Classical Lattice Vibrations as an Eigenvalue Problem

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I. COUPLED HARMONIC OSCILLATORS

We consider a chain of N particles of mass m interacting through harmonic springs (spring constant K). Different boundary conditions can also be considered, either closed ones (ens attached to walls), or boundary ones (a chain forms a circle). Ignoring, for a moment, boundary conditions, the Newton's equation of motion for the n-th particle ($n = 1, ..., N$) takes a form

$$m\frac{d^2}{dt^2}u_n(t) = -K(u_n(t) - u_{n-1}(t)) - K(u_n(t) - u_{n+1}(t))$$
$$= -K(2u_n(t) - u_{n-1}(t) - u_{n+1}(t)),$$

where $u_n(t)$ denote the particle displacements from the equilibrium (ground state) configuration.

II. MATRIX NOTATION

The notation is considerably simpler in matrix form, where a the particle displacements u_n are regarded as components of a column vector

$$\mathbf{u} = \begin{bmatrix} u_1 \\ . \\ . \\ . \\ u_N \end{bmatrix},$$

and the inter-site interactions form a matrix

$$M = \begin{bmatrix} 2K & -K & 0 & & & & -K \\ -K & 2K & -K & 0 & & 0 & \\ 0 & -K & . & . & & & \\ & 0 & . & . & . & 0 & \\ & & & . & . & -K & 0 \\ & 0 & & 0 & -K & 2K & -K \\ -K & & & & 0 & -K & 0 \end{bmatrix}.$$

This precise form corresponds to a circular chain, where the particle 1 interacts with the particle N on the other side of the chain. In other words, this is a band matrix, where only the diagonal and two neighboring rows have nonzero matrix elements (except for the matrix elements $M_{1N} = -K$ and $M_{N1} = -K$ which describe the spring between particles 1 and N).

In this notation, we can write the entire set of N equations as a single matrix equation

$$m\frac{d^2}{dt^2}\mathbf{u}(t) = -\mathbf{M}\mathbf{u}(t).$$

This perspective also gives us a nice geometric interpretation of the mechanical motion: as time evolves, the tip of the Ndimensional vector $\mathbf{u}(t)$ traces a trajectory in the Ndimensional space. As we will see, the sound modes, i.e. the eigenmodes of this problem, will correspond to motion along straight lines, while superposition of many sound modes can produce a very complicated trajectory that describes, for example, music!!!

How to solve such a set of equations? We already know the solution for the case $N = 1$, which reduces to a standard linear harmonic oscillator (LHO). In the following, we will see how the above more complicated problem can be reduced to solving a set of N independent LHOs, by an appropriate coordinate transformation.

III. EIGENVALUE ANALYSIS

We first note that, very generally, the matrix $\mathbf{M}$ is a real symmetric matrix (this is true even if the masses of different particles or different spring constants are no the same; note that the symmetry of the matrix follows from the 3rd Law of Newton: the action-reaction law). Rigorous results from linear algebra then tell us that there exist exactly N linearly independent ortho-normal (i.e. $\widehat{\mathbf{x}}_i \cdot \widehat{\mathbf{x}}_j = \delta_{ij}$) eigenvectors $\mathbf{x}_i$ that satisfy the following equation

$$\mathbf{M}\widehat{\mathbf{e}}_i = \lambda_i \widehat{\mathbf{e}}_i,$$

where the N eigenvalues λ_i ($i = 1, ..., N$) are real numbers.

Let us now assume that the initial condition is such that $\mathbf{u}(t = 0) = u_{oi}\widehat{\mathbf{e}}_i$, i.e. the initial direction is parallel to one (any) of the eigenvectors. Then the direction remains the same with time, and we can write

$$\mathbf{u}(t) = v_i(t)\widehat{\mathbf{e}}_i,$$

where $x(t = 0) = u_o$, and $x(t)$ satisfies the LHO equation

$$m\frac{d^2}{dt^2}v_i(t) = -\lambda_i v_i(t).$$

As we know from the well-known LHO solution $v_i(t) = \mathrm{Re}[v_i^o e^{-i\omega t}]$, where the complex amplitude v_i^o determine both the (scalar) amplitude and the phase of the oscillations, both of which are determined from the initial displacement and the initial velocity, etc. Plugging this in the above equation, we find the (eigen)frequency of oscillations for this mode

$$\omega_i = (\lambda_i/m)^{1/2}.$$

If the initial condition vector is not along on of the eigenvectors, then it can always be written as a linear

superposition of the eigenvectors

$$\mathbf{u}(t=0) = \sum_{i=1}^{N} u_{oi}\widehat{\mathbf{e}}_i,$$

and similarly for the initial velocities. Then the full solution takes the form of the superposition of modes

$$\mathbf{u}(t) = \sum_{i=1}^{N} v_i(t)\widehat{\mathbf{e}}_i,$$

where the N complex amplitudes are uniquely determined from the initial position and velocities of all particles.

IV. STRATEGIES FOR EIGENVALUE ANALYSIS

This solution is very generally valid for an arbitrary set of N particles interacting through elastic springs. The precise form of the solution depends on the form of these eigenmodes, i.e. the values for the eigenvalues and the form of the eigenvectors. Our main task will, therefore, be to solve the eigenvalue problem for a given system of particles (model). This can be accomplished by a variety of methods, numerical or analytical. When specific symmetries are present (e.g. translational symmetry as in a crystal), then the eigenvalue analysis can be done in close form. Most generally, it is sufficient to guess the form of the eigenvectors, plug them in the eigenvalue equation and see if the guess works. if it does, we immediately also get the corresponding eigenvalues.

The important question is, however, how do we know if we have found all the desired solutions? The answer is provided by theorems of linear algebra, which tell us that any real and symmetric matrix of dimension N has exactly N ortho-normal (this linearly independent) eigenvectors. If we can find them by guess, and verify that they satisfy these conditions, then we have rigorously solved the problem. This is precisely the strategy one uses in a periodic case, for example. One guesses that the eigenvectors take the form of plane waves, and then check if the guess "works". The rest of the analysis is easy, as we will see shortly.

V. TWO-ATOM MOLECULE IN A HARMONIC TRAP

We will consider a two atom molecule bound by a string of constant K. In addition, imagine that this molecule is confined to a quasi-one dimensional parabolic potential well, so that we pay energy even to move the entire molecule left or right. This system can be represented by introducing additional boundary conditions, such that each of the atoms is also attached by an additional spring to a nearby "wall", with corresponding spring constant Q. The equations of motion then assume the form

$$m\frac{d^2}{dt^2}u_1(t) = -Qu_1(t) - Ku_1(t) + Ku_2(t),$$
$$m\frac{d^2}{dt^2}u_2(t) = -Ku_2(t) + Ku_1(t) - Qu_2(t).$$

The corresponding interaction matrix assumes the form

$$\mathbf{M} = \begin{bmatrix} Q+K & -K \\ -K & Q+K \end{bmatrix}.$$

A. Diagonalization by a guess

Let us first try the following eigenvectors

$$\widehat{\mathbf{e}}_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}, \ \widehat{\mathbf{e}}_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

We then get

$$\mathbf{M}\widehat{\mathbf{e}}_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} Q+K & -K \\ -K & Q+K \end{bmatrix}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} Q \\ Q \end{bmatrix} = Q\widehat{\mathbf{e}}_1,$$

and

$$\mathbf{M}\widehat{\mathbf{e}}_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} Q+K & -K \\ -K & Q+K \end{bmatrix}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} Q+2K \\ -Q-2K \end{bmatrix} = (Q+2K)\widehat{\mathbf{e}}.$$

We conclude that these are indeed eigenvectors, and the corresponding eigenvalues are

$$\lambda_1 = Q, \ \lambda_1 = Q + 2K$$

Using the above formulas, we immediately find the oscillation frequencies of the two modes

$$\omega_1 = [Q/m]^{1/2}, \ \omega_1 = [(Q+2K)/m]^{1/2}.$$

One frequency is lower, corresponding to the "acoustic" mode, where $u_1(t) = u_2(t)$, meaning that the molecule moves as whole! Note that if we eliminate the harmonic trap confining the molecule, then $\omega_1 \to 0$, corresponding to inertial (free) motion of the molecule. The other mode has atoms moving "out of phase" $u_1(t) = -u_2(t)$, corresponding to internal vibrations of the molecule. The corresponding frequency $\omega_1 \to [2K/m]^{1/2}$ remain finite even for $Q \to 0$, since then the motion corresponds to a simple LHO. Note the factor of 2 in this expression. This reflects the fact that for such a molecule, we need to introduce a center-of-mass and relative coordinate; the equation describing the relative coordinate corresponds to a standard LHO, but with a reduced mass

$$m_r = \frac{m_1 m_2}{m_1 + m_2} = \frac{m}{2},$$

in our case where $m_1 = m_2$.

VI. FORMAL DIAGONALIZATION

We can also solve the characteristic equation

$$\det|\mathbf{M}-\lambda\mathbf{I}|=0,$$

or

$$\begin{vmatrix} Q+K-\lambda & -K \\ -K & Q+K-\lambda \end{vmatrix}=0,$$

giving

$$(Q+K-\lambda)^2=K^2,$$

or

$$Q+K-\lambda=\pm K,$$

i.e.

$$\lambda_{1/2}=\begin{cases} Q \\ Q+2K \end{cases},$$

just as we found before. We can no also find the eigenvectors from

$$\mathbf{M}\widehat{\mathbf{x}}_{1/2}=\lambda_{1/2}\widehat{\mathbf{x}}_{1/2},$$

giving

$$(Q+K-\lambda_{1/2})u_1=Ku_2,$$

and we recover the above results for $\widehat{\mathbf{x}}_1$ and $\widehat{\mathbf{x}}_2$ (note that they should also be normalized).

VII. PERIODIC ONE DIMENSIONAL SOLID

We can now use our "good guess" strategy, inspired by periodicity. We guess that the eigenvectors have a form of plane waves

$$u_n=Ce^{-ikna},$$

where a is the lattice spacing, and k labels different wavevectors. We will later determine precisely the allowed values for k. We plug this guess in the equation of motion

$$-m\omega^2u_n=-K(2u_n-u_{n-1}-u_{n+1}),$$

or

$$m\omega^2Ce^{-kna}=K(2Ce^{-ikna}-Ce^{-ik(n+1)a}-Ce^{-ik(n-1)a}).$$

Cancelling the factors -Ce^{-kna}, we get

$$\begin{aligned} m\omega^2&=K(2-Ce^{-ika}-Ce^{ika}) \\ &=2K(1-\cos(ka)), \end{aligned}$$

or

$$\omega=2\sqrt{\frac{K}{m}}\sin(ka).$$

VIII. BOUNDARY CONDITIONS

Note now that the plane wave solution $u_n(k)=Ce^{-ikna}$, is meaningful only for values of $|k|<\pi/a$, since

$$u_n(k+2\pi/a)=Ce^{-ikna-2\pi ni}=Ce^{-ikna}=u_n(k).$$

In other words, we find periodicity in k-space with period $2\pi/a$, and have to restrict the "physical solution" to the "first Brilloiun zone" $k\in(-\pi/a,\pi/a)$.

Furthermore, consider a finite system, so that

$$u_n=u_{n+N}.$$

The above plane wave form of our solution then gives

$$Ce^{-ikna}=Ce^{-ik(n+N)a},$$

or

$$1=e^{-ikNa}.$$

From this equation we conclude that the only allowed solution for the wavevector k are given by

$$k=\frac{2\pi}{Na}m,$$

where m is an integer in the range $|m|<N/2$, so k is restricted to the first Brilloiun zone. As we can see, we get "quantization" of sound modes - a phenomenon which lies behind all musical instruments and their "harmonics". In the thermodynamic limit $N\to\infty$, we get a continuum of sound modes.