FRONTIERS IN PHYSICS

A LECTURE NOTE & REPRINT SERIES

Quantum Theory of Many-Particle Systems

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Problems in Quantum Theory of Many-Particle Systems

A Lecture Note and Reprint Volume

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EDITOR'S FOREWORD

The problem of communicating in a coherent fashion the recent developments in the most exciting and active fields of physics seems particularly pressing today. The enormous growth in the number of physicists has tended to make the familiar channels of communication considerably less effective. It has become increasingly difficult for experts in a given field to keep up with the current literature; the novice can only be confused. What is needed is both a consistent account of a field and the presentation of a definite "point of view" concerning it. Formal monographs cannot meet such a need in a rapidly developing field, and, perhaps more important, the review article seems to have fallen into disfavor. Indeed, it would seem that the people most actively engaged in developing a given field are the people least likely to write at length about it.

"Frontiers in Physics" has been conceived in an effort to improve the situation in several ways. First, to take advantage of the fact that the leading physicists today frequently give a series of lectures, a graduate seminar, or a graduate course in their special fields of interest. Such lectures serve to summarize the present status of a rapidly developing field and may well constitute the only coherent account available at the time. Often, notes on lectures exist (prepared by the lecturer himself, by graduate students, or by postdoctoral fellows) and have been distributed in mimeographed form on a limited basis. One of the principal purposes of the "Frontiers in Physics" series is to make such notes available to a wider audience of physicists.

It should be emphasized that lecture notes are necessarily rough and informal, both in style and content, and those in the series will prove no exception. This is as it should be. The point of the series is to offer new, rapid, more informal, and, it is hoped, more effective ways for physicists to teach one another. The point is lost if only elegant notes qualify.

A second way to improve communication in very active fields of physics is by the publication of collections of reprints of recent articles. Such collections are themselves useful to people working in the field. The value of the reprints would, however, seem much enhanced if the collection would be accompanied by an introduction of moderate length, which would serve to tie the collection together and, necessarily, constitute a brief survey of the present status of the field. Again, it is appropriate that such an introduction be informal, in keeping with the active character of the field.

A third possibility for the series might be called an informal monograph, to connote the fact that it represents an intermediate step between lecture notes and formal monographs. It would offer the author an opportunity to present his views of a field that has developed to the point at which a summation might prove extraordinarily fruitful, but for which a formal monograph might not be feasible or desirable.

Fourth, there are the contemporary classics—papers or lectures which constitute a particularly valuable approach to the teaching and learning of physics today. Here one thinks of fields that lie at the heart of much of present-day research, but whose essentials are by now well understood, such as quantum electrodynamics or magnetic resonance. In such fields some of the best pedagogical material is not readily available, either because it consists of papers long out of print or lectures that have never been published.

"Frontiers in Physics" is designed to be flexible in editorial format. Authors are encouraged to use as many of the foregoing approaches as seem desirable for the project at hand. The publishing format for the series is in keeping with its intentions. Photo-offset printing is used throughout, and the books are paperbound, in order to speed publication and reduce costs. It is hoped that the books will thereby be within the financial reach of graduate students in this country and abroad.

Finally, because the series represents something of an experiment on the part of the editor and the publisher, suggestions from interested readers as to format, contributors, and contributions will be most welcome.

DAVID PINES

Urbana, Illinois
August 1961

PREFACE

In June, 1958, at the invitation of Professor J. C. Slater, I gave at the Massachusetts Institute of Technology a series of ten lectures entitled "Interactions of Elastic Waves in Solids." The aim was to present the application to a concrete physical problem of rather general techniques developed by N. M. Hugenholtz and me for the study of interaction effects in quantum systems of many particles. The first part of the present book contains an expanded version of these lectures, prepared by L. P. Howland and originally circulated as a Technical Report of the Solid State and Molecular Theory Group of M.I.T. A number of original papers by G. Placzek, N. M. Hugenholtz, and me, dealing with problems or methods discussed in the lectures, are represented in the second part.

By presenting first a detailed discussion of a special and rather simple physical system, an anharmonic crystal lattice at the absolute zero of temperature, and then a number of articles of greater generality, we hope to give the reader a convenient and self-contained introduction to one of the methods that has been developed and used in recent years for the study of interactions in quantum systems containing a large number of particles. In the study of anharmonic crystals we have considered among other things the effect of the interaction between elastic waves on slow neutron scattering by the crystal. It is for this reason that a few somewhat older papers on slow neutron scattering have been included.

On behalf of L. P. Howland and myself I gladly express our gratitude to Professor J. C. Slater for his stimulating interest in the lecture series and in the preparation of the lecture notes.

Authors and publishers are indebted to the Solid State and Molecular Theory Group of M.I.T., and to the editors of the *Physical Review* and *Physica*, for permission to republish the material contained in this book.

L. VAN HOVE

Geneva, Switzerland
August 1961

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Quantum Theory of Many-Particle Systems

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1. INTRODUCTION

In this report it is intended to discuss several problems in solid-state physics by means of a new perturbation method for many-particle, quantum-mechanical systems. The particular problems to be discussed concern effects of the interactions of elastic waves in ideal single crystals, especially non-conducting crystals. Some of these problems have been treated earlier by other methods, but they still serve well as illustrative applications of the new method.

The solid-state problems to be discussed have much in common with other many-particle problems. Examples of these are the Fermi gas with interactions (Brueckner and Levinson, 1955; Bethe, 1956; Goldstone, 1957) and the Bose gas with interactions (Bogolyubov, 1947; Huang and Yang, 1957; Brueckner and Sawada, 1957). The perturbation method presented here was actually developed in a treatment of the Fermi gas (Hugenholtz, 1957 a,b), but it is applicable to all of the problems mentioned above. Furthermore, the method is closely related to methods used in field theory, and, in fact, it was largely inspired by those methods (Van Hove, 1955 b and 1956; Frazer and Van Hove, 1958).

There are many types of waves in addition to elastic waves which are familiar in solid-state physics. Among these are the Bloch-type wave functions for electrons, the spin waves of magnetic materials at low temperatures, and the waves of x-rays and neutrons which are used to study solids in scattering experiments. In each of these examples the wave is a useful concept because it is relatively independent and long-lived in the total system. When the system is described in terms of such waves, there only remains the problem of treating small interactions between the waves to obtain a complete description of the system. When the interactions are not small, of course, the concept of the wave is not so useful. Even when the wave description is quite good, however, some of the most important properties of the system derive from the small interactions which remain. This is the case for all transport properties, for example, and the new method actually originated as a new approach to the related irreversible statistics (Van Hove, 1955 a and 1957).

In an ideal non-conducting crystal the vibrational problem is generally treated in the following way. The crystal is assumed to have a total potential energy which is only a function of nuclear positions (the electrons are assumed to follow the nuclei), and this energy is written as a series in powers of the displacements of nuclei from their equilibrium positions. The potential energy is therefore given by a constant plus quadratic and higher-order terms in the nuclear displacements. If only the quadratic, or harmonic, terms are significant, the crystal vibration problem can be completely solved in terms of independent elastic waves, each wave being characterized by a wave vector $\vec{q}$, a polarization vector $\vec{e}$, and a frequency ω. In a quantum-mechanical description of the vibrations, the energy of each elastic wave is quantized, and there is said to be one phonon present for each quantum of energy, $\hbar\omega$.

The higher-order or anharmonic terms in the expanded potential energy give rise to interactions between the elastic waves or phonons of the harmonic approximation. Except near the melting point of the solid, these interaction terms turn out to be small enough that the elastic waves or phonons still provide a good basis for treating the vibrational problem. Once the harmonic problem is solved, then, there remains the problem of calculating the effects of small phonon-phonon interactions. The calculation of such effects when the crystal is at equilibrium or in its ground state is the main problem which is treated in the present report.

In an ideal conducting crystal the vibrational problem is complicated by the presence of conduction electrons, which are not constrained to follow the vibrations of the nuclei (or the ionic cores). If the nuclei were fixed rigidly in their equilibrium positions, these conduction electrons could be described by Bloch-type one-electron wave functions, each of these functions being characterized by a wave vector, an energy, and a spin quantum number. If the nuclei make displacements from their equilibrium positions, however, as they do in an actual vibrating crystal, the crystal symmetry is no longer that appropriate to Bloch electrons, and, furthermore, the electrons cannot be assumed to follow the nuclei, as they do in a non-conducting crystal. In the usual treatment of this problem, the conduction electrons are described in terms of the Bloch functions of the non-vibrating crystal, and they are then allowed to interact with the lattice vibrations or phonons. When a conducting crystal is thus described in terms of phonons and Bloch electrons, there remains the problem of calculating the effects of three different types of interaction: phonon-phonon, phonon-electron, and electron-electron.

The interactions described above for non-conductors and conductors are responsible for important physical effects. The phonon-phonon interaction gives rise to heat conduction, and it also leads to the effect of thermal expansion. The phonon-electron interaction also gives rise to heat conduction, and it is responsible for electrical resistance and superconductivity. The electron-electron interaction gives rise to plasma oscillations. There are other effects, of course, but those given should be sufficient to illustrate the point.

Theoretical treatments of these and other interaction effects are generally quite difficult, and the best treatments of some are still far from satisfactory. Since the interactions of interest are small and non-singular, some form of perturbation theory is the natural basis for any treatment. Standard perturbation theory is generally inadequate for a large system, however, because some high-order terms may be quite large, even though the interaction forces are small.

There are also other difficulties which arise in treating many-particle systems by perturbation methods, and some of these can be related to certain physical characteristics of the interaction effects. In the first place, many of the interaction effects are at least partly dissipative in character. This is not surprising, of course, since a solid could not come to thermal equilibrium without such effects. Thermal conductivity is one dissipative effect, and electrical conductivity is another.

For a dissipative effect which is somewhat simpler theoretically, consider the decay of an extra phonon in a non-conducting solid. Such a phonon might have been excited by neutron bombardment, for example. In any case, the phonon decays with a finite lifetime into two or more phonons, and the secondary phonons and all the later products also decay. The original system containing the single extra phonon thus decays irreversibly into a system in which the energy of the original extra phonon is distributed among all the vibrational degrees of freedom of the system and thermal equilibrium is restored. Such effects are involved in many physical processes of interest, and one of the difficulties in many-particle perturbation theory is to account for them in a natural and practical way.

In the second place, some of the effects depend upon interaction-produced energy shifts and involve the physical characteristics of such shifts. The particular characteristic which is of interest here is the volume dependence of an energy shift, as will be seen below. Thermal expansion is an energy-shift effect, since it occurs because of an interaction-produced shift in the free energy of a crystal. The equilibrium value of the lattice constant at O°K also involves an energy-shift effect, since it depends upon an interaction-produced shift in the zero-point energy of a crystal. In both of these examples the energy shift is an extensive (bulk) quantity, and it should be proportional to the volume of the crystal.

For a different energy-shift effect, consider again the extra phonon in a non-conducting solid. The energy of this phonon (the energy required to excite it) is not exactly equal to $\hbar\omega$, as predicted by harmoinc theory, but it is shifted from this value by the anharmonic forces. This energy shift is an intensive (local) quantity, and it should be independent of the volume of the crystal.

One of the difficulties in many-particle perturbation theory is to obtain expressions for energy-shift effects which exhibit the expected volume-dependence in a simple way. For many of these effects a straightforward calculation leads to an expression in which intensive and extensive effects are intermixed, even though the effect itself is expected to be purely extensive or intensive.

Finally, many interaction effects involve both dissipative processes and energy shifts, and these mixed effects exhibit further difficulties. The extra phonon in a non-conducting solid again provides a good example. The lifetime of this phonon is a dissipative effect, but it is influenced by the energy-shift effect, since energy conservation is involved in each decay. The mixing of the effects is really more complete than this, however. In view of the finite lifetime of the phonon, its energy cannot be perfectly well defined. The phonon therefore has an energy spectrum, and the spectrum must have a width corresponding to an imaginary part of the phonon frequency and depending on the decay probability of the phonon. The spectrum may also have a peak position which depends upon the decay probability. If the mixing in such mixed effects is quantitatively important, intuitive perturbation treatments become impossible and a completely systematic perturbation method is required.

In this report a general many-particle perturbation method which handles the difficulties mentioned above is presented. The presentation is accomplished in the course of a discussion of a relatively simple system consisting of interacting phonons in a non-conducting crystal. The problems for this system which are discussed are the ground-state energy and wave function at O°K, the cross-section for neutron scattering at O°K, the free energy at an arbitrary temperature, and, very briefly, the cross-section for neutron scattering at an arbitrary temperature. In view of the purpose of this report the results presented are not in general those in which an experimentalist would be interested. Important factors such as the presence of impurities are neglected, mainly low-temperature properties are discussed, and many other simplifications are made. Results of interest to experimentalists can be obtained by the new perturbation method, but they will not be presented here. No quantitative calculations have as yet been made for any of the problems considered in this report, but the theory has reached a point where such calculations are feasible and desirable.