Quantum Many-Particle Systems

JOHN W. NEGELE

HENRI ORLAND

Quantum Many-Particle Systems

JOHN W. NEGELE
DEPARTMENT OF PHYSICS, MASSACHUSETTS INSTITUTE OF TECHNOLOGY

HENRI ORLAND
SERVICE DE PHYSIQUE THEORIQUE, CEA SACLAY, FRANCE

ADVANCED BOOK PROGRAM

ADDISON-WESLEY PUBLISHING COMPANY

THE ADVANCED BOOK PROGRAM
Redwood City, California • Menlo Park, California
Reading, Massachusetts • New York
Amsterdam • Don Mills, Ontario • Mexico City
Sydney • Bonn • Madrid • Singapore • Tokyo
San Juan • Wokingham, England

Publisher: Allan M. Wylde

Library of Congress Cataloging-in-Publication Data

Negele, John W.
Quantum many-particle systems.

(Frontiers in physics)
Bibliography: p.
Includes index.
1. Many-body problem. 2. Quantum field theory.
3. Integration, Functional 4. Stochastic processes.
5. Degree of freedom. I. Orland, Henri. II. Title.
III. Series.
QC174.17.P7N44 1987 530.1'44 87-17472
ISBN 0-201-12593-5

This book was typeset in TEX using the TEX sanserif font on a VAX 780 computer. Camera-ready copy output from an Imagen Image Station Laser Printer. TEXing was done by Roger Gilson.

BCDEFGHIJK-HA-898
0-201-12593-5

Frontiers in Physics

DAVID PINES / EDITOR

Volumes of the Series published from 1961 to 1973 are not officially numbered. The parenthetical numbers shown are designed to aid librarians and bibliographers to check the completeness of their holdings.

Titles published in this series prior to 1987 appear under either the W. A. Benjamin or the Benjamin/Cummings imprint; titles published since 1986 appear under the Addison-Wesley imprint.

(1)	N. Bloembergen	Nuclear Magnetic Relaxation: A Reprint Volume, 1961
(2)	G. F. Chew	S-Matrix Theory of Strong Interactions: A Lecture Note and Reprint Volume, 1961
(3)	R. P. Feynman	Quantum Electrodynamics: A Lecture Note and Reprint Volume, 1961 (8th printing, 1983).
(4)	R. P. Feynman	The Theory of Fundamental Processes: A Lecture Note Volume, 1961 (6th printing, 1980)
(5)	L. Van Hove, N. M. Hugenholtz, and L. P. Howland	Problems in Quantum Theory of Many-Particle Systems: A Lecture Note and Reprint Volume, 1961
(6)	D. Pines	The Many-Body Problem: A Lecture Note and Reprint Volume, 1961 (6th printing, 1982)
(7)	H. Frauenfelder	The Mössbauer Effect: A Review—with a Collection of Reprints, 1962
(8)	L. P. Kadanoff and G. Baym	Quantum Statistical Mechanics: Green's Function Methods in Equilibrium and Nonequilibrium Problems, 1962 (5th printing, 1981)
(9)	G. E. Pake	Paramagnetic Resonance: An Introductory Monograph, 1962 [cr. (42)—2nd edition]
(10)	P. W. Anderson	Concepts in Solids: Lectures on the Theory of Solids, 1963 (5th printing, 1982)
(11)	S. C. Frautschi	Regge Poles and S-Matrix Theory, 1963
(12)	R. Hofstadter	Electron Scattering and Nuclear and Nucleon Structure: A Collection of Reprints with an Introduction, 1963

(13)	A. M. Lane	Nuclear Theory: Pairing Force Correlations to Collective Motion, 1964
(14)	R. Omnès and M. Froissart	Mandelstam Theory and Regge Poles: An Introduction for Experimentalists, 1963
(15)	E. J. Squires	Complex Angular Momenta and Particle Physics: A Lecture Note and Reprint Volume, 1963
(16)	H. L. Frisch and J. L. Lebowitz	The Equilibrium Theory of Classical Fluids: A Lecture Note and Reprint Volume, 1964
(17)	M. Gell-Mann and Y. Ne'eman	The Eightfold Way: (A Review—with a Collection of Reprints), 1964
(18)	M. Jacob and G. F. Chew	Strong-Interaction Physics: A Lecture Note Volume, 1964
(19)	P. Nozières	Theory of Interacting Fermi Systems, 1964
(20)	J. R. Schrieffer	Theory of Superconductivity, 1964 (revised 3rd printing, 1983)
(21)	N. Bloembergen	Nonlinear Optics: A Lecture Note and Reprint Volume, 1965 (4th printing, 1981)
(22)	R. Brout	Phase Transitions, 1965
(23)	I. M. Khalatnikov	An Introduction to the Theory of Superfluidity, 1965
(24)	P. G. deGennes	Superconductivity of Metals and Alloys, 1966
(25)	W. A. Harrison	Pseudopotentials in the Theory of Metals, 1966 (2nd printing, 1971)
(26)	V. Barger and D. Cline	Phenomenological Theories of High Energy Scattering: An Experimental Evaluation, 1967
(27)	P. Choquàrd	The Anharmonic Crystal, 1967
(28)	T. Loucks	Augmented Plane Wave Method: A Guide to Performing Electronic Structure Calculations—A Lecture Note and Reprint Volume, 1967
(29)	Y. Ne'eman	Algebraic Theory of Particle Physics: Hadron Dynamics in Terms of Unitary Spin Currents, 1967
(30)	S. L. Adler and R. F. Dashen	Current Algebras and Applications to Particle Physics, 1968
(31)	A. B. Migdal	Nuclear Theory: The Quasiparticle Method, 1968
(32)	J. J. J. Kokkedee	The Quark Model, 1969
(33)	A. B. Migdal and V. Krainov	Approximation Methods in Quantum Mechanics, 1969
(34)	R. Z. Sagdeev and A. A. Galeev	Nonlinear Plasma Theory, 1969
(35)	J. Schwinger	Quantum Kinematics and Dynamics, 1970
(36)	R. P. Feynman	Statistical Mechanics: A Set of Lectures, 1972 (7th printing, 1982)
(37)	R. P. Feynman	Photo-Hadron Interactions, 1972
(38)	E. R. Caianiello	Combinatorics and Renormalization in Quantum Field Theory, 1973
(39)	G. B. Field, H. Arp, and J. N. Bahcall	The Redshift Controversy, 1973 (2nd printing, 1976)

(40)	D. Horn and F. Zachariasen	Hadron Physics at Very High Energies, 1973
(41)	S. Ichimaru	Basic Principles of Plasma Physics: A Statistical Approach, 1973 (2nd printing, with revisions, 1980)
(42)	G. E. Pake and T. L. Estle	The Physical Principles of Electron Paramagnetic Resonance, 2nd Edition, completely revised, enlarged, and reset, 1973 [cf. (9)—1st edition]

Volumes published from 1974 onward are being numbered as an integral part of the bibliography.

43	R. C. Davidson	Theory of Nonneutral Plasmas, 1974
44	S. Doniach and E. H. Sondheimer	Green's Functions for Solid State Physicists, 1974 (2nd printing, 1978)
45	P. H. Frampton	Dual Resonance Models, 1974
46	S. K. Ma	Modern Theory of Critical Phenomena, 1976 (5th printing, 1982)
47	D. Forster	Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions, 1975 (3rd printing, 1983)
48	A. B. Migdal	Qualitative Methods in Quantum Theory, 1977
49	S. W. Lovesey	Condensed Matter Physics: Dynamic Correlations, 1980
50	L. D. Faddeev and A. A. Slavnov	Gauge Fields: Introduction to Quantum Theory, 1980
51	P. Ramond	Field Theory: A Modern Primer, 1981 (4th printing, 1983)
52	R. A. Broglia and A. Winther	Heavy Ion Reactions: Lecture Notes Vol. I: Elastic and Inelastic Reactions, 1981
53	R. A. Broglia and A. Winther	Heavy Ion Reactions: Lecture Notes Vol. II, *in preparation*
54	Howard Georgi	Lie Algebras in Particle Physics: From Isospin to Unified Theories, 1982
55	P. W. Anderson	Basic Notions of Condensed Matter Physics, 1983
56	Chris Quigg	Gauge Theories of the Strong, Weak, and Electromagnetic Interactions, 1983
57	S. I. Pekar	Crystal Optics and Additional Light Waves, 1983
58	S. J. Gates, M. T. Grisaru, M. Roček, and W. Siegel	Superspace *or* One Thousand and One Lessons in Supersymmetry, 1983
59	R. N. Cahn	Semi-Simple Lie Algebras and Their Representations, 1984
60	G. G. Ross	Grand Unified Theories, 1984
61	S. W. Lovesey	Condensed Matter Physics: Dynamic Correlations, 2nd Edition, 1986
62	P. H. Frampton	Gauge Field Theories, 1986
63	J. I. Katz	High Energy Astrophysics, 1987
64	T. J. Ferbel	Experimental Techniques in High Energy Physics, 1987

T. Appelquist, A. Chodos, and P. G. O. Freund	Modern Kaluza-Klein Theories, 1987
G. Parisi	Statistical Field Theory, 1988
R. C. Richardson E. N. Smith	Techniques in Low-Temperature Condensed Matter Physics, 1988
J. W. Negele H. Orland	Quantum Many-Particle Systems, 1987

EDITOR'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 stochastic 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 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.

Portions of earlier drafts of the manuscript were typeset in TEX by Meredith Pollard, Karl Kowalski, and Dany Bunel. The majority of the TEX typesetting, as well as the final editing, improving the layout and appearance of formulas, and preparation of tables was performed by Roger L. Gilson, to whom the authors are particularly indebted for his outstanding work. We also wish to acknowledge the excellent technical art work by Don Souza and the work of the Addison-Wesley production department in providing the final copy.

JOHN NEGELE
HENRI ORLAND

CONTENTS

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 $\mathcal{H}$. This Hilbert space $\mathcal{H}$ is the vector space of complex, square integrable functions, defined in configuration space. Using Dirac notation, the scalar product of vectors in $\mathcal{H}$ 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 $\mathcal{H}$ if the norm of $|\phi\rangle$ is finite:

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

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 $\mathcal{H}$, because their norm is not finite, they span the whole Hilbert space $\mathcal{H}$. 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 $\mathcal{H}$.

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:

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

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

and

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

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:

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

and

$$\begin{aligned}\langle\vec{r}|\hat{\vec{p}}|\phi\rangle &= \int d^3p\langle\vec{r}|\hat{\vec{p}}|\vec{p}\rangle\langle\vec{p}|\phi\rangle \\ &= \int d^3p\vec{p}\langle\vec{r}|\vec{p}\rangle\langle\vec{p}|\phi\rangle \\ &= \frac{\hbar}{i}\frac{\vec{\partial}}{\partial r}\int d^3p\langle\vec{r}|\vec{p}\rangle\langle\vec{p}|\phi\rangle \\ &= \frac{\hbar}{i}\frac{\vec{\partial}}{\partial r}\phi(\vec{r}) \quad .\end{aligned} \tag{1.12}$$

Thus, in coordinate representation we may write:

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

and

$$\hat{\vec{p}} = \frac{\hbar}{i}\frac{\partial}{\partial\vec{r}} \quad . \tag{1.14}$$

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

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