Physics 106a: **3 December, 2013**

Lecture 18: Normal Modes

In this lecture I discuss small vibrations in systems with many degrees of freedom leading to the idea of normal modes.

General approach

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

Setup

We restrict our attention to systems of N degrees of freedom with generalized coordinates q_i with time independent holonomic constraints and a time independent Lagrangian. Under these restrictions the kinetic energy is a quadratic form in the $\dot{q}_i$, and the condition for a *stable equilibrium* is that the potential energy is a minimum. We arrange the minimum to be at $q_i = 0$.

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

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

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

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. Both $\boldsymbol{T}$ and $\boldsymbol{V}$ are symmetric. 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 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

$$\boldsymbol{V} \cdot \boldsymbol{\Phi} - \omega^2 \boldsymbol{T} \cdot \boldsymbol{\Phi} = 0 \,. \tag{6}$$

Because of the appearance of $\boldsymbol{T}$ in the second term this 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.

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
- the eigenvectors $\boldsymbol{\Phi}^{(\alpha)}$ may be chosen real (we will do this)
- 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*
- different eigenvectors can be chosen orthonormal (orthogonal and normalized to 1) in the sense

$$\tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \boldsymbol{\Phi}^{(\beta)} = \delta_{\alpha\beta} \,. \tag{8}$$

- the eigenvectors form a complete set and may be used as a 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. As usual, you can show that eigenvectors for different eigenvalues are necessarily orthogonal; for degenerate eigenvalues we can choose linear combinations within the degenerate subspace so that they are orthogonal (see Hand and Finch p367 for an example of this).

General solution

The normal modes provide a basis, and at any time we can write a general solution in terms of the normal modes

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

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!)

$$\tilde{\boldsymbol{R}}\cdot\boldsymbol{T}\cdot\boldsymbol{R} = \boldsymbol{I} \tag{13}$$

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.

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

$$\sum_\alpha(\ddot{\rho}_\alpha\boldsymbol{T}\cdot\boldsymbol{\Phi}^{(\alpha)} + \rho_\alpha\boldsymbol{V}\cdot\boldsymbol{\Phi}^{(\alpha)}) \tag{15}$$

and then using Eq. (6) to give

$$\sum_\alpha(\ddot{\rho}_\alpha + \omega_\alpha^2\rho_\alpha)\boldsymbol{T}\cdot\boldsymbol{\Phi}^{(\alpha)} = 0\,. \tag{16}$$

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

$$\ddot{\rho}_\beta + \omega_\beta^2\rho_\beta = 0 \tag{17}$$

so that the normal mode coordinates act as simple harmonic oscillators $\rho_\alpha(t) \propto \cos(\omega_\alpha t + \theta_\alpha)$, with θ_α an integration constant. Equation (17) 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 (16) would then have this force term on the right hand side, and Eq. (17) would become

$$\ddot{\rho}_\beta + \omega_\beta^2\rho_\beta = \mathcal{F}_\beta \quad \text{with} \quad \mathcal{F}_\beta = \tilde{\boldsymbol{\Phi}}^{(\beta)}\cdot\boldsymbol{F}. \tag{18}$$

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)

$$T = \tfrac{1}{2}\tilde{\dot{\boldsymbol{q}}}\cdot\boldsymbol{T}\cdot\dot{\boldsymbol{q}} = \tfrac{1}{2}\tilde{\dot{\boldsymbol{\rho}}}\cdot\dot{\boldsymbol{\rho}} \tag{19}$$

$$V = \tfrac{1}{2}\tilde{\boldsymbol{q}}\cdot\boldsymbol{V}\cdot\boldsymbol{q} = \tfrac{1}{2}\tilde{\boldsymbol{\rho}}\cdot\boldsymbol{\Omega}\cdot\boldsymbol{\rho} \tag{20}$$

so that the Lagrangian is

$$L = \tfrac{1}{2}\sum_\alpha(\dot{\rho}_\alpha^2 - \omega_\alpha^2\rho_\alpha^2)\,. \tag{21}$$

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

$$p_{\rho,\alpha} = \frac{\partial L}{\partial\dot{\rho}_\alpha} = \dot{\rho}_\alpha \tag{22}$$

gives the Hamiltonian

$$H = \tfrac{1}{2}\sum_\alpha(p_{\rho,\alpha}^2 + \omega_\alpha^2\rho_\alpha^2)\,. \tag{23}$$

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

Diagonalization

Equation (13) shows how to convert $\boldsymbol{T}$ to diagonal form. Also

$$(\tilde{\boldsymbol{R}} \cdot \boldsymbol{V} \cdot \boldsymbol{R})_{\alpha\beta} = \tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{V} \cdot \boldsymbol{\Phi}^{(\beta)} = \omega_\beta^2 \tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \boldsymbol{\Phi}^{(\beta)} = \omega_\beta^2 \delta_{\alpha\beta} \tag{24}$$

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

$$\tilde{\boldsymbol{R}} \cdot \boldsymbol{V} \cdot \boldsymbol{R} = \boldsymbol{\Omega} \tag{25}$$

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 $\tilde{\boldsymbol{R}} \neq \boldsymbol{R}^{-1}$).

Initial conditions

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

$$\rho_\alpha(t) = \mathrm{Re}[A_\alpha e^{i\omega_\alpha t}] \tag{26}$$

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. (17)).[1] The general solution Eq. (9) can now be written (remember $\boldsymbol{\Phi}^{(\alpha)}$ is real)

$$\boldsymbol{q}(t) = \sum_\alpha \mathrm{Re}[A_\alpha e^{i\omega_\alpha t}] \boldsymbol{\Phi}^{(\alpha)} \, . \tag{27}$$

and then

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

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

$$\mathrm{Re}\, A_\alpha = \tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \boldsymbol{q}(0) \, , \tag{29}$$

$$\omega_\alpha \, \mathrm{Im}\, A_\alpha = -\tilde{\boldsymbol{\Phi}}^{(\alpha)} \cdot \boldsymbol{T} \cdot \dot{\boldsymbol{q}}(0) \, . \tag{30}$$

Examples

Two coupled pendulums

See Hand and Finch §9.1 for the discussion.

[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.

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. See the slides for a discussion of ozone, a molecule with the shape of an equilateral triangle.

Michael Cross December 2, 2013