times. That being the case only  $N$  coordinates (rather than  $3N$ ) suffice to describe the state of the molecule. Only one equation is needed to express zero translational motion, and none are needed to express zero rotational motion. Thus there are  $N - 1$  internal coordinates, and hence  $N - 1$  normal vibrational modes. In the case of OCS,  $N = 3$ , so there are two normal vibrational modes.]

A molecule with  $n$  degrees of vibrational freedom can be described at some instant of time by  $n$  internal coordinates  $q_i$ . A typical such coordinate may be related to the external coordinates of two atoms, for example, by some expression of the form  $q = x_2 - x_1 - a$ , as we saw in our example of the molecule OCS. Its potential energy can be written in the form



$$\begin{aligned}
2V = & \kappa_{11}q_1^2 + \kappa_{12}q_1q_2 + \dots & + \kappa_{1n}q_1q_n \\
& + \kappa_{21}q_2q_1 + \kappa_{22}q_2^2 + \dots & + \kappa_{2n}q_2q_n \\
& + \dots & \\
& + \kappa_{n1}q_nq_1 + \kappa_{12}q_nq_2 + \dots & + \kappa_{nn}q_nq_n.
\end{aligned}
\tag{17.11.1}$$

Unless the  $q$  are the judiciously chosen "normal coordinates" (see our example of the transverse vibrations of three masses on an elastic string), there will in general be cross terms, such as  $q_1q_2$ . If both  $qs$  of a term are linear displacements, the corresponding  $\kappa$  is a force constant (dimensions  $MT^{-2}$ ). If both  $qs$  are angles,  $\kappa$  is a torsion constant (dimensions  $ML^2T^{-2}$ ). If one is a linear displacement and the other is an angular displacement,  $\kappa$  will be a coefficient of dimensions  $MLT^{-2}$ .

The matrix is symmetric, so that equation 17.11.1 could also be written

$$\begin{aligned}
2V = & \kappa_{11}q_1^2 + 2\kappa_{12}q_1q_2 + \dots & + 2\kappa_{1n}q_1q_n \\
& + \kappa_{22}q_2^2 & + \dots & + 2\kappa_{2n}q_2q_n \\
& & + \dots & \\
& & & + \kappa_{nn}q_nq_n.
\end{aligned}
\tag{17.11.2}$$

In matrix notation, the equation (i.e. equations 17.11.1 or 17.11.2) could be written:

$$2V = \tilde{\mathbf{q}} \boldsymbol{\kappa} \mathbf{q} . \tag{17.11.3}$$

or in vector/tensor notation,  $2V = \mathbf{q} \cdot \boldsymbol{\kappa} \mathbf{q} . \tag{17.11.4}$

The kinetic energy can be written in terms of the time rates of change of the external coordinates  $x_i$ :

$$2T = m_1\dot{x}_1^2 + m_2\dot{x}_2^2 + \dots + m_{3N}\dot{x}_{3N}^2 . \tag{17.11.5}$$

To make use of the Lagrangian equations of motion, we need to express  $V$  and  $T$  in terms of the same coordinates, and it is usually advantageous if these be the  $n$  internal coordinates rather than the  $3N$  external coordinates – so that we have to deal with only  $n$  rather than  $3N$  lagrangian equations. (Recall that  $n = 3N - 6$  or  $5$ .) The relations between the external and internal coordinates are given as a set of equations that express a choice of coordinates such that there is no pure translation and no pure rotation of the molecule. These equations are of the form

$$\mathbf{q} = \mathbf{A}\mathbf{x} . \tag{17.11.6}$$

Here  $\mathbf{q}$  is an  $n \times 1$  column matrix,  $\mathbf{x}$  a  $3N \times 1$  column matrix, and  $\mathbf{A}$  is a matrix with  $n$  rows and  $3N$  columns, and it may need a little trouble to set up. We could then use this to express  $V$  in terms of the external coordinates, so we would then have both  $V$  and  $T$  in terms of the external coordinates. We could then apply Lagrange's equation to each of the  $3N$  external coordinates and arrive at  $3N$  simultaneous differential equations of motion.

A better approach is usually to set up the equations connecting  $\dot{\mathbf{q}}$  and  $\dot{\mathbf{x}}$ :

$$\dot{\mathbf{q}} = \mathbf{B}\dot{\mathbf{x}}. \quad 17.11.7$$

(These correspond to equations 17.6.3 and 17.6.4 in our example of the linear triatomic molecule in Section 17.6.) We then want to invert equations 17.11.7 in order to express  $\dot{\mathbf{x}}$  in terms of  $\dot{\mathbf{q}}$ . But we can't do this, because  $\mathbf{B}$  is not a square matrix.  $\dot{\mathbf{x}}$  has  $3N$  elements while  $\dot{\mathbf{q}}$  has only  $n$ . We have to add an additional six (or five for linear molecules) equations to express zero pure translational and zero pure rotational motion. This adds a further 6 or 5 rows to  $\mathbf{B}$ , so that  $\mathbf{B}$  is now square (this corresponds to equation 17.6.6), and we can then invert equation 17.11.7:

$$\dot{\mathbf{x}} = \mathbf{B}^{-1}\dot{\mathbf{q}}. \quad 17.11.8$$

(This corresponds to equation 17.6.7.)

By this means we can express the kinetic energy in terms of the time rates of change of only the  $n$  internal coordinates:

$$\begin{aligned} 2T = & \mu_{11}\dot{q}_1^2 + \mu_{12}\dot{q}_1\dot{q}_2 + \dots + \mu_{1n}\dot{q}_1\dot{q}_n \\ & + \mu_{21}\dot{q}_2\dot{q}_1 + \mu_{22}\dot{q}_2^2 + \dots + \mu_{2n}\dot{q}_2\dot{q}_n \\ & + \dots \\ & + \mu_{n1}\dot{q}_n\dot{q}_1 + \mu_{n2}\dot{q}_n\dot{q}_2 + \dots + \mu_{nn}\dot{q}_n^2. \end{aligned} \quad 17.11.7$$

Since the matrix is symmetric, the equation could also be written in a form analogous to equation 17.11.2. The equation can also be written in matrix notation as

$$2T = \tilde{\mathbf{q}}\boldsymbol{\mu}\dot{\mathbf{q}}. \quad 17.11.8$$

or in vector/tensor notation, 
$$2T = \dot{\mathbf{q}} \cdot \boldsymbol{\mu} \dot{\mathbf{q}}. \quad 17.11.9$$

Here the  $\mu_{ij}$  are functions of the masses. If both  $q$ s in a particular term have the dimensions of a length, the corresponding  $\mu$  and  $\kappa$  will have dimensions of mass and force constant. If both  $q$ s are angles, the corresponding  $\mu$  and  $\kappa$  will have dimensions of rotational inertia and torsion constant.. If one  $q$  is a length and the other is an angle, the corresponding  $\mu$  and  $\kappa$  will have dimensions  $ML$  and  $MLT^{-2}$ .

Apply Lagrange's equation successively to  $q_1, \dots, q_n$  to obtain  $n$  equations of the form

$$\mu_{11}\ddot{q}_1 + \dots + \mu_{1n}\ddot{q}_n + \kappa_{11}q_1 + \dots + \kappa_{1n}q_n = 0. \quad 7.11.10$$

That is to say

$$\boldsymbol{\mu}\ddot{\mathbf{q}} = -\boldsymbol{\kappa}\mathbf{q}. \quad 17.11.11$$

Seek simple harmonic solutions of the form  $\ddot{q} = -\omega^2 q$

and we obtain  $n$  equations of the form

$$(\kappa_{11} - \mu_{11}\omega^2)q_1 + \dots + (\kappa_{1n} - \mu_{1n}\omega^2)q_n = 0. \quad 17.11.13$$

The frequencies of the normal modes can be obtained by equating the determinant of the coefficients to zero, and hence the displacement ratios can be determined.

If  $N$  is large, this could be a formidable task. The work can be very much reduced by making use of symmetry relations of the molecule, in which case the determinant of the coefficients may be factored into a number of much smaller subdeterminants. Further, if the configuration of the molecule could be expressed in terms of *normal coordinates* (combinations of the internal coordinates) such that the potential energy contained no cross terms, the equations of motion for each normal coordinate would be in the form  $\ddot{q} = -\omega^2 q$ .

### 17.12 A Driven System

It would probably be useful before reading this and the next section to review Chapters 11 and 12.

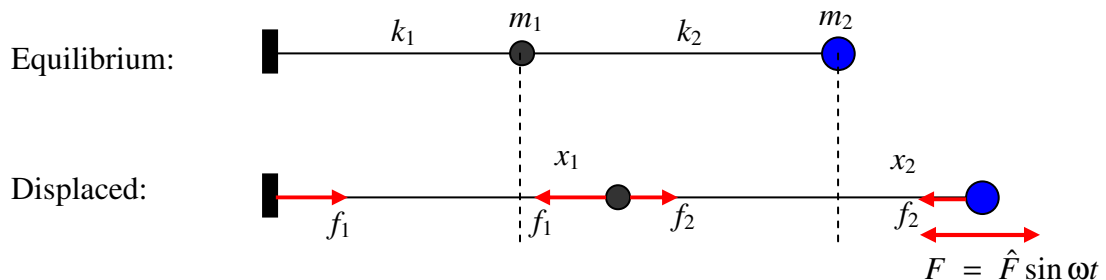


FIGURE XVII.12

Figure XVII.12 shows the same system as figure XVII.2, except that, instead of being left to vibrate on its own, the second mass is subject to a periodic force  $F = \hat{F} \sin \omega t$ . For the time being, we'll suppose that there is no damping. Either way, it is not a

conservative force, and Lagrange's equation will be used in the form of equation 13.4.12. As in section 17.2, the kinetic energy is

$$T = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2. \quad 17.12.1$$

Lagrange's equations are

$$\frac{d}{dt} \frac{\partial T}{\partial \dot{x}_1} - \frac{\partial T}{\partial x_1} = P_1 \quad 17.12.2$$

and

$$\frac{d}{dt} \frac{\partial T}{\partial \dot{x}_2} - \frac{\partial T}{\partial x_2} = P_2. \quad 17.12.3$$

We have to identify the generalized forces  $P_1$  and  $P_2$ .

In the nonequilibrium position, the extension of the left hand spring is  $x_1$  and so the tension in that spring is  $f_1 = k_1x_1$ . The extension of the right hand spring is  $x_2 - x_1$  and so the tension in that spring is  $f_2 = k_2(x_2 - x_1)$ . If  $x_1$  were to increase by  $\delta x_1$ , the work done on  $m_1$  would be  $(f_2 - f_1)\delta x_1$ , and therefore the generalized force associated with the coordinate  $x_1$  is  $P_1 = k_2(x_2 - x_1) - k_1x_1$ . If  $x_2$  were to increase by  $\delta x_2$ , the work done on  $m_2$  would be  $(F - f_2)\delta x_2$ , and therefore the generalized force associated with the coordinate  $x_2$  is  $P_2 = \hat{F} \sin \omega t - k_2(x_2 - x_1)$ . The lagrangian equations of motion therefore become

$$m_1\ddot{x}_1 + (k_1 + k_2)x_1 - k_2x_2 = 0 \quad 17.12.4$$

and

$$m_2\ddot{x}_2 + k_2(x_2 - x_1) = \hat{F} \sin \omega t. \quad 17.12.5$$

Seek solutions of the form  $\ddot{x}_1 = -\omega^2 x_1$  and  $\ddot{x}_2 = -\omega^2 x_2$ . The equations become

$$(k_1 + k_2 - m_1\omega^2)x_1 - k_2x_2 = 0 \quad 17.12.6$$

and

$$-k_2x_1 + (k_2 - m_2\omega^2)x_2 = \hat{F} \sin \omega t. \quad 17.12.7$$

We do not, of course, now equate the determinants of the coefficients to zero (why not?!), but we can solve these equations to obtain

$$x_1 = \frac{k_2 \hat{F} \sin \omega t}{(k_1 + k_2 - m_1\omega^2)(k_2 - m_2\omega^2) - k_2^2} \quad 17.12.8$$

and 
$$x_2 = \frac{(k_1 + k_2 - m_1\omega^2)\hat{F} \sin \omega t}{(k_1 + k_2 - m_1\omega^2)(k_2 - m_2\omega^2) - k_2^2}. \quad 17.12.9$$

The amplitudes of these motions (and how they vary with the forcing frequency  $\omega$ ) are

$$\hat{x}_1 = \frac{k_2\hat{F}}{m_1m_2\omega^4 - (m_1k_2 + m_2k_1 + m_2k_2)\omega^2 + k_1k_2} \quad 17.12.10$$

and 
$$\hat{x}_2 = \frac{(k_1 + k_2 - m_1\omega^2)\hat{F}}{m_1m_2\omega^4 - (m_1k_2 + m_2k_1 + m_2k_2)\omega^2 + k_1k_2}, \quad 17.12.11$$

where I have re-written the denominators in the form of a quadratic expression in  $\omega^2$ .

For illustration I draw, in figure XVII.13, the amplitudes of the motion of  $m_1$  (continuous curve, in black) and of  $m_2$  (dashed curve, in blue) for the following data:

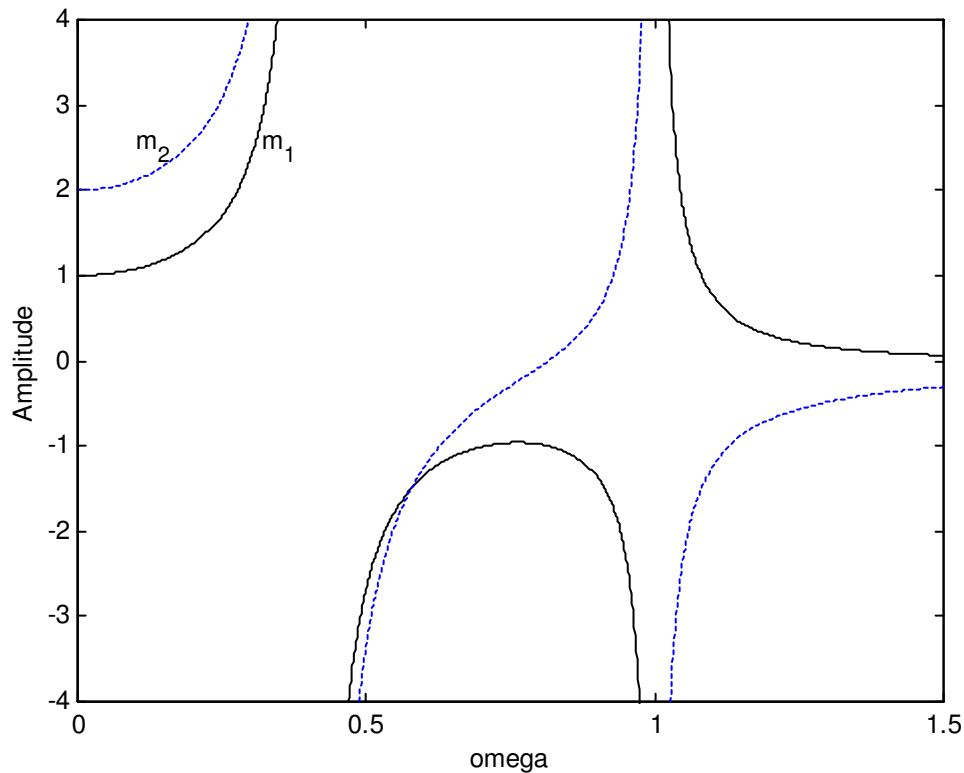
$$\hat{F} = 1, \quad k_1 = k_2 = 1, \quad m_1 = 3, \quad m_2 = 2,$$

when the equations become

$$\hat{x}_1 = \frac{1}{6\omega^4 - 7\omega^2 + 1} = \frac{1}{(6\omega^2 - 1)(\omega^2 - 1)} \quad 17.12.12$$

and 
$$\hat{x}_2 = \frac{2 - 3\omega^2}{6\omega^4 - 7\omega^2 + 1} = \frac{2 - 3\omega^2}{(6\omega^2 - 1)(\omega^2 - 1)}. \quad 17.12.13$$

FIGURE XVII.13



Where the amplitude is negative, the oscillations are out of phase with the force  $F$ . The amplitudes go to infinity (remember we are assuming here zero damping) at the two frequencies where the denominators of equations 17.12.10 and 11 are zero. The amplitude of the motion of  $m_2$  is zero when the numerator of equation 17.12.11 is zero. This is at an angular frequency of  $\sqrt{(k_1+k_2)/m_1}$ , which is just the angular frequency of the motion of  $m_1$  held by the two springs between two fixed points. In our numerical example, this is  $\omega = \sqrt{2/3} = 0.8165$ . This is an example of *antiresonance*.

### 17.13 A Damped Driven System

I'll leave the reader to add some damping to the system described in section 17.12. Let us here try it with the system described in section 17.7. We'll apply a periodic force to the left hand mass, and we'll suppose that the damping constant for each mass is  $\gamma = b/m$ . We could write the periodic force as  $F = \hat{F} \sin \omega t$ , but the algebra will be easier if we write it as  $F = \hat{F} e^{i\omega t}$ . If the initial condition is such that  $F = 0$  when  $t = 0$ , then we choose just the imaginary part of this in subsequent expressions.

The equations of motion are

$$\begin{aligned}
 m\ddot{x} = & \text{-- the damping force } b\dot{x} \\
 & \text{-- the tension in the left hand spring } k_1x
 \end{aligned}$$

+ the force  $F$   
 + the tension in the middle spring  $k_2(y - x)$   
 (this last is a thrust whenever  $y < x$ )

and  $m\ddot{y} =$  - the damping force  $b\dot{y}$   
 - the thrust in the right hand spring  $k_1y$   
 - the tension in the middle spring  $k_2(y - x)$

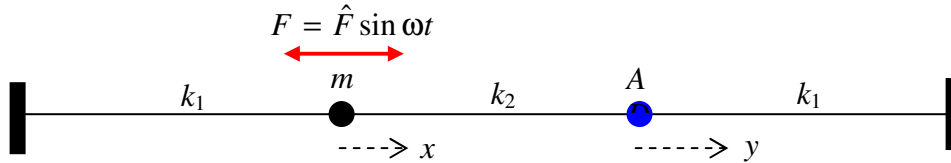


FIGURE XVII.14

That is,

$$m\ddot{x} + b\dot{x} + (k_1 + k_2)x - k_2y = \hat{F}e^{i\omega t} \quad 17.13.1$$

and

$$m\ddot{y} + b\dot{y} + (k_1 + k_2)y - k_2x = 0. \quad 17.13.2$$

For the steady-state motion, seek solutions of the form

$$\ddot{x} = -\omega^2 x, \quad \ddot{y} = -\omega^2 y, \quad \text{so that } \dot{x} = i\omega x \text{ and } \dot{y} = i\omega y.$$

The equations then become

$$(k_1 + k_2 - m\omega^2 + ib\omega)x - k_2y = \hat{F}e^{i\omega t} \quad 17.13.3$$

and

$$-k_2x + (k_1 + k_2 - m\omega^2 + ib\omega)y = 0. \quad 17.13.4$$

There is now a little algebra to be carried out. Solve these equations for  $x$  and  $y$ , and when, in doing so, there is a complex number in the denominator, multiply top and bottom by the conjugate in the usual way, so as to get  $x$  and  $y$  in the forms  $x' + ix''$  and  $y' + iy''$ . Then find expressions for the amplitudes  $\hat{x}$  and  $\hat{y}$ . After some algebra, the amount of which depends on one's skill, experience and luck (it is not always obvious how to gather terms in the most economical way, and you need some luck in this) you eventually get, for the amplitudes of the motion

$$\hat{x}^2 = \frac{((k_1 + k_2 - m\omega^2)^2 + b^2\omega^2)\hat{F}^2}{((k_1 - m\omega^2)^2 + b^2\omega^2)((k_1 + 2k_2 - m\omega^2)^2 + b^2\omega^2)} \quad 17.13.5$$

and

$$\hat{y}^2 = \frac{k_2^2 \hat{F}^2}{((k_1 - m\omega^2)^2 + b^2\omega^2)((k_1 + 2k_2 - m\omega^2)^2 + b^2\omega^2)}. \quad 17.13.6$$

There are many variables in these expressions, but in order to see qualitatively what the steady state motion is like, I'm going to put  $\hat{F}$ ,  $m$  and  $k_1 = 1$ . I think if I also put  $b = 1$ , this will give light damping in the sense described in Chapter 11. As for  $k_2$ , I am going to introduce a coupling coefficient  $\alpha$  defined by  $\alpha = \frac{k_2}{k_1 + k_2}$  or  $k_2 = \left(\frac{\alpha}{1-\alpha}\right)k_1$ . This coupling constant will be close to zero if the middle spring is very weak, and 1 if the middle connector is a rigid rod. The equations now become

$$\hat{x}^2 = \frac{\left(\frac{1}{1-\alpha} - \omega^2\right)^2 + \omega^2}{((1-\omega^2)^2 + \omega^2)\left(\frac{1+\alpha}{1-\alpha} - \omega^2\right)^2 + \omega^2}. \quad 17.13.7$$

and

$$\hat{y}^2 = \frac{\alpha/(1-\alpha)}{((1-\omega^2)^2 + \omega^2)\left(\frac{1+\alpha}{1-\alpha} - \omega^2\right)^2 + \omega^2}. \quad 17.13.8$$

For computational efficiency you might want to rewrite these equations a little. For example you could write  $(1 - \omega^2)^2 + \omega^2$  as  $1 - \Omega(1 - \Omega)$ , where  $\Omega = \omega^2$ . In any case, figure XVII.15 shows the amplitudes of the motions of the two masses as a function of frequency, for  $\alpha = 0.1, 0.5$  and  $0.9$ . The continuous black curves are for the left hand mass; the dashed blue curve is for the right hand mass.



FIGURE XVII.15

