

Vibrations of a one-dimensional, monoatomic lattice

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August 2019

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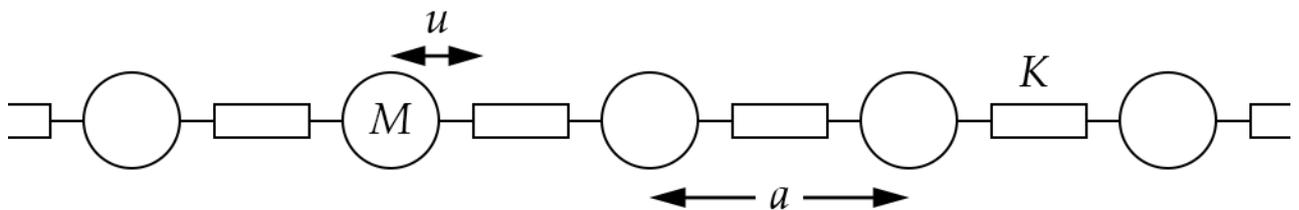
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Objectives. Basic ideas about phonons, vibrations of a linear chain of atoms, the first Brillouin zone, and phase and group velocities.

IN ANY LATTICE, the process of heating—that is, supplying any form of thermal energy—has a direct effect on the internal energy of the constituent atoms. This internal energy is manifest in two forms: first, we have lattice vibrations; and second, we have free electrons with some finite kinetic energy. Lattice vibrations are modelled on sound waves propagating through that lattice because, whether the vibrations are thermal or auditory, they share the same mechanism. Specifically, the frequency of vibrations in both cases is directly dependent on the elasticity of the object.

We say there is a collective excitation in a solid or other condensed matter when it behaves as if it is composed of several small, weakly interacting particles. A thermal wave or sound wave in a lattice is a classic example of this phenomenon: such waves in a lattice behave like quasiparticles called **phonons** which are excited states in quantised modes of vibration in lattices.

Phonons have lots of parallels with photons: they both have energies of $\epsilon = h\nu$ and are both bosons; they also both exhibit duality and are not conserved in interactions i.e. they can be created or destroyed. We have, so far, indirect evidence of their existence (hence the term *quasiparticle*) but the evidence—such as missing or added energy during interactions corresponding exactly to expected numbers of newly created or destroyed phonons—is quite convincing.



1 Vibrations of a one-dimensional lattice

Consider a chain of identical atoms of mass M with interatomic forces simplified as a connection of springs with force constant K and a common interatomic separation of a . We can imagine either an infinite chain or a ring of such atoms: this is to retain their one-dimensional nature while ensuring that all atoms are indistinguishable from one another. Assume that vibrations of any n^{th} atom over a displacement of u from the mean position occurs along the length of the atomic chain.

When heat is passed, sound waves are generated or some such

thermal energy is supplied to one part of the chain, the vibration created by it are propagated from atom to atom setting the entire chain in vibrational motion. We will now perform our discussion for some n^{th} atom in the chain.

Consider the force on the n^{th} atom due to the $(n-1)^{\text{th}}$ atom. Let us call this F' :

$$F' = K(U_n - U_{n-1})$$

Similarly we have the force F'' on the n^{th} atom due to the $(n+1)^{\text{th}}$ atom as

$$F'' = K(U_{n+1} - U_n)$$

These two forces are, at any given time, almost certain to be (at least on average across arbitrary atoms in the chain) in opposite directions or destructive to some degree². We will therefore algebraically sum them to get the net force F_n on the n^{th} atom as follows:

$$\begin{aligned} F_n &= F'' - F' \\ \implies F_n &= K(U_{n+1} - 2U_n + U_{n-1}) \\ \therefore M \left(\frac{d^2 U_n}{dt^2} \right) &= K(U_{n+1} - 2U_n + U_{n-1}) \end{aligned}$$

This equation is harmonic in nature and has the solution

$$\boxed{U_n = A e^{nka - \omega t}} \quad (1)$$

where k is the *wavenumber* related³ to the wavelength as $k = 2\pi/\lambda$, ω is the frequency, t the time period, and na is the length of the chain formed by the n atoms under consideration, equivalent to the maximum possible displacement.

Substituting this solution into the net force we get

$$\begin{aligned} \omega^2 M U_n &= K \left(e^{ika} - 2 + e^{-ika} \right) U_n \\ \omega^2 &= \frac{K}{M} (2 \cos ka - 2) \end{aligned}$$

where we have used $e^{i\theta} - e^{-i\theta} = 2i \sin \theta$. Going further we can use $(\cos \theta - 1) = 2 \sin^2(\theta/2)$ to get

$$\begin{aligned} \omega^2 &= \frac{2K}{M} \left(2 \sin^2 \left(\frac{ka}{2} \right) \right) \\ \implies \omega &= \left(\frac{4K}{M} \right)^{1/2} \left| \sin \left(\frac{ka}{2} \right) \right| \end{aligned}$$

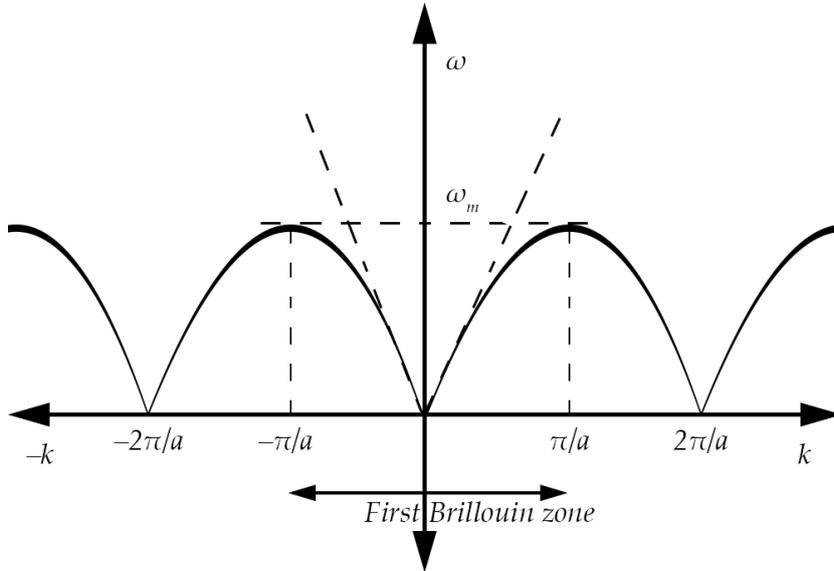
is the frequency of the wave i.e. that frequency ω and amplitude A with which all atoms in our set-up vibrate. However, note that ω hits its maximum value ω_m when $\omega = (4K/M)^{1/2}$ so we can simply write

$$\boxed{\omega = \omega_m \left| \sin \left(\frac{ka}{2} \right) \right|} \quad (2)$$

Equation (2) is called the **dispersion relation** and relates the frequency ω and wave vector \mathbf{k} as a sine curve (of absolute values only, hence making all peaks positive) of wavelength $2\pi/a$ as shown in the figure of the **dispersion curve** below.

² The simplest way to understand this is that such opposing forces are what cause the vibration in our atoms. Had these forces been completely constructive the entire chain may have undergone translational motion.

³ Generally the relation between the wavenumber k , the wave vector \mathbf{k} and the wavelength λ is $k = |\mathbf{k}| = 2\pi/\lambda$ but we simplify this in crystallography to simply $k = |\mathbf{k}| = 1/\lambda$ since a 2π factor almost always accompanies us thanks in part to Fourier transforms.



2 The First Brillouin Zone

2.1 Identifying the zone

We are now working in what is known as k -space or reciprocal space. This is an important tool used in X-ray diffraction experiments and across condensed matter physics as its reciprocal relation to real space length measurements, among other things, is helpful in studying and understanding lattice structure and properties. Observe that in the curve above we have two symmetries:

Translational symmetry. We notice that our absolute value sine curve $\omega \equiv \omega(k)$ has a common period of $2\pi/a$ and has several values of $\omega < \omega_m$ for various values of k . In turn, these several values of k arise from various possible values of λ thanks to the relation $k = 2\pi/\lambda$ that we already saw above.

Mirror symmetry. About the origin, in the positive y -axis region, we have a mirror symmetry as evinced by the fact that $\omega(-k) = \omega(k)$ i.e. two identical waves in opposite directions.

With such a set-up as above we conventionally choose the $-\pi/a < k < \pi/a$ region of k -space and call it the **First Brillouin Zone**.

2.2 On modes

For a ring of N atoms that is of length Na due to a spacing of a between atoms we observe that every $U_n(x = 0) = U_{N+n}(x = Na)$. This is also obviously true for an infinite, straight chain of atoms, not just a circular ring. We can substitute eq. (1) into such a $U_n \rightarrow U_{N+n}$ relation to arrive at

$$U_{N+n} = Ae^{i((N+n)ka - \omega t)} = Ae^{ikNa} e^{i(nka - \omega t)}$$

which can agree with the familiar equation for U_n given by eq. (1) iff

$$e^{ikNa} = 1 \quad (3)$$

In other words, only such values of k are permitted as those which obey eq. (3). This means, since $e^{ikNa} = 1$, $\cos kNa + i \sin kNa = 1$ which can only happen if

$$\begin{aligned} kNa &= 2n\pi \\ \therefore k &= n \left(\frac{2\pi}{Na} \right) \end{aligned}$$

On a number line this simply looks like a set of quantised values each separated by a distance of $2\pi/Na$. Such a quantisation is precisely what we expected when we described some properties of phonons at the start of this lecture.

From our sine curve pictured above—where the First Brillouin Zone is marked between $\pm\pi/a$ —we have a zone length of $2\pi/a$. We can combine this fact with the minimum quantised value $2\pi/Na$ of k , which we just obtained, to get the number of allowed values:

$$\frac{\text{Length}}{\text{Min. value}} = \frac{2\pi/a}{2\pi/Na} = N$$

That is to say, the number of values or allowed **vibrational modes** in the First Brillouin Zone is equal to N , the number of degrees of freedom in the lattice.

3 The dispersion curve

3.1 The long wavelength limit

There are some more important observations to be made in connection to the dispersion curve besides the already established facts that it is symmetric and periodic. Specifically, we are interested in what happens to the lattice when such a wave propagates.

While the wavelength is within the $0 < k < \pi/a$ window, we call the limit $k \rightarrow 0$ the **long wavelength limit**. Due to the reciprocal nature of k -space it is no surprise that as k drops λ increases. In this limit $\omega \propto k$ rather than $\omega \propto \sin(ka/2)$ as making appropriate changes to eq. (2) shows us:

$$\omega = \left(\frac{\omega_m a}{2} \right) k$$

Since ω is the frequency and k is proportional to the inverse of the wavelength, comparing this equation to the standard $v = f\lambda$ tells us that the term between the parentheses must be the velocity v_{sound} of the sound waves in question and can be related to its familiar equation with Young's modulus as follows:

$$v_{\text{sound}} = \frac{\omega_m a}{2} = \sqrt{\frac{Y}{\rho}}$$

Since $\omega_m = (4K/M)^{1/2}$ and $\rho = M/a^3$ by definition,

$$\begin{aligned} \implies v_{\text{sound}} &= \frac{a\sqrt{K}}{\sqrt{M}} = \frac{a\sqrt{Ya}}{\sqrt{M}} \\ \therefore K &= Ya \end{aligned}$$

Knowing Young's modulus for a solid—a quantity which can be measured comparatively easily by various experiments—we can determine the value of the spring constant K of our set-up.

Keep in mind, while the result that $\omega \propto k$ is true for small values of k (which is why we see a somewhat linear increase initially as indicated in the dispersion curve) it is not true as k becomes larger. When this happens, the relation between ω and k deviates from a linear path until k saturates at ω_m beyond which it falls off with the entire variation taking place over a length of π/a .

3.2 *Phase and group velocities*

A final observation to be made with respect to our dispersion curve are phase and group velocities of a sound wave. A single pure wave described by a frequency of ω and wave vector \mathbf{k} are said to travel with a **phase velocity** while wave packets with an average frequency of ω and wave vector \mathbf{k} are said to travel with a **group velocity**.