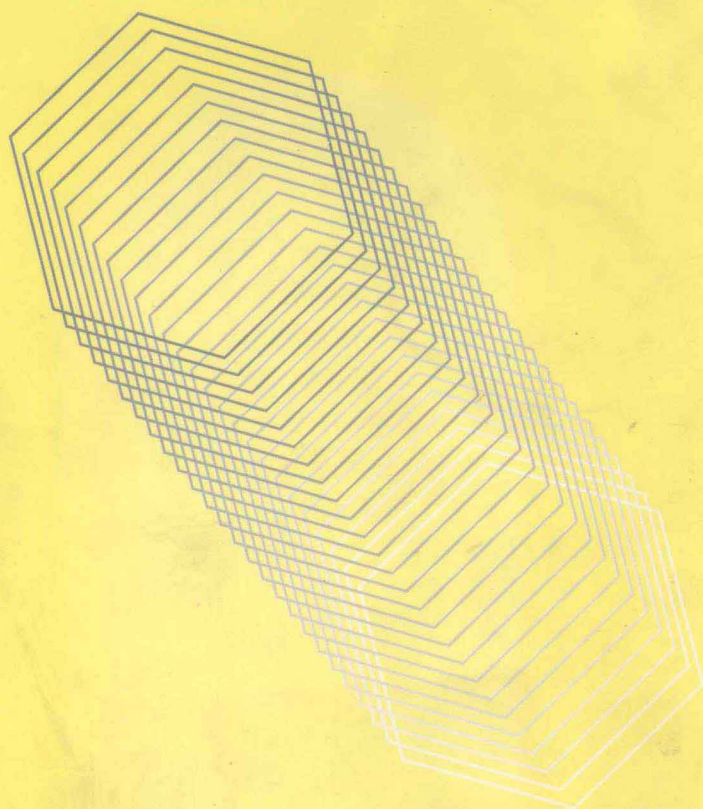


# A Quantum Approach to Condensed Matter Physics

凝聚态物理学的量子方法



Philip L. Taylor & Olle Heinonen

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# A Quantum Approach to Condensed Matter Physics

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## Preface

The aim of this book is to make the quantum theory of condensed matter *accessible*. To this end we have tried to produce a text that does not demand extensive prior knowledge of either condensed matter physics or quantum mechanics. Our hope is that both students and professional scientists will find it a user-friendly guide to some of the beautiful but subtle concepts that form the underpinning of the theory of the condensed state of matter.

The barriers to understanding these concepts are high, and so we do not try to vault them in a single leap. Instead we take a gentler path on which to reach our goal. We first introduce some of the topics from a semiclassical viewpoint before turning to the quantum-mechanical methods. When we encounter a new and unfamiliar problem to solve, we look for analogies with systems already studied. Often we are able to draw from our storehouse of techniques a familiar tool with which to cultivate the new terrain. We deal with BCS superconductivity in Chapter 7, for example, by adapting the canonical transformation that we used in studying liquid helium in Chapter 3. To find the energy of neutral collective excitations in the fractional quantum Hall effect in Chapter 10, we call on the approach used for the electron gas in the random phase approximation in Chapter 2. In studying heavy fermions in Chapter 11, we use the same technique that we found successful in treating the electron-phonon interaction in Chapter 6.

Experienced readers may recognize parts of this book. It is, in fact, an enlarged and updated version of an earlier text, *A Quantum Approach to the Solid State*. We have tried to preserve the tone of the previous book by emphasizing the overall structure of the subject rather than its details. We avoid the use of many of the formal methods of quantum field theory, and substitute a liberal amount of intuition in our effort to reach the goal of physical understanding with minimal mathematical complexity. For this we pay the penalty of losing some of the rigor that more complete analytical

treatments can yield. The methods used to demonstrate results are typically simple and direct. They are expedient substitutes for the more thorough approaches to be found in some of the bulkier and more specialized texts cited in the Bibliography.

Some of the problems at the ends of the chapters are sufficiently challenging that it took the authors a longer time to solve them than it did to create them. Instructors using the text may therefore find it a time-saver to see our versions of the solutions. These are available by sending to [solutions@cambridge.org](mailto:solutions@cambridge.org) an e-mail containing plausible evidence that the correspondent is in fact a busy instructor rather than a corner-cutting student pressed for time on a homework assignment.

The earlier version of this text owed much to Harold Hosack and Philip Nielsen for suggested improvements. The new version profits greatly from the comments of Harsh Mathur, Michael D. Johnson, Sankar Das Sarma, and Allan MacDonald. Any mistakes that remain are, of course, ours alone. We were probably not paying enough attention when our colleagues pointed them out to us.

Philip Taylor    Cleveland, Ohio  
Olle Heinonen    Minneapolis, Minnesota

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# Chapter 1

## Semiclassical introduction

### 1.1 Elementary excitations

The most fundamental question that one might be expected to answer is “why are there solids?” That is, if we were given a large number of atoms of copper, why should they form themselves into the regular array that we know as a crystal of metallic copper? Why should they not form an irregular structure like glass, or a superfluid liquid like helium?

We are ill-equipped to answer these questions in any other than a qualitative way, for they demand the solution of the many-body problem in one of its most difficult forms. We should have to consider the interactions between large numbers of identical copper nuclei – identical, that is, if we were fortunate enough to have an isotopically pure specimen – and even larger numbers of electrons. We should be able to omit neither the spins of the electrons nor the electric quadrupole moments of the nuclei. Provided we treated the problem with the methods of relativistic quantum mechanics, we could hope that the solution we obtained would be a good picture of the physical reality, and that we should then be able to predict all the properties of copper.

But, of course, such a task is impossible. Methods have not yet been developed that can find even the lowest-lying exact energy level of such a complex system. The best that we can do at present is to guess at the form the states will take, and then to try and calculate their energy. Thus, for instance, we might suppose that the copper atoms would either form a face-centered or body-centered cubic crystal. We should then estimate the relative energies of these two arrangements, taking into account all the interactions we could. If we found that the face-centered cubic structure had the lower energy we might be encouraged to go on and calculate the change in energy due to various small displacements of the atoms. But even though we found that all the small displacements that we tried only increased the energy of the

system, that would still be no guarantee that we had found the lowest energy state. Fortunately we have tools, such as X-ray diffraction, with which we can satisfy ourselves that copper does indeed form a face-centered cubic crystal, so that calculations such as this do no more than test our assumptions and our mathematics. Accordingly, the philosophy of the quantum theory of condensed matter is often to accept the crystal structure as one of the given quantities of any problem. We then consider the wavefunctions of electrons in this structure, and the dynamics of the atoms as they undergo small displacements from it.

Unfortunately, we cannot always take this attitude towards the electronic structure of the crystal. Because we have fewer direct ways of investigating the electron wavefunction than we had for locating the nuclei, we must sometimes spend time questioning whether we have developed the most useful picture of the system. Before 1957, for example, people were unsuccessful in accounting for the properties of superconductors because they were starting from a ground state that was qualitatively different from what it is now thought to be. Occasionally, however, a new technique is introduced by means of which the symmetry of electronic states can be probed. An example is shown on the cover of this book. There the effect on the electronic structure of an impurity atom at the surface of a high-temperature superconductor is shown. The clover-leaf symmetry of the superconducting state is clearly seen in the scanning-tunneling-microscope image.

The interest of the experimentalist, however, is generally not directed towards the energy of the ground state of a substance, but more towards its response to the various stimuli that may be applied. One may measure its specific heat, for example, or its absorption of sound or microwaves. Such experiments generally involve raising the crystal from one of its low-lying states to an excited state of higher energy. It is thus the task of the theorist not only to make a reasonable guess at the ground state, but also to estimate the energies of excited states that are connected to the ground state in a simple way. Because the ground state may be of little further interest once its form has been postulated, it is convenient to forget about it altogether and to regard the process of raising the system to a higher state as one of creating something where nothing was before. The simplest such processes are known as the creation of *elementary excitations* of the system.

The usefulness of the concept of elementary excitations arises from a simple property that most many-body systems have in common. Suppose that there are two excited states, and that these have energies above the ground state of  $\mathcal{E}_1$  and  $\mathcal{E}_2$ , respectively. Then it is frequently the case that there will also be one particular excited state whose energy,  $\mathcal{E}_3$ , is not far

removed from  $(\mathcal{E}_1 + \mathcal{E}_2)$ . We should then say that in the state of energy  $\mathcal{E}_3$  all the excitations that were present in the other two states are now present together. The difference  $\Delta\mathcal{E}$  between  $\mathcal{E}_3$  and  $(\mathcal{E}_1 + \mathcal{E}_2)$  would be ascribed to an interaction between them (Fig. 1.1.1). If the states of energy  $\mathcal{E}_1$  and  $\mathcal{E}_2$  could not themselves be considered as collections of other excitations of lower energy then we say that these states represent elementary excitations of the system. As long as the interaction energy remains small we can with reasonable accuracy consider most of the excited states of a solid as collections of elementary excitations. This is clearly a very useful simplification of our original picture in which we just had a spectrum of energy levels which had no particular relationship to one another.

At this point it is useful to consider a division of the possible types of elementary excitations into two classes, known as *quasiparticle excitations* and *collective excitations*. The distinction between these is best illustrated by some simple examples. We know that if we have a gas of noninteracting particles, we can raise the energy of one of these particles without affecting the others at all. Thus if the gas were originally in its ground state we could describe this process as creating an elementary excitation. If we were now to raise the energy of another particle, the energies of the excitations would clearly add up to give the energy of the doubly excited system above its ground state. We should call these *particle excitations*. If now we include some interactions between the particles of the gas, we should expect these particle excitations to decay, since now the excited particle would scatter off the unexcited ones, and its energy and momentum would gradually be lost. However, if the particles obeyed the Pauli Exclusion Principle, and the energy of the excitation was very low, there would be very few empty states into which the particle could be scattered. We should expect the excitation to have a sufficiently long lifetime for the description in terms of particles to

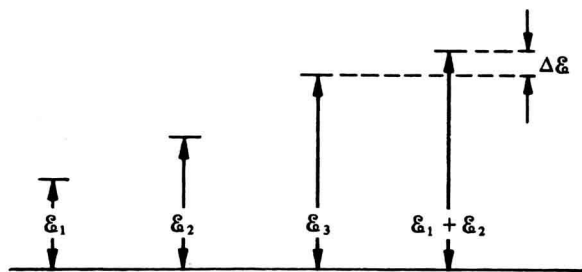


Figure 1.1.1. When two elementary excitations of energies  $\mathcal{E}_1$  and  $\mathcal{E}_2$  are present together the combined excitation has an energy  $\mathcal{E}_3$  that is close to  $\mathcal{E}_1 + \mathcal{E}_2$ .

be a useful one. The energies of such excitations will differ from those for noninteracting particles because of the interactions. It is excitations such as these that we call *quasiparticles*.

A simple example of the other class of excitation is that of a sound wave in a solid. Because the interatomic forces in a solid are so strong, there is little profit in considering the motion of an atom in a crystal in terms of particle motion. Any momentum we might give to one atom is so quickly transmitted to its neighbors that after a very short time it would be difficult to tell which atom we had initially displaced. But we do know that a sound wave in the solid will exist for a much longer time before it is attenuated, and is therefore a much more useful picture of an excitation in the material. Since a sound wave is specified by giving the coordinates not of just one atom but of every atom in the solid, we call this a collective motion. The amplitude of such motion is quantized, a quantum unit of traveling sound wave being known as a *phonon*. A phonon is thus an example of a collective excitation in a solid.

We shall now consider semiclassically a few of the more important excitations that may occur in a solid. We shall postpone the more satisfying quantum-mechanical derivations until a later chapter. By that time the familiarity with the concepts that a semiclassical treatment gives may reduce somewhat the opacity of the quantum-mechanical procedures.

## 1.2 Phonons

The simplest example of collective motion that we can consider is that of a linear chain of equal masses connected by springs, as illustrated in Fig. 1.2.1. The vibrational modes of this system provide some insight into the atomic motion of a crystal lattice.

If the masses  $M$  are connected by springs of force constant  $K$ , and we call the displacement of the  $n$ th mass from its equilibrium position  $y_n$ , the equations

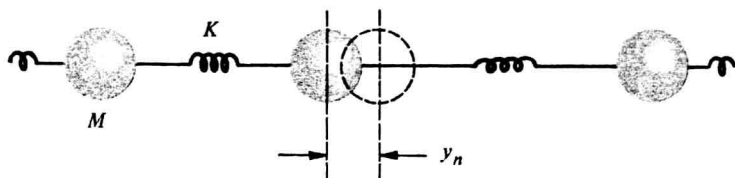


Figure 1.2.1. This chain of equal masses and springs supports collective motion in the form of traveling waves.

of motion of the system are

$$\begin{aligned} M \frac{d^2 y_n}{dt^2} &= K[(y_{n+1} - y_n) - (y_n - y_{n-1})] \\ &= K(y_{n+1} - 2y_n + y_{n-1}). \end{aligned} \quad (1.2.1)$$

These equations are easily solved for any boundary conditions if we remember the recursion formula for cylindrical Bessel functions,

$$\frac{dJ_n}{dt} = -\frac{1}{2} [J_{n+1}(t) - J_{n-1}(t)],$$

from which

$$\frac{d^2 J_n}{dt^2} = \frac{1}{4} [J_{n+2}(t) - 2J_n(t) + J_{n-2}(t)].$$

The problem we considered in Section 1.1 was to find the motion of the masses if we displaced just one of them ( $n = 0$ , say) and then released it. The appropriate solution is then

$$y_n(t) = J_{2n}(\omega_m t)$$

where  $\omega_m^2 = 4K/M$ . This sort of behavior is illustrated in Fig. 1.2.2. The displacement of the zeroth mass, being given by  $J_0(\omega_m t)$ , is seen to exhibit oscillations which decay rapidly. After just a few oscillations  $y_0(t)$  behaves as  $t^{-1/2} \cos(\omega_m t)$ . This shows that particle-like behavior, in which velocities are constant, has no relation to the motion of a component of such a system.

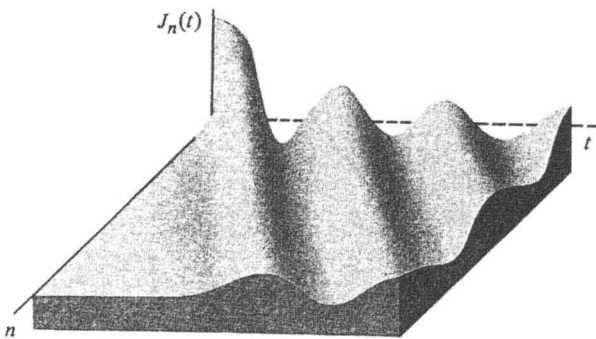


Figure 1.2.2. These Bessel functions are solutions of the equations of motion of the chain of masses and springs.

And this is quite apart from the fact that in a crystal whose atoms are vibrating we are not fortunate enough to know the boundary conditions of the problem. This direct approach is thus not very useful.

We find it more convenient to look for the normal modes of vibration of the system. We make the assumption that we can write

$$y_n \propto e^{i(\omega t + k n a)}, \quad (1.2.2)$$

where  $\omega$  is some function of the wavenumber  $k$ , and  $a$  is the spacing between masses. This satisfies the equations of motion if

$$-\omega^2 M = K(e^{ika} + e^{-ika} - 2),$$

that is, if

$$\omega = \pm \omega_m \sin\left(\frac{1}{2}ka\right).$$

The solution (1.2.2) represents traveling waves of frequency  $\omega$  and wave-number (defined for our purposes by  $2\pi/\lambda$ , where  $\lambda$  is the wavelength) equal to  $k$ . The group velocity  $v$  is given by  $d\omega/dk$ , the gradient of the curve shown in Fig. 1.2.3. We note that as  $\omega$  approaches its maximum value,  $\omega_m$ , the group velocity falls to zero. This explains why the Bessel function solution decayed to an oscillation of frequency  $\omega_m$  after a short time, if we realize that the original equation for  $y_n(t)$  can be considered as a superposition of waves of all wavenumbers. The waves of low frequency, having a large group velocity, travel quickly away from the zeroth site, leaving only the highest-frequency oscillations, whose group velocity is zero.

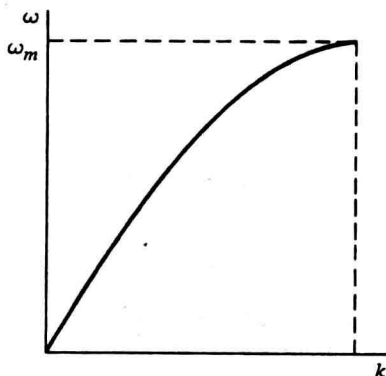


Figure 1.2.3. The dispersion curve for the chain of masses and springs.



It is formally straightforward enough to find the normal modes of vibration for systems more complicated than our linear chain of masses. The extension to three dimensions leads us to consider the *polarization* of the lattice waves, that is, the angle between  $\mathbf{k}$ , which is now a vector, and the direction of displacement of the atoms. We can also introduce forces between atoms other than nearest neighbors. This makes the algebra of finding  $\omega(\mathbf{k})$  more involved, but there are no difficulties of principle. Introduction of two or more different kinds of atom having different masses splits the graph of  $\omega(\mathbf{k})$  into two or more branches, but as long as the restoring forces are all proportional to the displacement, then solutions like Eq. (1.2.2) can be found.

A *phonon* is the quantum-mechanical analog of the lattice wave described by Eq. (1.2.2). A single phonon of angular frequency  $\omega$  carries energy  $\hbar\omega$ . A classical lattice wave of large amplitude corresponds to the quantum situation in which there are many phonons present in one mode. We shall see later that a collection of phonons bears some similarity to a gas of particles. When two particles collide we know that the total momentum is conserved in the collision. If we allow two phonons to interact we shall find that the total wavenumber is conserved in a certain sense. For this reason phonons are sometimes called quasiparticles, although we shall avoid this terminology here, keeping the distinction between collective and particle-like behavior.

### 1.3 Solitons

The chain of masses connected by Hookean springs that we considered in the previous section was a particularly easy problem to solve because the equations of motion (1.2.1) were linear in the displacements  $y_n$ . A real solid, on the other hand, consists of atoms or ions having hard, mutually repulsive cores. The equations of motion will now contain nonlinear (i.e., anharmonic) terms. How do these affect the type of excitation we may find?

If the amplitudes of the phonons are small then the effects of the anharmonic terms will be weak, and the problem can be treated as a system of interacting phonons. If the atomic displacements are large, on the other hand, then there arises a whole new family of elementary excitations known as solitary waves or *solitons*. In these excitations a localized wave of compression can travel through a solid, displacing the atoms momentarily but then leaving them as stationary as they were before the wave arrived.

The term soliton suggests by its word ending that it is a purely quantum-mechanical concept, but this is not the case. Solitary waves in classical systems had been observed as long ago as 1834, but it was only when their