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Applications of Quantum Mechanics

University of Cambridge Part II Mathematical Tripos

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Recommended Books and Resources

There are many good books on quantum mechanics. Here's a selection that I like:

- Griffiths, *Introduction to Quantum Mechanics*

An excellent way to ease yourself into quantum mechanics, with uniformly clear explanations. For this course, it covers both approximation methods and scattering.

- Shankar, *Principles of Quantum Mechanics*
- James Binney and David Skinner, *The Physics of Quantum Mechanics*
- Weinberg, *Lectures on Quantum Mechanics*

These are all good books, giving plenty of detail and covering more advanced topics. Shankar is expansive, Binney and Skinner clear and concise. Weinberg likes his own notation more than you will like his notation, but it's worth persevering.

This course also contains topics that cannot be found in traditional quantum textbooks. This is especially true for the condensed matter aspects of the course, covered in Sections 3, 4 and 5. Some good books include

- Ashcroft and Mermin, *Solid State Physics*
- Kittel, *Introduction to Solid State Physics*
- Steve Simon, *Solid State Physics Basics*

Ashcroft & Mermin and Kittel are the two standard introductions to condensed matter physics, both of which go substantially beyond the material covered in this course. I have a slight preference for the verbosity of Ashcroft and Mermin. The book by Steve Simon covers only the basics, but does so very well. (An earlier draft can be downloaded from his homepage; see below for a link.)

A number of lecture notes are available on the web. Links can be found on the course webpage: http://www.damtp.cam.ac.uk/user/tong/aqm.html

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Acknowledgements

This course is built on the foundation of previous courses, given in Cambridge by Ron Horgan and Nick Dorey. I'm supported by the Royal Society and Alex Considine Tong.

0. Introduction

Without wishing to overstate the case, the discovery of quantum mechanics is the single greatest achievement in the history of human civilisation.

Quantum mechanics is an outrageous departure from our classical, comforting, common sense view of the world. It is more baffling and disturbing than anything dreamt up by science fiction writers. And yet it is undoubtably the correct description of the Universe we inhabit and has allowed us to understand Nature with unprecedented accuracy. In these lectures we will explore some of these developments.

The applications of quantum mechanics are many and various, and vast swathes of modern physics fall under this rubric. Here we tell only a few of the possible stories, laying the groundwork for future exploration. There are two major topics.

Much of these lectures is devoted to *condensed matter physics* or, more precisely, *solid state physics*. This is the study of "stuff", of how the wonderfully diverse properties of solids can emerge from the simple laws that govern electrons and atoms. We will develop the basics of the subject, learning how electrons glide through seemingly impenetrable solids, how their collective motion is described by a Fermi surface, and how the vibrations of the underlying atoms get tied into bundles of energy known as phonons. We will learn that electrons in magnetic fields can do strange things and start to explore some of the roles that geometry and topology play in quantum physics.

The second major topic is *scattering theory*. In the past century, physicists have developed a foolproof and powerful method to understand everything and anything: you take the object that you're interested in and you throw something at it. This technique was pioneered by Rutherford who used it to understand the structure of the atom. It was used by Franklin, Crick and Watson to understand the structure of DNA. And, more recently, it was used at the LHC to demonstrate the existence of the Higgs boson. In fact, throwing stuff at other stuff is the single most important experimental method known to science. It underlies much of what we know about condensed matter physics and all of what we know about high-energy physics.

In many ways, these lectures are where theoretical physics starts to fracture into separate sub-disciplines. Yet areas of physics which study systems separated by orders of magnitude — from the big bang, to stars, to materials, to information, to atoms and beyond — all rest on a common language and background. The purpose of these lectures is to build this shared base of knowledge.

1. Scattering Theory

The basic idea behind *scattering theory* is simple: there's an object that you want to understand. So you throw something at it. By analysing how that something bounces off, you can glean information about the object itself.

A very familiar example of scattering theory is called "looking at things". In this section we're going to explore what happens when you look at things by throwing a quantum particle at an object.

1.1 Scattering in One Dimension

We start by considering a quantum particle moving along a line. The maths here will be simple, but the physics is sufficiently interesting to exhibit many of the key ideas.

The object that we want to understand is some potential $V(x)$. Importantly, the potential is localised to some region of space which means that $V(x) \to 0$ as $x \to \pm\infty$. An example is shown to the right. We will need the potential to fall-off to be suitably fast in what follows although, for now, we won't be careful about what this means. A quantum particle moving along the line is governed by the Schrödinger equation,

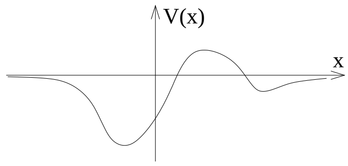


Figure 1:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{1.1}$$

Solutions to this equation are energy eigenstates. They evolve in time as $\psi(x,t) = e^{-iEt/\hbar}\psi(x)$. For any potential, there are essentially two different kinds of states that we're interested in.

- *Bound States* are states that are localised in some region of space. The wavefunctions are normalisable and have profiles that drop off exponentially far from the potential

  $$\psi(x) \sim e^{-\lambda|x|} \quad \text{as} \quad |x| \to \infty$$

  Because the potential vanishes in the asymptotic region, the Schrödinger equation (1.1) relates the asymptotic fall-off to the energy of the state,

  $$E = -\frac{\hbar^2\lambda^2}{2m} \tag{1.2}$$

  In particular, bound states have $E < 0$. Indeed, it is this property which ensures that the particle is trapped within the potential and cannot escape to infinity.

Bound states are rather special. In the absence of a potential, a solution which decays exponentially to the left will grow exponentially to the far right. But, for the state to be normalisable, the potential has to turn this behaviour around, so the wavefunction decreases at both $x \to -\infty$ and $x \to +\infty$. This will only happen for specific values of λ. Ultimately, this is why the spectrum of bound states is discrete, like in the hydrogen atom. It's where the name "quantum" comes from.

- *Scattering States* are not localised in space and, relatedly, the wavefunctions are not normalisable. Instead, asymptotically, far from the potential, scattering states take the form of plane waves. In one dimension, there are two possibilities

$$\text{Right moving:} \quad \psi \sim e^{ikx}$$
$$\text{Left moving:} \quad \psi \sim e^{-ikx}$$

where $k > 0$. To see why these are left or right moving, we need to put the time dependence back in. The wavefunctions then take the form $e^{\pm ikx - iEt/\hbar}$. The peaks and troughs of the wave move to the right with the plus sign, and to the left with the minus sign. Solving the Schrödinger equation in the asymptotic region with $V = 0$ gives the energy

$$E = \frac{\hbar^2 k^2}{2m}$$

Scattering states have $E > 0$. Note that, in contrast, to bound states, nothing special has to happen to find scattering solutions. We expect to find solutions for any choice of k.

This simple classification of solutions already tells us something interesting. Suppose, for example, that the potential looks something like the one shown in the figure. You might think that we could find a localised solution that is trapped between the two peaks, with $E > 0$. But this can't happen because if the wavefunction is to be normalisable, it must have $E < 0$. The physical reason, of course, is quantum tunnelling which allows the would-be bound state to escape to infinity. We will learn more about this situation in Section 1.1.5.

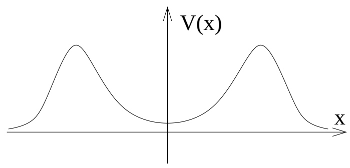


Figure 2:

1.1.1 Reflection and Transmission Amplitudes

Suppose that we stand a long way from the potential and throw particles in. What comes out? This is answered by solving the Schrödinger equation for the scattering states. Because we have a second order differential equation, we expect that there are two independent solutions for each value of k. We can think of these solutions physically as what you get if you throw the particle in from the left or in from the right. Let's deal with each in turn.

Scattering from the Left

We throw the particle in from the left. When it hits the potential, one of two things can happen: it can bounce back, or it can pass straight through. Of course, this being quantum mechanics, it can quite happily do both at the same time. Mathematically, this means that we are looking for a solution which asymptotically takes the form

$$\psi_R(x) \sim \begin{cases} e^{ikx} + re^{-ikx} & x \to -\infty \\ te^{ikx} & x \to +\infty \end{cases} \tag{1.3}$$

We've labelled this state ψ_R because the ingoing wave is *right*-moving. This can be seen in the first term e^{ikx} which represents the particle we're throwing in from $x \to -\infty$. The second term re^{-ikx} represents the particle that is reflected back to $x \to -\infty$ after hitting the potential. The coefficient $r \in \mathbf{C}$ is called the *reflection amplitude*. Finally, the term te^{ikx} at $x \to +\infty$ represents the particle passing through the potential. The coefficient $t \in \mathbf{C}$ is called the *transmission coefficient*. (Note: in this formula t is a complex number that we have to determine; it is not time!) There is no term e^{-ikx} at $x \to +\infty$ because we're not throwing in any particles from that direction. Mathematically, we have chosen the solution in which this term vanishes.

Before we proceed, it's worth flagging up a conceptual point. Scattering is clearly a dynamical process: the particle goes in, and then comes out again. Yet there's no explicit time dependence in our ansatz (1.3); instead, we have a solution formed of plane waves, spread throughout all of space. It's best to think of these plane waves as describing a beam of particles, with the ansatz (1.3) giving us the steady-state solution in the presence of the potential.

The probability for reflection R and transmission T are given by the usual quantum mechanics rule:

$$R = |r|^2 \quad \text{and} \quad T = |t|^2$$

In general, both R and T will be functions of the wavenumber k. This is what we would like to calculate for a given potential and we will see an example shortly. But, before we do this, there are some observations that we can make using general statements about quantum mechanics.

Given a solution $\psi(x)$ to the Schrödinger equation, we can construct a conserved probability current

$$J(x) = -i\frac{\hbar}{2m}\left(\psi^\star\frac{d\psi}{dx} - \psi\frac{d\psi^\star}{dx}\right)$$

which obeys $dJ/dx = 0$. This means that $J(x)$ is constant. (Mathematically, this is the statement that the Wronskian is constant for the two solutions to the Schrödinger equation). For our scattering solution ψ_R, with asymptotic form (1.3), the probability current as $x \to -\infty$ is given by

$$\begin{aligned} J(x) &= \frac{\hbar k}{2m}\Big[\left(e^{-ikx} + r^\star e^{+ikx}\right)\left(e^{ikx} - re^{-ikx}\right) + \left(e^{ikx} + re^{-ikx}\right)\left(e^{-ikx} - r^\star e^{+ikx}\right)\Big] \\ &= \frac{\hbar k}{m}\left(1 - |r|^2\right) \qquad \text{as } \ x \to -\infty \end{aligned}$$

Meanwhile, as $x \to +\infty$, we have

$$J(x) = \frac{\hbar k}{2m}|t|^2 \qquad \text{as } \ x \to +\infty$$

Equating the two gives

$$1 - |r|^2 = |t|^2 \quad \Rightarrow \quad R + T = 1 \tag{1.4}$$

This should make us happy as it means that probabilities do what probabilities are supposed to do. The particle can only get reflected or transmitted and the sum of the probabilities to do these things equals one.

Scattering from the Right

This time, we throw the particle in from the right. Once again, it can bounce back off the potential or pass straight through. Mathematically, we're now looking for solutions which take the asymptotic form

$$\psi_L(x) \sim \begin{cases} t'e^{-ikx} & x \to -\infty \\ e^{-ikx} + r'e^{+ikx} & x \to +\infty \end{cases} \tag{1.5}$$

where we've now labelled this state ψ_L because the ingoing wave, at $x \to +\infty$, is *left*-moving. We've called the reflection and transmission amplitudes r' and t'.

There is a simple relation between the two solutions ψ_R in (1.3) and ψ_L in (1.5). This follows because the potential $V(x)$ in (1.1) is a real function, so if ψ_R is a solution then so is $\psi_R^\star$. And, by linearity, so is $\psi_R^\star - r^\star \psi_R$ which is given by

$$\psi_R^\star(x) - r^\star\psi_R(x) \sim \begin{cases} (1-|r|^2)e^{-ikx} & x \to -\infty \\ t^\star e^{-ikx} - r^\star t e^{ikx} & x \to +\infty \end{cases}$$

This takes the same functional form as (1.5) except we need to divide through by $t^\star$ to make the normalisations agree. (Recall that scattering states aren't normalised anyway so we're quite at liberty to do this.) Using $1-|r|^2 = |t|^2$, this tells us that there is a solution of the form (1.5) with

$$t' = t \quad \text{and} \quad r' = -\frac{r^\star t}{t^\star} \tag{1.6}$$

Notice that the transition amplitudes are always the same, but the reflection amplitudes can differ by a phase. Nonetheless, this is enough to ensure that the reflection probabilities are the same whether we throw the particle from the left or right: $R = |r|^2 = |r'|^2$.

An Example: A Pothole in the Road

Let's compute r and t for a simple potential, given by

$$V(x) = \begin{cases} -V_0 & -a/2 < x < a/2 \\ 0 & \text{otherwise} \end{cases}$$

with $V_0 > 0$. This looks like a pothole in the middle of an, otherwise, flat potential.

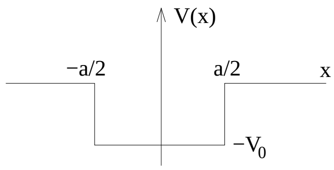


Figure 3:

Outside the potential, we have the usual plane waves $\psi \sim e^{\pm ikx}$. In the middle of the potential, the solutions to the Schrödinger equation (1.1) take the form

$$\psi(x) = Ae^{iqx} + Be^{-iqx} \qquad x \in [-a/2, a/2] \tag{1.7}$$

where

$$q^2 = \frac{2mV_0}{\hbar^2} + k^2$$

To compute the reflection and transmission amplitudes, r, r' and t, we need to patch the solution (1.7) with either (1.3) or (1.5) at the edges of the potential.

Let's start by scattering from the left, with the solution (1.3) outside the potential. Continuity of the wavefunction at $x = \pm a/2$ tells us that

$$e^{-ika/2} + re^{ika/2} = Ae^{-iqa/2} + Be^{iqa/2} \quad \text{and} \quad te^{ika/2} = Ae^{iqa/2} + Be^{-iqa/2}$$

Meanwhile, matching the derivatives of ψ at $x = \pm a$ gives

$$\frac{k}{q}\left(e^{-ika/2} - re^{ika/2}\right) = Ae^{-iqa/2} - Be^{iqa/2} \quad \text{and} \quad \frac{kt}{q}e^{ika/2} = Ae^{iqa/2} - Be^{-iqa/2}$$

These are four equations with four unknowns: A, B, r and t. One way to proceed is to add and subtract the two equations on the right, and then do the same for the two equations on the left. This allows us to eliminate A and B

$$A = t\left(1+\frac{k}{q}\right)e^{i(k-q)a/2} = \left(1+\frac{k}{q}\right)e^{-i(k-q)a/2} + r\left(1-\frac{k}{q}\right)e^{i(k+q)a/2}$$

$$B = t\left(1-\frac{k}{q}\right)e^{i(k+q)a/2} = \left(1-\frac{k}{q}\right)e^{-i(k+q)a/2} + r\left(1+\frac{k}{q}\right)e^{i(k-q)a/2}$$

We've still got some algebraic work ahead of us. It's grungy but straightforward. Solving these two remaining equations gives us the reflection and transmission coefficients that we want. They are

$$\begin{aligned} r &= \frac{(k^2-q^2)\sin(qa)e^{-ika}}{(q^2+k^2)\sin(qa)+2iqk\cos(qa)} \\ t &= \frac{2iqke^{-ika}}{(q^2+k^2)\sin(qa)+2iqk\cos(qa)} \end{aligned} \tag{1.8}$$

Even for this simple potential, the amplitudes are far from trivial. Indeed, they contain a lot of information. Perhaps the simplest lesson we can extract comes from looking at the limit $k \to 0$, where $r \to -1$ and $t \to 0$. This means that if you throw the particle very softly ($k \to 0$), then it won't make it through the potential; it's guaranteed to bounce back.

Conversely, in the limit $k \to \infty$, we have $r = 0$. (Recall that $q^2 = k^2 + 2mV_0/\hbar^2$ so we also have $q \to \infty$ in this limit.) By conservation of probability, we must then have $|t| = 1$ and the particle is guaranteed to pass through. This is what you might expect; if you throw the particle hard enough, it barely notices that the potential is there.

There are also very specific values of the incoming momenta for which $r = 0$ and the particle is assured of passage through the potential. This occurs when $qa = n\pi$ with $n \in \mathbf{Z}$ for which $r = 0$. Notice that you have to fine tune the incoming momenta so that it depends on the details of the potential which, in this example, means V_0 and a.

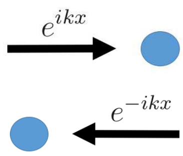
We can repeat the calculation above for scattering from the right. In fact, for our pothole potential, the result is exactly the same and we have $r = r'$. This arises because $V(x) = V(-x)$ so it's no surprise that scattering from the left and right are the same. We'll revisit this in Section 1.1.3.

1.1.2 Introducing the S-Matrix

The *S-matrix* is a convenient way of packaging the information about reflection and transmission coefficients. It is useful both because it highlights new features of the problem, and because it generalises to scattering in higher dimensions.

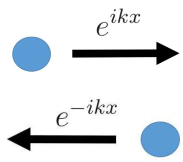
We will start by writing the above solutions in slightly different notation. We have two ingoing asymptotic wavefunctions, one from the left and one from the right

$$\text{Ingoing} \begin{cases} \text{right-moving:} \quad \mathcal{I}_R(x) = e^{+ikx} \quad x \to -\infty \\ \text{left-moving:} \quad \mathcal{I}_L(x) = e^{-ikx} \quad x \to +\infty \end{cases}$$



Similarly, there are two outgoing asymptotic wavefunctions,

$$\text{Outgoing} \begin{cases} \text{right-moving:} \quad \mathcal{O}_R(x) = e^{+ikx} \quad x \to +\infty \\ \text{left-moving:} \quad \mathcal{O}_L(x) = e^{-ikx} \quad x \to -\infty \end{cases}$$



The two asymptotic solutions (1.3) and (1.5) can then be written as

$$\begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} = \begin{pmatrix} \mathcal{I}_R \\ \mathcal{I}_L \end{pmatrix} + \mathcal{S} \begin{pmatrix} \mathcal{O}_R \\ \mathcal{O}_L \end{pmatrix} \tag{1.9}$$

where

$$\mathcal{S} = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix} \tag{1.10}$$

This is the *S-matrix*. As we've seen, for any given problem the entries of the matrix are rather complicated functions of k.

The S-matrix has many nice properties, some of which we will describe in these lectures. One of the simplest and most important is that $\mathcal{S}$ is unitary. To see this note that

$$\mathcal{S}\mathcal{S}^\dagger = \begin{pmatrix} |t'|^2 + |r|^2 & t'r'^\star + rt^\star \\ t'^\star r' + tr^\star & |t|^2 + |r'|^2 \end{pmatrix}$$

Unitarity then follows from the conservation of probability. The off-diagonal elements vanish by virtue of the relations $t' = t$ and $r' = -r^\star t/t^\star$ that we found in (1.6). Meanwhile, the diagonal elements are equal to one by (1.4) and so $\mathcal{S}\mathcal{S}^\dagger = \mathbf{1}$. The equivalence between conservation of probability and unitarity of the S-matrix is important, and will generalise to higher dimensions. Indeed, in quantum mechanics the word "unitarity" is often used synonymously with "conservation of probability".

One further property follows from the fact that the wavefunctions $\psi_R(x)$ and $\psi_L(x)$ do not change under complex conjugation if we simultaneously flip $k \to -k$. In other words $\psi(x;k) = \psi^\star(x;-k)$. This means that the S-matrix obeys

$$\mathcal{S}^\star(k) = \mathcal{S}(-k)$$

There are a number of other, more hidden properties of the S-matrix that we will uncover below.

1.1.3 A Parity Basis for Scattering

As we've seen above, for symmetric potentials, with $V(x) = V(-x)$, scattering from the left and right is the same. Let's first make this statement more formal.

We introduce the *parity* operator P which acts on functions $f(x)$ as

$$P : f(x) \to f(-x)$$

For symmetric potentials, we have $[P, H] = 0$ which means that eigenstates of the Hamiltonian can be chosen so that they are also eigenstates of P. The parity operator is Hermitian, $P^\dagger = P$, so its eigenvalues λ are real. But we also have $P^2 f(x) = f(x)$, which means that the eigenvalues must obey $\lambda^2 = 1$. Clearly there are only two possibilities: $\lambda = +1$ and $\lambda = -1$, This means that eigenstates of the Hamiltonian can be chosen to be either even functions ($\lambda = +1$) or odd functions ($\lambda = -1$).

Above we worked with scattering eigenstates ψ_R and ψ_L. These are neither odd nor even. Instead, for a symmetric potential, they are related by $\psi_L(x) = \psi_R(-x)$. This is the reason that symmetric potentials have $r = r'$. If we want to work with the parity eigenstates, we take

$$\begin{aligned}\psi_+(x) &= \psi_R(x) + \psi_L(x) = \psi_R(x) + \psi_R(-x)\\ \psi_-(x) &= -\psi_R(x) + \psi_L(x) = -\psi_R(x) + \psi_R(-x)\end{aligned}$$

which obey $P\psi_\pm(x) = \pm\psi_\pm(x)$.

Often, working with parity eigenstates makes the algebra a little easier. This is particularly true if our problem has a parity-invariant potential, $V(x) = V(-x)$.

The Pothole Example Revisited

Let's see how the use of parity eigenstates can make our calculations simpler. We'll redo the scattering calculation in the pothole, but now we'll take the asymptotic states to be ψ_+ and ψ_-. Physically, you can think of this experiment as throwing in particles from both the left and right at the same time, with appropriate choices of signs.

We start with the even parity wavefunction ψ_+. We want to patch this onto a solution in the middle, but this too must have even parity. This mean that the solution in the pothole takes the form

$$\psi_+(x) = A(e^{iqx} + e^{-iqx}) \qquad x \in [-a/2, a/2]$$

which now has only one unknown coefficient, A. As previously, $q^2 = k^2 + 2mV_0/\hbar^2$. We still need to make sure that both the wavefunction and its derivative are continuous at $x = \pm a/2$. But, because we're working with even functions, we only need to look at one of these points. At $x = a/2$ we get

$$\begin{aligned}e^{-ika/2} + (r+t)e^{ika/2} &= A(e^{iqa/2} + e^{-iqa/2})\\ \left(-e^{-ika/2} + (r+t)e^{ika/2}\right) &= \frac{q}{k}A(e^{iqa/2} - e^{-iqa/2})\end{aligned}$$

Notice that only the combination $(r + t)$ appears. We have two equations with two unknowns. If we divide the two equations and rearrange, we get

$$r + t = -e^{-ika}\ \frac{q\tan(qa/2) - ik}{q\tan(qa/2) + ik} \tag{1.11}$$

which is all a lot easier than the messy manipulations we had to do when working with ψ_L and ψ_R. Of course, we've only got an expression for $(r + t)$. But we can play the same game for the odd parity eigenstates to get a corresponding expression for $(r-t)$. Now, the solution in the pothole takes the form

$$\psi_-(x) = B(e^{iqx} - e^{-iqx}) \qquad x \in [-a/2, a/2]$$

Requiring continuity of the wavefunction and its derivative at $x = a/2$ we get

$$\begin{aligned} e^{-ika/2} + (r-t)e^{ika/2} &= B(e^{iqa/2} - e^{-iqa/2}) \\ \left(-e^{-ika/2} + (r-t)e^{ika/2}\right) &= \frac{q}{k}B(e^{iqa/2} + e^{-iqa/2}) \end{aligned}$$

Once again, dividing we find

$$r - t = e^{-ika}\frac{q + ik\tan(qa/2)}{q - ik\tan(qa/2)} \tag{1.12}$$

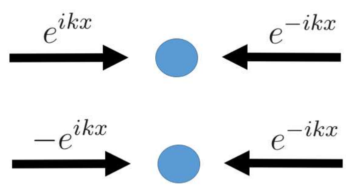
It's not immediately obvious that the expressions (1.11) and (1.12) are the same as those for r and t that we derived previously. But a little bit of algebra should convince you that they agree.

[A helping hand: this little bit of algebra is extremely fiddly if you don't go about it in the right way! Here's a reasonably a streamlined approach. First define the denominator of (1.8) as $D(k) = (q^2+k^2)\sin(qa) + 2iqk\cos(qa)$. Using the double-angle formula from trigonometry, we can write this as $D(k) = 2\cos^2(qa/2)(q\tan(qa/2) + ik)(q - ik\tan(qa/2))$. We can then add the two expressions in (1.8), and use the double-angle formula again, to get $r + t = 2e^{-ika}\cos^2(qa/2)(q\tan(qa/2) - ik)(ik\tan(qa/2) - q)/D(k)$ This coincides with our formula (1.11). Similar games give us the formula (1.12).]

The S-Matrix in the Parity Basis

We can also think about the S-matrix using our new basis of states. The asymptotic ingoing modes are even and odd functions, given at $|x| \to \infty$ by

$$\text{Ingoing} \begin{cases} \text{parity-even:} \qquad \mathcal{I}_+(x) = e^{-ik|x|} \\ \text{parity-odd:} \qquad \mathcal{I}_-(x) = \text{sign}(x)\, e^{-ik|x|} \end{cases}$$



The two asymptotic outgoing modes are

Outgoing $\begin{cases} \text{parity-even:} \qquad \mathcal{O}_+(x) = e^{+ik|x|} \\ \text{parity-odd:} \qquad \mathcal{O}_-(x) = -\text{sign}(x)\, e^{+ik|x|} \end{cases}$

These are related to our earlier modes by a simple change of basis,

$$\begin{pmatrix} \mathcal{I}_+ \\ \mathcal{I}_- \end{pmatrix} = \mathcal{M} \begin{pmatrix} \mathcal{I}_R \\ \mathcal{I}_L \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathcal{O}_+ \\ \mathcal{O}_- \end{pmatrix} = \mathcal{M} \begin{pmatrix} \mathcal{O}_R \\ \mathcal{O}_L \end{pmatrix} \quad \text{with} \quad \mathcal{M} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

We can define an S-matrix with respect to this parity basis. In analogy with (1.9), we write asymptotic solutions as

$$\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \begin{pmatrix} \mathcal{I}_+ \\ \mathcal{I}_- \end{pmatrix} + \mathcal{S}^P \begin{pmatrix} \mathcal{O}_+ \\ \mathcal{O}_- \end{pmatrix} \tag{1.13}$$

where we use the notation $\mathcal{S}^P$ to denote the S-matrix with respect to the parity basis. We write

$$\mathcal{S}^P = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix}$$

This is related to our earlier S-matrix by a change of basis. We have

$$\mathcal{S}^P = \mathcal{M}S\mathcal{M}^{-1} = \begin{pmatrix} t + (r+r')/2 & (r-r')/2 \\ (r'-r)/2 & t-(r+r')/2 \end{pmatrix}$$

As you may expect, this basis is particularly useful if the underlying potential is symmetric, so $V(x) = V(-x)$. In this case we have $r = r'$ and the S-matrix becomes diagonal. The diagonal components are simply

$$S_{++} = t + r \quad \text{and} \quad S_{--} = t - r$$

In fact, because $\mathcal{S}^p$ is unitary, each of these components must be a phase. This follows because r and t are not independent. First, they obey $|r|^2 + |t|^2 = 1$. Moreover, when $r' = r$, the relation (1.6) becomes

$$rt^\star + r^\star t = 0 \qquad \Rightarrow \qquad \text{Re}(rt\star) = 0$$

This is enough to ensure that both S_{++} and S_{--} are indeed phases. We write them as

$$S_{++} = e^{2i\delta_+(k)} \quad \text{and} \quad S_{--} = e^{2i\delta_-(k)}$$

We learn that for scattering off a symmetric potential, all the information is encoded in two momentum-dependent *phase shifts*, $\delta_\pm(k)$ which tell us how the phases of the outgoing waves $\mathcal{O}_\pm$ are changed with respect to the ingoing waves $\mathcal{I}_\pm$.

1.1.4 Bound States

So far we've focussed only on the scattering states of the problem. We now look at the bound states, which have energy $E < 0$ and are localised near inside the potential. Here, something rather magical happens. It turns out that the information about these bound states can be extracted from the S-matrix, which we constructed purely from knowledge of the scattering states.

To find the bound states, we need to do something clever. We take our scattering solutions, which depend on momentum $k \in \mathbf{R}$, and extend them to the complex momentum plane. This means that we analytically continue out solutions so that they depend on $k \in \mathbf{C}$.

First note that the solutions with $k \in \mathbf{C}$ still obey our original Schrödinger equation (1.1) since, at no point in any of our derivation did we assume that $k \in \mathbf{R}$. The only difficulty comes when we look at how the wavefunctions behave asymptotically. In particular, any putative solution will, in general, diverge exponentially as $x \to +\infty$ or $x \to -\infty$, rendering the wavefunction non-normalisable. However, as we will now show, there are certain solutions that survive.

For simplicity, let's assume that we have a symmetric potential $V(x) = V(-x)$. As we've seen above, this means that there's no mixing between the parity-even and parity-odd wavefunctions. We start by looking at the parity-even states. The general solution takes the form

$$\psi_+(x) = \mathcal{I}_+(x) + S_{++}\mathcal{O}_+(x) = \begin{cases} e^{+ikx} \ + \ S_{++}e^{-ikx} & x \to -\infty \\ e^{-ikx} \ + \ S_{++}e^{+ikx} & x \to +\infty \end{cases}$$

Suppose that we make k pure imaginary and write

$$k = i\lambda$$

with $\lambda > 0$. Then we get

$$\psi_+(x) = \begin{cases} e^{-\lambda x} \ + \ S_{++}e^{+\lambda x} & x \to -\infty \\ e^{+\lambda x} \ + \ S_{++}e^{-\lambda x} & x \to +\infty \end{cases} \tag{1.14}$$

Both terms proportional to S_{++} decay asymptotically, but the other terms diverge. This is bad. However, there's a get-out. For any fixed k (whether real or complex), S_{++} is simply a number. That means that we're quite at liberty to divide by it. Indeed, the wavefunction above isn't normalised anyway, so dividing by a constant isn't going to change anything. We get

$$\psi_+(x) = \begin{cases} S_{++}^{-1}\, e^{-\lambda x} \ + \ e^{+\lambda x} & x \to -\infty \\ S_{++}^{-1}\, e^{+\lambda x} \ + \ e^{-\lambda x} & x \to +\infty \end{cases} \tag{1.15}$$

Now we can see the loop-hole. The wavefunction above is normalisable whenever we can find a $\lambda > 0$ such that

$$S_{++}(k) \to \infty \quad \text{ as } k \to i\lambda$$

This, then, is the magic of the S-matrix. Poles in the complex momentum plane that lie on the positive imaginary axis (i.e. $k = i\lambda$ with $\lambda > 0$) correspond to bound states. This information also tells us the energy of the bound state since, as we saw in (1.2), it is given by

$$E = -\frac{\hbar^2\lambda^2}{2m}$$

We could also have set $k = -i\lambda$, with $\lambda > 0$. In this case, it is the terms proportional to S_{++} in (1.14) which diverge and the wavefunction is normalisable only if $S_{++}(k = -i\lambda) = 0$. However, since S_{++} is a phase, this is guaranteed to be true whenever $S_{++}(k = i\lambda)$ has a pole, and simply gives us back the solution above.

Finally, note that exactly the same arguments hold for parity-odd wavefunctions. There is a bound state whenever $S_{--}(k)$ has a pole at $k = i\lambda$ with $\lambda > 0$.

An Example: Stuck in the Pothole

We can illustrate this with our favourite example of the square well, of depth $-V_0$ and width a. We already computed the S-matrix in (1.11) and (1.12). We have,

$$S_{++}(k) = r + t = -e^{-ika}\,\frac{q\tan(qa/2) - ik}{q\tan(qa/2) + ik}$$

where $q^2 = 2mV_0/\hbar^2 + k^2$. Setting $k = i\lambda$, we see that this has a pole when

$$\lambda = q\tan\left(\frac{qa}{2}\right) \quad \text{ with } \quad \lambda^2 + q^2 = \frac{2mV_0}{\hbar^2}$$

These are the usual equations that you have to solve when finding parity-even bound states in a square well. The form of the solutions is simplest to see if we plot these equations, as shown in the left-hand of Figure 4. There is always at least one bound state, with more appearing as the well gets deeper.

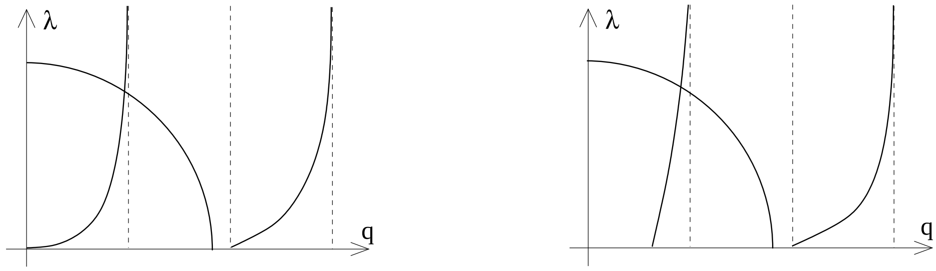


Figure 4: Bound state of even parity always exist, since the two equations shown on the left always have a solution with $\lambda, q > 0$. Bound states of odd parity, shown on the right, exist if the potential is deep enough.

Similarly, if we look at the parity-odd wavefunctions, we have

$$S_{--}(k) = t - r = e^{-ika}\frac{q + ik\tan(qa/2)}{q - ik\tan(qa/2)}$$

which has a pole at $k = i\lambda$ when

$$q = -\lambda\tan\left(\frac{qa}{2}\right) \qquad \text{with} \quad \lambda^2 + q^2 = \frac{2mV_0}{\hbar^2} \tag{1.16}$$

This too reproduces the equations that we found in earlier courses in quantum mechanics when searching for bound states in a square well. Now there is no guarantee that a bound state exists; this only happens if the potential is deep enough.

1.1.5 Resonances

We might wonder if there's any other information hidden in the analytic structure of the S-matrix. In this section, we will see that there is, although its interpretation is a little more subtle.

First, the physics. Let's think back again to the example shown on the right. One the one hand, we know that there can be no bound states in such a trap because they will have $E > 0$. Any particle that we place in the trap will ultimately tunnel out. On the other hand, if the walls of the trap are very large then we might expect that the particle stays there for a long time before it eventually escapes. In this situation, we talk of a *resonance*. These are also referred to as *unstable* or *metastable* states. Our goal is to show how such resonances are encoded in the S-matrix.

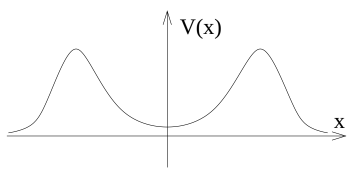


Figure 5:

Now, the maths. We'll restrict attention to parity-even functions. Suppose that the S-matrix S_{++} has a pole that lies on the complex momentum plane at position

$$k = k_0 - i\gamma$$

On general grounds, the wavefunction will have a second pole at $-k^\star = -k_0 - i\gamma$. We'd like to interpret these poles. First note that the energy is also imaginary

$$E = \frac{\hbar^2 k^2}{2m} \equiv E_0 - i\frac{\Gamma}{2} \tag{1.17}$$

with $E_0 = \hbar^2(k_0^2 - \gamma^2)/2m$ and $\Gamma = 2\hbar^2\gamma k_0/m$. An imaginary energy may sound strange, but it is has a very natural interpretation. Recall that the time dependence of the wavefunction is given by

$$e^{-iEt/\hbar} = e^{-iE_0 t/\hbar}\, e^{-\Gamma t/2\hbar} \tag{1.18}$$

This is the first clue that we need. We see that, for $\gamma > 0$, the overall form of the wavefunction decays exponentially with time. This is the characteristic behaviour of unstable states. A wavefunction that is initially supported inside the trap will be very small there at time much larger than $\tau = 1/\Gamma$. Here τ is called the *half-life* of the state, while Γ is usually referred to as the *width* of the state. (We'll see why in Section 1.2).

Where does the particle go? Including the time dependence (1.18), the same argument that led us to (1.15) now tells us that when $S_{++} \to \infty$, the solution takes the asymptotic form

$$\psi_+(x,t) = \begin{cases} e^{-iE_0 t/\hbar}\, e^{-ik_0 x}\, e^{-\gamma x - \Gamma t/2\hbar} & x \to -\infty \\ e^{-iE_0 t/\hbar}\, e^{+ik_0 x}\, e^{+\gamma x - \Gamma t/2\hbar} & x \to +\infty \end{cases} \tag{1.19}$$

The first two exponential factors oscillate. But the final factor varies as

$$e^{\pm\gamma(x \mp vt)} \quad \text{where} \quad v = \frac{\Gamma}{2\hbar\gamma} = \frac{\hbar k_0}{m}$$

This has the interpretation of a particle moving with momentum $\hbar k_0$. This, of course, is the particle which has escaped the trap.

Note that for fixed time t, these wavefunctions are not normalisable: they diverge at both $x \to \pm\infty$. This shouldn't concern us, because, although our wavefunctions are eigenstates of the Hamiltonian, they are not interpreted as stationary states. Indeed, it had to be the case. An unstable state has complex energy, but standard theorems in linear algebra tell us that a Hermitian operator like the Hamiltonian must have real eigenvalues. We have managed to evade this theorem only because these wavefunctions are non-normalisable and so do not, strictly speaking, live in the Hilbert space.

There's a lesson buried in all of this. If we were to take the standard axioms of quantum mechanics, we would simply throw away wavefunctions of the form (1.19) on the grounds that they do not lie in the Hilbert space and so are unphysical. But this would be a mistake: the wavefunctions do contain interesting physics, albeit of a slightly different variety than we are used to. Sometimes it's worth pushing our physical theories beyond our comfort zone to see what is lurking there.

The upshot of this discussion is that poles of the S-matrix in the lower-half complex plane correspond to resonances. It is often useful to write S_{++} as a function of energy rather than momentum. (They are related by (1.17)). Since S_{++} is a phase, close to a resonance it necessarily takes the form

$$S_{++} = \frac{E - E_0 - i\Gamma/2}{E - E_0 + i\Gamma/2}$$

An Example: A Pair of Delta-Functions

A pair of delta functions provide a simple and tractable example to illustrate the idea of resonances. The potential is given by

$$V(x) = V_0\Big[\delta(x-1) + \delta(x+1)\Big]$$

Recall that the effect of the delta-functions is simply to change the boundary conditions at $x = \pm 1$ when solving the Schrödinger equation. All wavefunctions should be continuous at $x = \pm 1$, but their derivatives are discontinuous. For example, at $x = +1$, solutions obey

$$\lim_{\epsilon \to 0}\Big[\psi'(1+\epsilon) - \psi'(1-\epsilon)\Big] = U_0\psi(1) \quad \text{with} \quad U_0 = \frac{2mV_0}{\hbar^2}$$

Working in the parity basis makes life simpler, not least because you only need to consider the matching at one of the delta-functions, with the other then guaranteed. The computation of the S-matrix is a problem on the exercise sheet. You will find

$$S_{++} = e^{-2ik}\left[\frac{(2k - iU_0)e^{ik} - iU_0 e^{-ik}}{(2k + iU_0)e^{-ik} + iU_0 e^{ik}}\right]$$

Note that the denominator is the complex conjugate of the numerator, ensuring that S_{++} is a phase, as expected. The poles of this S-matrix are given by solutions to the equation

$$e^{2ik} = -\left(1 - \frac{2ik}{U_0}\right) \tag{1.20}$$

To understand the physics behind this, let's first look at the situation where $U_0 \to \infty$, so that the weight of the delta-functions gets infinitely large. Then the poles sit at

$$e^{2ik} = -1 \quad \Rightarrow \quad k = k_n = \left(n + \frac{1}{2}\right)\pi$$

These correspond to bound states trapped between the two wavefunctions. For example, the $n = 0$ state is shown in the figure. Note that they're rather unusual because the poles sit on the real k-axis, rather than the imaginary k-axis. Correspondingly, these bound states have $E > 0$. This strange behaviour is only allowed because we have an infinitely large potential which forbids particles on one side of the barrier to cross to the other.

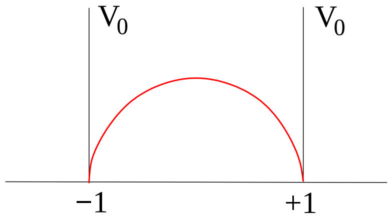


Figure 6:

As a side remark, we note that this same impenetrable behaviour is seen in scattering. When $U_0 \to \infty$, the S-matrix becomes $S_{++} \to -e^{2ik}$. This tells us that a particle coming from outside is completely reflected off the infinitely large barrier. The minus sign is the standard phase change after reflection. The factor of e^{2ik} is because the waves are forbidden from travelling through the region between the delta functions, which has width $x = 2$. As a result, the phase is shifted by e^{ikx} from what it would be if the barriers were removed.

Let's now look at what happens when U_0 is large, but finite? We'll focus on the lowest energy bound state with $n = 0$. We can expand (1.20) in $1/U_0$. (This too is left as a problem on the exercise sheet.) We find

$$k = \frac{\pi}{2} + \alpha - i\gamma$$

with

$$\alpha \approx -\frac{\pi}{2U_0} + \frac{\pi}{2U_0^2} + \mathcal{O}\left(\frac{1}{U_0^3}\right) \quad \text{and} \quad \gamma \approx \frac{\pi^2}{4U_0^2} + \mathcal{O}\left(\frac{1}{U_0^3}\right)$$

Note, in particular, that $\gamma > 0$, so the pole moves off the real axis and into the lower half-plane. This pole now has all the properties that we described at the beginning of this section. It describes a state, trapped between the two delta-functions, which decays with half-life

$$\tau = \frac{\hbar}{\Gamma} = \frac{4mU_0^2}{\hbar\pi^3}\left(1 + \mathcal{O}\left(\frac{1}{U_0}\right)\right)$$

This is the resonance.

1.2 Scattering in Three Dimensions

Our real interest in scattering is for particles moving in three spatial dimensions, with Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r})$$

Recall that there are two distinct interpretations for such a Hamiltonian

- We could think of this as the motion of a single particle, moving in a fixed background potential $V(\mathbf{r})$. This would be appropriate, for example, in Rutherford's famous experiment where we fire an alpha particle at a gold nucleus.

- Alternatively, We could think of this as the relative motion of two particles, separated by distance $\mathbf{r}$, interacting through the force $\mathbf{F} = -\nabla V(\mathbf{r})$. We could take $V(r)$ to be the Coulomb force, to describe the scattering of electrons, or the Yukawa force to describe the scattering of neutrons.

In this section, we will use language appropriate to the first interpretation, but everything we say holds equally well in the second. Throughout this section, we will work with rotationally invariant (i.e. central) potentials, so that $V(\mathbf{r}) = V(|\mathbf{r}|)$.

1.2.1 The Cross-Section

Our first goal is to decide what we want to calculate. The simple reflection and transmission coefficients of the one-dimensional problem are no longer appropriate. We need to replace them by something a little more complicated. We start by thinking of the classical situation.

Classical Scattering

Suppose that we throw in a single particle with kinetic energy E. Its initial trajectory is characterised by the *impact parameter* b, defined as the closest the particle would get to the scattering centre at $r = 0$ if there were no potential. The particle emerges with *scattering angle* θ, which is the angle between the asymptotic incoming and outgoing trajectories, as shown in the figure. By solving the classical equations of motion, we can compute $\theta(b; E)$ or, equivalently, $b(\theta; E)$.

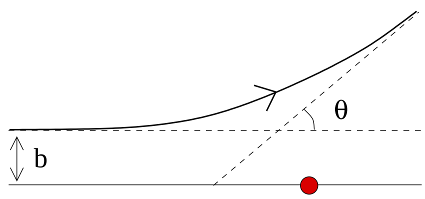


Figure 7:

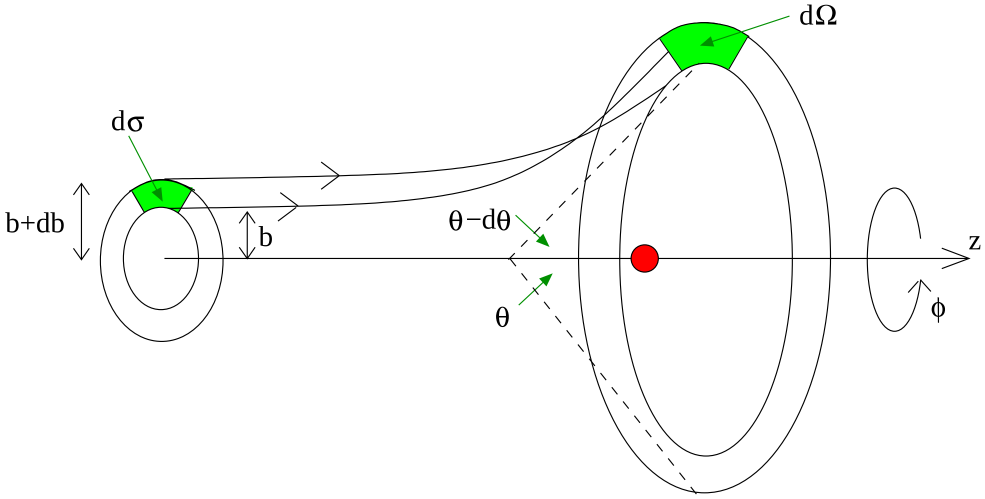


Figure 8: What becomes of an infinitesimal cross-sectional area after scattering.

Now consider a uniform beam of particles, each with kinetic energy E. We want to understand what becomes of this beam. Consider the cross-sectional area, denoted $d\sigma$ in Figure 8. We write this as

$$d\sigma = b\, d\phi\, db$$

The particles within $d\sigma$ will evolve to the lie in a cone of solid angle $d\Omega$, given by

$$d\Omega = \sin\theta\, d\phi\, d\theta$$

where, for central potentials, the infinitesimal angles $d\phi$ are the same in both these formulae. The *differential cross-section* is defined to be

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

The left-hand side should really be $|d\sigma/d\Omega|$, but we'll usually drop the modulus. The differential cross-section is a function of incoming momentum k, together with the outgoing angle θ.

More colloquially, the differential cross-section can be thought of as

$$\frac{d\sigma}{d\Omega}\, d\Omega = \frac{\text{Number of particles scattered into } d\Omega \text{ per unit time}}{\text{Number of incident particles per area } d\sigma \text{ per unit time}}$$

We write this in terms of *flux*, defined to be the number of particles per unit area per unit time. In this language, the differential cross-section is

$$\frac{d\sigma}{d\Omega} = \frac{\text{Scattered flux}}{\text{Incident flux}}$$

5. Phonons

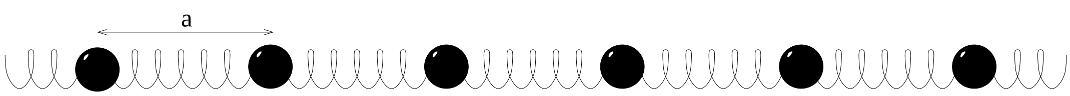
Until now, we've discussed lattices in which the atoms are fixed in place. This is, of course, somewhat unrealistic. In materials, atoms can jiggle, oscillating back and forth about their equilibrium position. The result of their collective effort is what we call sound waves or, at the quantum level,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

5.1 Lattices in One Dimension

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

5.1.1 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 $n = 1, \ldots, N$. 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^{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

$$H = \sum_n \frac{p_n^2}{2m} + \frac{\lambda}{2} \sum_n (u_n - u_{n-1})^2 \tag{5.1}$$

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

$$m\ddot{u}_n = -\lambda(2u_n - u_{n-1} - u_{n+1}) \tag{5.2}$$

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 (5.2) as

$$u_n = A\, e^{-i\omega t - ikna} \tag{5.3}$$

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 $k \to k + 2\pi/a$. 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

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

where, to make life somewhat easier, we will assume that N is even. 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 ω in terms of k. Substituting the ansatz into the formula (5.2), we have

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

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 73, with k ranging over the first Brillouin zone.

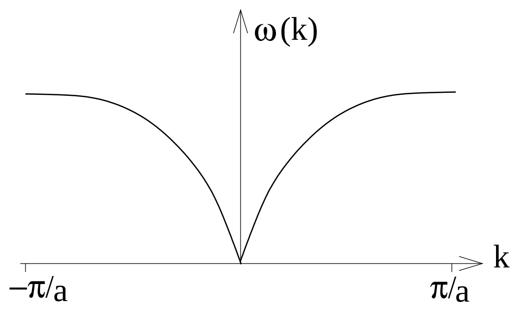


Figure 73: Phonon dispersion relation for a monatomic chain.

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

$$\omega \approx \sqrt{\frac{\lambda}{m}}\,ak$$

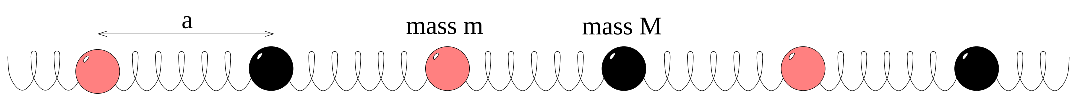
This is in contrast to the electron propagation where we get the dispersion relation for a non-relativistic, massive particle (3.6). Instead, the dispersion relation for phonons is more reminiscent of the massless, relativistic dispersion relation for light. For phonons, the ripples travel with speed

$$c_s = \sqrt{\frac{\lambda}{m}}a \tag{5.4}$$

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

5.1.2 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

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

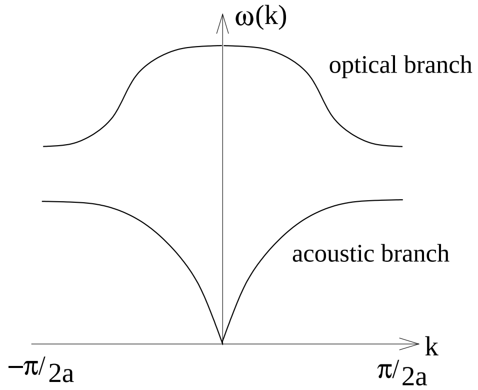


Figure 74: Phonon dispersion relation for a diatomic chain.

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 $k \to k + \pi/a$. 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

$$k \in \left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right) \tag{5.5}$$

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

$$\omega^2 \begin{pmatrix} m & 0 \\ 0 & M \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \lambda \begin{pmatrix} 2 & -(1+e^{-2ika}) \\ -(1+e^{2ika}) & 2 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \tag{5.6}$$

This is viewed as an eigenvalue equation. The frequency ω 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 74 in the first Brillouin zone (5.5). 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 ω_- part of the dispersion relation is called the *acoustic branch*. The upper ω_+ part is called the *optical branch*. To understand where these names come from, we need to look a little more closely at the the physical origin of these two branches. This comes from studying the eigenvectors of (5.6) which tells us the relative amplitudes of the two types of atoms.

This is simplest to do in the limit $k \to 0$. 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[10] and clearly exhibits these features.

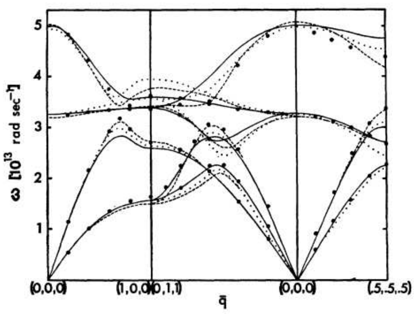


Figure 75:

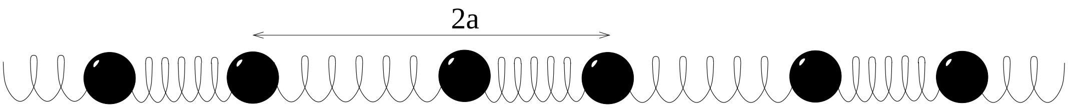
5.1.3 Peierls Transition

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.

[10]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 5.1.1 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 3.1. 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 δx, we expect that the total energy cost is of order

$$U_{\text{lattice}} \sim N\lambda(\delta x)^2 \tag{5.7}$$

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 3.1, 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 76. 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_{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

$$U_{\text{electron}} = -2\,\frac{Na}{2\pi} \int_{-\pi/2a}^{\pi/2a} dk\, \Big(E_0(k) - E_-(k)\Big) \tag{5.8}$$

Here the overall minus sign is because the electrons gain 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.

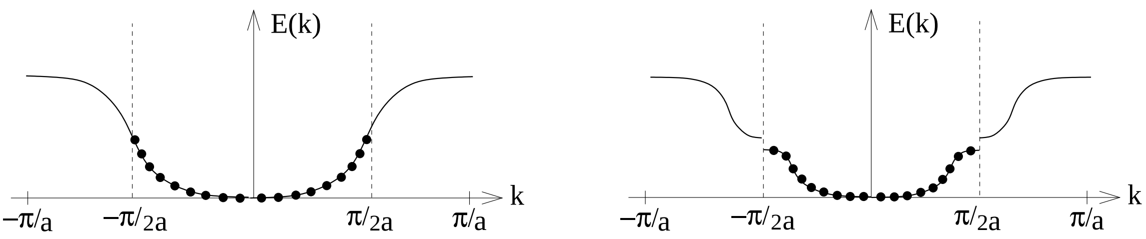


Figure 76: The distortion of the lattice reduces the energy of the Fermi sea of electrons.

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,

$$E_0(k) \approx \mu + \nu q \quad \text{ with } q = k - \frac{\pi}{2a} \tag{5.9}$$

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 3.1. Suppose that the distortion opens up a gap Δ at $k = \pi/2a$. Since there is no gap unless there is a distortion of the lattice, we expect that

$$\Delta \sim \delta x \tag{5.10}$$

(or perhaps δx to some power). To compute $E_-(k)$ in the vicinity of the gap, we can use our earlier result (3.16). Adapted to the present context, the energy E close to $k = \pi/2a$ is given by

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

Using our linearisation (5.9) 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 (5.8) is dominated by the regions $k = \pm\pi/2a$. By symmetry, it is the same in both and given by

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

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 Δ is small. In this limit, we have

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

Both terms contribute to the gain in energy of the electrons. The first term is of order Δ^2 and hence, through (5.10), of order δx^2. This competes with the energy cost from the lattice distortion (5.7), but there is no guarantee that it is either bigger or smaller. The second term with the log is more interesting. For small Δ, this always beats the quadratic cost of the lattice distortion (5.7).

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[11]. The resistivity – plotted on the vertical axis – rises sharply when the temperature drops to the scale Δ. (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.)

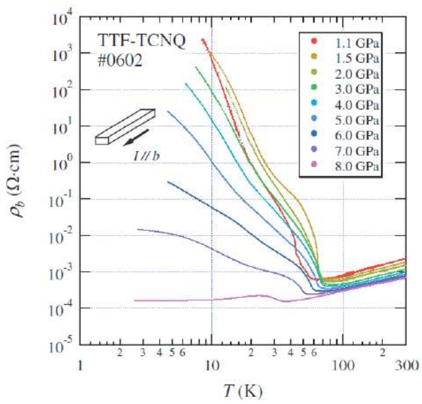


Figure 77:

5.1.4 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.

[11] 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 (5.3) for each $k_l = 2\pi l/Na$ with $l = -N/2, \ldots, N/2$. 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

$$u_n(t) = X_0(t) + \sum_{l\neq 0}\left[\alpha_l\, e^{-i(\omega_l t - k_l na)} + \alpha_l^\dagger\, e^{i(\omega_l t - k_l na)}\right] \tag{5.11}$$

This requires some explanation. First, we sum over all modes $l = -N/2, \ldots, +N/2$ with the exception of $l = 0$. This has been singled out and it 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 α_l. Finally, we have taken the real part of the solution because, ultimately, $u_n(t)$ should be real.

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

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

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 α_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

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

Similarly,

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

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

$$\begin{aligned}\alpha_l &= \frac{1}{2m\omega_l N}\sum_n e^{-ik_l na}\big(m\omega_l u_n + ip_n\big)\\ \alpha_l^\dagger &= \frac{1}{2m\omega_l N}\sum_n e^{ik_l na}\big(m\omega_l u_n - ip_n\big)\end{aligned} \tag{5.12}$$

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

$$X_0 = \frac{1}{N}\sum_n u_n \quad \text{and} \quad P_0 = \frac{1}{N}\sum_n p_n \tag{5.13}$$

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

$$\alpha_l = \sqrt{\frac{\hbar}{2m\omega_l N}}\, a_l \tag{5.14}$$

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 (5.1). Substituting in our expressions (5.12) and (5.13), 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 ω_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, $N \to \infty$, there are excited states with infinitesimally small energies. We say that the system is *gapless*, meaning that there is no gap betwen 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 5.1.2. We introduce two *polarization vectors*, $\mathbf{e}_\pm(k)$. These are eigenvectors obeying the matrix equation (5.6),

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

We then write the general solution as

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

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 $\hbar k$.

5.2 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 (5.2)

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

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

$$\rho\frac{\partial^2 u}{\partial t^2} = -\lambda' \frac{\partial^2 u}{\partial x^2} \tag{5.15}$$

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 (5.4) can be written purely in terms of these macroscopic parameters, $c_s^2 = \lambda'/\rho$.

The equation of motion (5.15) can be derived from the action

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

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

5.2.1 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

$$S = \int dtd^3x \, \frac{1}{2}\left[\rho\left(\frac{\partial u_i}{\partial t}\right)^2 - 2\mu \, u_{ij}u_{ij} - \lambda \, u_{ii}u_{jj}\right] \tag{5.16}$$

The coefficients μ and λ are called Lamé coeffcients; they characterise the underlying solid.

This action gives rise to the equations of motion

$$\rho \frac{\partial^2 u_i}{\partial t^2} = (\mu + \lambda) \frac{\partial^2 u_j}{\partial x^i \partial x^j} + \mu \frac{\partial^2 u_i}{\partial x^j \partial x^j} \tag{5.17}$$

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 ϵ_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

$$\omega^2 = \frac{2\mu + \lambda}{\rho} k^2 \tag{5.18}$$

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

$$\omega^2 = \frac{\mu}{\rho} k^2 \tag{5.19}$$

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 (5.17) is then

$$u_i(\mathbf{x}, t) = \sum_s \int \frac{d^3k}{(2\pi)^3} \, \frac{1}{2\rho\omega_s(k)} \, \epsilon_i^s \left(a_s(\mathbf{k}) \, e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_s t)} + a_s^\dagger(\mathbf{k}) \, e^{-i(\mathbf{k}\cdot\mathbf{x} - \omega_s t)} \right) \tag{5.20}$$

where the s sum is over the three polarisation vectors, two transverse and one longitudinal. The frequencies $\omega_s(k)$ correspond to either (5.18) or (5.19) depending on the choice of s.

5.2.2 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 (5.16). 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 5.1.4. 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 (5.20) 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 (5.20), we have

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

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

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

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 (5.12). We then use this to determine the commutation relations,

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

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 5.1.4. 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 $\boldsymbol{\epsilon}_s$ 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.