

## 4. Phonons

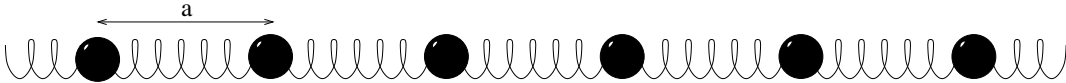
Until now, we've discussed lattices in which the atoms are fixed in place. This is, of course, somewhat unrealistic. In materials, atoms can jiggle, oscillating back and forth about their equilibrium position. The result of their collective effort is what we call sound waves or, at the quantum level, *phonons*. In this section we explore the physics of this jiggling.

### 4.1 Lattices in One Dimension

Much of the interesting physics can be illustrated by sticking to one-dimensional examples.

#### 4.1.1 A Monotonic Chain

We start with a simple one-dimensional lattice consisting of  $N$  equally spaced, identical atoms, each of mass  $m$ . This is shown below.



We denote the position of each atom as  $x_n$ , with  $n = 1, \dots, N$ . In equilibrium, the atoms sit at

$$x_n = na$$

with  $a$  the lattice spacing.

The potential that holds the atoms in place takes the form  $\sum_n V(x_n - x_{n-1})$ . For small deviations from equilibrium, a generic potential always looks like a harmonic oscillator. The deviation from equilibrium for the  $n^{\text{th}}$  atom is given by

$$u_n(t) = x_n(t) - na$$

The Hamiltonian governing the dynamics is then a bunch of coupled harmonic oscillators

$$H = \sum_n \frac{p_n^2}{2m} + \frac{\lambda}{2} \sum_n (u_n - u_{n-1})^2 \quad (4.1)$$

where  $p_n = m\dot{u}_n$  and  $\lambda$  is the spring constant. (It is not to be confused with the wavelength.) The resulting equations of motion are

$$m\ddot{u}_n = -\lambda(2u_n - u_{n-1} - u_{n+1}) \quad (4.2)$$

To solve this equation, we need to stipulate some boundary conditions. It's simplest to impose periodic boundary conditions, extending  $n \in \mathbf{Z}$  and requiring  $u_{n+N} = u_n$ . For  $N \gg 1$ , which is our interest, other boundary conditions do not qualitatively change the physics. We can then write the solution to (4.2) as

$$u_n = A e^{-i\omega t - ikna} \quad (4.3)$$

Because the equation is linear, we can always take real and imaginary parts of this solution. Moreover, the linearity ensures that the overall amplitude  $A$  will remain arbitrary.

The properties of the lattice put restrictions on the allowed values of  $k$ . First note that the solution is invariant under  $k \rightarrow k + 2\pi/a$ . This means that we can restrict  $k$  to lie in the first Brillouin zone,

$$k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right)$$

Next, the periodic boundary conditions  $u_{N+1} = u_1$  require that  $k$  takes values

$$k = \frac{2\pi}{Na}l \quad \text{with } l = -\frac{N}{2}, \dots, \frac{N}{2}$$

where, to make life somewhat easier, we will assume that  $N$  is even so  $l$  is an integer. We see that, as in previous sections, the short distance structure of the lattice determines the range of  $k$ . Meanwhile, the macroscopic size of the lattice determines the short distance structure of  $k$ . This, of course, is the essence of the Fourier transform. Before we proceed, it's worth mentioning that the minimum wavenumber  $k = 2\pi/Na$  was something that we required when discussing the Debye model of phonons in the [Statistical Physics](#) lectures.

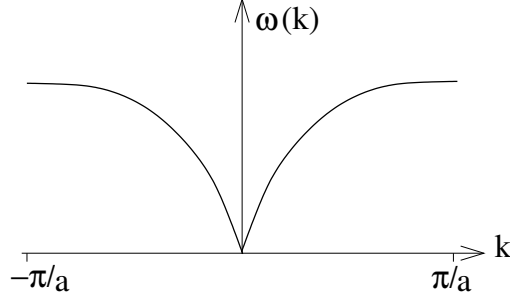
Our final task is to determine the frequency  $\omega$  in terms of  $k$ . Substituting the ansatz into the formula (4.2), we have

$$m\omega^2 = \lambda(2 - e^{ika} - e^{-ika}) = 4\lambda \sin^2\left(\frac{ka}{2}\right)$$

We find the dispersion relation

$$\omega = 2\sqrt{\frac{\lambda}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

This dispersion relation is sketched Figure 63, with  $k$  ranging over the first Brillouin zone.



**Figure 63:** Phonon dispersion relation for a monatomic chain.

Many aspects of the above discussion are familiar from the discussion of electrons in the tight-binding model. In both cases, we end up with a dispersion relation over the Brillouin zone. But there are some important differences. In particular, at small values of  $k$ , the dispersion relation for phonons is linear

$$\omega \approx \sqrt{\frac{\lambda}{m}} a k$$

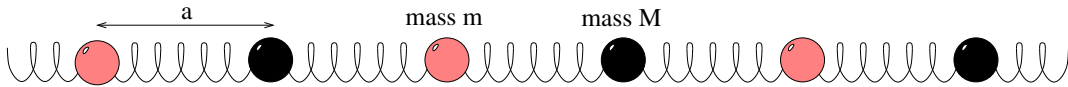
This is in contrast to the electron propagation where we get the dispersion relation for a non-relativistic, massive particle (2.6). Instead, the dispersion relation for phonons is more reminiscent of the massless, relativistic dispersion relation for light. For phonons, the ripples travel with speed

$$c_s = \sqrt{\frac{\lambda}{m}} a \quad (4.4)$$

This is the *speed of sound* in the material.

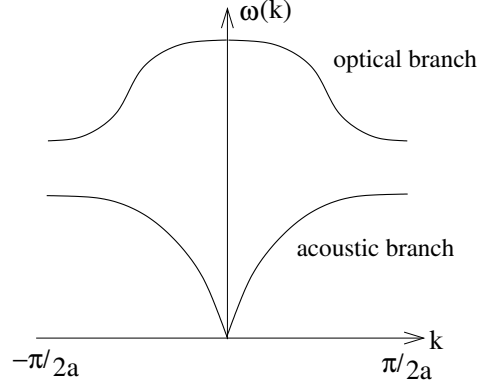
#### 4.1.2 A Diatomic Chain

Consider now a linear chain of atoms, consisting of alternating atoms of different types.



The atoms on even sites have mass  $m$ ; those on odd sites have mass  $M$ . For simplicity, we'll take the restoring forces between these atoms to be the same. The equations of motion are

$$\begin{aligned} m\ddot{u}_{2n} &= -\lambda(2u_{2n} - u_{2n-1} - u_{2n+1}) \\ M\ddot{u}_{2n+1} &= -\lambda(2u_{2n+1} - u_{2n} - u_{2n+2}) \end{aligned}$$



**Figure 64:** Phonon dispersion relation for a diatomic chain.

We make the ansatz

$$u_{2n} = A e^{-i\omega t - 2ikna} \quad \text{and} \quad u_{2n+1} = B e^{-i\omega t - 2ikna}$$

Note that these solutions are now invariant under  $k \rightarrow k + \pi/a$ . This reflects the fact that, if we take the identity of the atoms into account, the periodicity of the lattice is doubled. Correspondingly, the Brillouin zone is halved and  $k$  now lies in the range

$$k \in \left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right) \quad (4.5)$$

Plugging our ansatz into the two equations of motion, we find a relation between the two amplitudes  $A$  and  $B$ ,

$$\omega^2 \begin{pmatrix} m & 0 \\ 0 & M \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \lambda \begin{pmatrix} 2 & -(1 + e^{-2ika}) \\ -(1 + e^{2ika}) & 2 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \quad (4.6)$$

This is viewed as an eigenvalue equation. The frequency  $\omega$  is determined in terms of the wavenumber  $k$  by requiring that the appropriate determinant vanishes. This time we find that there are two frequencies for each wavevector, given by

$$\omega_{\pm}^2 = \frac{\lambda}{mM} \left[ m + M \pm \sqrt{(m - M)^2 + 4mM \cos^2(ka)} \right]$$

The resulting dispersion relation is sketched in Figure 64 in the first Brillouin zone (4.5). Note that there is a gap in the spectrum on the boundary of the Brillouin zone,  $k = \pm\pi/2a$ , given by

$$\Delta E = \hbar(\omega_+ - \omega_-) = \hbar\sqrt{2\lambda} \left| \frac{1}{\sqrt{m}} - \frac{1}{\sqrt{M}} \right|$$

For  $m = M$ , the gap closes, and we reproduce the previous dispersion relation, now plotted on half the original Brillouin zone.

The lower  $\omega_-$  part of the dispersion relation is called the *acoustic branch*. The upper  $\omega_+$  part is called the *optical branch*. To understand where these names come from, we need to look a little more closely at the physical origin of these two branches. This comes from studying the eigenvectors of (4.6) which tells us the relative amplitudes of the two types of atoms.

This is simplest to do in the limit  $k \rightarrow 0$ . In this limit the acoustic branch has  $\omega_- = 0$  and is associated to the eigenvector

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

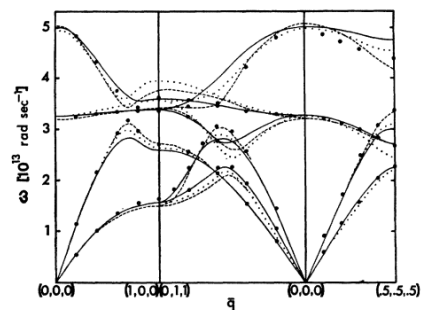
The atoms move in phase in the acoustic branch. Meanwhile, in the optical branch we have  $\omega_+^2 = 2\lambda(M^{-1} + m^{-1})$  with eigenvector

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} M \\ -m \end{pmatrix}$$

In the optical branch, the atoms move out of phase.

Now we can explain the name. Often in a lattice, different sites contain ions of alternating charges: say,  $+$  on even sites and  $-$  on odd sites. But alternating charges oscillating out of phase create an electric dipole of frequency  $\omega_+(k)$ . This means that these vibrations of the lattice can emit or absorb light. This is the reason they are called “optical” phonons.

Although our discussion has been restricted to one-dimensional lattices, the same basic characterisation of phonon branches occurs for higher dimensional lattices. Acoustic branches have linear dispersion  $\omega \sim k$  for low momenta, while optical branches have non-vanishing frequency, typically higher than the acoustic branch. The data for the phonon spectrum of *NaCl* is shown on the right<sup>6</sup> and clearly exhibits these features.



**Figure 65:**

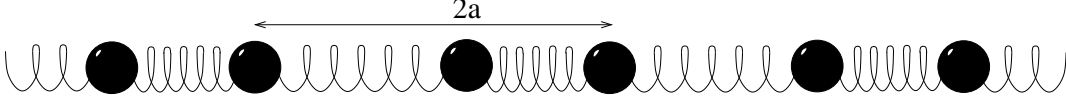
### 4.1.3 Peierls Transition

We now throw in two separate ingredients: we will consider the band structure of electrons, but also allow the underlying atoms to move. There is something rather special and surprising that happens for one-dimensional lattices.

<sup>6</sup>This was taken from “*Phonon Dispersion Relations in NaCl*”, by G. Raumo, L. Almqvist and R. Stedman, Phys Rev. 178 (1969).

We consider the simple situation described in Section 4.1.1 where we have a one-dimensional lattice with spacing  $a$ . Suppose, further, that there is a single electron per lattice site. Because of the spin degree of freedom, it results in a half-filled band, as explained in Section 2.1. In other words, we have a conductor.

Consider a distortion of the lattice, in which successive pairs of atoms move closer to each other, as shown below.



Clearly this costs some energy since the atoms move away from their equilibrium positions. If each atom moves by an amount  $\delta x$ , we expect that the total energy cost is of order

$$U_{\text{lattice}} \sim N\lambda(\delta x)^2 \quad (4.7)$$

What effect does this have on the electrons? The distortion has changed the lattice periodicity from  $a$  to  $2a$ . This, in turn, will halve the Brillouin zone so the electron states are now labeled by

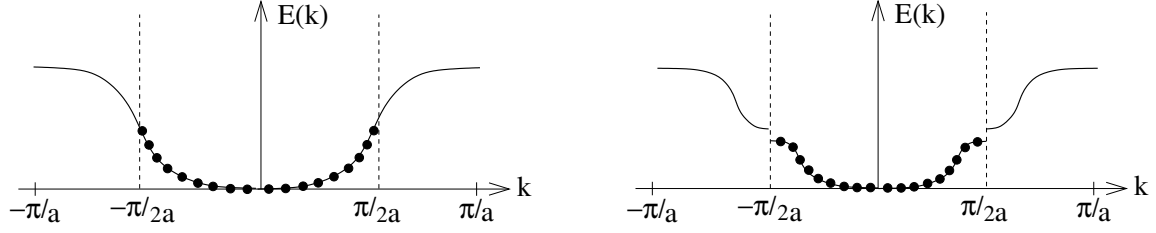
$$k \in \left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right)$$

More importantly, from the analysis of Section 2.1, we expect that a gap will open up in the electron spectrum at the edges of the Brillouin zone,  $k = \pm\pi/2a$ . In particular, the energies of the filled electron states will be pushed down; those of the empty electron states will be pushed up, as shown in the Figure 66. The question that we want to ask is: what is the energy reduction due to the electrons? In particular, is this more or less than the energy  $U_{\text{lattice}}$  that it cost to make the distortion in the first place?

Let's denote the dispersion relation before the distortion as  $E_0(k)$ , and the dispersion relation after the distortion as  $E_-(k)$  for  $|k| \in [0, \pi/2a)$  and  $E_+(k)$  for  $|k| \in [\pi/2a, \pi/a)$ . The energy cost of the distortion due to the electrons is

$$U_{\text{electron}} = -2 \frac{Na}{2\pi} \int_{-\pi/2a}^{\pi/2a} dk \left( E_0(k) - E_-(k) \right) \quad (4.8)$$

Here the overall minus sign is because the electrons lose energy, the factor of 2 is to account for the spin degree of freedom, while the factor of  $Na/2\pi$  is the density of states of the electrons.



**Figure 66:** The distortion of the lattice reduces the energy of the Fermi sea of electrons.

To proceed, we need to get a better handle on  $E_0(k)$  and  $E_-(k)$ . Neither are particularly nice functions. However, for a small distortion, we expect that the band structure is changed only in the immediate vicinity of  $k = \pi/2a$ . Whatever the form of  $E_0(k)$ , we can always approximate it by a linear function in this region,

$$E_0(k) \approx \mu + \nu q \quad \text{with } q = k - \frac{\pi}{2a} \quad (4.9)$$

where  $\mu = E_0(\pi/2a)$  and  $\nu = \partial E_0 / \partial k$ , again evaluated at  $k = \pi/2a$ . Note that  $q < 0$  for the filled states, and  $q > 0$  for the unfilled states.

We can compute  $E_-(k)$  in this region by the same kind of analysis that we did in Section 2.1. Suppose that the distortion opens up a gap  $\Delta$  at  $k = \pi/2a$ . Since there is no gap unless there is a distortion of the lattice, we expect that

$$\Delta \sim \delta x \quad (4.10)$$

(or perhaps  $\delta x$  to some power). To compute  $E_-(k)$  in the vicinity of the gap, we can use our earlier result (2.16). Adapted to the present context, the energy  $E$  close to  $k = \pi/2a$  is given by

$$\left(E_0(\pi/2a + q) - E\right) \left(E_0(\pi/2a - q) - E\right) - \frac{\Delta^2}{4} = 0$$

Using our linearisation (4.9) of  $E_0$ , we can solve this quadratic to find the dispersion relation

$$E_{\pm}(q) = \mu \pm \sqrt{\nu^2 q^2 + \frac{\Delta^2}{4}}$$

Note that when evaluated at  $q = 0$ , we find the gap  $E_+ - E_- = \Delta$ , as expected. The filled states sit in the lower branch  $E_-$ . The energy gained by the electrons (4.8) is

dominated by the regions  $k = \pm\pi/2a$ . By symmetry, it is the same in both and given by

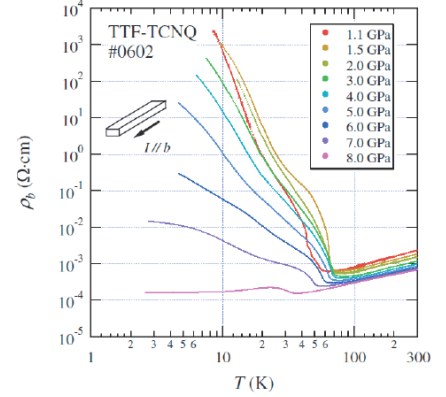
$$U_{\text{electron}} \approx -\frac{Na}{\pi} \int_{-\Lambda}^0 dq \left( \nu q + \sqrt{\nu^2 q^2 + \frac{\Delta^2}{4}} \right)$$

Here we have introduced a lower cut-off  $-\Lambda$  on the integral; it will not ultimately be important where we take this cut-off, although we will require  $\nu\Lambda \gg \Delta$ . The integral is straightforward to evaluate exactly. However, our interest lies in what happens when  $\Delta$  is small. In this limit, we have

$$U_{\text{electron}} \approx -\frac{Na}{\pi} \left[ \frac{\Delta^2}{16\nu} - \frac{\Delta^2}{8\nu} \log \left( \frac{\Delta}{4\nu\Lambda} \right) \right]$$

Both terms contribute to the decrease in energy of the electrons. The first term is of order  $\Delta^2$  and hence, through (4.10), of order  $\delta x^2$ . This competes with the energy cost from the lattice distortion (4.7), but there is no guarantee that it is either bigger or smaller. The second term with the log is more interesting. For small  $\Delta$ , this always beats the quadratic cost of the lattice distortion (4.7).

We reach a surprising conclusion: a half-filled band in one-dimension is unstable. The lattice rearranges itself to turn the metal into an insulator. This is known as the Peierls transition; it is an example of a metal-insulator transition. This striking behaviour can be seen in one-dimensional polymer chains, such as the catchily named TTF-TCNQ shown in the figure<sup>7</sup>. The resistivity – plotted on the vertical axis – rises sharply when the temperature drops to the scale  $\Delta$ . (The figure also reveals another feature: as the pressure is increased, the resistivity no longer rises quite as sharply, and by the time you get to 8 *GPa* there is no rise at all. This is because of the interactions between electrons become important.)



**Figure 67:**

#### 4.1.4 Quantum Vibrations

Our discussion so far has treated the phonons purely classically. Now we turn to their quantisation. At heart this is not difficult – after all, we just have a bunch of harmonic oscillators. However, they are coupled in an interesting way and the trick is to disentangle them. It turns out that we’ve already achieved this disentangling by writing down the classical solutions.

<sup>7</sup>This data is taken from “*Recent progress in high-pressure studies on organic conductors*”, by S. Yasuzuka and K. Murata (2009)



We have a classical solution (4.3) for each  $k_l = 2\pi l/Na$  with  $l = -N/2, \dots, N/2$ . We will call the corresponding frequency  $\omega_l = 2\sqrt{\lambda/m}|\sin(k_l a/2)|$ . We can introduce a different amplitude for each  $l$ . The most general classical solution then takes the form

$$u_n(t) = X_0(t) + \sum_{l \neq 0} \left[ \alpha_l e^{-i(\omega_l t - k_l n a)} + \alpha_l^\dagger e^{i(\omega_l t - k_l n a)} \right] \quad (4.11)$$

This requires some explanation. First, we sum over all modes  $l = -N/2, \dots, +N/2$  with the exception of  $l = 0$ . This has been singled out and written as  $X_0(t)$ . It is the centre of mass, reflecting the fact that the entire lattice can move as one. The amplitudes for each  $l \neq 0$  mode are denoted  $\alpha_l$ . Finally, we have taken the real part of the solution because, ultimately,  $u_n(t)$  should be real. Note that we've denoted the complex conjugation by  $\alpha_l^\dagger$  rather than  $\alpha_l^*$  in anticipation of the quantisation that we will turn to shortly.

The momentum  $p_n(t) = m\dot{u}_n$  is given by

$$p_n(t) = P_0(t) + \sum_{l \neq 0} \left[ -im\omega_l \alpha_l e^{-i(\omega_l t - k_l n a)} + im\omega_l \alpha_l^\dagger e^{i(\omega_l t - k_l n a)} \right]$$

Now we turn to the quantum theory. We promote  $u_n$  and  $p_n$  to operators acting on a Hilbert space. We should think of  $u_n(t)$  and  $p_n(t)$  as operators in the Heisenberg representation; we can get the corresponding operators in the Schrödinger representation simply by setting  $t = 0$ .

Since  $u_n$  and  $p_n$  are operators, the amplitudes  $\alpha_l$  and  $\alpha_l^\dagger$  must also be operators if we want these equations to continue to make sense. We can invert the equations above by setting  $t = 0$  and looking at

$$\sum_{n=1}^N u_n e^{-ik_l n a} = \sum_n \sum_{l'} \left[ \alpha_{l'} e^{-i(k_l - k_{l'}) n a} + \alpha_{l'}^\dagger e^{-i(k_l + k_{l'}) n a} \right] = N(\alpha_l + \alpha_{-l}^\dagger)$$

Similarly,

$$\sum_{n=1}^N p_n e^{ik_l n a} = \sum_n \sum_{l'} \left[ -im\omega_{l'} \alpha_{l'} e^{-i(k_l - k_{l'}) n a} + im\omega_{l'} \alpha_{l'}^\dagger e^{-i(k_l + k_{l'}) n a} \right] = -iNm\omega_l(\alpha_l - \alpha_{-l}^\dagger)$$

where we've used the fact that  $\omega_l = \omega_{-l}$ . We can invert these equations to find

$$\begin{aligned} \alpha_l &= \frac{1}{2m\omega_l N} \sum_n e^{-ik_l n a} (m\omega_l u_n + ip_n) \\ \alpha_l^\dagger &= \frac{1}{2m\omega_l N} \sum_n e^{ik_l n a} (m\omega_l u_n - ip_n) \end{aligned} \quad (4.12)$$

Similarly, we can write the centre of mass coordinates — which are also now operators — as

$$X_0 = \frac{1}{N} \sum_n u_n \quad \text{and} \quad P_0 = \frac{1}{N} \sum_n p_n \quad (4.13)$$

At this point, we're ready to turn to the commutation relations. The position and momentum of each atom satisfy

$$[u_n, p_{n'}] = i\hbar \delta_{n,n'}$$

A short calculation using the expressions above reveals that  $X_0$  and  $P_0$  obey the expected relations

$$[X_0, P_0] = i\hbar$$

Meanwhile, the amplitudes obey the commutation relations

$$[\alpha_l, \alpha_{l'}^\dagger] = \frac{\hbar}{2m\omega_l N} \delta_{l,l'} \quad \text{and} \quad [\alpha_l, \alpha_{l'}] = [\alpha_l^\dagger, \alpha_{l'}^\dagger] = 0$$

This is something that we've seen before: they are simply the creation and annihilation operators of a simple harmonic oscillator. We rescale

$$\alpha_l = \sqrt{\frac{\hbar}{2m\omega_l N}} a_l \quad (4.14)$$

then our new operators  $a_l$  obey

$$[a_l, a_{l'}^\dagger] = \delta_{l,l'} \quad \text{and} \quad [a_l, a_{l'}] = [a_l^\dagger, a_{l'}^\dagger] = 0$$

## Phonons

We now turn to the Hamiltonian (4.1). Substituting in our expressions (4.12) and (4.13), and after a bit of tedious algebra, we find the Hamiltonian

$$H = \frac{P_0^2}{2M} + \sum_{l \neq 0} \left( a_l^\dagger a_l + \frac{1}{2} \right) \hbar \omega_l$$

Here  $M = Nm$  is the mass of the entire lattice. Since this is a macroscopically large object, we set  $P_0 = 0$  and focus on the Hilbert space arising from the creation operators  $a_l^\dagger$ . After our manipulations, these are simply  $N$ , decoupled harmonic oscillators.

The ground state of the system is a state  $|0\rangle$  obeying

$$a_l|0\rangle = 0 \quad \forall l$$

Each harmonic oscillator gives a contribution of  $\hbar\omega_l/2$  to the zero-point energy  $E_0$  of the ground state. However, this is of no interest. All we care about is the energy difference between excited states and the ground state. For this reason, it's common practice to redefine the Hamiltonian to be simply

$$H = \sum_{l \neq 0} \hbar\omega_l a_l^\dagger a_l$$

so that  $H|0\rangle = 0$ .

The excited states of the lattice are identical to the excited states of the harmonic oscillators. For each  $l$ , the first excited state is given by  $a_l^\dagger|0\rangle$  and has energy  $E = \hbar\omega_l$ . However, although the mathematics is identical to that of the harmonic oscillator, the physical interpretation of this state is rather different. That's because it has a further quantum number associated to it: this state carries crystal momentum  $\hbar k_l$ . But an object which carries both energy and momentum is what we call a particle! In this case, it's a particle which, like all momentum eigenstates, is not localised in space. This particle is a quantum of the lattice vibration. It is called the *phonon*.

Note that the coupling between the atoms has lead to a quantitative change in the physics. If there was no coupling between atoms, each would oscillate with frequency  $m\lambda$  and the minimum energy required to excite the system would be  $\sim \hbar m\lambda$ . However, when the atoms are coupled together, the normal modes now vibrate with frequencies  $\omega_l$ . For small  $k$ , these are  $\omega_l \approx \sqrt{\frac{\lambda\pi^2}{m}} \frac{l}{N}$ . The key thing to notice here is the factor of  $1/N$ . In the limit of an infinite lattice,  $N \rightarrow \infty$ , there are excited states with infinitesimally small energies. We say that the system is *gapless*, meaning that there is no gap between the ground state and first excited state. In general, the question of whether a bunch interacting particles is gapped or gapless is one of the most basic (and, sometimes, most subtle) questions that you can ask about a system.

Any state in the Hilbert space can be written in the form

$$|\psi\rangle = \prod_l \frac{(a_l^\dagger)^{n_l}}{\sqrt{n_l!}} |0\rangle$$

and has energy

$$H|\psi\rangle = \sum_l \hbar n_l \omega_l$$

This state should be thought of as described  $\sum_l n_l$  phonons and decomposes into  $n_l$  phonons with momentum  $\hbar k_l$  for each  $l$ . The full Hilbert space constructed in this way contains states consisting of an arbitrary number of particles. It is referred to as a *Fock space*.

Because the creation operators  $a_l^\dagger$  commute with each other, there is no difference between the state  $|\psi\rangle \sim a_l^\dagger a_{l'}^\dagger |0\rangle$  and  $|\psi\rangle \sim a_{l'}^\dagger a_l^\dagger |0\rangle$ . This is the statement that phonons are bosons.

The idea that harmonic oscillator creation operators actually create particles sometimes goes by the terrible name of *second quantisation*. It is misleading — nothing has been quantised twice.

## Quantisation of Acoustic and Optical Phonons

It is not difficult to adapt the discussion above to vibrations of a diatomic lattice that we met in Section 4.1.2. We introduce two *polarization vectors*,  $\mathbf{e}_\pm(k)$ . These are eigenvectors obeying the matrix equation (4.6),

$$\begin{pmatrix} 2 & -(1 + e^{-2ika}) \\ -(1 + e^{2ika}) & 2 \end{pmatrix} \mathbf{e}_\pm(k) = \frac{\omega_\pm^2}{\lambda} \begin{pmatrix} m & 0 \\ 0 & M \end{pmatrix} \mathbf{e}_\pm(k)$$

We then write the general solution as

$$\begin{pmatrix} u_{2n}(t) \\ u_{2n+1}(t) \end{pmatrix} = \sum_{k \in BZ} \sum_{s=\pm} \sqrt{\frac{\hbar}{2N\omega_s(k)}} \left[ a_s(k) \mathbf{e}_s(k) e^{i(\omega_s t + 2kna)} + a_s^\dagger(k) \mathbf{e}_s^*(k) e^{-i(\omega_s t + 2kna)} \right]$$

where the creation operators obey

$$[a_s(k), a_{s'}(k')^\dagger] = \delta_{s,s'} \delta_{k,k'} \quad \text{and} \quad [a_s(k), a_{s'}(k')] = [a_s^\dagger(k), a_{s'}(k')^\dagger] = 0$$

Now the operators  $a_-^\dagger(k)$  create acoustic phonons while  $a_+^\dagger(k)$  create optical phonons, each with momentum  $\hbar k$ .

### 4.1.5 The Mössbauer Effect

There's a rather nice application of phonons that goes by the name of the *Mössbauer effect*. This is to do with how nuclei in solids absorb gamma rays.

To understand this, we first need to think about atoms absorb light, and then contrast this with how nuclei absorb light. To this end, consider a gas of atoms, all sitting in the ground state. If we shine light on the atoms at very specific frequencies, then the atoms will absorb the light by jumping to excited states. The frequency should be

$$E_\gamma = \hbar\nu = E_{\text{excite}}$$

where  $E_{\text{excite}}$  is the energy difference between the excited state and the ground state. Once the atom absorbs a photon, it will sit in the excited state for some time and then decay. If it drops back down to the ground state, the emitted photon will again have energy  $E_\gamma$  and can be absorbed by another atom. This then repeats, a process known as *resonant absorption*.

However, a little thought shows that the situation is slightly more complicated than we've made out. Suppose, for simplicity, that the original atom was at rest. In the collision with the atom, both energy and momentum must be conserved. The momentum of the incoming photon is  $p_\gamma = E_\gamma/c$  and, after the collision, this is transferred to the atom, so  $p_{\text{atom}} = E_\gamma/c$ . This means that the atom has kinetic energy from the recoil,

$$E_{\text{recoil}} = \frac{p_{\text{atom}}^2}{2M} = \frac{E_\gamma^2}{2Mc^2} \quad (4.15)$$

where  $M$  is the mass of the atom. (The speed of the atom is small enough that we can use the non-relativistic form of kinetic energy.) So we see that it's not quite right to say that the energy of the photon should be tuned to the energy difference  $E_{\text{excite}}$  because this ignores the energy that goes into the recoil. Instead, the incoming photon should have slightly higher energy,  $E_\gamma = E_{\text{excite}} + E_{\text{recoil}}$ , or

$$E_\gamma = E_{\text{excite}} + \frac{E_\gamma^2}{2Mc^2} \quad \Rightarrow \quad E_\gamma \approx E_{\text{excite}} + \frac{(E_{\text{excite}})^2}{2Mc^2} + \dots \quad (4.16)$$

Meanwhile, when the atom now decays back to the ground state, it will emit the photon in a random direction. This means that the atom typically remains in motion; indeed, it's quite possible that the kinetic energy of atom increases yet again if it emits the photon back in the direction it came. All of this means that the energy of the emitted photon that the atom emits is smaller than the energy of the photon that it absorbed.

The question is: what happens next? In particular, is it possible for this emitted photon to be re-absorbed by a different atom so that we get resonant absorption? This is now a quantitative question, rather than a qualitative question. The key point is that you don't need to tune the frequency of light exactly to  $E_{\text{excite}}$  in order to excite

an atom. Instead, there is a range of energies – a so-called *line width* – that will do the job. This line width is related to the lifetime  $\tau$  of the excited state by  $\Delta E \sim \hbar/\tau$ . (See the chapter on scattering in the lectures on [Topics in Quantum Mechanics](#) for more details.)

Let's put in some numbers. The energy needed to excite an electron from one level to another is measured in  $E_{\text{excite}} \approx \text{eV}$ . Meanwhile the mass of, say, an iron atom is around  $Mc^2 \sim 5 \times 10^4 \text{ MeV}$ . This means that the correction term (4.16) in the photon energy is of order  $\Delta E_\gamma \approx 10^{-11} \text{ eV}$ . This is significantly smaller than the line width of atomic excitations, and the discussion above has no relevance to absorption of light due to transitions of electrons from one energy level to another.

However, things are very different when it comes to nuclear transitions. Now the relevant excitation energy is of order  $E_{\text{excite}} \approx 10^4 \text{ eV}$ , corresponding to soft gamma rays, and the correction term (4.16) in the photon energy due to recoil effects is  $\Delta E \approx 10^{-3} \text{ eV}$ . This time the energy is significantly larger than the line width: a typical nuclear excitation has lifetime  $\tau \sim 10^{-7}$  seconds and a width  $\Gamma \sim 10^{-8} \text{ eV}$ . The upshot of this argument is that, while X-ray absorption lines are seen corresponding to atomic excitations, we should not expect to see a repeat in the gamma-ray spectrum associated to nuclear excitations.

And yet. . . while it's true that gamma ray resonant absorption lines are not seen in gasses, they are seen in solids. This is the *Mössbauer effect*. The important point is that a nucleus in an atom is coupled to all the other atoms through the bonds in a solid. A nucleus will recoil when hit by a photon, as in the discussion above, but now the atom will bounce back into position and the energy  $E_{\text{recoil}}$  will typically be distributed into phonon degrees of freedom. When there are a large number of phonons excited, the story is not different from that told above, and the emitted photon has a sufficiently different frequency to kill resonant absorption. However, there is some probability that no phonons are created, but instead the entire solid moves and absorbs the momentum of the photon. In this case, the recoil energy is still given by (4.15) but with  $M$  is the mass of the solid, rather than the mass of a single atom. This gives an extra factor of around  $10^{23}$  in the denominator, and the recoil energy becomes negligible. For this to happen, the entire solid must react coherently as a single quantum object! The resulting gamma ray resonant absorption spectrum is indeed observed.

## 4.2 From Atoms to Fields

If we look at a solid at suitably macroscopic distances, we don't notice the underlying atomic structure. Nonetheless, it's still straightforward to detect sound waves. This suggests that we should be able to formulate a continuum description of the solid that is ignorant of the underlying atomic make-up.

With this in mind, we define the *displacement field* for a one-dimensional lattice. This is a function  $u(x, t)$ . It is initially defined only at the lattice points

$$u(x = na) = u_n$$

However, we then extend this field to all  $x \in \mathbf{R}$ , with the proviso that our theory will cease to make sense if  $u(x)$  varies appreciably on scales smaller than  $a$ .

The equation governing the atomic displacements is (4.2)

$$m\ddot{u}_n = -\lambda(2u_n - u_{n-1} - u_{n+1})$$

In the continuum limit, this difference equation becomes the wave equation

$$\rho \frac{\partial^2 u}{\partial t^2} = -\lambda' \frac{\partial^2 u}{\partial x^2} \quad (4.17)$$

where  $\rho = m/a$  is the density of our one-dimensional solid, and  $\lambda' = \lambda a$ . These are the macroscopic parameters. Note, in particular, that the speed of sound (4.4) can be written purely in terms of these macroscopic parameters,  $c_s^2 = \lambda'/\rho$ .

The equation of motion (4.17) can be derived from the action

$$S = \int dt dx \left[ \frac{\rho}{2} \left( \frac{\partial u}{\partial t} \right)^2 - \frac{\lambda'}{2} \left( \frac{\partial u}{\partial x} \right)^2 \right]$$

This is the field theory for the phonons of a one-dimensional solid.

### 4.2.1 Phonons in Three Dimensions

For three-dimensional solids, there are three displacement fields,  $u_i(\mathbf{x})$ , one for each direction in which the lattice can deform. In general, the resulting action can depend on various quantities  $\partial u_i / \partial x^j$ . However, if the underlying lattice is such that the long-wavelength dynamics is rotationally invariant, then the action can only be a function of the symmetric combination

$$u_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x^j} + \frac{\partial u_j}{\partial x^i} \right)$$

If we want an equation of motion linear in the displacement, then the most general action is a function of  $u_{ij}u_{ij}$  or  $u_{kk}^2$ . (The term  $u_{kk}$  is a total derivative and does not affect the equation of motion). We have

$$S = \int dt d^3x \frac{1}{2} \left[ \rho \left( \frac{\partial u_i}{\partial t} \right)^2 - 2\mu u_{ij}u_{ij} - \lambda u_{ii}u_{jj} \right] \quad (4.18)$$

The coefficients  $\mu$  and  $\lambda$  are called Lamé coefficients; they characterise the underlying solid.

This action gives rise to the equations of motion

$$\rho \frac{\partial^2 u_i}{\partial t^2} = (\mu + \lambda) \frac{\partial^2 u_j}{\partial x^i \partial x^j} + \mu \frac{\partial^2 u_i}{\partial x^j \partial x^j} \quad (4.19)$$

We can look for solutions of the form

$$u_i(\mathbf{x}, t) = \epsilon_i e^{i(\mathbf{k} \cdot \mathbf{x} + \omega t)}$$

where  $\epsilon_i$  determines the polarisation of the wave. Plugging this ansatz into the equation of motion gives us the relation

$$\rho \omega^2 \epsilon_i = \mu k^2 \epsilon_i + (\mu + \lambda) (\boldsymbol{\epsilon} \cdot \mathbf{k}) k_i$$

The frequency of the wave depends on the polarisation. There are two different options. Longitudinal waves have  $\mathbf{k} \sim \boldsymbol{\epsilon}$ . These have dispersion

$$\omega^2 = \frac{2\mu + \lambda}{\rho} k^2 \quad (4.20)$$

Meanwhile, transverse waves have  $\boldsymbol{\epsilon} \cdot \mathbf{k} = 0$  and dispersion

$$\omega^2 = \frac{\mu}{\rho} k^2 \quad (4.21)$$

Note that both of these dispersion relations are linear. The continuum approximation only captures the low- $k$  limit of the full lattice system and does not see the bending of the dispersion relation close to the edge of the Brillouin zone. This is because it is valid only at long wavelengths,  $ka \ll 1$ .

The general solution to (4.19) is then

$$u_i(\mathbf{x}, t) = \sum_s \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\rho\omega_s(k)} \epsilon_i^s \left( a_s(\mathbf{k}) e^{i(\mathbf{k} \cdot \mathbf{x} - \omega_s t)} + a_s^\dagger(\mathbf{k}) e^{-i(\mathbf{k} \cdot \mathbf{x} - \omega_s t)} \right) \quad (4.22)$$

where the  $s$  sum is over the three polarisation vectors, two transverse and one longitudinal. The frequencies  $\omega_s(k)$  correspond to either (4.20) or (4.21) depending on the choice of  $s$ .



### 4.2.2 From Fields to Phonons

Although we have discarded the underlying atoms, this does not mean that we have lost the discrete nature of phonons. To recover them, we must quantise the field theory defined by the action (4.18). This is the subject of *Quantum Field Theory*. You will learn much (much) more about this in [next year's lectures](#). What follows is merely a brief taster for things to come.

To quantise the field, we need only follow the same path that we took in Section 4.1.4. At every step, we simply replace the discrete index  $n$  with the continuous index  $\mathbf{x}$ . Note, in particular, that  $\mathbf{x}$  is not a dynamical variable in field theory; it is simply a label.

First, we turn the field  $u(\mathbf{x})$  into an operator. This means that the amplitudes  $a_s(\mathbf{k})$  and  $a_s^\dagger(\mathbf{k})$  in (4.22) also become operators. To proceed, we need the momentum conjugate to  $u_i(\mathbf{x}, t)$ . This too is now a field, and is determined by the usual rules of classical dynamics,

$$\pi_i(\mathbf{x}) = \frac{\partial L}{\partial \dot{u}_i} = \rho \dot{u}_i$$

Written in terms of the solution (4.22), we have

$$\pi_i(\mathbf{x}, t) = \rho \sum_s \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\rho\omega_s(k)} \epsilon_i^s \left( -i\omega_s a_s(\mathbf{k}) e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_s t)} + i\omega_s a_s^\dagger(\mathbf{k}) e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega_s t)} \right)$$

The canonical commutation relations are the field-theoretical analog of the usual position-momentum commutation relations,

$$[u_i(\mathbf{x}), \pi_j(\mathbf{x}')] = i\hbar \delta_{ij} \delta^3(\mathbf{x} - \mathbf{x}')$$

At this point we have some straightforward but tedious calculations ahead of us. We will skip these on the grounds that you will see them in glorious detail in later courses. The first is an inverse Fourier transform, which expresses  $a_s(\mathbf{k})$  and  $a_s^\dagger(\mathbf{k})$  in terms of  $u_i(\mathbf{x})$  and  $\pi_i(\mathbf{x})$ . The result is analogous to (4.12). We then use this to determine the commutation relations,

$$[a_s(\mathbf{k}), a_{s'}^\dagger(\mathbf{k}')] = \delta_{s,s'} \delta^3(\mathbf{k} - \mathbf{k}') \quad \text{and} \quad [a_s(\mathbf{k}), a_{s'}(\mathbf{k}')] = [a_s^\dagger(\mathbf{k}), a_{s'}^\dagger(\mathbf{k}')] = 0$$

This is the statement that these are creation and annihilation operators for harmonic oscillators, now labelled by both a discrete polarisation index  $s = 1, 2, 3$  as well as the continuous momentum index  $\mathbf{k}$ .

The next fairly tedious calculation is the Hamiltonian. This too follows from standard rules of classical dynamics, together with a bunch of Fourier transforms. When the dust settles, we find that, up to an irrelevant overall constant,

$$H = \sum_s \int \frac{d^3k}{(2\pi)^3} \hbar\omega_s(k) a_s^\dagger(\mathbf{k}) a_s(\mathbf{k})$$

This is simply the Hamiltonian for an infinite number of harmonic oscillators.

The interpretation is the same as we saw in Section 4.1.4. We define the ground state of the field theory to obey  $a_s(\mathbf{k})|0\rangle = 0$  for all  $s$  and for all  $\mathbf{k}$ . The Fourier modes of the field  $a_s^\dagger(\mathbf{k})$  are then to be viewed as creating and destroying phonons which carry momentum  $\hbar\mathbf{k}$ , polarisation  $\epsilon_s$  and energy  $\hbar\omega_s(k)$ . In this way, we see particles emerging from an underlying field.

### Lessons for the Future

This has been a very quick pass through some basic quantum field theory, applied to the vibrations of the lattice. Buried within the mathematics of this section are two, key physical ideas. The first is that a coarse grained description of atomic vibrations can be described in terms of a continuous field. The second is that quantisation of the field results in particles that, in the present context, we call phonons.

There is a very important lesson to take from the second of these ideas, a lesson which extends well beyond the study of solids. All of the fundamental particles that we know of in Nature – whether electrons, quarks, photons, or anything else — arise from the quantisation of an underlying field. This is entirely analogous to the way that phonons arose in the discussion above.

Is there also a lesson to take away from the first idea above? Could it be that the fundamental fields of Nature themselves arise from coarse-graining something smaller? The honest answer is that we don't know. However, perhaps surprisingly, all signs point towards this *not* being the case. First, and most importantly, there is no experimental evidence that the fundamental fields in our Universe have a discrete underpinning. But at the theoretical level, there are some deep mathematical reasons — to do with chiral fermions and topology — which suggest that it is not possible to find a discrete system from which the known laws of physics emerge. It would appear that our Universe does not have something akin to the atomic lattice which underlies the phonon field. Understanding these issues remains a vibrant topic of research, both in condensed matter physics and in high energy physics.