Non-rigid bodies

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Small displacements from equilibrium

For a system with D degrees of freedom, q_i, the Lagrangian is

$$L = \frac{1}{2}\sum_{i=1}^{D} m_i \dot{q}_i^2 - V(q_1, q_2, \cdots, q_D).$$

If the coordinates at the minimum of the potential are Q_i then

$$\left.\frac{\partial V}{\partial q_i}\right|_{Q_i} = 0.$$

As a result, for small displacements around the minimum, $q_i = Q_i + \xi_i$, one can write

$$V(\{\xi_i\}) = V(\{Q_i\}) + \frac{1}{2}\left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_{Q_i} \xi_i \xi_j + \mathcal{O}(\xi_i^3).$$

As long as the displacements are small, the cubic and higher terms can be neglected. This is the problem of small oscillations.

The Hessian

A constant in the potential has no effect on the force and can always be dropped. Then this expansion, gives an effective Lagrangian

$$L = \frac{1}{2}\sum_{i=1}^{D} m_i \dot{\xi}_i^2 - \frac{1}{2}\sum_{ij=1}^{D} \Omega_{ij}\xi_i\xi_j,$$

where Ω_{ij} is the Hessian matrix, *i.e.*, the square matrix each element of which is one of the second derivatives of the original potential. Clearly the Hessian is symmetric.

A theorem

At stable equilibrium the Hessian has non-negative eigenvalues. Proof: The potential, V, has a minimum at $\xi_i = 0$. However, if one or more of the eigenvalues were negative, then a smaller value of V could be obtained by moving away from the origin in the direction of the corresponding eigenvectors.

Normal modes

We show now that the generic result of a small displacement is oscillation.

It is useful to make a canonical transformation which diagonalizes the Hessian. The eigendirections of the Hessian, ξ_i are called normal modes. Since the Hessian is symmetric, this transformation is orthogonal. As a result, in the new coordinates, ξ_i, the Lagrangian is

$$L = \frac{1}{2}\sum_{i=1}^{D} m_i[\dot{\xi}_i^2 - \omega_i^2\xi_i^2].$$

This is the Lagrangian of D independent oscillators; the frequency of each normal mode is given by the eigenvalue of the Hessian, λ_i, through the relation $\omega_i^2 m_i = \lambda_i$.

A special case is worth noting: if one or more of the eigenvalues of the Hessian vanish then the cubic and quartic terms have to be investigated.

Some problems

Problem 63: Vibrations of diatomic molecules

The atoms in a diatomic molecule need not sit at the equilibirum positions. Set up and solve the problem of small oscillations: identify the number of degrees of freedom, write the Lagrangian, find the generalized momenta and forces, set up the equations of motion, and solve them. Build a table of the values of the free parameters in the Lagrangian for different molecules.

Problem 64: Vibrations of triatomic molecules

Triatomic molecules may be linear (ozone) or not (water). Solve the problem of small oscillations in both cases: identify the number of degrees of freedom, write the Lagrangian, find the generalized momenta and forces, set up the equations of motion, and solve them. Build a table which lists the values of each free parameter for every molecule you can find.

Solving the equations

The equations of motion are

$$\ddot{\xi}_i = \omega_i^2 \xi_i.$$

The general solution is

$$\begin{aligned} \xi_i(t) &= \mathrm{Re}\left[A e^{i\omega_i t} + B e^{-i\omega_i t}\right] \\ &= A' \cos\omega_i t + B' \sin\omega_i t. \end{aligned}$$

Clearly this whole topic is a development of the simple pendulum. In that case there is one degree of freedom, which is the angle of the pendulum from the vertical, ϕ. The shape of the potential is $\cos\phi$. For small oscillations one needs to keep only the quadratic term. Since there is only one mode, the diagonalization of the Hessian is trivial, and one gets the oscillatory solution above.

A chain

Consider N particles all laid out in a chain, each connected to its neighbour by a spring. The equilibrium distances are $q_i = Q_i$. Now suppose the i-th particle is displaced from its equilibrium position to the right by an amount ξ_i. Then the distance between the i-th and the $i+1$-st particles are $Q_i - \xi_i + \xi_{i+1}$.
As a result, the quadratic part of the potential becomes

$$V_2 = \frac{\omega^2}{2} \sum_{i=1}^{N} (\xi_i - \xi_{i+1})^2.$$

Solving the problem

The Hessian is a regular $N \times N$ matrix

$$\Omega = \begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & -1 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ 0 & 0 & -1 & 2 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \cdots & \vdots \\ -1 & 0 & 0 & 0 & \cdots & 2 \end{pmatrix}.$$

Notice the corner elements: their values are dictated by periodic boundary conditions.
All that is needed to solve this problem is to diagonalize this.

Introducing a new matrix

Introduce the $N \times N$ square matrix

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \cdots & \vdots \\ 1 & 0 & 0 & 0 & \ddots & 0 \end{pmatrix}, \qquad i.e., \qquad A_{ij} = \delta_{i+1,j} + \delta_{iN}\delta_{j1}.$$

As a result,

$$A^2_{ij} = \delta_{i+2,j} + \delta_{i+1,N}\delta_{j1} + \delta_{iN}\delta_{j2}.$$

Continuing in this way, we find $A^N = 1$.

Diagonalizing the Hessian

Since the only algebraic relation involving the N-th power of an $N \times N$ matrix is the Cayley-Hamiliton equation, we find the eigenvalues of A,

$$z^N = 1 \qquad i.e. \qquad z = \exp\left[\frac{2\pi ik}{N}\right],$$

where $0 \leq k < N_1$. The corresponding eigenvectors are the Fourier modes.

The Hessian is given by $\Omega = 2I - A - A^{N-1}$. Since all powers of A commute with each other and any matrix commutes with I, all three matrices on the right can be simultaneously diaginalized. Since we know the eigenvalues and eigenvctors of A, those of Ω are

$$\lambda_k = 2 - \exp\left[\frac{2\pi ik}{N}\right] - \exp\left[\frac{-2\pi ik}{N}\right] = 2\left[1 - \cos\left(\frac{2\pi k}{N}\right)\right].$$

When $N \to \infty$ then $\lambda_k \propto k^2$.

Next-to-nearest neighbour couplings

The Hessian becomes

$$\Omega = \begin{pmatrix} 2 & -1 & -1 & 0 & \cdots & -1 \\ -1 & 2 & -1 & -1 & \cdots & 0 \\ -1 & -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & -1 & 2 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \cdots & \vdots \\ -1 & -1 & 0 & 0 & \cdots & 2 \end{pmatrix} = 2I - A - A^2 - A^{N-1} - A^{N-2}.$$

The eigenvectors turn out to be the same as before, but the eigenvalues are different. Find them Coupling further number of neighbours does not change the problem essentially: the simplifying assumption is that of translation invariance.

The continuum limit

The Lagrangian of the discrete (lattice) problem that we just solved was

$$L = \frac{m}{2}\sum_i \dot{\xi}_i^2 - \frac{KQ^2}{2}\sum_i \left(\frac{\xi_{i+1}-\xi_i}{Q^2}\right)^2,$$

where K is the spring constant, m the mass of the particles, and Q is the equilibrium distance for each oscillator. The equilibrium size of the system is QN. Now we take $N \to \infty$ keeping the total size fixed. The equilibrium position of the i-th oscillator is at $x = iQ/N$. In the limit as $N \to \infty$, we find

$$L = \int dx \left\{ \left[\frac{\partial \xi(x,t)}{\partial t}\right]^2 - \omega^2 \left[\frac{\partial \xi(x,t)}{\partial x}\right]^2 \right\} \equiv \int dx \mathcal{L}$$

The sum over i in the expression on top becomes the integral over x, and the difference between nearest neighbours becomes the spatial derivative. $\mathcal{L}$ is called the Lagrangian density.

Keywords and References

Keywords

small oscillations, Hessian matrix, canonical transformation, normal modes, Lagrangian density

References

Appropriate chapters of Goldstein, and Landau