Physics 106a, Caltech — 29 October, 2019

Lectures 9 & 10: Normal Modes

Here we discuss small vibrations in systems with many degrees of freedom, leading to the idea of normal modes.

General approach

You have learned about simple harmonic oscillators in Ph 12a and in Lecture 6 of this class. You have learned about systems on N coupled oscillators (pendula, masses on springs, molecules, LC circuit chains) in Ph 12a. You've taken the continuum limit (eg, transverse oscillations of a continuous string, transverse and longitudinal oscillations of masses on springs, in 1-D and 3-D, sound waves) in Ph 12a. (If you need a review, Georgi's *Physics of Waves* is available for free on the web). And, you have applied this to crystalline solids in the Debye theory of specific heats, in Ph 12c.

In Ph 12a you learned about normal modes: N distinct oscillators (pendulum bobs, masses on springs) that are coupled to one another, when viewed individually, have complicated motion, at many different frequencies; but in their collective motion, they move in a superposition of N normal modes, with each normal mode behaving like an independent (uncoupled) SHO at one specific frequency. Because the equations of motion are linear in the displacement, the normal modes are each a specific superposition of the motion of the N individual oscillators, and the individual oscillators are a superposition of the normal modes. Normal mode analysis makes it easy to understand the complicated motion of individual oscillators when they are coupled to others. (Although vibrations of molecules and crystals require quantum mechanics to fully describe them, the classical theory is sufficient for enumerating normal modes, except at low temperatures, when $k_bT < (n + 1/2)\hbar\omega$ is insufficient to support even $n = 1$; those modes "freeze out", resulting in the Debye theory of heat capacity of solids).

Linear superposition leads us to use the formal notation and computational power of linear algebra. In the *basis* of coupled displacement coordinates, the Lagrangian is not diagonal; in the *normal mode basis*, it is diagonal, and we get a set of uncoupled oscillators. Linar algebra shows us how to rotate from one basis to the other, to *diagonalize* the degrees of freedom.

Linear algebra has an elegant and compact notation and conceptual structure. Hidden under the hood is the nitty gritty of how to actually solve problems: inverting $N \times N$ matrices, diagonalizing them, solving eigenvalue problems, and so on. This is all pretty easy for $N = 2$ and maybe even $N = 3$, after which, you'd have to be crazy to try to do it analytically. However, the techniques are well-established, if exceedingly tedious; textbooks are filled with the details, and computers handle the tedium (numerically, not analytically). We even have an entire computing language, MATLAB, designed specifically to solve these problems numerically with very efficient algorithms. For any problem with $N > 3$, turn to MATLAB (or any other computing language that has the same capabilities, such as numpy.linalg for python).

Examples

Simple examples of the collective (normal mode) motion of N coupled SHO's include:

- a 1-dim chain of N masses connected by springs, of equilibrium length L that can oscillate about their equilibrium position (either longitudinally, along the chain; or transversely, perpendicular to the chain).
  - The ends can be fixed, or free to move.

  - In either case, the collective motion of the normal modes are the familiar configurations with wavelengths $\lambda_n = 2L/n$, where n is an integer that counts the number of nodes along the chain (including one but not both endpoints). The shortest wavelength corresponds to the "zigzag" mode, where $n = N$.
  - The spatial frequency is $k_n = 2\pi/\lambda_n$ and the temporal frequency is $\omega_n = 2\pi\nu_n = vk_n$, or $\nu_n = v/\lambda_n$ (which is the physicist's answer to the question "What's nu?".)
  - Here, v is the "speed of sound" in the material; if it doesn't depend of the frequency, then all frequencies travel at the same speed; the material is "dispersionless". If v depends on frequency, then different frequency components of a travelling pulse will travel at different speeds, and the pulse will "disperse".
  - Chains connected by springs have "nearest neighbor" couplings; but one can imagines systems with next-to-nearest-neighbor couplings (or beyond).
  - If the chain has *free* ends, the whole thing can translate and rotate as well; these are modes with $\omega = 0$.
  - in the continuum limit ($N \to \infty$, $Nm/L \to \rho$, the mass per unit length), we have a massive elastic string, and the transverse normal modes of oscillation are the modes of a violin string.

- Instead of masses and springs, we can have coupled pendula, free to move in one or two dimensions.

- A crystalline solid elastic body can be envisioned as a 3-dimensional lattice of masses and "springs" (ionic bonds). Here, $N \sim 10^{24}$ (Avogadro's number). A cubic or rectangular lattice is simple enough to visualize, but many crystalline solids have more complex structure (which can be categorized and enumerated in group theory, as you will study in crystallography.)

- Diatomic and tri-atomic molecules ($N = 2$ or $N = 3$ atoms with molecular bonds). Triatomic molecules can be linear (like carbon dioxide, CO_2: O-C-O) or planar triangles (like ozone, O_3).

- Thus, the formalism developed below works for $N =$ few (like, 2 or 3), $N = 10^{24}$ (Avogadro's number), or $N = \infty$ (the continuum limit), and for systems in 1 spatial dimension, or 2, or 3 (or more!).

Notation

Note that we use a different convention than Hand and Finch for defining the kinetic and potential energy matrices. Here, we keep an explicit factor of $\frac{1}{2}$ in the definition of the kinetic energy (or mass) matrix and the potential energy matrix. We use different symbols $\boldsymbol{T}, \boldsymbol{V}$ instead of $\boldsymbol{t}, \boldsymbol{v}$ in Hand and Finch (then $\boldsymbol{T} = 2\boldsymbol{t}, \boldsymbol{V} = 2\boldsymbol{v}$). This convention is the one used by Goldstein et al. The choice of convention does not change the equations of motion. We also use $\boldsymbol{q}$ for the generalized coordinates as usual, instead of $\boldsymbol{\phi}$ as in Hand and Finch. We use bold for a vector of generalized coordinates, to contrast with the arrow symbol for a vector in three dimensional coordinate space. Finally, it should always be clear from the context what is a scalar and what is a column vector, matrix, or row vector.

Setup

We restrict our attention to systems of N degrees of freedom with generalized coordinates q_i. There can be time independent holonomic constraints (so that the $3M$ "Newtonian" degrees of

freedom for M particles in 3-D can be reduced to $N < 3M$ generalized coordinates). Assume a time independent Lagrangian. Under these restrictions the kinetic energy is a quadratic form in the $\{\dot{q}_i\}$'s, and $H = T + V$ is a conserved energy.

The condition for a *stable equilibrium* is that the potential energy is a minimum, and we arrange the minimum to be at $q_i = 0$, so that the potential V is quadratic in the $\{q_i\}$'s.

Expand to quadratic order in $q_i, \dot{q}_i$ for small displacements from the equilibrium: using matrix notation (with $\boldsymbol{q}$ the column vector with components q_j, $\tilde{\boldsymbol{q}}$ the row vector, etc.) this gives

$$T = \tfrac{1}{2}\tilde{\dot{\boldsymbol{q}}} \cdot \boldsymbol{T} \cdot \dot{\boldsymbol{q}} \qquad \text{with} \qquad T_{ij} = \left.\frac{\partial^2 T}{\partial \dot{q}_i \partial \dot{q}_j}\right|_{\{q_j\}=0,\{\dot{q}_j\}=0} \tag{1}$$

$$V = \tfrac{1}{2}\tilde{\boldsymbol{q}} \cdot \boldsymbol{V} \cdot \boldsymbol{q} \qquad \text{with} \qquad V_{ij} = \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_{\{q_j\}=0,\{\dot{q}_j\}=0} \tag{2}$$

Note that H&F instead put the 1/2 into the $\boldsymbol{T}$, which they write as $\boldsymbol{t}$, and the same for $\boldsymbol{V}$.

Both $\boldsymbol{T}$ and $\boldsymbol{V}$ are symmetric, $N \times N$ matrices, with elements that are constant (not functions of time, or of $\boldsymbol{q}$ or $\dot{\boldsymbol{q}}$), at least, to quadratic order.

We will assume that the kinetic energy is positive for all $\dot{\boldsymbol{q}}$ in which case the matrix $\boldsymbol{T}$ is said to be positive definite (T cannot be negative, and if there are any "directions" $\dot{\boldsymbol{q}}$ for which T is zero, there are no dynamics for this direction, and we can eliminate it from the discussion).

Also the potential matrix $\boldsymbol{V}$ is positive definite for expansion about a *stable* equilibrium (V increases for any $\boldsymbol{q}$). Sometimes, in the case of symmetries such as translational or rotational, there may be directions of *neutral stability* — the potential change is zero to quadratic order. In that case, as we will see, the mode frequencies are $\omega = 0$; they correspond not to oscillations, but to translations or rotations.

Recall from Lecture 6 that, for a single SHO, the equilibrium is stable if $V \propto q^2$ so that $L \propto (\dot{q}^2 - \omega^2 q^2)$ and $H \propto (p^2 + \omega^2 q^2)$. The same is true for $N > 1$. For unstable equilibria, $L \propto (\dot{q}^2 + \omega^2 q^2)$ and $H \propto (p^2 - \omega^2 q^2)$. We will not consider that case here.

In these expressions, and those below, if you don't understand what they mean, write out in terms of components using the summation convention, or compare with the treatment of the two coupled oscillators.

Equations of motion and eigenvalue problem

The Lagrangian (ignoring, for now, damping or driving force terms) becomes

$$L = \tfrac{1}{2}\tilde{\dot{\boldsymbol{q}}} \cdot \boldsymbol{T} \cdot \dot{\boldsymbol{q}} - \tfrac{1}{2}\tilde{\boldsymbol{q}} \cdot \boldsymbol{V} \cdot \boldsymbol{q} \ . \tag{3}$$

The Euler-Lagrange equations give

$$\boldsymbol{T} \cdot \ddot{\boldsymbol{q}} + \boldsymbol{V} \cdot \boldsymbol{q} = 0 \ . \tag{4}$$

We look for a solution varying sinusoidally, which in complex notation is

$$\boldsymbol{q}(t) = \boldsymbol{\Phi} e^{i\omega t} \tag{5}$$

with $\boldsymbol{\Phi}$ a column vector giving the amplitudes of each coordinate q_i in the oscillation. Substituting into Eq. (4) gives

$$\boldsymbol{V} \cdot \boldsymbol{\Phi} - \omega^2 \boldsymbol{T} \cdot \boldsymbol{\Phi} = 0 = \left(\boldsymbol{V} - \omega^2 \boldsymbol{T}\right) \cdot \boldsymbol{\Phi} \ . \tag{6}$$

Because of the appearance of $\boldsymbol{T}$ in the second term (instead of a unit matrix) this is not exactly an eigenvalue problem; it is called a *generalized eigenvalue problem.* The procedure is basically the same as for a regular eigenvalue problem, and many of the theorems on the eigenvalues and eigenvectors

carry over, with slight modifications. The condition for a solution to these N homogeneous linear equations is

$$\det(\boldsymbol{V} - \omega^2 \boldsymbol{T}) = 0. \tag{7}$$

Expanding this out gives an Nth order polynomial in ω^2, and so there are N solutions ω_α^2, the eigenvalues, which give the *normal mode frequencies*. For each of these, substitution in Eq. (6) gives the corresponding eigenvectors $\boldsymbol{\Phi}^{(\alpha)}$ which we call the *normal modes* (the components give the size of the displacements q_i in each mode, up to an overall constant factor since the equations are linear). There are as many normal modes as original coordinates. We will use latin indices (i, j, k) for the generalized coordinates and greek indices (α, β, γ) for the normal modes. One is a linear superposition of the other, and we will learn how to "rotate" from one to the other.

The following results can be proved. The method follows the scheme for the eigenvalues and eigenvectors of a real symmetric matrix (see for example Hand and Finch §9.6).

- the eigenvalues ω_α^2 are real.
- there may be more than one eigenvalue with the same value; this is called a *degeneracy*.
- the eigenvectors $\boldsymbol{\Phi}^{(\alpha)}$ may be chosen real (we will do this); this is easy to see from Eq. (6).
- assuming $\boldsymbol{T}$ is positive definite, then if $\boldsymbol{V}$ is positive definite, corresponding to a stable equilibrium, $\omega_\alpha^2 > 0$ and the mode frequencies ω_α are real so that the solutions are oscillatory rather than exponentially growing/decaying.
- a symmetry may lead to no change in potential energy for some displacement: this will give a zero eigenvalue and a *zero frequency mode*. For example, collective motion of the $\boldsymbol{q}$'s can be simple translational or rotational motion (for an elastic but otherwise rigid body, these are 6 degrees of freedom), with $\omega = 0$.
- different eigenvectors can be chosen orthonormal (orthogonal and normalized to 1); in the sense

  $$\tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \boldsymbol{\Phi}^{(\beta)} = \delta_{\alpha\beta} \ , \quad \textit{not the usual} \quad \tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{\Phi}^{(\beta)} = \delta_{\alpha\beta} \ . \tag{8}$$

  This is easy to prove for the case of non-degenerate eigenvalues; for degenerate eigenvalues we can choose linear combinations within the degenerate subspace so that they are orthogonal (see Hand and Finch pp 365-367 for an example of this). There are many ways to do this, but often, symmetries suggest simple solutions.
- the eigenvectors form a complete set, spanning all possible values of $\boldsymbol{q}$ (the *coupled* basis), and may be used as an alternative, *uncoupled* basis.

  Note the appearance of $\boldsymbol{T}$ in Eq. (8) — we can think of $\boldsymbol{T}$ as playing the role of the "metric" for defining scalar products in the vector space of the generalized coordinates. This is the main difference from the regular eigenvalue problem.

General solution

The normal modes provide a basis, and at any time we can write a general solution for the motion in the coupled basis $\boldsymbol{q}(t)$ in terms of the normal modes:

$$\boldsymbol{q}(t) = \sum_\alpha \rho_\alpha(t) \boldsymbol{\Phi}^{(\alpha)} \tag{9}$$

(where both $\boldsymbol{q}$ and $\boldsymbol{\Phi}^{(\alpha)}$ are column vectors with N rows), or in component form:

$$q_i(t) = \sum_\alpha \rho_\alpha(t) \Phi_i^{(\alpha)} \ . \tag{10}$$

The $\rho_\alpha(t)$ are called *normal mode coordinates.* Define the matrix $\boldsymbol{R}$ as

$$R_{i\alpha} = \Phi_i^{(\alpha)} \tag{11}$$

(the *columns* of $\boldsymbol{R}$ are the eigenvectors). Then we can write

$$q_i(t) = \sum_\alpha R_{i\alpha} \rho_\alpha(t) \qquad \text{or} \qquad \boldsymbol{q}(t) = \boldsymbol{R} \cdot \boldsymbol{\rho}\ (t). \tag{12}$$

The orthogonality Eq. (8) can be expressed as (check components!)

$$R_{\alpha i} T_{ij} R_{j\beta} = \delta_{\alpha\beta} \qquad \text{or} \qquad \tilde{\boldsymbol{R}} \cdot \boldsymbol{T} \cdot \boldsymbol{R} = \boldsymbol{I} \qquad \text{or} \qquad \tilde{\boldsymbol{R}} \cdot \boldsymbol{T} = \boldsymbol{R}^{-1} \ , \tag{13}$$

with $\boldsymbol{I}$ the unit $N \times N$ matrix. Using this we can calculate the inverse relation

$$\boldsymbol{\rho}(t) = \tilde{\boldsymbol{R}} \cdot \boldsymbol{T} \cdot \boldsymbol{q}(t) \qquad \text{or} \qquad \rho_\alpha(t) = \tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \boldsymbol{q}(t) \ . \tag{14}$$

This is useful for calculating $\boldsymbol{\rho}(0)$ in terms of initial conditions on $\boldsymbol{q}$, for example.

Diagonalization

Equation (13) shows how to convert $\boldsymbol{T}$ to diagonal form (uncoupled basis). Also, using Eq. (6)

$$(\tilde{\boldsymbol{R}} \cdot \boldsymbol{V} \cdot \boldsymbol{R})_{\alpha\beta} = \tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{V} \cdot \boldsymbol{\Phi}^{(\beta)} = \omega_\beta^2 \tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \boldsymbol{\Phi}^{(\beta)} = \omega_\beta^2 \delta_{\alpha\beta} \tag{15}$$

so that $\boldsymbol{R}$ also diagonalizes $\boldsymbol{V}$

$$\tilde{\boldsymbol{R}} \cdot \boldsymbol{V} \cdot \boldsymbol{R} = \boldsymbol{\Omega} \tag{16}$$

where $\boldsymbol{\Omega}$ is the diagonal matrix with entries ω_α^2. Thus the *congruence transformation* $\tilde{\boldsymbol{R}} \cdot \boldsymbol{?} \cdot \boldsymbol{R}$ diagonalizes both $\boldsymbol{T}$ and $\boldsymbol{V}$.

You will remember, or encounter later, the important result in quantum mechanics that only matrices that *commute* can be simultaneously diagonalized by a unitary transformation. The difference in the present work is that $\boldsymbol{R}$ is *not* in general an orthogonal matrix (the real equivalent of a unitary matrix) $\tilde{\boldsymbol{R}} \cdot \boldsymbol{R} \neq \boldsymbol{I}$. The extra flexibility allows *any* pair of matrices to be simultaneously diagonalized by the congruence transformation (not a similarity transform since $\tilde{\boldsymbol{R}} \neq \boldsymbol{R}^{-1}$).

Equations of motion

The equations of motion for $\boldsymbol{\rho}(t)$ are given by substituting Eq. (9) into Eq. (4)

$$\sum_\alpha (\ddot{\rho}_\alpha \boldsymbol{T}\cdot\boldsymbol{\Phi}^{(\alpha)} + \rho_\alpha \boldsymbol{V}\cdot\boldsymbol{\Phi}^{(\alpha)}) = 0 \ , \tag{17}$$

and then using Eq. (6) to give

$$\sum_\alpha (\ddot{\rho}_\alpha + \omega_\alpha^2 \rho_\alpha)\boldsymbol{T}\cdot\boldsymbol{\Phi}^{(\alpha)} = 0 \ . \tag{18}$$

Now multiply on the left by $\tilde{\boldsymbol{\Phi}}_\beta$ and use the orthonormality to get

$$\ddot{\rho}_\beta + \omega_\beta^2 \rho_\beta = 0 \tag{19}$$

so that the normal mode coordinates act as simple harmonic oscillators

$$\rho_\alpha(t) = \rho_\alpha(0)\cos(\omega_\alpha t + \theta_\alpha) \ , \tag{20}$$

with $\rho_\alpha(0)$ and θ_α set by initial conditions. Equation (19) is for undriven motion. We could add oscillating force terms $\boldsymbol{F}(t)$ to Eq. (4), with each component corresponding to the generalized force for that generalized coordinate. Equation (18) would then have this force term on the right hand side, and Eq. (19) would become

$$\ddot{\rho}_\beta + \omega_\beta^2 \rho_\beta = \mathcal{F}_\beta \quad \text{with} \quad \mathcal{F}_\beta = \tilde{\boldsymbol{\Phi}}^{(\beta)}\cdot\boldsymbol{F}. \tag{21}$$

Then if the force is sinusoidal with frequency ω, we would get a resonance response whenever ω is at each mode frequency (assuming the force is not orthogonal to that normal mode vector). To get a finite response on resonance, we would need to add dissipative terms to the equations of motion.

Lagrangian and Hamiltonian

It is straightforward to show (using the vector form in Eq. (12) and Eq. (13) is easiest)

$$T = \tfrac{1}{2}\tilde{\dot{\boldsymbol{q}}}\cdot\boldsymbol{T}\cdot\dot{\boldsymbol{q}} = \tfrac{1}{2}\tilde{\dot{\boldsymbol{\rho}}}\cdot\dot{\boldsymbol{\rho}} \tag{22}$$

$$V = \tfrac{1}{2}\tilde{\boldsymbol{q}}\cdot\boldsymbol{V}\cdot\boldsymbol{q} = \tfrac{1}{2}\tilde{\boldsymbol{\rho}}\cdot\boldsymbol{\Omega}\cdot\boldsymbol{\rho} \tag{23}$$

so that the Lagrangian is

$$L = \tfrac{1}{2}\sum_\alpha (\dot{\rho}_\alpha^2 - \omega_\alpha^2\rho_\alpha^2) \ . \tag{24}$$

Note that all the variables $\boldsymbol{q}, \boldsymbol{\rho}$ must be real variables in these expressions—care must be taken since we are forming nonlinear quantities. Defining the momentum conjugate to the normal mode coordinate in the usual way

$$p_{\rho,\alpha} = \frac{\partial L}{\partial \dot{\rho}_\alpha} = \dot{\rho}_\alpha \tag{25}$$

gives the Hamiltonian

$$H = \tfrac{1}{2}\sum_\alpha (p_{\rho,\alpha}^2 + \omega_\alpha^2\rho_\alpha^2) \ . \tag{26}$$

The expressions for the Lagrangian and Hamiltonian are the sum of N independent harmonic oscillators.

Initial conditions

It is often convenient, as for a single simple harmonic oscillator, to use complex notation for the oscillations

$$\rho_\alpha(t) = \mathrm{Re}[A_\alpha e^{i\omega_\alpha t}] \tag{27}$$

with A_α a complex amplitude that sets the magnitude and the phase of the oscillations (this then contains both the $e^{i\omega_\alpha t}$ and $e^{-i\omega_\alpha t}$ time dependencies solving Eq. (19)).[1] The general solution Eq. (9) can now be written (remember $\mathbf{\Phi}^{(\alpha)}$ is real)

$$\boldsymbol{q}(t) = \sum_\alpha \mathrm{Re}[A_\alpha e^{i\omega_\alpha t}]\mathbf{\Phi}^{(\alpha)} \ . \tag{28}$$

and then

$$\dot{\boldsymbol{q}}(t) = \sum_\alpha \mathrm{Re}[i\omega_\alpha A_\alpha e^{i\omega_\alpha t}]\mathbf{\Phi}^{(\alpha)} \ . \tag{29}$$

The initial conditions are usually known in terms of the initial coordinates $\boldsymbol{q}(0)$ and velocities $\dot{\boldsymbol{q}}(0)$. Using the orthogonality relation to invert the above equations at time zero as in Eq. (14) gives

$$\mathrm{Re}\, A_\alpha = \tilde{\mathbf{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \boldsymbol{q}(0) \ , \tag{30}$$

$$\mathrm{Im}\, A_\alpha = -\tilde{\mathbf{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \dot{\boldsymbol{q}}(0)/\omega_\alpha \ . \tag{31}$$

From this we can compute the magnitude and phase of all of the A_α's for any initial condition.

Examples

Two coupled pendulums

See Hand and Finch §9.1 for the discussion. Make sure you understand the patterns of the two normal modes.

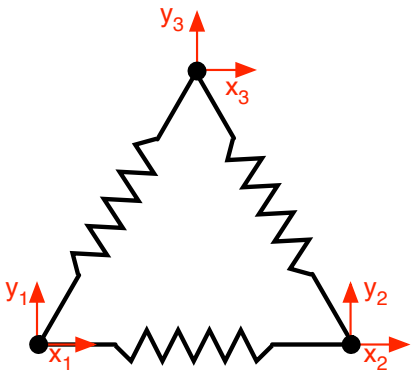
Molecular vibrations

The vibrations of ball-and-spring descriptions of molecules provide nice examples of the use of normal modes, important in spectroscopy, statistical mechanics, etc. See Hand and Finch §9.5 for the discussion of the linear triatomic molecule (e.g. CO_2), although in class I suggest using symmetry-based intuitive understanding and the orthogonality of the modes might be an easier way to proceed in general than diagonalizing large matrices.

[1] Often, as for the single oscillator, we might write "$\rho_\alpha(t) = A_\alpha e^{i\omega_\alpha t}$", thinking of the normal mode coordinate as complex, and then remember to take the real part to give the physical solution. This is OK for linear manipulations, but not for nonlinear ones such as calculating the kinetic and potential energies.

Vibrations of Ozone

Ozone (O_3) is a tri-atomic molecule with the shape of an equilateral triangle. Out of lack of inspiration, we will use six cartesian degrees of freedom to describe the dynamics, even through there clearly are translational and rotational symmetries in the problem that should inspire us to reduce the problem to three generalized coordinates. As we will see, we'll end up with zero frequency modes.



Normal mode analysis of vibrations of Ozone

The potential energy is only non-zero when springs are stretched or compressed; that is, when the masses move with the projection of their displacements *along* a spring. In terms of the coordinates

$$\mathbf{q} = (x_1, y_1, x_2, y_2, x_3, y_3),$$

the potential energy is:

$$V = \tfrac{1}{2}K\left\{\left[\tfrac{1}{2}(x_2 - x_3) + \tfrac{\sqrt{3}}{2}(y_3 - y_2)\right]^2 + \left[\tfrac{1}{2}(x_3 - x_1) + \tfrac{\sqrt{3}}{2}(y_3 - y_1)\right]^2 + (x_2 - x_1)^2\right\}$$

and the *matrix* V_{ij} is

$$V_{14} = \frac{\partial^2 V}{\partial x_1 \partial y_2} \quad \text{etc.}$$

$$\mathbf{V} = K\begin{pmatrix} 5/4 & \sqrt{3}/4 & -1 & 0 & -1/4 & -\sqrt{3}/4 \\ \sqrt{3}/4 & 3/4 & 0 & 0 & -\sqrt{3}/4 & -3/4 \\ -1 & 0 & 5/4 & -\sqrt{3}/4 & -1/4 & \sqrt{3}/4 \\ 0 & 0 & -\sqrt{3}/4 & 3/4 & \sqrt{3}/4 & -3/4 \\ -1/4 & -\sqrt{3}/4 & -1/4 & \sqrt{3}/4 & 1/2 & 0 \\ -\sqrt{3}/4 & -3/4 & \sqrt{3}/4 & -3/4 & 0 & 3/2 \end{pmatrix}$$

$$\mathbf{T} = m\mathbf{I}$$

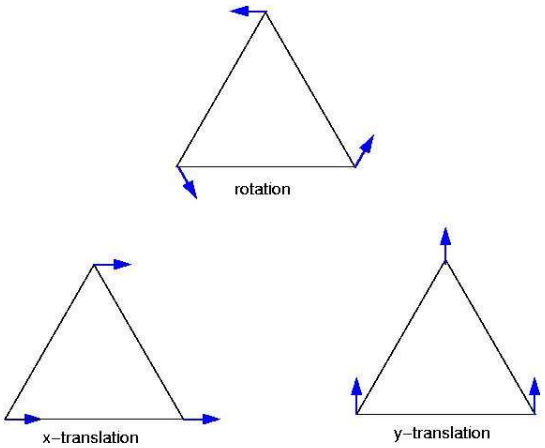
The kinetic energy matrix is $T = mI$, where I is the 6×6 unit matrix in the $\mathbf{q}$ basis. Linear algebra with Eq. (6) gives the normal mode eigenvalues ω_α^2 and eigenvectors:

$$\text{Eigenvalues}[\mathbf{V}/m]: \quad \left\{0, 0, 0, \frac{3k}{2m}, \frac{3k}{2m}, \frac{3k}{m}\right\}$$

The general motion is a linear superposition of the 6 normal eigenmodes, with coefficients that are the *normal mode coordinates*.

Zero frequency modes

How do we identify the eigenvectors associated with the three degenerate zero frequency modes? We can invoke symmetries to convince ourselves that they correspond to two translational and one rotational degrees of freedom (in the 2-D $x-y$ plane). These have to be mutually orthogonal eigenvectors (convince yourself that they are!):



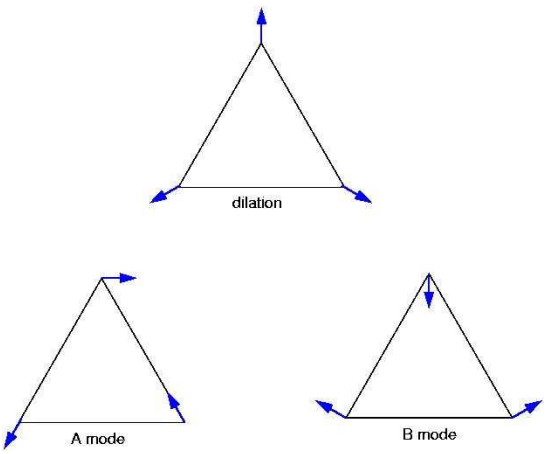
Vibrational modes

The three other modes are vibrational. Standard but tedious linear algebra (use MATLAB or Mathematica) gives us the orthonormal eigenvectors (two of which are degenerate):

$$\text{Eigenvectors[V][[6]]:} \quad \left\{-\frac{\sqrt{3}}{2}, -\frac{1}{2}, \frac{\sqrt{3}}{2}, -\frac{1}{2}, 0, 1\right\}$$

$$\text{Eigenvectors[V][[5]]:} \quad \left\{-\frac{1}{2}, -\frac{\sqrt{3}}{2}, -\frac{1}{2}, \frac{\sqrt{3}}{2}, 1, 0\right\}$$

$$\text{Eigenvectors[V][[4]]:} \quad \left\{\frac{-\sqrt{3}}{2}, \frac{1}{2}, \frac{\sqrt{3}}{2}, \frac{1}{2}, 0, -1\right\}$$



A and B modes are *degenerate*. These solutions are the generators of symmetry transformations (rotations about 120°), as described by group theory for $\bar{6}m2$ point group.