Quantum Many-Particle Systems

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FOITOR'S FOREWORD

The problem of communicating in a coherent fashion recent developments in the most exciting and active fields of physics continues to be with us. 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, while 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 was conceived in 1961 in an effort to improve the situation in several ways. Leading physicists 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, by graduate students, or by postdoctoral fellows) and are distributed in the mimeographed form on a limited basis. One of the principal purposes of the FRONTIERS OF 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 in content; and those in the series will prove no exception. This is as it should be. One 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.

As FRONTIERS OF PHYSICS has evolved, a third category of book, the informal text/monograph, an intermediate step between lecture notes and formal texts or monographs, has played an increasingly important role in the series. In an informal text or monograph an author has reworked his her lecture notes to the point at which the manuscript represents a coherent summation of a newly-developed field, complete with references and problems, suitable for either classroom teaching or individual study.

During the past two decades, the study of many-particle systems has become an essential part of the education of graduate students in physics and chemistry, while the application of nonperturbative approaches, functional integral techniques, and stcchastic methods to these systems has led to an improved qualitative and quantitative understanding of their behavior. In the present volume, John Negele and Henri Orland, two pioneers in these developments, provide the nonspecialist with a lucid introduction to these nonperturbative approaches, as well as to the "traditional" techniques of many-body theory, perturbation theory, and general arguments using order parameters, symmetry, and Fermi liquid theory. Given its emphasis on pedagogy and physical

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understanding, their book will be welcomed by all scientists interested in understanding many-body physics, from the beginning graduate student to the practitioner in universities, industry, or government. I share their view that "Quantum Many-Particle Systems" conveys the essential ideas of the field, and that it will assist students and professionals alike in reading, understanding, and contributing to the literature.

DAVID PINES Urbana, Illinois April, 1987

PREFACE

The problem of understanding the properties of quantum systems possessing large or infinite numbers of degrees of freedom pervades all of theoretical physics. Hence, the theoretical methods and the physical insight which have been developed over the years for quantum many-particle systems comprise an essential part of the education of students in disciplines as diverse as solid state physics, field theory, atomic physics, condensed matter physics, quantum chemistry and nuclear physics. During the past decade, we have taught one- and two-semester courses on the quantum theory of many-particle systems to graduate students in these disciplines at the Massachusetts Institute of Technology, and this book is an outgrowth of these lectures.

Compared to the texts that appeared in the early 1970's, we have presented standard topics from a different perspective and included a number of new developments. Because of the physical appeal and utility of the Feynman path integral, we have used functional integrals as the foundation of our presentation. Functional integral techniques provide an economical formalism for deriving familiar results, such as perturbation expansions, and yield valuable new approximations and insight into such problems as quantum collective motion, tunneling decay, and phase transitions. Because of the power and physical insights provided by these techniques and their prevalence in the literature, we believe it is essential to teach them to students at this level.

Order parameters and broken symmetry play crucial roles in characterizing and understanding the phases in which matter exists and the transitions between these phases. These concepts, which are familiar from the Landau theory of phase transitions, arise quite naturally from our general development in terms of functional integrals, and are discussed in detail in this text.

Another new topic is the use of stochastic methods for many-body problems. Techniques have existed for a long time to use Markov random walks and Monte Carlo evaluation of integrals to calculate quantum mechanical observables of physical interest to any desired degree of accuracy. In the past, such techniques have received less attention than analytic methods involving summations of diagrams having undetermined convergence properties or other ultimately uncontrolled approximations. We believe that stochastic methods are intellectually interesting in their own right and that they provide a powerful tool to obtain definitive answers to certain classes of otherwise insolvable problems. Hence, we have included a pedagogical introduction to stochastic methods, showing how to calculate observables of interest, stressing the physical connection with path integrals, and demonstrating how to tailor the method to the physics of the problem under consideration.

The scope of this book is intended to be sufficiently broad to serve as a text for a one-or, two-semester graduate course. Thus, in addition to these new topics, we have also included the basic body of methodology found in older texts, such as perturbation theory, Green's function techniques, and the Landau theory of Fermi liquids.

Our pedagogical objective is to convey the essential ideas and to prepare the student to read and understand the relevant research literature. We have attempted to present the formalism tersely, without undue emphasis on technical details and to show how it applies to a broad variety of interesting physical systems.

Homework problems are provided at the end of each chapter, and are crucial to a thorough mastery of the subject. Instructive alternative treatments of formal developments in the text are often presented as problems, as well as detailed calculations which are too lengthy for the text. One model system, particles in one dimension interacting via a δ -function two-body potential, is used extensively to illustrate methods presented in the text. For this system, both exact solutions and a multitude of common approximations can be worked out in detail analytically.

Finally, the organization of the book is as follows: We assume only an understanding of elementary quantum mechanics and statistical mechanics, so we begin in Chapter 1 with a thorough, self-contained treatment of second quantization and coherent states. Chapter 2 presents the general formalism of path integrals, perturbation theory and its resummations, and non-perturbative approximations in the formally simple case of the grand canonical ensemble at finite temperature. Specialization to zero temperature and the canonical ensemble is discussed in Chapter 3. Chapter 4 addresses the role of order parameters and broken symmetry in many-body theory and shows how mean field theory embodies the essential physical content of the Landau theory of order parameters and phase transitions. The next chapter develops the general properties of Green's functions, and their application in describing fundamental excitations and physical observables. The phenomenological description and microscopic foundation of the Landau theory of Fermi liquids are presented in Chapter 6. Chapter 7 describes a number of further developments of functional integral techniques, including alternative functional integral representations, the treatment of quantum mean field theory and tunneling decay, and the study of high orders of perturbation theory. The final chapter presents stochastic methods.

As in all such efforts, we are indebted to many people for their invaluable assistance in writing this book. This book was originally stimulated by David Pines and benefited from the editorial guidance of Rick Mixter and Allan Wylde. Although it is impossible to list all of the teachers, colleagues, and students whose insights have contributed to this work, we would particularly like to acknowledge the contributions of R. Balian, J. P. Blaizot, E. Brezin, C. De Dominicis, C. Itzykson, S. E. Koonin, S. Leibler, S. Levit, G. Ripka, and R. Schaeffer.

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JOHN NEGELE HENRI ORLAND

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CHAPTER 1

SECOND QUANTIZATION AND COHERENT STATES

The quantum mechanics of a single particle is usually formulated in terms of the position operator \hat{x} and the momentum operator \hat{p} . All other operators of physical interest may be expressed in terms of these operators, and a natural representation for quantum mechanics, the coordinate representation, is defined in terms of eigenfunctions of the position operator. In this chapter, an analogous formalism is developed for systems composed of many identical particles. For these systems it is useful to define operators which create or annihilate a particle in specified states. Operators of physical interest may be expressed in terms of these creation and annihilation operators, in which case they are said to be expressed in "second quantized" form. The eigenstates of the annihilation operators are coherent states. A natural representation for the quantum mechanics of many-particle systems, the holomorphic representation, is defined in terms of these coherent states.

As a prelude to the formalism for many-particle systems, it is useful to begin by reviewing some elementary aspects of quantum mechanics.

1.1 QUANTUM MECHANICS OF A SINGLE PARTICLE

Quantum mechanics describes the state of a particle by a state vector $|\phi\rangle$, which belongs to a Hilbert space $\mathcal X$. This Hilbert space $\mathcal X$ is the vector space of complex, square integrable functions, defined in configuration space. Using Dirac notation, the scalar product of vectors in $\mathcal X$ is:

$$\langle \phi | \psi \rangle = \int d^3r \phi^*(\vec{r}) \psi(\vec{r}) \quad . \tag{1.1}$$

Then by definition, a vector $|\phi\rangle$ belongs to the Hilbert space $\mathcal X$ if the norm of $|\phi\rangle$ is finite:

 $\langle \phi | \phi \rangle = \int d^3 r \left| \phi(\vec{r}) \right|^2 < +\infty \quad .$ (1.2)

Of particular importance are the vectors $|\vec{r}\rangle$ and $|\vec{p}\rangle$, eigenvectors of the quantum position operator $\hat{\vec{r}}$ and momentum operator $\hat{\vec{p}}$

$$\hat{\vec{r}}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle \tag{1.3}$$

$$\hat{\vec{p}}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle \quad . \tag{1.4}$$

Although these vectors do not belong to \mathcal{X} , because their norm is not finite, they span the whole Hilbert space \mathcal{X} . This is reflected by the following closure relations:

$$\int d^3r |\vec{r}\rangle\langle \vec{r}| = 1 \tag{1.5}$$

$$\int d^3p|\vec{p}\rangle\langle\vec{p}|=1 \tag{1.6}$$

where 1 denotes the unit operator in X.

A state vector $|\vec{r}\rangle$ represents a state in which the particle is localized at point \vec{r} , and a state vector $|\vec{p}\rangle$ represents a particle with a momentum \vec{p} . The overlap of these vectors is given by:

$$\langle \vec{r} | \vec{r}' \rangle = \delta^{(3)} (\vec{r} - \vec{r}') \tag{1.7}$$

$$\langle \vec{p} | \vec{p}' \rangle = \delta^{(3)} (\vec{p} - \vec{p}')$$
 (1.8)

and

$$\langle \vec{r} \, | \vec{p} \rangle \, = \left(\frac{1}{2\pi\hbar} \right)^{\frac{3}{2}} \, e^{\frac{i\vec{p} \cdot \vec{r}}{\hbar}} \quad . \tag{1.9}$$

The wave function of a particle in a state $|\phi\rangle$ is given in coordinate representation by:

$$\phi(\vec{r}) = \langle \vec{r} | \phi \rangle \tag{1.10}$$

and represents the probability amplitude for finding the particle at point \vec{r} . In coordinate representation, the operators $\hat{\vec{r}}$ and $\hat{\vec{p}}$ act as follows:

$$\langle \vec{r}|\hat{\vec{r}}|\phi\rangle = \vec{r}\langle \vec{r}|\phi\rangle = \vec{r}\phi(\vec{r})$$
 (1.11)

and

$$\langle \vec{r} | \vec{p} | \phi \rangle = \int d^3 p \langle \vec{r} | \hat{\vec{p}} | \vec{p} \rangle \langle \vec{p} | \phi \rangle$$

$$= \int d^3 p \vec{p} \langle \vec{r} | \vec{p} \rangle \langle \vec{p} | \phi \rangle$$

$$= \frac{\hbar}{i} \frac{\vec{\partial}}{\partial r} \int d^3 p \langle \vec{r} | \vec{p} \rangle \langle \vec{p} | \phi \rangle$$

$$= \frac{\hbar}{i} \frac{\vec{\partial}}{\partial r} \phi (\vec{r}) . \qquad (1.12)$$

Thus, in coordinate representation we may write:

$$\hat{\vec{r}} = \vec{r} \tag{1.13}$$

and

$$\hat{\vec{p}} = \frac{\hbar}{4} \frac{\partial}{\partial \vec{r}} \tag{1.14}$$

For a particle of mass m in a local potential $V(\vec{r})$, the Hamiltonian is

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + V(\vec{r}) \tag{1.15}$$

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