Chapter 6

Small Oscillations

We start by considering a system with one degree of freedom, described by the Lagrangian,

$$L = \frac{1}{2}m(q)\dot{q}^2 - V(q), \qquad (6.1)$$

which yields the canonical momentum

$$p = \frac{\partial L}{\partial \dot{q}} = m(q)\dot{q},\tag{6.2}$$

which satisfies the equation of motion

$$\dot{p} = m(q)\ddot{q} + m'(q)\dot{q}^2 = \frac{\partial L}{\partial q} = \frac{1}{2}m'(q)\dot{q}^2 - V'(q), \tag{6.3}$$

or

$$m(q)\ddot{q} + \frac{1}{2}m'(q)\dot{q}^2 + V'(q) = 0.$$
(6.4)

The only property will will assume about the function m(q) is that it is positive. If we have an equilibrium solution of this system, q_0 , for which

$$\ddot{q}_0 = \dot{q}_0 = 0$$
, and $V'(q_0) = 0$, $V''(q_0) > 0$, (6.5)

that is, the particle is sitting at a minimum of the potential, we can consider small oscillations about this equilibrium position. That is, write

$$q = q_0 + \delta q, \tag{6.6}$$

and expand the equation of motion (6.4) to first order in δq . Because of the equilibrium conditions, the differential equation satisfied by δq is

$$m(q_0)\frac{d^2}{dt^2}\delta q + V''(q_0)\delta q = 0.$$
 (6.7)

Since both $m(q_0)$ and $V''(q_0)$ are positive constants, we may write them as

$$m = m(q_0), \quad k = V''(q_0),$$
 (6.8)

47 Version of October 27, 2015

and then the small-fluctuation equation of motion reads

$$m\frac{d^2}{dt^2}\delta q + k\delta q = 0. \tag{6.9}$$

This is the familiar equation for the harmonic oscillator, which has solution

$$\delta q = a\cos(\omega t + \alpha), \quad \omega^2 = \frac{k}{m},$$
(6.10)

where a and α are arbitrary real constants. We can also write this as

$$\delta q = \operatorname{Re} a e^{i(\omega t + \alpha)} = \operatorname{Re} A e^{i\omega t}, \quad A = a e^{i\alpha}, \tag{6.11}$$

where A is called the complex amplitude.

6.1 Driven Harmonic Oscillator

Now suppose we add a force, or driving, term to the Lagrangian of the harmonic oscillator,

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2 + xF(t), \qquad (6.12)$$

where the force F is some prescribed function of t. The equation of motion is

$$\ddot{x} + \omega^2 x = \frac{F(t)}{m}.\tag{6.13}$$

A general way to solve this equation is through a Green's function, a function which satisfies

$$\left(\frac{d^2}{dt^2} + \omega^2\right)g(t,t') = \delta(t-t').$$
(6.14)

Then the solution to Eq. (6.13) is a particular solution plus a general solution of the homogeneous equation (without the F term):

$$x(t) = x_0(t) + \int_{-\infty}^{\infty} dt' g(t, t') \frac{F(t')}{m},$$
(6.15)

where

$$x_0(t) = a\cos(\omega t + \alpha). \tag{6.16}$$

This is because

$$\left(\frac{d^2}{dt^2} + \omega^2\right)x(t) = \int_{-\infty}^{\infty} dt' \delta(t - t')\frac{F(t')}{m} = \frac{F(t)}{m},$$
(6.17)

because of the defining property of the δ function.

So we must find the Green's function satisfying Eq. (6.14). We seek a solution that is retarded, that is, we want the effect to come after the cause. Thus we

6.1. DRIVEN HARMONIC OSCILLATOR 49 Version of October 27, 2015

want g(t, t') = 0 for t < t'. On the other hand, for t > t', the δ function is not present, and so with some complex amplitudes A and B,

$$t > t': \quad g(t, t') = Ae^{i\omega t} + Be^{-i\omega t}.$$
 (6.18)

To solve the differential equation we see that g must be continuous at t = t' (if it were not, the second derivative would be more singular than a δ function), or

$$g(t,t')\Big|_{t=t'-\epsilon}^{t=t'+\epsilon} = Ae^{i\omega t'} + Be^{-i\omega t'} = 0.$$
(6.19)

But the derivative of g must be discontinuous at t = t', as we can see by integrating the differential equation (6.14) over a small interval around t':

$$\int_{t'-\epsilon}^{t'+\epsilon} dt \left(\frac{d^2}{dt^2} + \omega^2\right) g(t,t') = \int_{t'-\epsilon}^{t'+\epsilon} dt \,\delta(t-t') = 1. \tag{6.20}$$

Because g is continuous, this says from the fundamental theorem of calculus

$$\frac{d}{dt}g(t,t')\Big|_{t=t'-\epsilon}^{t=t'+\epsilon} = 1.$$
(6.21)

Because g vanishes when t < t' this reads

$$i\omega A e^{i\omega t'} - i\omega B e^{-i\omega t'} = 1. \tag{6.22}$$

We solve the set of simultaneous equations (6.19) and (6.22) as follows. Multiply Eq. (6.19) by $i\omega$ and add to Eq. (6.22) to obtain

$$A = \frac{1}{2i\omega} e^{-i\omega t'}; \tag{6.23a}$$

on the other hand, if we subtract Eq. (6.22) from $i\omega$ times Eq. (6.19), we get

$$B = -\frac{1}{2i\omega}e^{i\omega t'}.$$
 (6.23b)

Now, when we combine these results with the form (6.18), we get

$$g(t,t') = \theta(t-t')\frac{1}{\omega}\sin\omega(t-t').$$
(6.24)

Here, appears the Heaviside step-function,

$$\theta(t - t') = \begin{cases} 1, \ t > t', \\ 0, \ t < t'. \end{cases}$$
(6.25)

We can easily check that this satisfies the required differential equation (6.14):

$$\frac{\partial}{\partial t}g(t,t') = \delta(t-t')\frac{1}{\omega}\sin\omega(t-t') + \theta(t-t')\cos\omega(t-t')$$

= $\theta(t-t')\cos\omega(t-t'),$ (6.26a)

$$\frac{\partial^2}{\partial t^2}g(t,t') = \delta(t-t') - \theta(t-t')\omega\sin\omega(t-t'), \qquad (6.26b)$$

which used

$$\frac{\partial}{\partial t}\theta(t-t') = \delta(t-t'), \qquad (6.27)$$

which, in turn, can be verified by integrating over t from $t = t' - \epsilon$ to $t = t' + \epsilon$. Now let's use this Green's function in Eq. (6.15) for the case of a sinusoidally

varying force,

$$F(t) = f\cos(\gamma t + \beta). \tag{6.28}$$

Then

$$\begin{aligned} x(t) - x_0(t) &= \int_{-\infty}^t dt' \frac{f}{m\omega} \sin \omega(t - t') \cos(\gamma t' + \beta) \\ &= \frac{f}{m\omega} \frac{1}{4i} \int_{-\infty}^t dt' \left(e^{i\omega(t - t')} - e^{-i\omega(t - t')} \right) \left(e^{i(\gamma t' + \beta)} + e^{-i(\gamma t' + \beta)} \right) \\ &= \frac{f}{4im\omega} \left[e^{i\omega t} e^{i\beta} \frac{1}{i(\gamma - \omega)} e^{i(\gamma - \omega)t} - e^{-i\omega t} e^{i\beta} \frac{1}{i(\gamma + \omega)} e^{i(\gamma + \omega)t} \right. \\ &\quad + e^{i\omega t} e^{-i\beta} \frac{1}{i(-\gamma - \omega)} e^{-i(\gamma + \omega)t} - e^{-i\omega t} e^{-i\beta} \frac{1}{i(-\gamma + \omega)} e^{-i(\gamma - \omega)t} \right] \\ &= \frac{f}{4im\omega} \left[\frac{1}{i(\gamma - \omega)} - \frac{1}{i(\gamma + \omega)} \right] \left[e^{i(\beta + \gamma t)} + e^{-i(\beta + \gamma t)} \right] \\ &= \frac{f}{m} \frac{1}{\omega^2 - \gamma^2} \cos(\beta + \gamma t). \end{aligned}$$
(6.29)

Thus the motion of the oscillator is given by

$$x(t) = a\cos(\omega t + \alpha) + \frac{f}{m}\frac{1}{\omega^2 - \gamma^2}\cos(\gamma t + \beta).$$
(6.30)

When the two frequencies are close together, we see the phenomenon of *beats*. That is, if $\gamma = \omega + \epsilon$, we can write the coordinate in complex form,

$$x(t) = \operatorname{Re}\left[Ae^{i\omega t} + Be^{i(\omega+\epsilon)t}\right] = \operatorname{Re}\left[A + Be^{i\epsilon t}\right]e^{i\omega t},\tag{6.31}$$

so, effectively, there is a slowly varying amplitude

$$C = A + Be^{i\epsilon t},\tag{6.32}$$

which varies only slightly over the short period of oscillation, $2\pi/\omega$. With $A = ae^{i\alpha}$, $B = be^{i\beta}$,

$$|C|^{2} = a^{2} + b^{2} + 2ab\cos(\epsilon t + \beta - \alpha);$$
(6.33)

the amplitude varies periodically with frequency ϵ between the limits |a - b| < |C| < a + b.

The limit $\epsilon \to 0$ corresponds to *resonance*, when the driving frequency is the natural frequency of the oscillator. To take that limit, we expand the expression

(6.30):

$$\begin{aligned} x(t) &= a\cos(\omega t + \alpha) + \frac{f}{m} \frac{1}{\omega^2 - (\omega + \epsilon)^2} \cos((\omega + \epsilon)t + \beta) \\ &= a\cos(\omega t + \alpha) - \frac{f}{2m\omega\epsilon} \left[\cos(\omega t + \beta) - \epsilon t\sin(\omega t + \beta)\right] \\ &= \tilde{a}\cos(\omega t + \alpha) + \frac{f}{2m\omega} t\sin(\omega t + \beta), \end{aligned}$$
(6.34)

where the first term involves both a rescaling and a phase shift of the free oscillator term,

$$\tilde{a}e^{i\tilde{\alpha}} = ae^{i\alpha} - \frac{f}{2m\omega\epsilon}e^{i\beta}.$$
(6.35)

The driving force results in an oscillation whose amplitude grows linearly with t.

Perhaps a more convincing argument for this effect is obtained by returning to Eq. (6.15), and setting $\gamma = \omega$ from the outset. Then

$$\begin{aligned} x(t) - x_0(t) &= \frac{f}{m\omega} \int_{-\infty}^t dt' \frac{1}{2i} \left(e^{i\omega(t-t')} - e^{-i\omega(t-t')} \right) \frac{1}{2} \left(e^{i(\omega t'+\beta)} + e^{-i(\omega t'+\beta)} \right) \\ &= \frac{f}{4im\omega} \left(T e^{i(\omega t+\beta)} - \frac{1}{2i\omega} e^{-i(\omega t+\beta)} - \frac{1}{2i\omega} e^{i(\omega t+\beta)} - T e^{-i(\omega t+\beta)} \right) \\ &= \frac{f}{2m\omega} \left[T \sin(\omega t+\beta) + \frac{1}{2\omega} \cos(\omega t+\beta) \right]. \end{aligned}$$
(6.36)

Here T is the time from when the driving force was turned on; so again we see the linear growth in the oscillation amplitude with time, together with a "renormalization" of the original free oscillation.

These results can be given in somewhat simpler form if we introduce complex coordinates. The driven harmonic oscillator equation (6.12) can be written as

$$\frac{d}{dt}(\dot{x} + i\omega x) - i\omega(\dot{x} + i\omega x) = \frac{F}{m},$$
(6.37)

or, if we define $\xi = \dot{x} + i\omega x$,

$$\dot{\xi} - i\omega\xi = \frac{F}{m}.\tag{6.38}$$

Then our Green's function solution,

$$x(t) = x_0(t) + \int_{-\infty}^t dt' \frac{1}{\omega} \sin \omega (t - t') \frac{F(t')}{m}$$
(6.39)

implies

$$\dot{x}(t) = \dot{x}_0(t) + \int_{-\infty}^t dt' \cos \omega (t - t') \frac{F(t')}{m},$$
(6.40)

 \mathbf{SO}

$$\xi = \xi_0 + \int_{-\infty}^t dt' e^{i\omega(t-t')} \frac{F(t')}{m}.$$
 (6.41)

The energy of the harmonic oscillator is easily expressed in terms of this complex coordinate:

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 = \frac{m}{2}(\dot{x} - i\omega x)(\dot{x} + i\omega x) = \frac{m}{2}|\xi|^2.$$
 (6.42)

Because of the driving force, the energy is not constant, but changes with time. Suppose the particle is at rest before the application of the force, so $x_0 = \dot{x}_0 = \xi_0 = 0$. Then, in view of the time evolution equation (6.41), the energy acquired over the course of the action of the force is proportional to the square of the Fourier transform of the force:

$$E(t = \infty) = \frac{1}{2m} \left| \int_{-\infty}^{\infty} dt' e^{-i\omega t'} F(t') \right|^{2}.$$
 (6.43)

Example: Consider the above case with a sinusoidally varying driving force, but which is only applied for a finite time T. That is, let

$$F(t) = f\cos(\gamma t + \beta)\theta(t)\theta(T - t).$$
(6.44)

Then the Fourier transform is

$$F(\omega) = \int_0^T dt \, e^{-i\omega t} f \frac{1}{2} \left(e^{i(\gamma t+\beta)} + e^{-i(\gamma t+\beta)} \right)$$

$$= \frac{f}{2} \left[e^{i\beta} \frac{1}{i(\gamma-\omega)} \left(e^{i(\gamma-\omega)T} - 1 \right) + e^{-i\beta} \frac{1}{-i(\omega+\gamma)} \left(e^{-i(\omega+\gamma)T} - 1 \right) \right]$$

$$= \frac{f}{(\gamma-\omega)} e^{i\beta} e^{i(\gamma-\omega)T/2} \sin(\gamma-\omega)T/2$$

$$+ \frac{f}{(\omega+\gamma)} e^{-i\beta} e^{-i(\omega+\gamma)T/2} \sin(\omega+\gamma)T/2.$$
(6.45)

As γ approaches ω , the second term remains oscillatory, while if $(\omega - \gamma)T/2 \ll 1$, the first term grows linearly with T. Therefore if T is not too large,

$$|F(\omega)| \approx \frac{\sin(\omega - \gamma)T/2}{\omega - \gamma} f \approx \frac{T}{2} f, \qquad (6.46)$$

and the energy imparted to the oscillator is

$$E(T) = \frac{f^2}{8m}T^2,$$
 (6.47)

reflecting the linear growth in the amplitude we saw previously.

6.2 Normal Modes

Now suppose we have a system with s degrees of freedom, and a general Lagrangian of the form

$$\frac{1}{2}\sum_{ij}M_{ij}(\{q\})\dot{q}_i\dot{q}_j - V(\{q\}), \tag{6.48}$$

6.2. NORMAL MODES

53 Version of October 27, 2015

that is, the kinetic energy term is quadratic in velocities, multiplied by coefficients depending on $\{q_1, q_2, \ldots, q_s\}$, and with a potential depending on all the generalized coordinates q_i . Now consider an equilibrium position, where all the \dot{q}_i are zero, and the potential is a minimum, $\frac{\partial}{\partial q_i}V(q_i)\Big|_{q_i=q_{0i}} = 0$. We want to examine small oscillations about the equilibrium position,

$$q_i = q_{0i} + x_i, \quad \dot{q}_i = \dot{x}_i,$$
 (6.49)

where q_{0i} represents the coordinate at equilibrium. Then, assuming that all the second derivatives of the potential do not vanish at equilibrium, we can write, to second order in x_i 's,

$$L = \frac{1}{2} \sum_{ij} \left(M_{ij} \dot{x}_i \dot{x}_j - K_{ij} x_i x_j \right), \qquad (6.50)$$

where

$$M_{ij} = M_{ij}(\{q_0\}), \quad K_{ij} = \frac{\partial^2}{\partial q_i \partial q_j} V(\{q_0\}), \tag{6.51}$$

which are symmetric

$$M_{ij} = M_{ji}, \quad K_{ij} = K_{ji}.$$
 (6.52)

Both matrices are positive, in the sense that all their eigenvalues are positive numbers. This is true of K_{ij} because it corresponds to a *minimum* of the potential. The corresponding equations of motion are

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} - \frac{\partial L}{\partial x_i} = 0, \quad \text{or} \quad \sum_j M_{ij} \ddot{x}_j = \sum_j K_{ij} x_j, \tag{6.53}$$

which, although linear, are rather complicated since they constitute a system of s coupled equations. Can we decouple these?

To do so, it is convenient to adopt matrix notation. Introduce a column vector

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_s \end{pmatrix}, \tag{6.54}$$

and a corresponding row vector (T = transpose)

$$\mathbf{x}^T = (x_1, x_2, x_3, \dots, x_s).$$
 (6.55)

Also define an $s \times s$ mass matrix, **M**, such that

$$(\mathbf{M})_{ij} = M_{ij}, \tag{6.56}$$

and a corresponding "spring-constant" matrix, K,

$$(\mathbf{K})_{ij} = K_{ij},\tag{6.57}$$

and then the Lagrangian has the more compact-looking form,

$$L = \frac{1}{2} \dot{\mathbf{x}}^T \mathbf{M} \dot{\mathbf{x}} - \frac{1}{2} \mathbf{x}^T \mathbf{K} \mathbf{x}.$$
 (6.58)

Because of the symmetrical structure of the Lagrangian in the x's and \dot{x} 's, without loss of generality we may assume, as noted above, that **M** and **K** are symmetric,

$$\mathbf{M}^T = \mathbf{M}, \quad \mathbf{K}^T = \mathbf{K}, \tag{6.59}$$

and furthermore they are real. Therefore, we know that \mathbf{M} can be brought into diagonal form, and we shall assume that all the diagonal elements then, the eigenvalues, are strictly positive. This means we can invert the matrix \mathbf{M} , and take its square root. So let us define new coordinates \mathbf{y} by

$$\mathbf{y} = \mathbf{M}^{1/2} \mathbf{x}, \quad \mathbf{y}^T = \mathbf{x}^T \mathbf{M}^{1/2} \tag{6.60}$$

and then the Lagrangian can be written as

$$L = \frac{1}{2} \dot{\mathbf{y}}^T \dot{\mathbf{y}} - \frac{1}{2} \mathbf{y}^T \mathbf{\Omega}^2 \mathbf{y}, \quad \mathbf{\Omega}^2 = \mathbf{M}^{-1/2} \mathbf{K} \mathbf{M}^{-1/2} > 0,$$
(6.61)

where the last inequality means that the eigenvalues of the Ω^2 matrix are all greater than zero. The equation of motion can be written as

$$\ddot{\mathbf{y}} = -\mathbf{\Omega}^2 \mathbf{y}.\tag{6.62}$$

Since Ω^2 is a real, symmetric matrix, we know it can be diagonalized. That is, we want to find the eigenvalues of this matrix, which are all positive, denoted by ω_n^2 , $n = 1, 2, \ldots, s$, which are solutions of the eigenvalue equation

$$\mathbf{\Omega}^2 \mathbf{Q}^{(n)} = \omega_n^2 \mathbf{Q}^{(n)}. \tag{6.63}$$

This is a set of s linear homogeneous equations for the components of $\mathbf{Q}^{(n)} = (\{y_i^{(n)}\})$; there can be a nonzero solution only if

$$\det(\mathbf{\Omega}^2 - \omega_n^2 \mathbf{1}) = 0, \tag{6.64}$$

which, because **M** is nonsingular, det $\mathbf{M} \neq 0$, is equivalent to

$$\det(\mathbf{K} - \omega_n^2 \mathbf{M}) = 0. \tag{6.65}$$

Once we have found the eigenvectors $\mathbf{Q}^{(n)}$ and eigenvalues ω_n^2 , the Lagrangian can be recast in diagonal form,

$$L = \sum_{n} \left(\frac{1}{2} \dot{Q}^{(n)2} - \frac{1}{2} \omega_n^2 Q^{(n)2} \right), \tag{6.66}$$

just a sum of harmonic oscillators, which satisfy the equations of motion

$$\ddot{Q}^{(n)} = -\omega_n^2 Q^{(n)}.$$
(6.67)

Here we have expressed $Q^{(n)}$ as linear combinations of the original x_i corrdinates, $\mathbf{Q}^{(n)T}\mathbf{Q}^{(n)} = Q^{(n)2}$ and likewise for the $\dot{Q}^{(n)}$'s and supplied a suitable normalization factor.

To see how this works preceisely, define a matrix

$$\mathbf{Q} = (\mathbf{Q}^{(1)}, \mathbf{Q}^{(2)}, \dots, \mathbf{Q}^{(s)}), \tag{6.68}$$

that is, the matrix constructed by placing in the kth column the column vector $\mathbf{Q}^{(k)}$. Note that, with a suitable choice of normalization, the $\mathbf{Q}^{(k)}$ vectors are orthonormal:

$$\mathbf{Q}^{(i)T}\mathbf{Q}^{(j)} = \delta_{ij},\tag{6.69}$$

because they are eigenvectors of a real symmetric matrix (which is therefore also Hermitian):

$$\mathbf{Q}^{(i)T}\mathbf{\Omega}^2\mathbf{Q}^{(j)} = \omega_j^2\mathbf{Q}^{(i)T}\mathbf{Q}^{(j)} = \omega_i^2\mathbf{Q}^{(i)T}\mathbf{Q}^{(j)}, \qquad (6.70)$$

since Ω^2 can act either to the left or right. Therefore, if the eigenvalues are different, $\omega_i^2 \neq \omega_j^2$, we conclude that

$$\mathbf{Q}^{(i)T}\mathbf{Q}^{(j)} = 0. \tag{6.71}$$

If, by chance, two distinct eigenvectors have the same eigenvalue ("degeneracy"), we can always choose the eigenvectors to be orthogonal, since they space a twodimensional space. And we choose the vectors to be of unit length, so Eq. (6.69) is satisfied. This means that the matrix \mathbf{Q} satisfies

$$\mathbf{Q}^T \mathbf{Q} = \mathbf{1},\tag{6.72}$$

where **1** is the unit matrix; that is, $\mathbf{Q}^T = \mathbf{Q}^{-1}$. The matrix **Q** brings $\mathbf{\Omega}^2$ into diagonal form:

(1)

$$\mathbf{Q}^T \mathbf{\Omega}^2 \mathbf{Q} = \operatorname{diag}(\omega_1^2, \omega_2^2, \dots, \omega_s^2).$$
(6.73)

Let us define new normal mode coordinates $\boldsymbol{\zeta}$ by

$$\mathbf{y} = \mathbf{Q}\boldsymbol{\zeta},\tag{6.74}$$

where

$$\boldsymbol{\zeta} = \begin{pmatrix} \zeta^{(1)} \\ \zeta^{(2)} \\ \vdots \\ \vdots \\ \zeta^{(s)} \end{pmatrix}.$$
(6.75)

Then the Lagrangian becomes

$$L = \frac{1}{2} \dot{\mathbf{y}}^T \dot{\mathbf{y}} - \frac{1}{2} \mathbf{y}^T \mathbf{\Omega}^2 \mathbf{y} = \sum_{n=1}^s \frac{1}{2} (\dot{\zeta}^{(n)2} - \omega_n^2 \zeta^{(n)2}).$$
(6.76)

This is what is meant by Eq. (6.66). In terms of the original coordinates,

$$\zeta^{(n)} = \mathbf{Q}^{(n)T} \mathbf{y} = \mathbf{Q}^{(n)T} \mathbf{M}^{1/2} \mathbf{x}.$$
(6.77)



Figure 6.1: Three equal mass particles, connected to each other by two springs as shown. The coordinates x, y, and z are relative to the equilibrium positions of the particles. Only motion along the line shown is considered.

6.2.1 Vibrations of a linear molecule

Consider three equal mass points, connected by two massless springs, as shown in Fig. 6.1. This is a simple model of a linear molecule consisting of three atoms each of mass m with harmonic restoring forces, represented by the spring constant k. Let the positions of the atoms, relative to their equilibrium positions, be x, y, and z, respectively; we only consider motion along the line. The Lagrangian is

$$\frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\dot{y}^2 + \frac{1}{2}m\dot{z}^2 - \frac{k}{2}(x-y)^2 - \frac{k}{2}(y-z)^2.$$
(6.78)

Thus the mass matrix is diagonal, but the spring constant matrix is not:

$$\mathbf{M} = m \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{K} = k \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}.$$
 (6.79)

It is simple to calculate

$$\det(\mathbf{K} - \omega^2 \mathbf{M}) = m\omega^2 (k - m\omega^2)(m\omega^2 - 3k).$$
(6.80)

Thus, there are three normal modes, with characteristic squared-frequencies

$$\omega^2 = 0, \quad \omega^2 = \frac{k}{m}, \quad \omega^2 = 3\frac{k}{m}.$$
 (6.81)

And the (redundant) equations for the components of $Q^{(n)}=\{q_i^{(n)}\}$ are

$$(k - m\omega^2)q_1 - kq_2 = 0, (6.82a)$$

$$-kq_1 + (2k - m\omega^2)q_2 - kq_3 = 0, (6.82b)$$

$$-kq_2 + (k - m\omega^2)q_3 = 0. (6.82c)$$

The zero frequency mode has solution $q_1 = q_2 = q_3$, so the normalized eigenvector is

$$\mathbf{Q}^{(1)} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1\\1\\1 \end{pmatrix}. \tag{6.83}$$

The corresponding normal coordinate is

$$\zeta^{(1)} = \frac{1}{\sqrt{3}}(1,1,1)\sqrt{m} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \sqrt{\frac{m}{3}}(x+y+z).$$
(6.84)

This evidently corresponds to the rigid center of mass motion of the entire system, which moves with constant velocity since there is no force acting on the molecule as a whole. The $\omega^2 = k/m$ mode has solution $q_2 = 0$, $q_1 = -q_3$, that is the center of the molecule is at rest, and the two outlying atoms move oppositely to each other:

$$\mathbf{Q}^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ 0\\ -1 \end{pmatrix}, \tag{6.85}$$

which means that the corresponding normal coordinate is

$$\zeta^{(2)} = \frac{1}{\sqrt{2}} (1, 0, -1) \sqrt{m} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \sqrt{\frac{m}{2}} (x - z).$$
(6.86)

Finally, the $\omega^2 = 3k/m$ mode has solution $q_1 = q_3 = -1/2q_2$, so

$$\mathbf{Q}^{(3)} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1\\ -2\\ 1 \end{pmatrix}, \tag{6.87}$$

so the corresponding normal coordinate is

$$\zeta^{(3)} = \frac{1}{\sqrt{6}} (1, -2, 1) \sqrt{m} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \sqrt{\frac{m}{6}} (x + z - 2y).$$
(6.88)

Then the Lagrangian (6.78) is equal to

$$L = \frac{1}{2} \left[\dot{\zeta}^{(1)2} + \dot{\zeta}^{(2)2} + \dot{\zeta}^{(3)2} - \frac{k}{m} \zeta^{(2)2} - \frac{3k}{m} \zeta^{(3)2} \right], \tag{6.89}$$

which explicitly displays the frequencies found in Eq. (6.81).

6.3 Damped Harmonic Oscillator

There is no such thing as a harmonic oscillator in nature. A real pendulum, say, is subject to frictional forces at the point of support, and with the air. These forces are difficult to describe in detail. However, for many purposes, we can describe them by saying there is a damping term in the equation of motion, described by a force proportional to the particle's velocity, $\mathbf{F}_{\text{friction}} = -\alpha \dot{\mathbf{r}}$, where α is a positive constant. For a one-dimensional oscillator, this implies that the differential equation

$$m\ddot{x} + kx + \alpha \dot{x} = 0, \tag{6.90}$$

or with

$$\omega_0^2 = \frac{k}{m}, \quad \gamma = \frac{\alpha}{m}, \tag{6.91}$$

we obtain

$$\ddot{x} + \gamma \dot{x} + \omega_0^2 x = 0. \tag{6.92}$$

Let us write the solution in terms of a complex exponential,

$$x(t) = \operatorname{Re} A e^{i\omega t}, \quad A = a e^{i\alpha}, \tag{6.93}$$

where a and α are real. The frequency then is given by the quadratic equation

$$-\omega^2 + i\gamma\omega + \omega_0^2 = 0, \qquad (6.94)$$

or, completing the square,

$$\left(\omega - i\frac{\gamma}{2}\right)^2 + \frac{\gamma^2}{4} = \omega_0^2. \tag{6.95}$$

The roots are

$$\omega = \frac{i\gamma}{2} \pm \sqrt{\omega_0^2 - \frac{\gamma^3}{4}}.$$
(6.96)

The solution to the original differential equation can then be written as

$$x(t) = e^{-\gamma t/2} \operatorname{Re} A e^{i \sqrt{\omega_0^2 - \gamma^2/4t}}.$$
 (6.97)

We assume here the usual case that $\gamma/2 < |\omega_0|$. The main effect of the friction is the exponential damping term; whatever motion was originally present will damp out with the square of the amplitude, which is proportional to the energy, decreasing like $e^{-\gamma t}$. In addition there is a shift in the frequency, which is small if, as usual, $\gamma/2 \ll \omega_0$. The frequency is decreased as a result of the dissipative force, as one would expect.

Now suppose we add a driving force, so the Eq. (6.90) is replaced by

$$m\ddot{x} + \alpha\dot{x} + kx = F(t), \tag{6.98}$$

or

$$\left(\frac{d^2}{dt^2} + \gamma \frac{d}{dt} + \omega_0^2\right) x(t) = \frac{F(t)}{m}.$$
(6.99)

A general solution of this equation is a general solution of the homogeneous part, $x_0(t)$, which will have the form (6.97), which will damp out in a characteristic time of order $1/\gamma$, and a particular solution which will respond to the driving force. In particular, if the driving force is oscillatory with frequency ν ,

$$F(t) = \operatorname{Re} f e^{i\nu t}, \qquad (6.100)$$

the steady state solution we seek has also the same frequency,

$$x(t) = \operatorname{Re} B e^{i\nu t}.$$
(6.101)

The equation relating the amplitudes B and f is

$$(-\nu^2 + i\nu\gamma + \omega_0^2)B = \frac{f}{m},$$
 (6.102)

which is immediately solved:

$$B = \frac{f}{m} \frac{1}{\omega_0^2 - \nu^2 + i\nu\gamma} = \frac{f}{m} \frac{\omega_0^2 - \nu^2 - i\nu\gamma}{(\omega_0^2 - \nu^2)^2 + \nu^2\gamma^2}.$$
 (6.103)

In this equation, without loss of generality, we can choose f to be real and positive, so that $B = be^{i\beta}$, where β is the relative phase between B and f. The magnitude of B is

$$b = \frac{f}{m} \frac{1}{\sqrt{(\omega_0^2 - \nu^2)^2 + (\nu\gamma)^2}},$$
(6.104)

and its phase is given by

$$\tan \beta = \frac{\operatorname{Im} B}{\operatorname{Re} B} = \frac{-\nu\gamma}{\omega_0^2 - \nu^2}.$$
(6.105)

Note that if $\nu < \omega_0$, this is in the 4th quadrant, so the phase $\beta \in [-\pi/2, 0]$. If $\nu > \omega_0$, this is in the 3rd quadrant, and $\beta \in [-\pi, -\pi/2]$. At resonance, $\nu = \omega$, $\beta = -\pi/2$. The behavior is perhaps most easily seen near resonance, where $\nu = \omega_0 + \epsilon$, $\epsilon \ll \omega_0$. Then

$$b = \frac{f}{2m\omega_0} \frac{1}{\sqrt{\epsilon^2 + \gamma^2/4}},$$
 (6.106)

and

$$\tan \beta = \frac{-\gamma}{-2\epsilon}.\tag{6.107}$$

The negative relative phase means that the response lags behind the driving force. The phase goes from zero to $-\pi$ over a small range of detuning,

$$\Delta \epsilon \sim \gamma. \tag{6.108}$$



Figure 6.2: The phase shift β given by Eq. (6.105) as a function of the driving frequency ν . What's plotted here is for $\gamma = 0.1$, $\omega_0 = 1$, that is, everything is expressed in units of ω_0 .

Because of the damping, the amplitude at resonance is finite:

$$b(\nu = \omega_0) = \frac{f}{m\omega_0\gamma}.$$
(6.109)

Fig. 6.2 shows how the phase changes as the driving frequency passes through resonance.

6.3.1 Energy absorbed by oscillator

The power, the energy supplied by the force per unit time, is given by

$$P = F\dot{x}.\tag{6.110}$$

In the above, we calculated x(t) in terms of a complex amplitude,

$$x(t) = \operatorname{Re} B e^{i\nu t} \tag{6.111}$$

in terms of

$$F(t) = \operatorname{Re} f e^{i\nu t} \tag{6.112}$$

 \mathbf{SO}

$$P = \operatorname{Re}\left(fe^{i\nu t}\right)\operatorname{Re}\left(Bi\nu e^{i\nu t}\right) = \frac{1}{4}\left(fe^{i\nu t} + f^*e^{-i\nu t}\right)\left(i\nu Be^{i\nu t} - i\nu B^*e^{-i\nu t}\right)$$

6.4. PROBLEMS FOR CHAPTER 6

$$= \frac{1}{4}(-i\nu fB^* + i\nu f^*B) + \text{ rapidly oscillating terms}, \qquad (6.113)$$

where the rapidly oscillating terms are proportional to either $e^{2i\nu t}$ or $e^{-i2\nu t}$. The latter disappear when we average the power over one cycle. So the timeaveraged power is, when we insert Eq. (6.103)

$$\bar{P} = \frac{1}{2} \operatorname{Re} f(-i\nu) \frac{f^*}{m} \frac{\omega_0^2 - \nu^2 + i\nu\gamma}{(\omega_0^2 - \nu^2)^2 + \nu^2\gamma^2} = \frac{|f|^2}{2m} \frac{\nu^2\gamma}{(\omega_0^2 - \nu^2)^2 + \nu^2\gamma^2}.$$
(6.114)

When we are near resonance, $\nu = \omega_0 + \epsilon$, this becomes

$$\bar{P} = \frac{|f|^2}{4m} \frac{\gamma/2}{\epsilon^2 + \gamma^2/4}.$$
(6.115)

At the peak,

$$\bar{P}_m = \frac{|f|^2}{2m\gamma},\tag{6.116}$$

which gets very large for small γ , and the power drops to half this value at $\epsilon = \pm \gamma/2$. The following figures shown that the approximation (6.115) is not really very good compared to the exact formula (6.114) away from the resonance.

We can calculate the total power absorbed at all frequencies by integrating over all ν : Using the approximation (6.115) we find

$$\int d\epsilon \bar{P}(\epsilon) = \frac{|f|^2}{4m} \frac{\gamma}{2} \int_{-\infty}^{\infty} d\epsilon \frac{1}{\epsilon^2 + (\gamma/2)^2} = \frac{|f|^2}{4m} \int_{-\infty}^{\infty} \frac{dy}{y^2 + 1} = \frac{|f|^2 \pi}{4m}.$$
 (6.117)

Remarkably, this is independent of the damping parameter. The same result is obtained if the exact formula (6.114) is used.

6.4 Problems for Chapter 6

- 1. Verify by direct calculation that the Lagrangian (6.78) takes on the diagonal form (6.89) when the normal coordinates (6.84), (6.86), (6.88) are substituted.
- 2. Show that when the exact formula for the time-averaged power (6.114) is integrated over all frequencies, the same result found in Eq. (6.117) is obtained. Hint: Use the residue theorem.





Figure 6.3: Comparison of the exact formula (6.114) for the power absorbed by a damped oscillator with the approximate formula (6.115), for $\omega_0 = 1$, $\nu = 0.1$, as a function of the driving frequency ν .



Figure 6.4: Same as previous figure, except looking away from the peak.



Figure 6.5: Relative error of the approximation (6.115) compared to the exact result (6.114) for the same parameters.