Lecture notes

Small oscillations

V.H. Belvadi

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These notes are based on a series of lectures on classical mechanics given to graduate physics students at YCM, University of Mysore, during the academic year 2016–2017. This document represents only a part of the entire course on classical mechanics.

Please e-mail `hello@vhbelvadi.com` with your thoughts or suggestions, or if you spot any errors. These notes are—and will probably always remain—a work in progress. They may be updated and, if they are, the latest version of this document will always be available for download at `http://vhbelvadi.com/notes/`.

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Changelog:

v.1.0	Initial.
v.2.0	Added two new sections (§5 and §8.2.1)
	Various minor corrections.

P.S. If any of you sitting for your exam in PHYS101 are reading this, note that you have nothing to do with §5 as far as your curriculum is concerned. It is, nevertheless, worth going over, if only out of interest. The discussion in §8.2.1, although apparent from our discussions in §8.2, has been mentioned separately but briefly.

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Oscillations play an important role in physics. This is not really surprising considering they are present in so many places and at so many instances in nature; and this sort of omnipresence has translated into their gaining incredible importance across various branches of physics, from quantum mechanics to solid state physics to astrophysics to high energy physics. In effect, one may treat oscillations as a class of motion into which various problems may be reduced for simplicity of solution as well as understanding.

What we will treat here will be a specific case that is often of considerable interest, called *small oscillations*. We are also interested in various equilibria, the kinetic and potential energies of a small oscialltor, its equations of motion, and some specific examples of small oscillators. Small oscillations are a general class of systems to which any body moving in the vicinity of its point of stable equilibrium may be reduced. In this, further, the one-dimensional (one degree of freedom) case is of importance since both an ensemble or a single particle with multiple dimensions of motion (multiple degrees of freedom) may be shown to simply be multiple applications of the one-dimensional case.

1 Introduction

Simple harmonic motion is a repetitive, periodic oscillation about an equilibrium point such that the restoring force at any instant is directly proportional to the displacement from the equilibrium position and acts in the direction opposite to that of the displacement.

Small oscillations are those where the deviation from the equilibrium position is small. While the exact extent of this, or how "small" is small enough, is not explicitly defined, it is best judged following an examination of the cases where small oscillations most often come into play: atomic and molecular oscillations in nature, electric circuits, acoustic studies etc. The most convenient approach to studying small oscillations is to use Lagrangian mechanics.

2 Equilibria

If one were to assume that the potential energy (V) of an oscillator was dependent only on its position (i.e. the ideal case), and that the generalised coördinates, (q_i) are all time-independent, then the equilibrium may be defined as,

$$F_i(q_i) = -\left(\frac{\partial V}{\partial q_i}\right)_0 = 0$$

which brings the oscillator to equilibrium at $q_i = 0$, as denoted by the subscript.[1] (F is a conservative force, i.e. it is dependent only on the position of the oscillator

[1] This helps us define potential energy as well: $V(q_i) = -\int_{q_0}^{q_i} F(x)dx + V(q_0)$. The fact that the integral depends on the constant term, $V(q_0)$, means the point of minimum potential can be defined wherever convenient — see the end of §3.1.

and not its path.) We know too that V is at its minimum in the equilibrium position.

Any small deviation from equilibrium will introduce a force $-\frac{\partial V}{\partial q}$ which attempts to restore the oscillator to its equilibrium position. We can use the disturbance which removes an oscillator from equilibrium to define two types of equilibria:

1. **Stable equilibrium** is that state of equilibrium from which an infinitesimal disturbance produces a small, bounded oscillation, i.e. one that sees $V \leftarrow 0$ and an eventual return to equilibrium with little deviation.

   Mathematically, for $\frac{dV}{dq_i} = 0$ at equilibrium, stable equilibrium puts the potential at a miminum, implying that $\frac{d^2V}{dq_i^2} > 0$. Graphically, this means the potential energy is at a minima and therefore has bounds.

2. **Unstable equilibrium** is that state of equilibrium from which an infinitesimal disturbance produces, over time, a large, unbounded oscillation.

   Mathematically, like in the case of stable equilibria, for $\frac{dV}{dq_i} = 0$ at equilibrium, unstable equilibrium puts the potential at a maxima, implying that $\frac{d^2V}{dq_i^2} < 0$. Graphically, this means the potential energy is at a maxima and is therefore unbounded.

There is a third kind of equilibrium called **neutral equilibrium** which we will discuss in context in §3.1.

3 Kinetic and potential energies

3.1 Potential energy

Suppose that the deviation from equilibrium takes q_0 to some q_i. Let us call this deviation x, such that $x_i = q_i - q_0$ or $q_i = q_0 + x_i$. We now use Taylor series, under the condition that small oscillations occur, to expand the potential of the oscillator.

$$V(q_1, q_2 ... q_n) = V(0, 0 ... 0) + \left(\frac{\partial V}{\partial q_i}\right)_0 x_i + \frac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right) x_i x_j + ...$$

with summations removed as per Einstein's convention[2].

The equilibrium condition, $\left(\frac{\partial V}{\partial q_i}\right)_0 = 0$, causes all terms linear in x_i to vanish, and the first term, which denotes the equilibrium, may be made to vanish by shifting the zero of the potential to coincide with the equilibrium point, leaving us with a quadratic equation for potential energy,

[2]The Einstein notation, or Einstein summation convention, when an index appears at least twice in a term, summation over that index is implicit. So, $x_1y_1 + x_2y_2 + x_3y_3$, which is often written as $\sum_{i=0}^{3} x_i y_i$, may simply be written as $x_i y_i$ and the summation is understood as implied.

$$V = \frac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right) x_i x_j = \frac{1}{2} V_{ij} x_i x_j \tag{1}$$

The higher order terms are neglected thanks to these being small oscillations. Also note that $V_{ij} = V_{ji}$ according to equation (1). And, since the equilibrium state can occur at any general coördinate q_i (we have taken it as some $q_k = 0$ with $i = k$ when we shifted the zero of the potential), we call this state of equilibrium **neutral** or **indifferent equilibrium**.

3.2 Kinetic energy

Calculations similar to those in §3.1 yield an expression for the kinetic energy (T) of the oscillator as well. We are aware of the standard expression for kinetic energy,

$$T = \tfrac{1}{2} m_{ij} \dot{q}_i \dot{q}_j = \tfrac{1}{2} m_{ij} \dot{x}_i \dot{x}_j$$

which arises, for any system of n points positioned at $\mathbf{r}_i$ where $i = 1, 2...n$ and governed by k equations of constraints $\phi_j(x_1, y_1, z_1 ... x_n, y_n, z_n)$ where $j = 1, 2...k$ that therefore has $3n - k$ degrees of freedom described by a set of f generalised coördinates, $q_1, q_2 ... q_f$. Once again, here, we use the summation convention.

How we arrived at this is not obvious, though, and warrants examination: we start with the more fundamental version of the equation for kinetic energy:

$$T = \frac{1}{2} \sum_{i=1}^{n} m_i \dot{\mathbf{r}}_i \dot{\mathbf{r}}_i$$

where the velocity of the i^{th} point, $\mathbf{v}_i = \dot{\mathbf{r}}_i$, and, since $\mathbf{r}_i = \mathbf{r}_i(q_1, q_2 ... q_f)$ as discussed above, we can write $\dot{\mathbf{r}}$ as $\frac{\partial \mathbf{r}_i}{\partial q_k} \dot{q}_k$, giving us,

$$T = \frac{1}{2} \sum_{i=1}^{n} m_i \left(\sum_{k=1}^{f} \frac{\partial \mathbf{r}_i}{\partial q_k} \dot{q}_k \cdot \sum_{l=1}^{f} \frac{\partial \mathbf{r}_i}{\partial q_l} \dot{q}_l \right)$$

or, written more simply with $T_{kl} = \sum_{i=1}^{n} m_i \frac{\partial \mathbf{r}_i}{\partial q_k} \cdot \frac{\partial \mathbf{r}_i}{\partial q_l}$ we arrive at,

$$T = \frac{1}{2} \sum_{k=1}^{f} \sum_{l=1}^{f} T_{kl}\, \dot{q}_k\, \dot{q}_l$$

$$\Rightarrow T = \frac{1}{2} T_{ij} \dot{x}_i \dot{x}_j$$

using the summation convention again.

Alternatively, Taylor expanding $m_{ij}(q_1, q_2 ... 1_n)$ gives us,

$$m_{ij} = m_{ij}(0, 0...0) + \left(\frac{\partial m_{ij}}{\partial q_k}\right) x_k + ...$$

This is parallel to what we worked out in the case of potential energy in §3.1 and leaves us with some T_{ij} (say), called the **mass matrix** (a diagonal matrix that establishes a relationship between the kinetic energy and the time-derivative of the generalised coördinate), for all the constant m_{ij} values from the first term in the expansion. The higher order terms are dropped as they will vanish anyway.

$$T = \frac{1}{2} T_{ij} \dot{x}_i \dot{x}_j \tag{2}$$

This quadratic equation gives us the kinetic energy of the body undergoing small oscillations. The T_{ij} term, like V_{ij}, is symmetric.

4 The equation of motion

For any point with s degrees of freedom, i.e. represented by generalised s coördinates, $(q_1, q_2 ... q_s)$, with generalised velocities, $\dot{q}_i$, and accelerations, $\ddot{q}_i$, an *equation of motion* is simply any equation relating these quantities to help us better predict the motion of said point.

For this purpose, the expressions in equations (1) and (2) for kinetic and potential energies may be used in the Lagrangian, $L = T - V$ as,

$$L = \frac{1}{2} T_{ij} \dot{x}_i \dot{x}_j - \frac{1}{2} V_{ij} x_i x_j \tag{3}$$

For the generalised coördinate, x, we know that $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) - \frac{\partial L}{\partial x_i} = 0$, which means,

$$\frac{d}{dt}\left(T_{ij}\dot{x}_j\right) - V_{ij}x_j = 0$$

which gives us a series of equations of motion for the oscillator:

$$T_{ij}\ddot{x}_j + V_{ij}x_j = 0 \tag{4}$$

5 Understanding the Lagrangian more generally

Our discussion from §3 – 4 is worth examining in greater detail before we set up our eigenvalue problem, even if only for a better understanding of our Lagrangian. This section is a digression from our main problem, so it can be read out of sequence or skipped entirely. However it is extremely interesting and worth reading for that alone at some point.

We started off with the kinetic and potential energies in terms of generalised coördinates, x_i and $\dot{x}_i$. We can do the same thing with the Lagrangian itself, although not explicitly, i.e. we cannot simply *assume* the form of equation (4) with no justification. Indeed we do not have to: keeping in tune with our displacement by some x_i giving us $x_i' = (x_i)_0 + x_i$ and, in turn, $\dot{x_i}' = \dot{x}_i$ since $(x_i)_0$ is small enough

for this approximation (we are talking about small oscillaitons after all, about an equilibirum position at some $(x_i)_0$ with $\dot{x_i} = 0$).

We can now Taylor expand our Lagrangian along the same lines as we expanded the energies, V and T, earlier.

$$\begin{aligned} L[x_i, \dot{x_i}] = L[(x_i)_0, 0] + \frac{\partial L}{\partial x_i}[(x_i)_0, 0]x_i' + \frac{\partial L}{\partial \dot{x_i}}[(x_i)_0, 0]\dot{x_i'} \\ + \frac{1}{2}\frac{\partial^2 L}{\partial x_i \partial x_j}[(x_i)_0, 0]x_i'x_j' + \frac{1}{2}\frac{\partial^2 L}{\partial \dot{x_i}\partial \dot{x_j}}[(x_i)_0, 0]\dot{x_i'}\dot{x_j'} \\ + \frac{\partial^2 L}{\partial x_i \partial \dot{x_j}}[(x_i)_0, 0]x_i'\dot{x_j'} + \cdots \end{aligned}$$

We simplify this in anticipation of its use in the Euler's equation, $\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x_i}}\right) - \frac{\partial L}{\partial x_i} = 0$. Therefore we can safely drop the $L[(x_i)_0, 0]$ term, representing the stable equilibrium position and being a timewise constant. Suppose our equilibrium occurs at the origin (or, in reverse, suppose we define our origin at the equilibrium position) then $\frac{\partial L}{\partial x_i} = 0$ and the second term can be dropped as well. The third term, being a time-derivative already will also not affect the Euler-Lagrange equation (where it will become the time-derivative of a time-derivative). An alternative reasoning would be that the third term is a total derivative, given that $\dot{x_i'} = \dot{x_i}$ as we saw already, and has no place in the Euler-Lagrange equation. It would be helpful, at this point, to write down what terms we have left in our Lagrangian expansion:

$$L[x_i, \dot{x_i}] = \frac{1}{2}\frac{\partial^2 L}{\partial x_i \partial x_j}[(x_i)_0, 0]x_i'x_j' + \frac{1}{2}\frac{\partial^2 L}{\partial \dot{x_i}\partial \dot{x_j}}[(x_i)_0, 0]\dot{x_i'}\dot{x_j'} + \frac{\partial^2 L}{\partial x_i \partial \dot{x_j}}[(x_i)_0, 0]x_i'\dot{x_j'} \quad (5)$$

The first two terms in equation (5) have symmetric $\frac{\partial L}{\partial \square_i \partial \square_j}$ coefficients. We will later see (in §8.1) that these are the two symmetric matrices that help us defined the potential and kinetic energies. Indeed if we define[3]

$$\frac{\partial^2 L}{\partial x_i \partial x_j}[(x_i)_0, 0] = -V_{ij} \quad \text{and} \quad \frac{\partial^2 L}{\partial \dot{x_i}\partial \dot{x_j}}[(x_i)_0, 0] = T_{ij}$$

we can quickly arrive at equation (3). The term we are interested in right now is the term we will have to ignore in equation (5) to arrive at equation (3) using our definition of $\mathbf{V}$ and $\mathbf{T}$ as stated above, i.e. it is the last term, $\frac{\partial^2 L}{\partial x_i \partial \dot{x_j}}[(x_i)_0, 0]x_i'\dot{x_j'}$ which we will now focus on.

In the case of small oscillations, given that equation (3) is indeed correct, we realise that $\frac{\partial^2 L}{\partial x_i \partial \dot{x_j}}[(x_i)_0, 0]x_i'\dot{x_j'} = 0$. But what about its non-zero case? This term has the form $\Phi_{ij}q_i'\dot{q_j'}$ which we can always write as

$$\Phi_{ij}q_i'\dot{q_j'} = \frac{1}{2}\left(\Phi_{ij}q_i'\dot{q_j'} + \Phi_{ij}\dot{q_i'}q_j'\right) + \frac{1}{2}\left(\Phi_{ij}q_i'\dot{q_j'} - \Phi_{ij}\dot{q_i'}q_j'\right)$$

[3]In fact, when we discuss more specific examples in §8.1 and §8.2, it will become clear that we can define the matrices $\mathbf{T}$ abd $\mathbf{V}$ in this form. In §8 we will be calling them as $\mathbf{B}$ and $\mathbf{A}$ instead.

The first term is, once again, a total derivative we can drop. It is simply one-half of $\Phi_{ij}\frac{\mathrm{d}}{\mathrm{d}t}(q'_i q'_j)$ implying that the symmetric part vanishes and our non-zero case requires that we focus on the anti-symmetric part $[\Phi_{ij} - \Phi_{ji}]q'_i\dot{q'_j}$ and ask ourselves under what circumstances this term comes into the picture.

The Lagrangian of a point charge, q, of mass m, moving under a z-directional magnetic field with vector potential, $\mathbf{A}$, is given by[4]

$$L = \frac{1}{2}m[\dot{x_i}^2 + \dot{x_j}^2] + q[A_{x_i}\dot{x_i} + A_{x_j}\dot{x_j}]$$

assuming that our point charge is restricted to the two dimensions of the x-y plane.

Here, $\Phi_{ij} = \frac{\partial A_{x_i}}{\partial x_j}$ (and Φ is *not* to be mistaken for the scalar potential) and, as we discussed earlier, we are interested in the $\Phi_{ij} - \Phi_{ji}$ term, which is nothing but

$$\frac{\partial A_{x_i}}{\partial x_j} - \frac{\partial A_{x_j}}{\partial x_i} \cong \boldsymbol{\nabla} \times \mathbf{A} = \mathbf{B}$$

We can arrive at this fairly easily by substituting L into Euler's equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x_i}}\right) - \frac{\partial L}{\partial x_i} = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(m\dot{x_i} + qA_{x_i}) - q(\Phi_{ii}\dot{x_i} + \Phi_{ji}\dot{x_j}) = 0$$

Expanding $\frac{\mathrm{d}}{\mathrm{d}t}A_{x_i} = \frac{\partial A_{x_i}}{\partial x_i}\frac{\mathrm{d}x_i}{\mathrm{d}t} + \frac{\partial A_{x_i}}{\partial x_j}\frac{\mathrm{d}x_j}{\mathrm{d}t}$ as a total derivative[5] in two-dimensions,

$$m\ddot{x_i} + q\left(\frac{\partial A_{x_i}}{\partial x_i}\frac{\mathrm{d}x_i}{\mathrm{d}t} + \frac{\partial A_{x_i}}{\partial x_j}\frac{\mathrm{d}x_j}{\mathrm{d}t}\right) - q(\Phi_{ii}\dot{x_i} + \Phi_{ji}\dot{x_j}) = 0$$

$$m\ddot{x_i} + q(\Phi_{ii}\dot{x_i} + \Phi_{ij}\dot{x_j}) - q(\Phi_{ii}\dot{x_i} + \Phi_{ji}\dot{x_j}) = 0$$

$$m\ddot{x_i} + q\mathbf{B}\dot{x_j} = 0 \tag{6}$$

$x_i = 0 = x_j$ therefore describes the equilibrium position. The general oscillatory solution (which we will soon make us of in §6.1) gives us $x_i = a_i e^{-i\omega t}$ which, on substitution in equation (6), gives us

$$-m\omega^2 a_i + i\omega q\mathbf{B}a_j = 0$$

This equation has two solutions, both of which can be arrived at simply by inspection: $\omega = 0$, representing a particle that is not oscillating; and the more interesting case of $\omega^2 = \frac{q\mathbf{B}}{m}$ with $a_i = \pm\, i a_j$, which has the eigenvalues $\omega = \pm\sqrt{\frac{q\mathbf{B}}{m}}$ representing a particle moving in circular orbits at cyclotron frequency.

[4] A discussion of how the second term in this equation arises is beyond the scope of this lecture. For a full discussion see Hornberger, Benjamin: *Electric and magnetic forces in Lagrangian and Hamiltonian formalism*, §3, PHY505, Stony Brook University, New York, available as a .pdf file at `http://insti.physics.sunysb.edu/itp/lectures/01-Fall/PHY505/09c/notes09c.pdf`.

[5] Total derivative in three dimensions: $\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t} + \frac{\partial f}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t}$.

6 The eingenvalue problem

6.1 The eigenvalue equation

For the equations of motion (4), which are linear and of second order type, we try the usual oscillatory solution, $y = e^{-i\omega t}$, in terms of our generalised coördinates:

$$x_i = a_i e^{-i\omega t}$$

where a_i is the complex amplitude of the oscillatory waveform.

Substituting this into equation (4) we arrive at,

$$-\omega^2 T_{ij} a_j + V_{ij} a_j = 0$$

or,

$$[V_{ij} - \omega^2 T_{ij}] a_j = 0 \tag{7}$$

in matrix form, whcih represents the generalised eigenvalue problem[6].

The matrix in the above equation has a non-trivial solution if its determinant vanishes:

$$\begin{vmatrix} V_{11} - \omega^2 T_{11} & \cdots & V_{1n} - \omega^2 T_{1n} \\ \vdots & & \vdots \\ V_{n1} - \omega^2 T_{n1} & \cdots & V_{nn} - \omega^2 T_{nn} \end{vmatrix} = 0$$

What we are interested in, though, is the fact that this equation may be written as an eigenvalue equation in the form,

$$V_{ij} a_j = \lambda T_{ij} a_j \tag{8}$$

where $\omega^2 = \lambda$. That is, $\mathbf{V}$ acting on a_j produces a multiple of the effect of $\mathbf{T}$ acting on a_j. Equation (8) is called the **eigenvalue equation**. Both $\mathbf{V}$ and $\mathbf{T}$, as seen above, are $n \times n$ matrices.

6.2 Solving for the eigenvalues

We now make use the fact that the matrices $\mathbf{V}$ and $\mathbf{T}$ are symmetric[7], i.e. $\mathbf{T}^T = \mathbf{T}$ and $\mathbf{V}^T = \mathbf{V}$. If equation (8) is satisfied by some $\mathbf{a}_k$, a column matrix representing some k^{th} eigenvector, we have,

$$\mathbf{V}\mathbf{a}_k = \lambda_k \mathbf{T}\mathbf{a}_k \tag{9}$$

[6]The idea behind eigenvalues is to find a value λ which satisfies, for the matrices A and B, the equation $Ax = \lambda Bx$. The generalised solution involves defining $\lambda = \frac{\alpha}{\beta}$ such that $[A\beta + B\alpha]x = 0$. Note that this resembles the equation we have arrived at at this point. The generalised solution is preferred, in part, because it works even when $\beta = 0$ despite $\lambda \to \infty$.

[7]Remember that T is the kinetic energy and $\mathbf{T}$ is the *matrix which helps us describe the kinetic energy.* The use of the same letter, T, may be confusing, so note that the kinetic energy, being a scalar, is represented as T, while the mass matrix is represented as $\mathbf{T}$, in bold.

and its transposed complex conjugate equation, or its *adjoint* equation, becomes,

$$\mathbf{a}_l^\dagger \mathbf{V} = \lambda_l^* \mathbf{a}_l^\dagger \mathbf{T} \tag{10}$$

because of the symmetry of $\mathbf{V}$ and $\mathbf{T}$. And $\mathbf{a}_l^\dagger$ is, of course, a row matrix with the complex conjugate elements of $\mathbf{a}_k$, or the *adjoint* vector.

Multiplying equation (9) from the left by $\mathbf{a}_l^\dagger$ and equation (10) from the right by $\mathbf{a}_k$ and subtracting the two to get rid of $\mathbf{V}$ we are left with,

$$0 = (\lambda_k - \lambda_l^*)\, \mathbf{a}_l^\dagger \mathbf{T} \mathbf{a}_k$$

which, when $l = k$, becomes,

$$0 = (\lambda_l - \lambda_l^*)\, \mathbf{a}_l^\dagger \mathbf{T} \mathbf{a}_l$$

and the matrices can be shown as real.

If $k \neq l$, then $\mathbf{a}_l^\dagger \mathbf{T} \mathbf{a}_k = 0$, which means that the amplitudes, a, are mutually orthogonal.

If $k = l$, then $\left(\mathbf{a}_k^\dagger \mathbf{T} \mathbf{a}_k\right)^\dagger = \mathbf{a}_k^\dagger \mathbf{T} \mathbf{a}_k \equiv \mathbf{a}_k^\dagger \mathbf{T} \mathbf{a}_k$, which implies that the product is *real*. Further, if $a_i = \alpha_i + i\beta_i$, the right hand side becomes,

$$\begin{aligned} \mathbf{a}_k^\dagger \mathbf{T} \mathbf{a}_k &= (\alpha_i + i\beta_i)^\dagger\, \mathbf{T}\, (\alpha_i + i\beta_i) \\ &= \left(\alpha_i^T \mathbf{T} \alpha_i + \beta_i^T \mathbf{T} \beta_i\right) + i\left(\alpha_i^T \mathbf{T} \beta_i - \beta_i^T \mathbf{T} \alpha_i\right) \end{aligned}$$

where, since $\mathbf{a}_k^\dagger \mathbf{T} \mathbf{a}_k$ has been shown to be real, the complex part is zero and,

$$\mathbf{a}_k^\dagger \mathbf{T} \mathbf{a}_k = \alpha_i^T \mathbf{T} \alpha_i + \beta_i^T \mathbf{T} \beta_i \tag{11}$$

The matrix form of $T = \frac{1}{2}\, T_{ij}\, \dot{x}_i\, \dot{x}_j$ is $T = \frac{1}{2} \dot{\mathbf{x}}^T \mathbf{T} \dot{\mathbf{x}}$. From this and our definition of α_i, which tells us that $x \propto \alpha$, we realise that equation (11) represents twice the kinetic energy and is positive. Thus $(\lambda_k - \lambda_k^*) = 0$, or $\lambda_k = \lambda_k^*$, and the eigenvector in equation (9) is real.

An alternate way of arriving at the same conclusion involves starting with the eigenvalue equation, equation (8), with $\lambda = \omega^2$, and multiplying by $a_j^\dagger$ from the left. Therefore,

$$\begin{aligned} a_j^\dagger V_{ij} a_j &= \omega^2 a_j^\dagger T_{ij} a_j \\ \Rightarrow \omega^2 &= \frac{a_j^\dagger V_{ij} a_j}{a_j^\dagger T_{ij} a_j} \end{aligned}$$

which tells us that ω is *real* so long as the potential energy is greater than the kinetic energy. This is expected for stable equilibrium.

If $a_j^\dagger \mathbf{T} a_j = 1$, and using $a_j^\dagger \mathbf{T} a_i = 0$ from the $k \neq l$ case above, the column matrix formed by the elements a_i gives us,

$$\mathbf{A}^T \mathbf{T} \mathbf{A} = \mathbf{1}$$

7 Normal coördinates

The set η_i of time-dependent coördinates, which arise due to a transformation on the set x_i of time-independent coördinates, are known as the **normal coördinates** of the small oscillator system.

The transformation in question uses the matrix $\mathbf{O}$ which diagonalises T_{ij}. Let us suppose this gives us some $\mathbf{t}$ such that $\mathbf{t} = \mathbf{OTO}^T$, with $\mathbf{t}$ being a diagonal matrix with positive, real elements as examined before. Thus,

$$\begin{aligned} T &= \frac{1}{2}\dot{\mathbf{x}}^T\mathbf{T}\dot{\mathbf{x}} \\ &= \frac{1}{2}\dot{\mathbf{x}}^T\left(\mathbf{O}^T\,\mathbf{t}\,\mathbf{O}\right)\dot{\mathbf{x}} \\ &= \frac{1}{2}\left(\dot{\mathbf{x}}^T\mathbf{O}^T\right)\,\mathbf{t}\,\left(\mathbf{O}\dot{\mathbf{x}}\right) \\ &= \frac{1}{2}\dot{\eta}^T\,\mathbf{t}\,\dot{\eta} \end{aligned} \tag{12}$$

The potential energy may be similarly solved to get $V = \frac{1}{2}\mathbf{x}^T\left(\mathbf{O}^T\mathbf{vO}\right)\mathbf{x}$.

Next, we define the diagonal matrix $S_{ii} = \sqrt{t_{ii}}\,\delta_{ij}$, which is mass-weighted, and a corresponding mass-weighted coördinate is deinfed as $y_i = \Sigma_j S_{ij}x_j$ (or $\mathbf{y} = \mathbf{Sx}$).

Conversely, $\mathbf{t} = S^2 = S^TS$, giving us,

$$\begin{aligned} T &= \frac{1}{2}\dot{\eta}^T S^T S\dot{\eta} \\ &= \frac{1}{2}\left(\dot{\eta}^T S^T\right)\left(S\dot{\eta}\right) \\ &= \dot{\mathbf{y}}^T\dot{\mathbf{y}} \end{aligned}$$

In case of the potential energy, we now have a similar expression: $V = \frac{1}{2}\mathbf{y}^T\mathbf{By}$, where $\mathbf{B} = \mathbf{S}^T\mathbf{O}^T\mathbf{v}\,\mathbf{O}\,\mathbf{S}$.

Let us finally define an orthogonal matrix P that diagonalises $\mathbf{B}$ as some $\mathbf{C} = \mathbf{PBP}^T$, which gives us the potential energy, $V = \frac{1}{2}\mathbf{y}^T\mathbf{P}^T\mathbf{CPy}$. If we define $\mathbf{Py} = \xi$ for simplicity, then we have the following potential and kinetic energies:

$$\begin{aligned} V &= \frac{1}{2}\,\xi^T\mathbf{C}\,\xi \quad \text{and} \\ T &= \frac{1}{2}\xi^T\xi \end{aligned}$$

For $\omega_i \coloneqq \sqrt{\mathbf{C}_{ii}}$, our equations, in terms of normalise coördinates, become—

for the kinetic energy,

$$T = \frac{1}{2}\Sigma_j\dot{\xi}_j^2 \tag{13}$$

for the potential energy,

$$V = \frac{1}{2}\Sigma_j \omega_j^2 \xi_j^2 \tag{14}$$

and for the Lagrangian,

$$\ddot{\xi}_j + \omega_j^2 \xi_j = 0 \tag{15}$$

In normalising thusly, we have reduced our problem of small oscillations to one of diagonalising symmetric, real matrices. This is a solution that is found to work for nearly all classes of systems that can be reduced to small oscillations.

There is an important term associated with oscillations which is worth introducing at this point: a **normal mode** of oscillation is one wherein all components of the system in question oscillate at the *same frequency* and *in phase*, thereby arriving at their equilibrium positions at the same time.

8 Examples

8.1 Longitudinal vibrations in a particle pair

Consider two masses, m, connected to each other and to a rigid support on either side to form a collinear system. Let us suppose that they are displaced by x_1 and x_2 along the spring system and that these displacements serve as our generalised coördinates, q_1 and q_2. We neglect gravity for simplicity (and also because the masses are assumed to be small enough that this assumption is permissible). We further suppose that the spring connecting the first mass from its rigid support has a spring constant of k, the spring connecting the two masses has $2k$, and the spring connecting the second mass to its rigid support has k again.

$$\begin{aligned} T &= \frac{1}{2}m(\dot{x_1}^2 + \dot{x_2}^2) \\ &= \begin{pmatrix} \dot{x_1} & \dot{x_2} \end{pmatrix} \begin{pmatrix} m/2 & 0 \\ 0 & m/2 \end{pmatrix} \begin{pmatrix} \dot{x_1} \\ \dot{x_2} \end{pmatrix} \end{aligned} \tag{16}$$

For simplicity, we may assign $\mathbf{B} = m\,\mathbf{I}$, thereby making $\mathbf{B}$ a *positive definite, real diagonal matrix.*

Likewise, the potential energy for the spring system can be written using the general formula, $V = \frac{1}{2}kx^2$, as follows:

$$\begin{aligned} V &= \frac{1}{2}kx_1^2 + \frac{1}{2}\cdot 2k(x_2 - x_1)^2 + \frac{1}{2}kx_2^2 \\ &= \frac{3}{2}kx_1^2 + \frac{3}{2}kx_2^2 - 2kx_1x_2 \end{aligned}$$

The terms, in order, refer to the potential energy in the spring on one end (rigid support to the first mass), the middle spring (between the masses), and the spring

on the other end (rigid support to the second mass). And, in a matrix form similar to equation (16), we get,

$$V = \begin{pmatrix} x_1 & x_2 \end{pmatrix} \begin{pmatrix} \frac{3}{2}k & -k \\ -k & \frac{3}{2}k \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \tag{17}$$

where we may assign to the second matrix the label $\mathbf{A}$.

Now, $\mathbf{B}^{-1}\mathbf{A} = \begin{pmatrix} \frac{3k}{m} & \frac{-2k}{m} \\ \frac{-2k}{m} & \frac{3k}{m} \end{pmatrix}$ and its eigenvalue equation[8], $\left|\mathbf{B}^{-1}\mathbf{A} - \lambda\mathbf{I}\right| = 0$ leaves us with,

$$\left(\frac{3k}{m} - \lambda\right)^2 - \left(\frac{2k}{m}\right)^2 = 0$$

which has the roots/eigenvalues $\lambda_1 = \frac{5k}{m}$ and $\lambda_2 = \frac{k}{m}$.

We know from §7 that there exists some matrix $\mathbf{P}$ such that,

$$\mathbf{P}^{-1}(\mathbf{B}^{-1}\mathbf{A})\mathbf{P} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} = \begin{pmatrix} \frac{5k}{m} & 0 \\ 0 & \frac{k}{m} \end{pmatrix}$$

and this is related to the normalised coördinates, ξ, as $\ddot{\xi}_1 + \lambda_1\xi_1 = 0$ and $\ddot{\xi}_2 + \lambda_2\xi_2 = 0$. If we define $\xi = \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}$, then $\ddot{\xi} + \left[\mathbf{P}^{-1}(\mathbf{B}^{-1}\mathbf{A})\mathbf{P}\right]\xi = \mathbf{0}$, which is like the normalised Lagrangian equation of motion (see equation (15)) which was discussed in §7.

In other words, we have two values[9] for ω given by $\omega_1 = \sqrt{\frac{5k}{m}}$ and $\omega_2 = \sqrt{\frac{k}{m}}$, or their corresponding frequencies, $f_1 = \frac{1}{2\pi}\sqrt{\frac{5k}{m}}$ and $f_2 = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$.

The next question then is all about what $\mathbf{P}$ is. This matrix may be determined using the eigenvectors, one of which, say, is $\mathbf{X}_1 = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$. Therefore,

$$\mathbf{B}^{-1}\mathbf{A} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{5k}{m} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

from the standard equation[10]. That is,

$$\begin{pmatrix} \frac{3k}{m} & \frac{-2k}{m} \\ \frac{-2k}{m} & \frac{3k}{m} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{5k}{m} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

or,

[8] We use $\mathbf{B}^{-1}\mathbf{A}$ to find the eigenvectors since the equation of motion (see equation (4)) tells us that $\mathbf{T}\ddot{\mathbf{x}} - \mathbf{V}\mathbf{x} = 0$, or, equivalently, $\ddot{\mathbf{x}} - \mathbf{T}^{-1}\mathbf{V}\mathbf{x} = 0$. By the same reasoning as in §7 we have some matrix, $\mathbf{P}$, such that $\ddot{\mathbf{x}} - (\mathbf{P}^{-1}\mathbf{T}^{-1}\mathbf{V}\mathbf{P})\mathbf{x} = 0$ where the matrix product in parentheses is the diagonal matrix made of the eigenvalues of $\mathbf{B}^{-1}\mathbf{A}$.

[9] Recall that we defined $\omega = \sqrt{\mathbf{C}}$ in §7.

[10] Basic maths: for eigenvalue λ and eigenvector $\mathbf{v}$ of some square matrix, $\mathbf{M}$, we have $\mathbf{M}\mathbf{v} = \lambda\mathbf{v}$.

$$\frac{3k}{m}a_1 - \frac{2k}{m}a_2 = \frac{5k}{m}a_1$$
$$\Rightarrow a_1 = -a_2$$

and,

$$\frac{3k}{m}a_2 - \frac{2k}{m}a_1 = \frac{5k}{m}a_2$$
$$\Rightarrow a_1 = -a_2$$

which is to say, the two Eigenvalues are of the type of, say, -1 and 1.

Indeed we can use this simplest of cases[11]: $X_1 \propto \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ to determine $\mathbf{P}$.

While the two equations above, which determined the components of the eigenvector, $\mathbf{X}_1$, used the eigenvalue $\sqrt{\frac{5k}{m}}$, we can work on the same lines with the eigenvalue $\sqrt{\frac{k}{m}}$ to arrive at $X_2 \propto \begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

These form the columns of $\mathbf{P}$ giving us,

$$\mathbf{P} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

For the normalised coördinates, ξ_i, we have $\mathbf{x} = \mathbf{P}\xi$, or, $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}$ giving us,

$$x_1 = \xi_1 + \xi_2$$
$$x_2 = -\xi_1 + \xi_2$$

from which the **first** and **second normal modes** may be obtained at $\xi_1 = 0$ and $\xi_2 = 0$. That the frequencies are $f_1 = \frac{1}{2\pi}\sqrt{\frac{5k}{m}}$ corresponding to the coördinate ξ_1 and $f_2 = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$ corresponding to ξ_2 is already known[12]. Therefore, when $\xi_1 = 0$, we have $x_1 = x_2$ and, similarly, when $\xi_2 = 0$, we have $x_1 = -x_2$.

Physically, this means that our first mode is simply the motion of the masses m along the same direction (since $x_1 = x_2$) at frequency $\frac{1}{2\pi}\sqrt{\frac{k}{m}}$ (since this is for $\xi_2 \neq 0$). And, similarly, the second mode is the motion of the masses in opposite directions (since $x_1 = -x_2$) at frequency $\frac{1}{2\pi}\sqrt{\frac{5k}{m}}$ (since this is for $\xi_1 \neq 0$).

[11]This is not strictly correct in that the components of X_1 may not be 1 and -1. We still need to *normalise* this eigenvector to determine what it actually is, but we will skip this for now since we are only interested in the relative displacements of the masses. In the second example discussed in §8.2 we will be normalising the eigenvectors.

[12]Consider the component ξ_1 from the matrix form of this equation, $\ddot{\xi} + \omega^2\xi = 0$. That is to say, $\ddot{\xi_1} + \omega^2\xi = 0$. This means the frequency, $f_i = \frac{\omega_i}{2\pi}$ is for the motion described by ξ_i.

8.2 Linear, triatomic molecules

One might be interested in moving on to a more real-world scenario working along the same lines as the last one. A good example is that of a linear, triatomic molecule. We might want to study this, for example, to see how the various modes of oscillation in such an atom affect its energies and, in turn, its radiation output. Specifically, think of a triatomic molecule with two types of atoms, in which two atoms of the *first* type lie on either side of one atom of the *second* type. Imagine, therefore, that we have two atoms of mass m on either side of an atom of mass M. Carbon dioxide is a common example of this design.

We consider a spring of stiffness k between these atoms and assume, once again, that any motion is restricted to the line connecting the three atoms of the molecule. Our approach is similar to the previous example (but is presented slightly differently, indeed as steps, for clarity). We will also make tiny changes to the way we solve equations in a bid to avoid having to compute the inverse of the mass matrix, $\mathbf{B}$, since we will soon find that this is a 3×3 matrix in our current example and not a simple 2×2 matrix like in the last one.

1. **Find the kinetic energy.**
   If the atoms of mass m are displaced by x_1 and x_2 while that of mass M is displaced by x_3, we have the kinetic energy of the entire system as,
   $$T = \frac{1}{2}m(\dot{x}_1^2 + \dot{x}_2^2) + \frac{1}{2}M\dot{x}_3^2$$
   which, in matrix form, gives us the mass matrix, $\mathbf{B}$, as[13],
   $$\mathbf{B} = \begin{pmatrix} m & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & M \end{pmatrix}$$

2. **Find the potential energy.**
   The molecule, in two parts, gives us two terms for the potential energy (i.e. one for the first atom and the middle one, and one for the middle atom and the last one).
   $$V = \frac{1}{2}k\left[(x_3 - x_1)^2 + (x_2 - x_3)^2\right]$$
   which, in its matrix form, gives us the matrix[14],
   $$\mathbf{A} = \begin{pmatrix} k & 0 & -k \\ 0 & k & -k \\ -k & -k & 2k \end{pmatrix}$$

[13] The steps are the same as in §8.1.

[14] To arrive at this matrix, $\mathbf{A}$, or the previous matrix $\mathbf{B}$, as well as their counterparts from §8.1, first simplify the equations for T and V. Next, write them in their expected matrix form: from equation (12) in §7, we know this looks like $T = \frac{1}{2}\dot{\mathbf{x}}^T\mathbf{B}\dot{\mathbf{x}}$. (Note that we used $\mathbf{T}$ to represent the mass matrix in this equation before.) In other words, this must look like,
$$T = \frac{1}{2}\begin{pmatrix} \dot{x}_1 & \dot{x}_2 & \dot{x}_3 \end{pmatrix}\begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix}\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix}$$

3. **Solve the characteristic equation**[15].
We can solve the characteristic equation $|\mathbf{B}^{-1}\mathbf{A}-\lambda\mathbf{I}|=0$ as we did before[16] in §8.1 or we can employ a much simpler method. Since this is derived from the eigenvalue equation $\mathbf{Aa}=\lambda\mathbf{Ba}$, (i.e. equation(9)), where $\mathbf{a}$ is the eigenvector for the eigenvalue λ, we can also solve this simply as $(\mathbf{A}-\lambda\mathbf{B})\mathbf{a}=0$, knowing, as in the previous example, that $\lambda := \omega^2$.

   Either way we find that we end up with,

$$\omega^2(k-\omega^2 m)[k(2m+M)-\omega^2 mM]=0$$

   The three roots of this equation[17] are

$$\omega_1 = 0 \tag{18}$$

$$\omega_2 = \sqrt{\frac{k}{m}} \tag{19}$$

$$\omega_3 = \sqrt{\frac{k}{m}\left(1+\frac{2m}{M}\right)} \tag{20}$$

4. **Use the eigenfrequencies to compute the normalised eigenvectors.**
We know that $(\mathbf{A}-\omega^2\mathbf{B})\mathbf{a}=0$. That is to say, for a given ω_j we can get our eigenvector $\mathbf{a}$ with the components a_{ij}. In matrix form,

$$\begin{pmatrix} k-\omega_j^2 m & 0 & -k \\ 0 & k-\omega_j^2 m & -k \\ -k & -k & 2k-\omega_j^2 M \end{pmatrix} \begin{pmatrix} a_{1j} \\ a_{2j} \\ a_{3j} \end{pmatrix} = 0$$

   giving us three equations for the three eigenvectors associated with each of three normal modes of vibration.

$$\begin{aligned} a_{1j}k - a_{1j}\omega_j^2 m - a_{3j}k &= 0 \\ a_{2j}k - a_{2j}\omega_j^2 m - a_{3j}k &= 0 \\ -a_{1j}k - a_{2j}k + 2a_{3j}k - a_{3j}\omega_j^2 M &= 0 \end{aligned}$$

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for kinetic energy and the equation $V=\frac{1}{2}\mathbf{x}^T\mathbf{Ax}$ for potential energy (in which we used $\mathbf{V}$ to represent the matrix before) in its matrix form looks like,

$$V = \frac{1}{2}\begin{pmatrix} x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

which we can use to solve for the elements of the matrices $\mathbf{B}$ and $\mathbf{A}$.

[15] See the footnote under §8.1 for an explanation of why we need this.

[16] Recollect the basics of matrices: for a matrix $\mathbf{B}$, the inverse is given by $\mathbf{B}^{-1} = \frac{1}{|\mathrm{B}|}\,\mathrm{adj}.\mathbf{B}$, where adj.$\mathbf{B}$ is the transpose of the co-factors of the minor matrix of $\mathbf{B}$. Given that $\mathbf{B}$ is a 3×3 matrix, this is best left as exercise lest these notes get unusually thick.

[17] Note that ω_3 mentioned here will simply be $\sqrt{\frac{3k}{m}}$ if the three atoms are of the same mass, m.

First normal mode. When $j = 1$, for $\omega_1 = 0$, we arrive at $a_{11} = a_{22} = a_{33}$. In other words, for $\omega_1 = 0$, the eigenvector is,

$$\mathbf{a}_1 = a_1 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Note that in the last example (see §8.1), for simplicity, we had ignored the normalisation conditions and thus the **amplitudes** given by the **normalisation constants** a_i for their corresponding eigenvectors, $\mathbf{a}_i$. As a result, we knew how the masses in our system would move relative to each other but we did not know much else, *e.g. by how much did they move?* This was also why we used the proportionality symbol ($\propto$) instead of an outright equals sign.

To normalise is to solve $\mathbf{a}_i^T \mathbf{B} \mathbf{a}_i = 0$. Thus,

$$0 = a_1 \begin{pmatrix} 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} m & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & M \end{pmatrix} a_1 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$0 = a_1^2 \begin{pmatrix} 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} m & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & M \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$a_1 = \frac{1}{\sqrt{2m + M}}$$

To sum up, we have, so far, the eigenfrequency $\omega_1 = 0$ which has the eigenvector,

$$\mathbf{a}_1 = \frac{1}{\sqrt{2m + M}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \tag{21}$$

Second and third normal modes. We repeat the above steps to arrive at the other two normal modes:

$$\mathbf{a}_2 = \frac{1}{\sqrt{2m}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \text{ and,} \tag{22}$$

$$\mathbf{a}_3 = \frac{1}{\sqrt{2m(1 + 2m/M)}} \begin{pmatrix} 1 \\ -2m/M \\ 1 \end{pmatrix} \tag{23}$$

5. **Examine the results.**
   As we did in §8.1, we can now use the eigenvectors to form our matrix $\mathbf{P}$ in the equation $\mathbf{P}\mathbf{x} = \xi$, or,

$$\mathbf{x} = \mathbf{P}^{-1} \xi$$

Knowing[18] that $\mathbf{P}$ is formed by the eigenvectors, $\mathbf{a}_i$, we realise that computing $\mathbf{P}^{-1}$ is going to be complicated. Alternatively, recall that we defined the oscillatory solution in §6.1 as $x_i = a_i e^{-i\omega_i t}$, or, more generally,

$$x_i = a_i(Ce^{i\omega_i t} + C^* e^{-i\omega_i t})$$

Observe that these two equarions are, in fact, the same. The left hand side gives us the matrix $\mathbf{x}$; the right hand side has the components a_i which form the matrix $\mathbf{P}$; and that leaves us with $(Ce^{i\omega_i t} + C^* e^{-i\omega_i t}) = \xi_i$.

Therefore, our solutions[19] look simply like $x_i = a_{ij}\xi_j$ leaving us with,

$$\begin{aligned}
x_1 &= \left(\frac{1}{\sqrt{2m+M}}\right)\xi_1 + \left(\frac{1}{\sqrt{2m}}\right)\xi_2 \qquad + \left(\frac{1}{\sqrt{2m(1+2m/M)}}\right)\xi_3 \\
x_2 &= \left(\frac{1}{\sqrt{2m+M}}\right)\xi_1 + (0)\,\xi_2 \qquad + \left(\frac{-2}{\sqrt{2M(2+2M/m)}}\right)\xi_3 \\
x_3 &= \left(\frac{1}{\sqrt{2m+M}}\right)\xi_1 + \left(\frac{-1}{\sqrt{2m}}\right)\xi_2 \qquad + \left(\frac{1}{\sqrt{2m(1+2m/M)}}\right)\xi_3
\end{aligned}$$

(Note how the terms in parentheses are our a_{ij} terms.)

Hereon we can either invert the matrix $\mathbf{a}$, which is the same as inverting $\mathbf{P}$, and was something we wanted to avoid. This is best done as an exercise and will leave us with values for each ξ_i in terms of three x_i. Each normal coördinate, ξ_i, is an independent oscillator.

However, for our interest in understanding how the system in question will vibrate, i.e. in understanding its *modes of vibration*, we need only look to equations (18, 19 and 20) for the frequencies of vibrations and to equations (21, 22 and 23) for the relative amplitudes.

Note that we will be writing the eigenvector in terms of its components only and we will simply be representing the normalisation constant by some N_i for simplicity.

[18] In §8.1 we took the liberty, albeit inaccurately, of using the eigenvectors *without* normalising them, relying instead only on proportionality. Having only ± 1 as elements allowed us to be somewhat careless in using $x = \mathbf{P}\xi$ to avoid computing $\mathbf{P}^{-1}$ and arrive at the solution in a simpler manner because it was obvious from experience that $x = \mathbf{P}^{-1}\xi$ would have given us the same answer. Here, however, we have normalised our eigenvectors and no longer have the convenience of a matrix with only ± 1 as its elements, which means we will have to compute $\mathbf{P}^{-1}$.

[19] Einstein's summation convention is used here.

(a) **Mode 1.** For $\omega_1 = 0$ with $\mathbf{a}_1 = N_1 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$, where $N_1 = \frac{1}{\sqrt{2m+M}}$.

Although having no frequency might sound unusual, it really just refers to there being no vibration (or oscillation) and this, coupled with the fact that there occurs an *equal displacement* of all masses (as denoted by the components of the vector $\mathbf{a}_1$), means the molecule undergoes translation.

(b) **Mode 2.** For $\omega_2 = \sqrt{\frac{k}{m}}$ with $\mathbf{a}_2 = N_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$, where $N_1 = \frac{1}{\sqrt{2m}}$.

In this case we see that a non-trivial frequency of oscillation does exist, but the eigenvector tells us that the central mass, M, does *not* oscillate. Further, the two masses, m, on either side vibrate exactly out of phase with each other, with the same amplitude.

(c) **Mode 3.** For $\omega_3 = \sqrt{\frac{k}{m}\left(1 + \frac{2m}{M}\right)}$ with $\mathbf{a}_3 = \begin{pmatrix} 1 \\ -2m/M \\ 1 \end{pmatrix}$, where $N_3 = \frac{1}{\sqrt{2m(1+2m/M)}}$.

In this last mode of oscillation, we observe that all three masses oscillate (since neither ω nor any a_{ij} goes to zero). The two masses, m, that flank the central mass oscillate *in phase* with each other and do so with the *same amplitude*. The central mass, M, remains *out of phase* with the other two masses and oscillates with a *different amplitude* as well.

While this tells us enough about our linear triatomic molecule, there are some observations worth noting. On the one hand, had the masses all been equal, we would have had much simpler calculations all through. On the other, had we not restricted all molecular vibrations to the line of the three atoms, we would have had many more degrees of freedom to deal with.

A triatomic molecule, i.e. $n = 3$, generally has $3n = 9$ degrees of freedom. This includes motion perpendicular to the axis, which we have prohibited in our examination of this system, but which nonetheless occurs. This more general case can be studied as an extension building atop of what we have worked out so far.

There will be three translations along the three axes which will all have $\omega = 0$ like in the first mode above. There will also be three rigid rotations about the three axes[20]. We are therefore left with three more degrees of freedom in a *general* triatomic molecule, all of which are vibrational. In our example of a *linear* triatomic

[20]This is for a generic triatomic molecule. For a linear, triatomic molecule, such as the one we have considered in our example, there are only two rotational degrees of freedom; the one along the axis co-inciding with the triatomic arrangement is ruled out since rotation about the axis of such a molecule makes no difference. As such, the total translational and rotational degrees of freedom are five in number and the total vibrational degrees of freedom are therefore $3n - 5 = 4$.

molecule, we are left with *four* vibrational degrees of freedom[21].

Two of these are *longitudinal* (in the x direction, say) as given by the second and third modes above, leaving two other modes in the y and z directions. That said, since the molecule is symmetric, any motions in the y and z directions are indistinguishable, making the two modes degenerate.

8.2.1 The case of a linear triatomic molecule with atoms of equal mass

Seeing how having three linearly arranged atoms of equal mass constituting a molecule is simply a specific case of our discussion in §8.2, there is no need to, once again, show all calculations here minutely. In fact, we can simply focus on what differences arise as a result of having all three masses constant. One of the first is a simpler mass matrix: $B_{ij} = m\delta_{ij}$ in terms of the Kronecker delta. The matrix, $\mathbf{A}$, remains unchanged thanks to its being independent of mass.

In computing the eigenvalues by solving $(\mathbf{A} - \lambda\mathbf{B})\mathbf{a} = (\mathbf{A} - \omega^2\mathbf{B})\mathbf{a} = 0$ we get $\omega^2(k - \omega^2 m)(3k - \omega^2 m) = 0$ with solutions $\omega_1 = 0$, $\omega_2 = \sqrt{\frac{k}{m}}$ (both as in §8.2), and $\omega_3 = \sqrt{\frac{3k}{m}}$, which is a simpler case of the value for ω_3 we arrived at in §8.2.

Of course we can always choose to rid ourselves of all trouble and substitute $M = m$ in equation (20) to arrive at the same result: $\omega_3 = \sqrt{\frac{k}{m}\left(1 + \frac{2m}{M}\right)} = \sqrt{\frac{3k}{m}}$ but our interest is in arriving at this from first principles. The remainder of our reasoning for the physical consequences of this follows as in §8.2, given that our eigenvectors (and their normalisation constants) have now become

$$\mathbf{a}_1 = \frac{1}{\sqrt{3m}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad \mathbf{a}_2 = \frac{1}{\sqrt{2m}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \quad \text{and} \quad \mathbf{a}_3 = \frac{1}{\sqrt{6m}}\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$

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