Many-Particle Physics

Gerald D. Mahan

Many-Particle Physics

Gerald D. Mahan
Indiana University
Bloomington, Indiana

PLENUM PRESS · NEW YORK AND LONDON

Library of Congress Cataloging in Publication Data

Mahan, Gerald D
Many-particle physics.

Includes bibliographical references and index.
1. Solid state physics. 2. Many-body problem. 3. Green's functions. I. Title.
QC176.M24 530.4'1 80-24834
ISBN 0-306-40411-7

A Division of Plenum Publishing Corporation
227 West 17th Street, New York, N.Y. 10011

Printed in the United States of America

Preface

This textbook is for a course in advanced solid-state theory. It is aimed at graduate students in their third or fourth year of study who wish to learn the advanced techniques of solid-state theoretical physics. The method of Green's functions is introduced at the beginning and used throughout. Indeed, it could be considered a book on practical applications of Green's functions, although I prefer to call it a book on physics. The method of Green's functions has been used by many theorists to derive equations which, when solved, provide an accurate numerical description of many processes in solids and quantum fluids. In this book I attempt to summarize many of these theories in order to show how Green's functions are used to solve real problems. My goal, in writing each section, is to describe calculations which can be compared with experiments and to provide these comparisons whenever available.

The student is expected to have a background in quantum mechanics at the level acquired from a graduate course using the textbook by either L. I. Schiff, A. S. Davydov, or I. Landau and E. M. Lifshiftz. Similarly, a prior course in solid-state physics is expected, since the reader is assumed to know concepts such as Brillouin zones and energy band theory. Each chapter has problems which are an important part of the lesson; the problems often provide physical insights which are not in the text. Sometimes the answers to the problems are provided, but usually not. It is hoped that the student can learn the subject by using the book as a study guide, since small enrollments often restrict the availability of courses at the advanced level.

I am often asked why I wrote this book. The questioner usually has an understanding of the work involved and so regards my effort as reflecting poorly upon my sanity. On the whole I agree, and if I knew at the beginning the actual investment of time, I probably would not have started. The actual time is about four to five hours per page, which is roughly divided equally among writing, editing, and library searching. My reason for undertaking this project was the great need for someone to do it and the disinclination of anyone else to write a comprehensive advanced textbook on solid-state theory. My own graduate students kept asking me for the standard reference on a number of topics, and I became tired of replying that none exist. My objective was to take standard subjects, such as the electron gas or polaron theory, and to summarize what is generally known. All the steps are retained in the derivation, so that the answers are obtained by starting from the beginning and working through to the end.

The volume is restricted to a description of the many-particle theory of solids. There is also some discussion of quantum fluids, which have historically been part of solid-state theory. The important subject of classical fluids is omitted entirely. In solids and liquids, the forces between pairs of particles are well understood, and the starting Hamiltonian for the problem is accurate. Here we are better off than our brethren in nuclear or stellar physics, since they are often groping for the Hamiltonian. In solids, the only problem is that there are usually 10^{23} particles in the system. Thus we have a well-defined many-body problem which is easy to state: We have simple forces between particles, and the only complication is the large number of particles. In this regard, the atomic theorists have an easier task since they usually have fewer than one hundred electrons in their theoretical system. Consequently, they have been more successful in achieving a quantitative description of atoms. However, solid-state theory has a richer variety of phenomena: magnetism, superconductivity, superfluidity, phase transitions, etc. We have been successful in describing most of these phenomena with great accuracy—magnetism is probably the greatest exception. There is no doubt that solid-state theory has been the center of developments in many-body theory, and our successes are followed by exporting these ideas to other disciplines; e.g., the plasma theory of metals becomes the giant dipole resonance of nuclei.

The topics chosen for discussion were selected on the basis of what every well-rounded theorist should know. Thus basic subjects such as the electron gas, electron–phonon interactions, transport theory, linear response, superconductivity, and superfluidity are covered. Other subjects were deemed equally important, but I ran out of energy, and the book became too long anyway; the important subjects which were omitted are the Kondo effect, Hubbard models, Anderson models, and magnetic systems. Also omitted were two important subjects which deserve large textbooks of their own: renormalization group and the Hohenberg–Kohn–Sham theory of the inhomogeneous electron gas.

Anyone writing an advanced book is going to receive some criticism. No one is expert in all advanced subjects. There are many topics on which I am not an expert and not even well informed. In this situation any choice of action will be criticized. If the topic is omitted, I am criticized for regarding it as unimportant. If it is included, then I am criticized for not providing the expert viewpoint. The only solution is to do one's best and to challenge critics to write their own book.

Historians of science have described numerous and competing models for how science advances. One model is the Ortega hypothesis which suggests that science advances by a large number of mediocre scientists each making a small incremental contribution. On the opposite end of the spectrum is a quite different view that science advances by great leaps forward by the intellectual giants such as Newton and Einstein. The rest of us merely fill in the details they overlook. In preparing this manuscript, I became aware that solid-state theory has advanced by a process intermediate between these extremes. In each chapter, usually six or eight theorists seem to dominate the subject and to provide most of the major concepts and understanding. But in the next chapter, on another subject, it is usually another entirely different group of six to eight theorists who provide the progress. Thus the advance of science appears to occur by a large number of talented workers, although in each topic only a few are important.

Quite often in the text it is necessary to evaluate standard integrals from tables. I use *Table of Integrals, Series and Products* by I. S. Gradshteyn and I. M. Ryzhik (Academic Press, New York, 1965). It seems to be available worldwide. All special integrals are referred to in this present book as "G&R" followed by the integral number.

It is a pleasure to thank many associates for the substantial assistance I have received in the preparation of the book. About half of the writing was done while I was on leave, from Indiana University, as visiting Professor at Chalmers University of Technology in Gothenburg, Sweden. I wish to thank Professor A. Sjölander and S. Lundqvist for this stimulating and very pleasant year. My financial support was provided by the Nordic Institute for Theoretical Astrophysics (NORDITA) in Copenhagen, and I wish to thank Professors A. Bohr, A. Luther, and J. W. Wilkins for arranging my visiting professorship. The entire draft was read by S. M. Girvin, who deserves special thanks for catching many lapses in the first draft. Additional proofreading was also provided by M. Jonson and P. Tua.

Finally, I wish to thank my family—Sally, Chris, Susie, and Roy—for their understanding and quietness during the eighteen months of preparation.

Indiana University Gerald D. Mahan

Contents

Chapter 1

Introductory Material

1.1. HARMONIC OSCILLATORS AND PHONONS

First quantization in physics refers to the property of particles that certain operators do not commute:

$$[x, p_x] = i\hbar$$
$$E \rightarrow \hbar i \frac{\partial}{\partial t} \tag{1.1.1}$$

Later it was realized that forces between particles were caused by other particles: Photons caused electromagnetic forces, pions caused some nuclear forces, etc. These particles are also quantized, and this leads to second quantization. The basic idea is that forces are caused by particles and that the number of particles is quantized: one, two, three, etc. This imparts a quantum nature to the classical force fields.

In solids the vibrational modes of the atoms are quantized because of first quantization (1.1.1). These quantized vibrational modes are called *phonons*. An electron can interact with a phonon, and this phonon can travel to another electron, interact, and thereby cause an indirect interaction between electrons. Indeed, the phonon does not need to move but can vibrate until the next electron comes by. In any case, phonons play a role in solids similar to that in the classical fields of physics. They cause quantized interactions between electrons.

Phonons in solids can usually be adequately described as harmonic oscillators. Later we shall have a fuller description of the effects of anharmonicity. But, for the moment, this should be sufficient motivation to study the harmonic oscillator. The one-dimensional harmonic oscillator has the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{K}{2} x^2$$

To solve it we introduce some dimensionless coordinates ξ:

$$\omega^2 = \frac{K}{m}$$

$$\xi = x\left(\frac{m\omega}{\hbar}\right)^{1/2}$$

$$\frac{1}{i}\frac{\partial}{\partial \xi} = p(\hbar m\omega)^{-1/2}$$

and

$$H = \frac{\hbar\omega}{2}\left(-\frac{\partial^2}{\partial \xi^2} + \xi^2\right) \tag{1.1.2}$$

The harmonic oscillator Hamiltonian has a solution in terms of Hermite polynomials. The states are quantized such that

$$H\psi_n = \hbar\omega(n + \tfrac{1}{2})\psi_n \tag{1.1.3}$$

where n is an integer. One can also learn by direct calculation that the following matrix elements exist for the operators x and p:

$$\begin{aligned} \langle n' \mid x \mid n\rangle &= \left(\frac{\hbar}{2m\omega}\right)^{1/2}[(n')^{1/2}\delta_{n'=n+1} + (n)^{1/2}\delta_{n'=n-1}] \\ \langle n' \mid p \mid n\rangle &= -\frac{1}{i}\left(\frac{m\hbar\omega}{2}\right)^{1/2}[(n')^{1/2}\delta_{n'=n+1} - (n)^{1/2}\delta_{n'=n-1}] \end{aligned} \tag{1.1.4}$$

It is customary to define two dimensionless operators as follows:

$$\begin{aligned} a &= \frac{1}{2^{1/2}}\left(\xi + \frac{\partial}{\partial \xi}\right) = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x + \frac{ip}{m\omega}\right) \\ a^\dagger &= \frac{1}{2^{1/2}}\left(\xi - \frac{\partial}{\partial \xi}\right) = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x - \frac{ip}{m\omega}\right) \end{aligned} \tag{1.1.5}$$

They are Hermitian conjugates of each other. They are sometimes called *raising* and *lowering operators*, but we shall call them *creation* ($a^\dagger$) and *destruction operators* (a). The Hamiltonian (1.1.2) may be written with them as

$$H = \frac{\hbar\omega}{2}[aa^\dagger + a^\dagger a]$$
$$= \frac{\hbar\omega}{2}\left[\frac{1}{2}\left(\xi + \frac{\partial}{\partial\xi}\right)\left(\xi - \frac{\partial}{\partial\xi}\right) + \frac{1}{2}\left(\xi - \frac{\partial}{\partial\xi}\right)\left(\xi + \frac{\partial}{\partial\xi}\right)\right]$$
$$= \frac{\hbar\omega}{2}\left(-\frac{\partial^2}{\partial\xi^2} + \xi^2\right)$$

A very important property of these operators is called *commutation relations.* These are derived by considering how they act, sequentially, on any function $f(\xi)$. The two operations a and $a^\dagger$ in turn give

$$aa^\dagger f(\xi) = \frac{1}{2}\left(\xi + \frac{\partial}{\partial\xi}\right)\left(\xi - \frac{\partial}{\partial\xi}\right)f(\xi) = \frac{1}{2}(\xi^2 f + f - f'')$$

while the reverse order gives

$$a^\dagger a f(\xi) = \frac{1}{2}\left(\xi - \frac{\partial}{\partial\xi}\right)\left(\xi + \frac{\partial}{\partial\xi}\right)f(\xi) = \frac{1}{2}(\xi^2 f - f - f'')$$

These two results are subtracted,

$$[aa^\dagger - a^\dagger a]f(\xi) = f(\xi) \tag{1.1.6}$$

and yield the original function. The operator in brackets is replaced by a bracket with a comma,

$$[aa^\dagger - a^\dagger a] \equiv [a, a^\dagger]$$

which means the same thing. The relationship (1.1.6) is usually expressed by omitting the function $f(\xi)$:

$$[a, a^\dagger] = 1 \tag{1.1.7}$$

In a similar way, one can prove that

$$\begin{aligned}[a, a] &= 0 \\ [a^\dagger, a^\dagger] &= 0\end{aligned} \tag{1.1.8}$$

These three commutators, plus the Hamiltonian

$$H = \frac{\hbar\omega}{2}[aa^\dagger + a^\dagger a] = \frac{\hbar\omega}{2}[aa^\dagger - a^\dagger a + 2a^\dagger a] = \hbar\omega[a^\dagger a + \tfrac{1}{2}] \tag{1.1.9}$$

completely specify the harmonic oscillator problem in terms of operators. With these four relationships, one can show that the eigenvalue spectrum is indeed (1.1.3), where n is an integer. The eigenstates are

$$|n\rangle = \frac{(a^\dagger)^n}{(n!)^{1/2}}|0\rangle$$

where $|0\rangle$ is the state which obeys

$$a|0\rangle = 0$$

and where the $n!$ is for normalization. If one operates on this state by a creation operator, one gets

$$a^\dagger|n\rangle = \frac{1}{(n!)^{1/2}}(a^\dagger)^{n+1}|0\rangle = \frac{(n+1)^{1/2}}{[(n+1)!]^{1/2}}(a^\dagger)^{n+1}|0\rangle$$
$$= (n+1)^{1/2}|n+1\rangle$$

the state with the next highest integer. Thus the only matrix element between states is

$$\langle n'|a^\dagger|n\rangle = (n+1)^{1/2}\delta_{n'=n+1}$$

If we take the Hermitian conjugate of this matrix element,

$$\langle n|a|n'\rangle = (n+1)^{1/2}\delta_{n'=n+1}$$

and exchange dummy variables n and n', we obtain

$$\langle n'|a|n\rangle = (n)^{1/2}\delta_{n'=n-1}$$

or

$$a|n\rangle = (n)^{1/2}|n-1\rangle$$

So the destruction operator a lowers the quantum number. Thus operating by the sequence

$$a^\dagger a|n\rangle = a^\dagger(n)^{1/2}|n-1\rangle) = (n)^{1/2}a^\dagger|n-1\rangle = n|n\rangle$$

gives an eigenvalue n, which verifies the Hamiltonian (1.1.3). Furthermore, using the original definitions (1.1.5) permits us to express x and p in terms