19. Dynamics of a One-Dimensional Crystal

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The Model

Notation! In this lecture, I use κ for the spring constant (k is a wave number) and Ω for frequency (ω is a root of unity).

A good classical model for a crystal is to represent the atoms by balls held in place by light springs, representing valence bonds, between nearest neighbors. The simplest such crystal that has some realistic features is a single chain of connected identical atoms. To make the math easy, we'll connect the ends of the chain to make it a circle. This is called "imposing periodic boundary conditions". It is common practice in condensed matter theory, and makes little difference to the physics for a large system.

We'll take the rest positions of the atoms to be uniformly spaced, a apart, with the first atom at a, the nth atom at na, the final N^{th} atom at the origin.

Away from the lowest energy state, we denote the position of the nth atom $na + x_n$, so, as in our earlier discussion of oscillating systems, x_n is the displacement from equilibrium (which we take to be along the line—we are not considering transverse modes of vibration at this time).
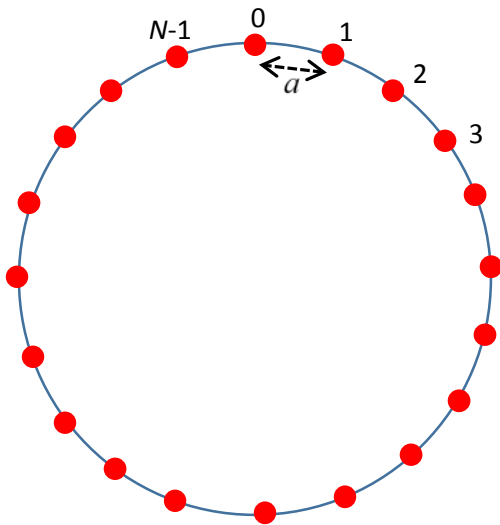
The Lagrangian of this circular chain system is:

$$L = \sum_{n=1}^{N} \tfrac{1}{2} m \dot{x}_n^2 - \sum_{n=1}^{N} \tfrac{1}{2}\kappa\left(x_{n+1} - x_n\right)^2, \quad N+1 \equiv 1.$$

We're going to call the spring constant κ, we'll need k for something else. We'll also call the frequency Ω.

Looking for eigenstates with frequency Ω, we find the set of equations

$$m\ddot{x}_n = -\kappa\left(2x_n - x_{n-1} - x_{n+1}\right).$$

Taking a solution $x_n = A_n e^{i\Omega t}$, with the understanding that A_n may be complex, and at the end x_n is just the real part of the formal solution, we find the eigenvalue equation for a chain of four atoms (the biggest Mathtype can handle!)

$$-m\Omega^2 \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix} = \begin{pmatrix} -2\kappa & \kappa & 0 & \kappa \\ \kappa & -2\kappa & \kappa & 0 \\ 0 & \kappa & -2\kappa & \kappa \\ \kappa & 0 & \kappa & -2\kappa \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix}.$$

Actually we'd have a much bigger matrix, with lots of zeroes, but hopefully the pattern is already clear: -2κ for each diagonal element and κ's in two diagonal-slanting lines flanking the main diagonal (corresponding to the links between nearest neighbors) and finally κ's in the two far corners, these coming from the spring joining N to 1 to complete the circle.

Notice first that if $\Omega = 0$ there is an eigenvector $(1,1,1,1)^T$, since the sum of the elements in one row is zero (the T means transpose, that is, it's really a column vector, but row vectors are a lot easier to fit into the text here).

This eigenvector is just uniform displacement of the whole system, which costs zero energy since the system isn't anchored to a particular place on the ring. We'll assume, though, that the system as a whole is at rest, meaning the center of mass is stationary, and the atoms have well-defined rest positions as in the picture at $a, 2a, 3a, \ldots, Na$, $Na \equiv 0$.

The Circulant Matrix: Nature of its Eigenstates

The matrix we've constructed above has a very special property: each row is identical to the preceding row with the elements moved over one place, that is, it has the form

$$\begin{pmatrix} c_0 & c_1 & c_2 & c_3 \\ c_3 & c_0 & c_1 & c_2 \\ c_2 & c_3 & c_0 & c_1 \\ c_1 & c_2 & c_3 & c_0 \end{pmatrix}$$

Such matrices are called *circulants*, and their properties are well known. In particular, we'll show that the *eigenvectors* have the form

$$\left(1, \omega_j, \omega_j^2, \omega_j^3, \ldots, \omega_j^{N-1}\right)^T \text{ where } \omega_j^N = 1.$$

unit circle $|z| = 1$

Recall the roots of the equation $z^N = 1$ are N points equally spaced around the unit circle,
$e^{2\pi i n/N}, n = 0, 1, 2, \ldots N-1.$

The standard mathematical notation is to label these points $1, \omega_1, \omega_2, \omega_3, \ldots, \omega_{N-1}$ as shown in the figure, but notice that $\omega_j = \omega_1^j$.
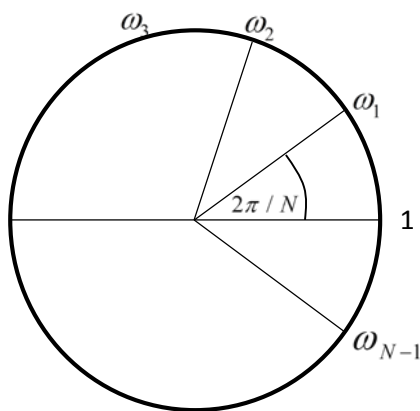
Comparison with Raising Operators

Actually these matrices are related to the raising and lowering operator for angular momentum (and simple harmonic oscillators) in quantum mechanics. For example, the 4×4 matrices would be for a spin 3/2, with four S_z eigenstates.

The quantum mechanical raising and lowering matrices look like

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

They move the spin S_z component up (and down) by one notch, except that on applying the raising operator, the top state $S_z = 3/2$ is annihilated, similarly the lowering operator on the bottom state.

Our circular generalizations have one extra element:

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

This makes the matrices circulants, and gives them a "recycling" property: the top element isn't thrown away, it just goes to the bottom of the pile.

(And bear in mind that the standard notation for a vector has the lowest index (0 or 1) for the top element, so when we bend the ladder into a circle, the "raising" operator actually moves to the next *lower* number, in other words, it's a shift to the *left*.)

We'll take this shift operator P as our basic matrix:

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \text{ from which } P^2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

It should be evident from this that the circulant matrix having top row c_0, c_1, c_2, c_3 is just the matrix $c_0 I + c_1 P + c_2 P^2 + c_3 P^3$.

This generalizes trivially to $N \times N$ matrices.

Finding the Eigenvectors
Now let's look at the eigenvectors, we'll start with those of P. Let's call the eigenvalue λ.

Then for an eigenstate of the shift operator, the shifted vector must be just a multiple of the original vector:

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix} = \begin{pmatrix} A_2 \\ A_3 \\ A_4 \\ A_1 \end{pmatrix} = \lambda \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix}.$$

Reading off the element by element equivalence of the two vectors,

$$A_2 = \lambda A_1, \ A_3 = \lambda A_2, \ A_4 = \lambda A_3, \ A_1 = \lambda A_4.$$

The first three equalities tell us the eigenvector has the form $\left(1, \lambda, \lambda^2, \lambda^3\right)^T$, the last tells us that $\lambda^4 = 1$.

From our earlier discussion of circulant matrices, writing the smallest phase nontrivial N^{th} root of unity as $\omega = e^{2\pi i/N}$, *the roots of the equation* $\lambda^N = 1$ *are just this basic root raised to* N *different powers*: the roots are $1, \omega, \omega^2, \omega^3, \ldots, \omega^{N-1}$.

This establishes that the eigenvectors of P have the form $\left(1, \omega^j, \left(\omega^j\right)^2, \left(\omega^j\right)^3, \ldots, \left(\omega^j\right)^{N-1}\right)^T$ where

$j = 0, 1, 2, 3, \ldots, N-1$ with corresponding eigenvalue the basic root raised to the jth power, $\omega^j = e^{2\pi ij/N}$.

Try it out for 3×3: the eigenvalues are given by $\begin{vmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ 1 & 0 & -\lambda \end{vmatrix} = 0, \ \lambda^3 = 1, \ \lambda = 1, \omega, \omega^2; \ \omega^3 = 1.$

The corresponding eigenvectors are found to be $\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ \omega \\ \omega^2 \end{pmatrix}, \begin{pmatrix} 1 \\ \omega^2 \\ \omega \end{pmatrix}.$

For the $N \times N$ case, there are N different, linearly independent, vectors of this form, so this is a complete set of eigenvectors of P.

They are also, of course, eigenvectors of P^2, P^3 all $N-1$ powers of P, and therefore of *all* the circulant matrices! *This means that all* $N \times N$ *circulant matrices commute.*

Eigenvectors of the Linear Chain

Let's get back to our chain, with eigenfunction equation of motion the N dimensional equivalent of

$$-m\Omega^2 \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix} = \begin{pmatrix} -2\kappa & \kappa & 0 & \kappa \\ \kappa & -2\kappa & \kappa & 0 \\ 0 & \kappa & -2\kappa & \kappa \\ \kappa & 0 & \kappa & -2\kappa \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix}.$$

We see the matrix is a circulant, so we know the eigenvectors are of the form

$\left(1, \omega^j, \left(\omega^j\right)^2, \left(\omega^j\right)^3, \ldots, \left(\omega^j\right)^{N-1}\right)^T$, which we'll now write $\left(1, e^{2\pi ij/N}, e^{2\pi i2\,j/N}, e^{2\pi i3\,j/N}, \ldots, e^{2\pi ij(N-1)/N}\right)$.

What does this mean for our chain system? Remember that the nth element of the eigenvector represents the displacement of the nth atom of the chain from its equilibrium position, that would be proportional to $e^{2\pi ijn/N}$.

The steady phase progression on going around the chain $n = 0, 1, 2, 3, \ldots$ makes clear that this is essentially a (longitudinal) wave. (The actual n^{th} particle displacement is the real part of the nth element, but there could be an overall complex factor fixing the phase.)

Allowed Wavenumbers from Boundary Conditions

The usual way of representing a wave on a line in physics is to have displacement proportional to e^{ikx}, and k is called the *wavenumber*. For our discretized system, the displacement parameter for the nth atom, at position na, would therefore be proportional to e^{ikna}.

But we know this is an eigenvector of a circulant, so we must have $e^{iNka} = 1$, and the allowed values of k are

$$k_n = \frac{2\pi}{Na}n = \frac{2\pi}{L}n$$

with n an integer.

The circulant structure of the matrix has determined the eigenvectors, but not the eigenvalues ω_n.

Finding the Eigenvalues

The eigenvalues are found by operating on the eigenvector we just found with the matrix, meaning the N dimensional generalization of

$$-m\Omega^2 \begin{pmatrix} 1 \\ e^{ik_n a} \\ e^{ik_n 2a} \\ e^{ik_n 3a} \end{pmatrix} = \begin{pmatrix} -2\kappa & \kappa & 0 & \kappa \\ \kappa & -2\kappa & \kappa & 0 \\ 0 & \kappa & -2\kappa & \kappa \\ \kappa & 0 & \kappa & -2\kappa \end{pmatrix} \begin{pmatrix} 1 \\ e^{ik_n a} \\ e^{ik_n 2a} \\ e^{ik_n 3a} \end{pmatrix}.$$

Applying the matrix to the column vector $\left(1, e^{ik_n a}, e^{2ik_n a}, e^{3ik_n a}, \ldots, e^{i(N-1)k_n a}\right)^T$, and cancelling out the common $e^{ik_n na}$ factor, we have

$$-m\Omega_n^2 = \kappa\left(e^{ik_n a} + e^{-ik_n a} - 2\right).$$

(Of course, this same result comes from every row.)

The complete set of eigenvalues is given by inserting in the above expression

$$k_n = 2\pi n / Na, \quad n = 0, 1, 2, \ldots, N-1 \text{ so } e^{ik_n a} = e^{2\pi in/N},$$

so $n = 0$ is displacement of the system as a whole, as is $n = N$.

Wavenumber values k_n beyond $n = N$ repeats the eigenstates we already have, since

$$e^{ik_{N+n} a} = e^{i\frac{2\pi(N+n)a}{Na}} = e^{2\pi i} e^{2\pi in/N} = e^{2\pi in/N} = e^{ik_n a}.$$

This means that the values of k are restricted to

$$\Omega_n = 2\sqrt{\frac{\kappa}{m}} \sin\left(\frac{k_n a}{2}\right) = 2\sqrt{\frac{\kappa}{m}} \sin\left(\frac{n\pi}{N}\right).$$

$$0 \le k < 2\pi / a$$

or equivalently

$$-\pi / a < k \le \pi / a.$$

The eigenvalue equation is

$$\Omega_n^2 = 2(\kappa / m)(1 - \cos k_n a),$$

or

$$\Omega_n = 2\sqrt{\frac{\kappa}{m}} \sin\left(\frac{k_n a}{2}\right) = 2\sqrt{\frac{\kappa}{m}} \sin\left(\frac{n\pi}{N}\right).$$

To see the dynamics of this eigenstate $\left(1, e^{ik_n a}, e^{2ik_n a}, e^{3ik_n a}, \ldots, e^{ik_n(N-1)a}\right)$, we need to multiply by the time dependence $e^{i\Omega_n t}$, then finally take the real part of the solution:

$$\left(\cos\Omega_n t, \ \cos(k_n a + \Omega_n t), \ \cos(2k_n a + \Omega_n t), \ \cos(3k_n a + \Omega_n t), \ldots, \cos((N-1)k_n a + \Omega_n t)\right).$$

Notice that in the continuum limit, meaning large N and small a, the atom displacement as a function of position has the form $\cos(kx + \Omega t)$, in other words we're looking at a sinusoidal wave disturbance with wavenumber k_n here.

Now, $-k_n$ is also a solution, but that is the same as $n' = N - n$, so one must be careful not to overcount. The two frequencies $\pm\Omega_n$ correspond to waves going in opposite directions.

The Discrete Fourier Transform

It's worth looking over this one more time from a slightly different perspective. In finding the energy of an oscillating continuous string, a standard approach is to analyze the motion of the string in terms of an infinite Fourier series of shorter and shorter wavelength oscillations, find the energy in each of these

modes, and add to find the total energy. We'll apply the same approach here—but with a difference. Since the waves only have meaning in our chain at a discrete set of uniformly spaced points, the set of waves needed to fully account for all possible motions is finite. In fact, it's the same as the number of points. As we've discussed above, a wave with a higher wavenumber gives an identical set of displacements of the atoms as some lower one. So a complete Fourier analysis of the displacements at these N equally spaces points only needs linear combinations of N waves. This is the *Discrete Fourier Transform (DFT)*.

Writing the complex (amplitude and phase) coefficient of the nth frequency eigenstate X_n, the position of the jth atom in a superposition of such waves (with the standard normalization convention)

$$x_j = \frac{1}{N}\sum_{n=0}^{N-1} X_n e^{ik_n ja} = \frac{1}{N}\sum_{n=0}^{N-1} X_n e^{i2\pi nj/N}$$

Given the positions x_j of the atoms, the amplitude coefficients can be found using the inverse mapping:

$$X_n = \sum_{j=0}^{N-1} x_j e^{-i2\pi jn/N} = \sum_{j=0}^{N-1}\frac{1}{N}\sum_{n'=0}^{N-1} X_{n'} e^{i2\pi n'j/N} e^{-i2\pi jn/N},$$

then using

$$\sum_{j=1}^{N} e^{-i2\pi nj/N} e^{i2\pi n'j/N} = \sum_{j=1}^{N} e^{i2\pi(n'-n)j/N} = N\delta_{n'n},$$

gives $X_n = X_n$, establishing that we have the correct form for the inverse transformation.

The instantaneous configuration of the system is completely defined by the set $(x_1, x_2,\ldots, x_N)$ and equally by the set $(X_1, X_2,\ldots, X_N)$. All possible particle displacements at the N equally spaced sites can be mapped into N amplitudes of the N distinct waves (eigenvectors).

(This DFT mapping is widely used in the time domain in signal processing: the signal amplitude is sampled, say every millisecond, then the data can be DFT'd to give the wave components down to a minimum frequency around one millisecond. A good quality voice signal would need a shorter time interval, maybe 0.2 milliseconds.)

Now, from $x_j = \frac{1}{N}\sum_{n=0}^{N-1} X_n e^{i2\pi nj/N}$,

$$\sum_{j=1}^{N} x_j^* x_j = \frac{1}{N^2}\sum_{j=1}^{N}\sum_{m=0}^{N-1} X_m^* e^{-i2\pi mj/N}\sum_{n=0}^{N-1} X_n e^{i2\pi nj/N},$$

and again using

$$\sum_{j=1}^{N} e^{-i2\pi mj/N} e^{i2\pi nj/N} = \sum_{j=1}^{N} e^{i2\pi(n-m)j/N} = N\delta_{mn},$$

we find

$$\sum_{j=1}^{N} x_j^* x_j = \frac{1}{N}\sum_{n=1}^{N} X_n^* X_n.$$

Back to our chain: for a physical configuration of the atoms, all the x_j must be real, so from

$X_n = \sum_{j=0}^{N-1} x_j e^{-i2\pi jn/N}$ we see that $X_n^* = X_{-n} = X_{N-n}$. (This reduces the number of apparent degrees of

freedom in the X representation to the correct N. X_0 is real, $X_1^* = X_{N-1}$, etc., and if there is a middle

X_n, it must be real.)

The kinetic energy of the chain particles, $\sum_{j=1}^{N} |\dot{x}_j|^2 = \frac{1}{N}\sum_{n=1}^{N} |\dot{X}_n|^2.$

We can find potential energy similarly:

$$\sum_{j=1}^{N}\left(x_{j+1} - x_j\right) = \sum_{j=1}^{N}\sum_{n=0}^{N-1} X_n e^{i2\pi nj/N}\left(e^{2\pi in/N} - 1\right),$$

and using the same routine as before,

$$\sum_{j=1}^{N}\left(x_{j+1} - x_j\right)^2 = \sum_{n=0}^{N-1}|X_n|^2\left|e^{2\pi in/N} - 1\right|^2 = \sum_{n=0}^{N-1}|X_n|^2\left|e^{ik_n a} - 1\right|^2.$$

Finally, $\left|e^{ik_n a} - 1\right|^2 = 4\sin^2\left(\dfrac{k_n a}{2}\right).$

Putting all this together, the Lagrangian can be written in terms of the transformed variables:

$$L = \frac{1}{N}\sum_{n=1}^{N}\left[\tfrac{1}{2}m|\dot{X}_n|^2 - 2\kappa\sin^2\left(\frac{k_n a}{2}\right)|X_n|^2\right].$$

The equation of motion is then

$$m\ddot{X}_n = -4\kappa\sin^2\left(\frac{k_n a}{2}\right)X_n,$$

with eigenvalues

$$\Omega_n = \sqrt{\frac{\kappa}{m}}\cdot 2\sin\left(\frac{k_n a}{2}\right) = \sqrt{\frac{\kappa}{m}}\cdot 2\sin\left(\frac{n\pi}{N}\right).$$

This is of course the same result we found earlier, but it is perhaps worth seeing how it comes from the (mathematically equivalent) DFT analysis.

A Note on the Physics of These Waves

For wavelength long compared to the interparticle spacing, $\Omega \cong vk$, these are like sound waves (and indeed they are what are called acoustic phonons in a crystal). As the wavelength shortens, the wave eigenstates are moving more slowly, remember the group velocity of a wavepacket goes as $d\Omega / dk$. This is because there is some Bragg reflection of the waves by the lattice. At $ka = \pi$, we have a standing wave. This is the highest energy mode, with even numbered sites all in sync with each other, and the odd numbered sites all half a cycle behind, so the restoring force experienced by an atom as a function of displacement is the maximum possible.