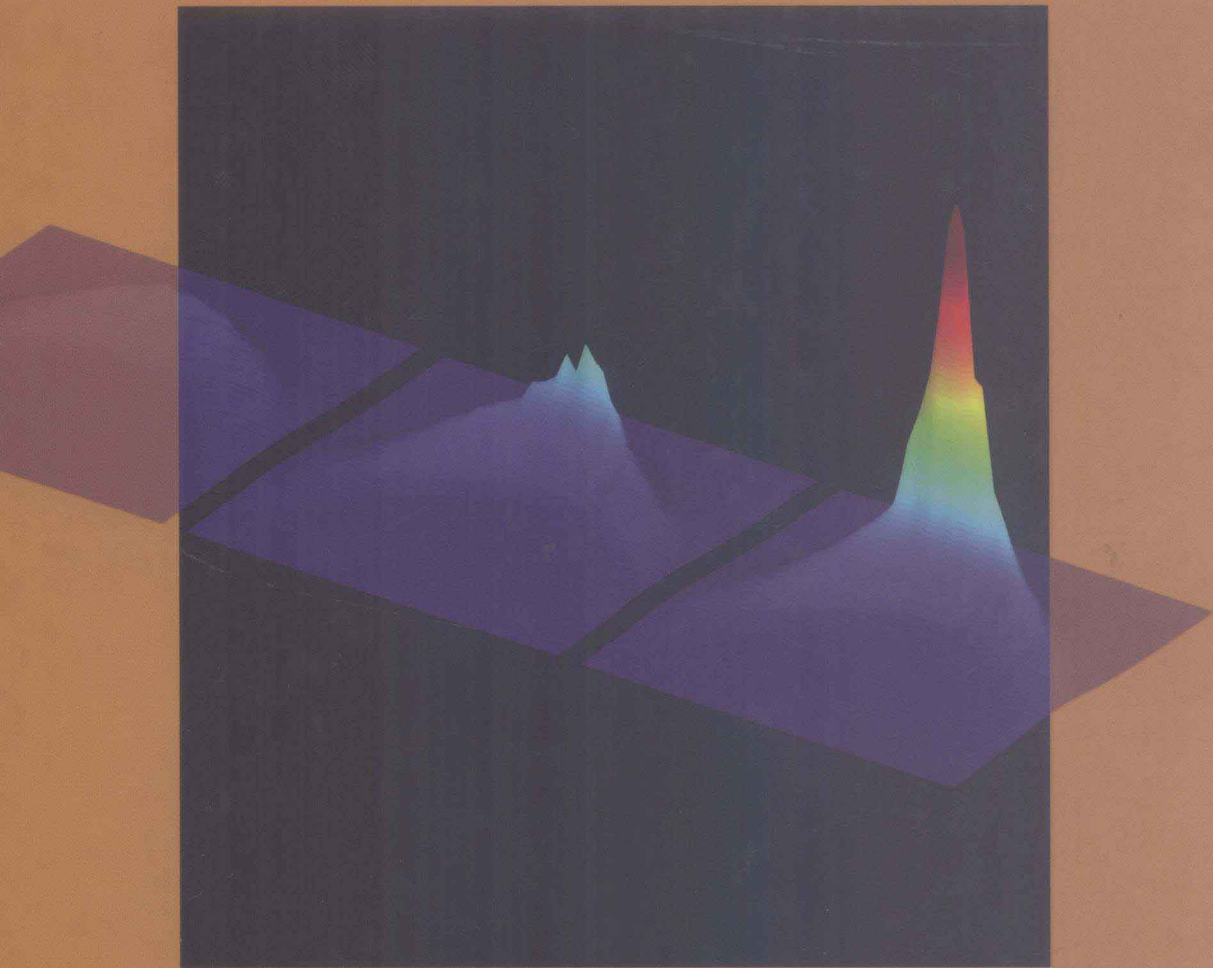
SOLID STATE PHYSICS
ESSENTIAL CONCEPTS



DAVID W. SNOKE

SOLID STATE PHYSICS
Essential Concepts

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USEFUL CONSTANTS AND UNIT CONVERSIONS

The natural energy unit in solid state physics is the electron volt, and the standard length is the centimeter. We stick with the MKS unit system in this entire book.

Numbers here are given only to two or three significant digits.

- $c = 3.0 \times 10^{10}$ cm/s
- $\hbar = 6.6 \times 10^{-16}$ eV-s
- $\hbar c = 2.0 \times 10^{-5}$ eV-cm
- $hc = 1.24 \times 10^{-4}$ eV-cm
- $k_B = 8.6 \times 10^{-5}$ eV/K
- $e = 1.6 \times 10^{-19}$ C
- $\dfrac{e^2}{4\pi\epsilon_0} = 1.44 \times 10^{-7}$ eV-cm
- $\dfrac{h}{e^2} = 2560\ \Omega$
- $m_0 = 5.1 \times 10^5$ eV/c^2
- $m_P = 9.4 \times 10^8$ eV/c^2
- $\epsilon_0 = 8.9 \times 10^{-14}$ C/V-cm
- $\mu_0 = 4\pi \times 10^{-9}$ V-s^2/C-cm
- 1 g $= 5.6 \times 10^{32}$ eV/c^2
- 1 J $= 6.2 \times 10^{18}$ eV (1 C $= 6.2 \times 10^{18}$ e)
- 1 T $= 10^{-4}\ \dfrac{\text{V-s}}{\text{cm}^2}$

SOLID STATE PHYSICS
Essential Concepts

There is beauty even in the solids.

I tell you, if these were silent, the very stones would cry out!

—Luke 19:40

For his invisible attributes, namely, his eternal power and divine nature, have been clearly perceived, ever since the creation of the world, in the things that have been made.

—Romans 1:20

Preface

Imagine teaching a physics course on classical mechanics in which the syllabus is organized around a survey of every type of solid shape and every type of mechanical device. Or imagine teaching thermodynamics by surveying all of the phenomenology of steam engines, rockets, heating systems, and such things. Not only would that be tedious, but much of the beauty of the unifying theories would be lost. Or imagine teaching a course on electrodynamics that begins with a lengthy discussion of all the faltering attempts to describe electricity and magnetism before Maxwell. Thankfully, we don't do this in most courses in physics. Instead, we present the main elements of the unifying theories and then use a few of the specific applied and historical cases as examples of working out the theory.

Yet in solid state physics courses, many educators seem to feel a need to survey every type of solid and every significant development in phenomenology. Students are left with the impression that solid state physics has no unifying, elegant theories and is just a grab bag of various effects.

Nothing could be further from the truth. There are many unifying concepts in solid state physics. But any book on solid state physics that focuses on fundamental theories must leave out some of the many specialized topics that crowd solid state physics books. In response, some educators will say, "You can't possibly leave that topic out!"

This book represents a departure from previous approaches to teaching solid state physics. Previous books have attempted to survey the phenomenology of the entire field, but solid state physics is now too large for any book to do a meaningful survey of all the important effects. The survey approach is also generally unsatisfying for the student. Teaching condensed matter physics by surveying the properties of various materials sacrifices the essential beauty of the topic.

Instead of surveying the phenomology, this book centers on *essential theoretical concepts* that are used in all types of solid state physics. Each chapter focuses on a different set of theoretical tools. The intent here is to survey the unifying concepts and refer the reader to appropriate volumes for greater depth. "Solid state" physics is particularly intended, because "condensed matter" physics includes liquids and gases, and this book does not include in-depth discussions of those states. These are covered amply, for example, in *Principles of Condensed Matter Physics*, by Chaikin and Lubensky.

Some people may raise their eyebrows at including group theory and many-body theory in a textbook aimed at second-year graduate students. In my experience, workers in the field do not need to know all the proofs and theorems of these highly mathematical topics; often, just some basic rules of thumb enable one to do useful calculations. On the other hand, some people may be surprised to see "engineering" topics such as semiconductor structures, optics, and stress and strain matrices included. In my opinion, the lack of understanding of these topics among physicists is appalling. A lot of basic physics relies on understanding these ideas.

In this book I have tried to focus on unifying and fundamental theories. This raises a question: Does solid state physics really involve fundamental physics? Are there really any important questions at stake? Many physics students think that astrophysics and particle physics deal with fundamental questions, but solid state physics doesn't. Perhaps this is because of the way we teach it. Astrophysics and particle physics courses tend to focus much more on unifying, grand questions, especially at the introductory level, while solid state physics courses often focus on a grab bag of various phenomena. If we can get past the listing of material properties, solid state physics does deal with fascinating questions.

One deep philosophical issue is the question of "reductionism" versus "emergent behavior." Since the time of Aristotle and Democritus, philosophers have debated whether matter can be reduced to "basic building blocks" or if it is infinitely divisible. For the past two centuries, many scientists have tended to assume that Democritus was right—that all matter is built from a few indivisible building blocks, and once we understand these, we can deduce all other behavior of matter from the laws that govern these underlying building blocks. In the past few decades, a number of solid state physicists have vociferously rejected this view. They would argue that possibly every quantum particle is divisible, but it doesn't matter at all for understanding the essential properties of things.

At one time, people thought atoms were indivisible, but it was found that they are made of subatomic particles. Then people thought subatomic particles were indivisible, but it was found that at least some of them are made of smaller particles such as quarks. Are quarks indivisible? Many physicists believe there is at least one level lower. As the distance scale gets smaller, the energy cost gets higher. This debate came to a head in the 1980s when the high-energy physics community proposed to spend billions of dollars on the Superconducting Supercollider in Texas, far more than the total budget for condensed matter physics. If such a project would reveal the basic building blocks of all nature, it might be worth it. If all particles are divisible, it seems less interesting to go on endlessly dividing particles to go to ever-smaller scales.

Two solid-state concepts support the anti-reductionist view. One is the idea of "renormalization." This very general concept appears in many different areas. Essentially, it means that often we can redefine a system at a higher level, ignoring the component parts from which it is made. We can work entirely at the higher level, ignoring the underlying complexities. The properties at this level depend only on a few basic properties of the system, which could arise from any number of different microscopic properties. The other idea is the closely-related concept of "universality." Certain classes of systems all have the same properties, despite having quite different underlying microscopic laws.

Another deep topic is the foundations of statistical mechanics. Although statistical mechanics courses are presented with great rigor, there was enormous controversy at the founding of the field, and much of this controversy was simply swept under the rug in later years. These questions re-emerge when we deal with nonequilibrium systems in quantum mechanics, a major topic of solid state physics.

This connects to another important philosophical question, the "measurement" problem of quantum mechanics—that is, what leads to "collapse" of the wavefunction, and what constitutes a measurement. In both quantum statistical mechanics and quantum collapse, we have irreversible behavior arising from an underlying system that is essentially reversible. In both cases there is a connection to the notion of *dephasing*, or decoherence, which has become a major topic of solid state physics in recent years. The essential paradoxes of quantum mechanics all arise in the context of condensed matter, and going to smaller particles does not help at all in the resolution of the paradoxes, nor does it raise new paradoxes.

One of the deepest issues of our day is the question of emergent phenomena. Is life as we know it essentially a generalization of condensed matter physics, in which structure arises entirely from simple interactions at the microscopic level, or do we need entirely new ways of thinking when approaching biophysics, with concepts such as feedback, systems engineering, and transmission and processing of information? Phase transitions are often viewed as examples of order coming out of disorder, through the process known as spontaneous symmetry breaking. The effects that come about in solid state physics due to phase transitions can be dramatic, but we are a long way from extrapolating these to an explanation of the origin of life.

There has been an increasing separation between "hard" condensed matter physics, or solid state physics, and "soft" condensed matter physics. The latter is well represented by Chaikin and Lubensky's book, mentioned above. A good preparation in condensed matter physics could therefore look like the following: a senior undergraduate solid state physics course, or first-year graduate course, using Kittel's *Introduction to Solid State Physics*, to survey the phenomenology; a first-year graduate course in quantum mechanics; followed by graduate courses in solid state physics using this book and in soft condensed matter physics using Chaikin and Lubensky. After this, those disposed toward theory should begin with many-body physics using Mahan's *Many-Particle Physics*, Doniach and Sondheimer's *Green's Functions for Solid State Physicists*, and *Statistical Physics, Part II*, by Lifshitz and Pitaevskii.

Many people contributed to improving this book. I would like to thank, in particular, David Citrin, Dan Boyanovsky, and Zoltan Vörös for their critical reading of the manuscript. I would also like to thank my wife Sandra for many years of warm support and encouragement.

David Snoke
Pittsburgh, 2008

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CHAPTER 1

Electron Bands

1.1 ■ WHERE DO BANDS COME FROM? WHY SOLID STATE PHYSICS REQUIRES A NEW WAY OF THINKING.

When we start out learning quantum mechanics, we usually think in terms of single particles, such as electrons in atoms or molecules. This is historically how quantum mechanics was first developed as a rigorous theory.

In a sense, all of atomic, nuclear, and particle physics are similar, because they all involve interactions of just a few particles. Typically in these fields, one worries about scattering of one particle with one or two others, or bound states of just a few particles. In large nuclei, there may be around 100 particles.

Solid state physics requires a completely new way of thinking. In a typical solid, there are more than 10^{23} particles. It is hopeless to try to keep track of the interactions of all of these particles individually. The beauty of solid state physics, however, lies in the old physics definition of simplicity: "one, two, infinity." In many cases, infinity is simpler to study than three; we can often find exact solutions for an infinite number of particles, and 10^{23} is infinite for all intents and purposes.

Not only that, but new phenomena arise when we deal with many particles. Various effects arise that we would never guess just from studying the component particles such as electrons and nuclei. These "emergent" or "collective" effects are truly *fundamental* physical laws in the sense that they are universal paradigms. In earlier generations, many physicists took a reductionist view of nature, which says that we understand all things better when we break them into their constituent parts. In modern physics, however, we see some fundamental laws of nature arising only when many parts interact together.

1.1.1 ■ Energy Splitting Due to Wavefunction Overlap

To see why a solid is different from all other states of matter, we can use a very simple model. We start with the well-known example of a particle in a square potential, potential as shown in Figure 1.1. From introductory quantum mechanics we know that the wave nature of the particle allows only discrete wavelengths. The time-independent Schrödinger equation for a particle with mass m is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) + V(x)\psi(x) = E\psi(x), \qquad (1.1)$$

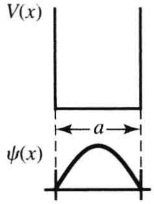

FIGURE 1.1 A square well and its ground state wavefunction.

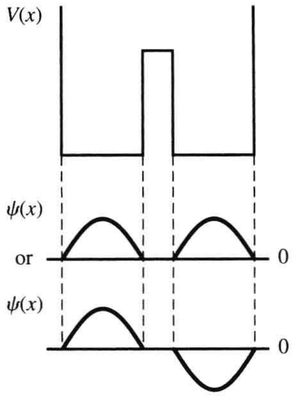

FIGURE 1.2 Two independent square wells and their ground state wavefunctions.

which has the eigenstates

$$\psi(x) = A\sin(kx)$$

in the region where $V(x) = 0$, and is zero at the boundaries. The energies are

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

where $k = N\pi/a$ and $N = 1, 2, 3, \ldots$.

Next consider the case of two square potentials separated by a barrier, as shown in Figure 1.2. If the barrier is high enough, or if the square-well potentials are far enough apart, then a particle cannot go from one well to the other, and we simply have two independent eigenstates of $\psi(x)$, one for each well, with the same energies. The eigenstate for each well is the same if we multiply $\psi(x)$ by -1 or i or any other phase factor, since an overall phase factor does not change the energy or probabilities, which depend only on the magnitude of the wavefunction.

Suppose now that we bring the wells closer together, so that the barrier does not completely prevent a particle in one well from going to the other well, as shown in Figure 1.3. In this case, we say that the two regions are *coupled*. Then elementary quantum mechanics tells us that we cannot solve two separate Schrödinger equations for the two wells; we must solve one Schrödinger equation for the whole