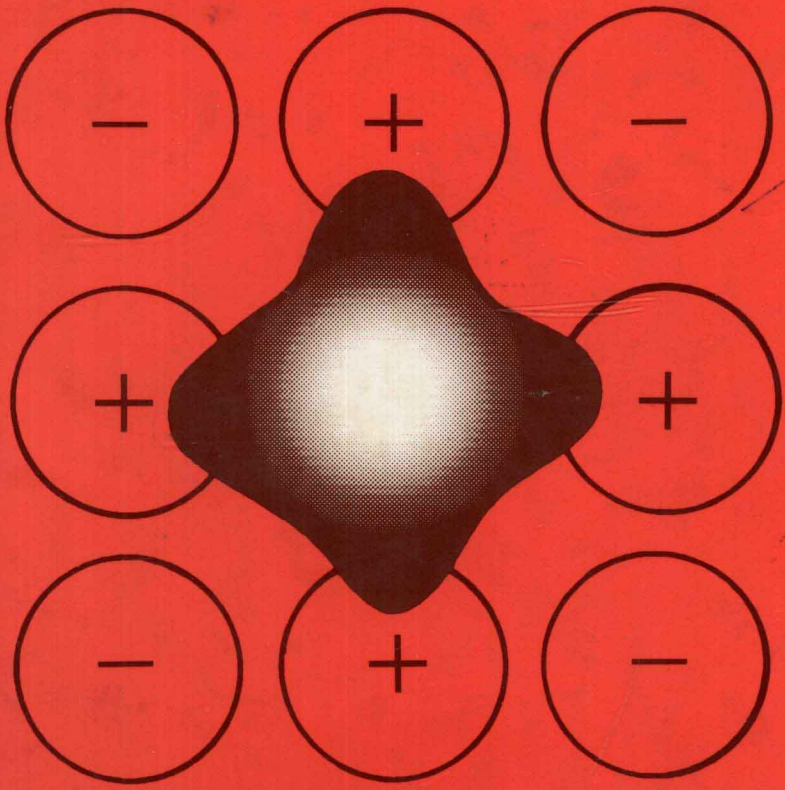
Brian K. Tanner

Introduction to the Physics of Electrons in Solids



INTRODUCTION TO THE PHYSICS OF ELECTRONS IN SOLIDS

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This book aims to introduce the reader to the behaviour of electrons in solids, starting with the simplest possible model, and introducing higher-level models only when the simple model is inadequate.

Unlike other solid state physics texts, this book does not begin with complex crystallography, but instead builds up from the simplest possible model of a free electron in a box. The approach is to introduce the subject through its historical development, and to show how quantum mechanics is necessary for an understanding of the properties of electrons in solids. It does not treat the dynamics of the crystal lattice, but proceeds to examine the consequences of collective behaviour in the phenomena of magnetism and superconductivity. Throughout the mathematics is straightforward and uses standard notation.

This text is suitable for a second- or third-year undergraduate course in physics, and would also be suitable for an introductory solid state course in materials science or materials chemistry.

INTRODUCTION TO THE PHYSICS OF ELECTRONS IN SOLIDS

To my mother
In memoriam

Preface

Most textbooks on solid state physics begin the exposition from what might be called a 'structural position'. Space and point groups are discussed, followed by consideration of the Bravais lattice. The reader is thus led on to elementary ideas about crystallography and the use of diffraction techniques for the solution of crystal structures. Having laid the foundation of how atoms and molecules order to form crystalline structures, electron motion in such periodic structures is treated and band theory developed. The free electron model is seen as an approximation of the more general band theory. In many, rather formal, ways this approach is very satisfying. It would seem obvious that in the first instance one must understand the structure of the material on which one is working before attempting to understand its other physical properties. However, in practice, it proves rather hard to teach solid state physics this way and to retain student enthusiasm in the early stages of the teaching of crystallography where one is dealing with rather difficult geometrical concepts and very little physics. There is a very real danger of making the introduction to the subject so unexciting that the inspiration is lost and students come to regard solid state physics as the 'dull and dirty' branch of their physics course. However, elementary quantum mechanics, including the one-dimensional solution of the time independent Schrödinger equation, is included quite early in many undergraduate courses and there is much attraction in illustrating at this early stage the important technological context of the apparently abstruse quantum mechanics. Further, in solid state physics one is dealing with very many particles, and one is forced to make approximations. Exact solution of the equations of motion of 10^{22} particles is clearly out of the question despite the fact that we understand the electromagnetic interaction so well! Thus in the first solid

state physics course at Durham we have tried both to utilize quantum mechanics at as early a stage as possible and also to introduce some concepts of model building. To this end we have taken the results of the solution of Schrödinger's equation for a single particle in a one-dimensional potential well, extended them and applied them to the problem of an electron in a solid. In this way, the student meets first the simplest possible model for the behaviour of electrons in solids, the free electron approximation where the potential well is flat bottomed and infinitely deep. The results are compared with experimental observations, and only when there is clear discrepancy between theory and experiment is the model made more complex. In many respects this represents a historical approach and one which is all too rarely adopted. There is a great danger that undergraduates come to regard their physics as the ultimate description of the universe which somehow appeared abruptly as a complete, well formulated, entity. While the teaching of relativity goes some way to correcting this impression, students rarely appreciate how physics is a constantly evolving science and how one is all the time building models to describe the physical world. Model building is at the heart of modern physics and is not just restricted to elementary particle physics. Accordingly the approach to the teaching of the physics of solids adopted in this book hinges on two principles. Firstly to illustrate something of the historical development of this subject and to show how necessary is quantum mechanics to understanding the behaviour of electrons in solids. Secondly, to begin with the simplest possible model and gradually increase the complexity. Thus the Drude classical free electron theory is followed by quantum mechanical free electron theory which in turn leads into elementary band theory as a perturbing periodic potential is introduced. The first six chapters are concerned with itinerant electrons under the independent particle approximation, developing the free electron model into elementary band models. In order to illustrate the technological application of the results, Chapter 7 is devoted to an examination of the physical properties of several solid state electronic devices. Chapter 8 examines the behaviour of localized electrons while the last two chapters are devoted to phenomena resulting from breakdown of the independent electron approximation, namely ferromagnetism and superconductivity.

The book is aimed at first or second year undergraduate level and a genuine attempt is made to keep the mathematical discussion as simple as is consistent with clarity. It will, it is hoped, have appeal not only to

students of physics but also of chemistry, metallurgy, geology and engineering. The text is based on a lecture course given originally to a mixed class of physicists, chemists, mathematicians and geologists at Durham University and the general response to the approach has been favourable. In restricting the scope and length of the text, it is hoped that individual students will be able to use it as a genuine introduction to the physics of solids, before graduating to one of the more weighty and comprehensive 'introductory' texts on the market.

Brian Tanner

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My sincere thanks are expressed to the many people who have assisted me in the preparation of this book. I am particularly grateful to Pauline Russell who patiently drew the diagrams from my spider-like sketches, to Nikki Bingham who has deciphered my handwriting with patience and care, to Vikki Greener who has uncomplainingly photocopied large quantities of material and Mike Lee whose skills with the camera continue to amaze us. Of my colleagues, Dick Fong has been particularly assiduous in pointing out errors in problems set over the years and I am indebted to the generations of students who have acted as stoical guinea pigs for my ideas, explanations and exercises. Finally, I acknowledge the love and support of my wife Ruth and sons Rob and Tom, who have tolerated my eccentricities and obsessions with equanimity and humour.

Contents

1

The classical free electron model

In practical terms, the enormous range of values of resistivity of solids is something which we take for granted. Every day, we happily touch the polymer sleeving or fitments surrounding conductors bearing potentially lethal currents at quite high voltages. Only when one is reminded that the difference of almost 30 orders of magnitude found between the resistivity of the noble metals and some synthetic polymers represents the largest variation of any physical parameter does this apparently mundane phenomenon suddenly appear intriguing. It is tempting to enquire whether the same physical process can be responsible for electrical conduction in all materials. Even if the same process extends over half the range it would be a remarkable achievement. Perhaps we would then appreciate why so much time and effort is devoted to measurements of electrical conductivity.

It is hard to conceive that, prior to the turn of the century, very little was known about the physics of solids. Some ideas on crystal structure had been anticipated from the morphology of natural and synthetic crystals but there existed little understanding of the electrical, thermal or magnetic properties of solids. Solid state physics is a twentieth century branch of science and as such deserves recognition as an important section of 'modern physics'. As we shall see later, it was not until quantum mechanics was applied to the physics of solids that many real advances were made.

The first major step in our understanding of the electrical properties of solids was taken by Drude in 1905. Around this time, J. J. Thompson had been performing his classic experiments on the properties of cathode rays. These cathode rays, which were electrically negative, were produced by heating a metallic filament. Somehow, the cathode rays were 'boiled off' from the metal. What was most

important was that the properties of the cathode rays were independent of the metal used for the filament. They seemed to be contained in all metallic solids. Drude's suggestion was that these cathode rays, which we now know as electrons, might be responsible for the electrical conduction in metals. As it turned out, this was a very perceptive insight.

The theory which Drude developed was, naturally, based on classical principles. In it is made an important assumption which is implicit throughout the first eight chapters of this book. This is the INDEPENDENT ELECTRON APPROXIMATION. Drude himself made the approximation, but it is so important that it deserves highlighting here before any further discussion takes place. From what we know about the spacing of atoms in solids, following the pioneering X-ray diffraction experiments of Friedrich and Knipping in 1912, it becomes obvious that a 1 cm cube of metal contains a very large number of electrons. In principle we should consider the interaction of each electron with all the others in the solid via the Coulomb electrostatic interaction. This is clearly impossible to do in practice, so what is done is to assume that each electron moves in an average potential created by all the other electrons, as well as the positive ions in the crystal. Thus we can treat the motion of one electron independently and simply add the contributions of the individual electrons to get the collective response. We can handle the physics of one particle in an average potential well but we cannot handle many particles simultaneously. The independent electron approximation underlies the whole treatment of electronic behaviour developed in the first eight chapters. When it breaks down, as discussed in the last two chapters, very important phenomena arise.

In the classical free electron theories, including that formulated by Drude, one makes the following assumptions in addition to the independent electron approximation.

1 Conduction is entirely by electrons.
2 The sample defines a flat bottomed potential well within which the electrons are constrained and within which they are free to move.
3 The electrons behave as a classical gas, i.e.
   (a) they are distinguishable
   (b) they are small and take up negligible volume
   (c) they have random motion
   (d) they are perfectly elastic.

4 There are no quantum restrictions on the electron energy i.e. the energy distribution of the electrons is a perfect continuum.

1.1 Drude theory

In addition to the above assumptions, Drude made the assumption that all electrons have the average energy. As can be seen in Appendix 2, application of statistical mechanics to a large ensemble of classical particles predicts a probability distribution for the electron energy known as the Boltzmann distribution and the Drude assumption is clearly a very drastic approximation. However, the Drude model is the *simplest possible* model for the behaviour of electrons in metals and therefore we examine it first.

1.1.1 Electrical conductivity (σ)

Suppose that an electron, labelled i, mass m^* is acted upon by a field $\mathscr{E}_x$ in the x direction. This results in a force of $e\mathscr{E}_x$ acting on the electron in the x direction, where e is the charge on an electron. From Newton's Second Law, this equals the rate of change of momentum in the x direction. Thus, if v_x is the x component of velocity of the electron, we have

$$m^* \mathrm{d}v_{ix}/\mathrm{d}t = e\mathscr{E}_x. \tag{1.1}$$

Now the right hand side of this equation is the same for all electrons and hence we can write

$$m^* \mathrm{d}\langle v \rangle/\mathrm{d}t = e\mathscr{E}_x, \tag{1.2}$$

where $\langle v \rangle$ is known as the drift velocity in the x direction and is given by

$$\langle v \rangle = \frac{1}{n}\sum_{i=1}^{n} v_{ix} \tag{1.3}$$

and n is the number of electrons considered.

The drift velocity is essentially different from the random velocities of the individual electrons as it represents a net motion in the field direction superimposed upon such random motion. Fig. 1.1 gives an example of such a drift in the x direction. In zero electric field, on average the electron does not change its position despite its random motion. In a non-zero electric field, the position in the field direction changes, and the electron drifts in this direction. Clearly this leads to a

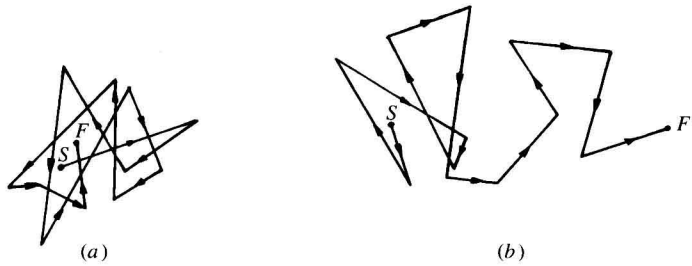

Fig. 1.1 Concept of drift velocity. Schematic electron motion in (*a*) zero (*b*) non-zero electric field. In an electric field, the start, S, and finish, F, positions differ, leading to a net flow of charge.

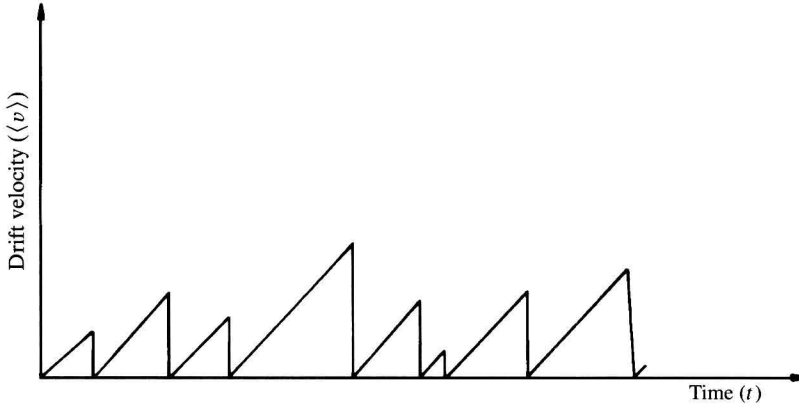

Fig. 1.2 Variation of drift velocity with time. Average time between collisions is τ, the relaxation time.

net flow of charge and hence the passage of an electric current. According to Equation (1.2), the drift velocity $\langle v \rangle$ should increase linearly with time if the electric field is constant. This implies a linear increase of current in a constant field, which is at odds with experimental observation.

The dilemma is resolved by the assumption that the electrons encounter obstacles to their motion and that after such collisions, the motion is randomized and the drift velocity destroyed. After a collision all memory of the previous motion is lost. In effect the clock is set back to zero. The drift velocity will then vary with time in a manner illustrated in Fig. 1.2. On average, collisions occur every time interval of τ, which is known as the relaxation time. As $m^*\langle v \rangle$ of momentum is destroyed at each collision, the rate of destruction of momentum is