

Henk T.C. Stoof
Koos B. Gubbels
Dennis B.M. Dickerscheid

Theoretical and Mathematical Physics

Ultracold Quantum Fields

 Springer

Theoretical and Mathematical Physics

The series founded in 1975 and formerly (until 2005) entitled *Texts and Monographs in Physics* (TMP) publishes high-level monographs in theoretical and mathematical physics. The change of title to *Theoretical and Mathematical Physics* (TMP) signals that the series is a suitable publication platform for both the mathematical and the theoretical physicist. The wider scope of the series is reflected by the composition of the editorial board, comprising both physicists and mathematicians.

The books, written in a didactic style and containing a certain amount of elementary background material, bridge the gap between advanced textbooks and research monographs. They can thus serve as basis for advanced studies, not only for lectures and seminars at graduate level, but also for scientists entering a field of research.

Editorial Board

W. Beiglböck, Institute of Applied Mathematics, University of Heidelberg, Germany
J.-P. Eckmann, Department of Theoretical Physics, University of Geneva, Switzerland
H. Grosse, Institute of Theoretical Physics, University of Vienna, Austria
M. Loss, School of Mathematics, Georgia Institute of Technology, Atlanta, GA, USA
S. Smirnov, Mathematics Section, University of Geneva, Switzerland
L. Takhtajan, Department of Mathematics, Stony Brook University, NY, USA
J. Yngvason, Institute of Theoretical Physics, University of Vienna, Austria

For other titles published in this series, go to
www.springer.com/series/720

Henk T.C. Stoof • Koos B. Gubbels •
Dennis B.M. Dickerscheid

Ultracold Quantum Fields

 Springer

Henk T.C. Stoof
Utrecht University
Institute for Theoretical Physics
Leuvenlaan 4
3584 CE Utrecht
The Netherlands

Koos B. Gubbels
Utrecht University
Institute for Theoretical Physics
Leuvenlaan 4
3584 CE Utrecht
The Netherlands

Dennis B.M. Dickerscheid
Utrecht University
Institute for Theoretical Physics
Leuvenlaan 4
3584 CE Utrecht
The Netherlands

Library of Congress Control Number: 2008936953

ISSN 1864-5879
ISBN-13 978-1-4020-8762-2 (HB)
ISBN-13 978-1-4020-8763-9 (e-book)

Published by Springer Science+Business Media B.V.
P.O. Box 17, 3300 AA Dordrecht, The Netherlands
In association with
Canopus Publishing Limited,
27 Queen Square, Bristol BS1 4ND, UK

www.springer.com and www.canopusbooks.com

All Rights Reserved
© 2009 Canopus Academic Publishing Limited
No part of this work may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, microfilming, recording or otherwise, without written permission from the Publisher, with the exception of any material supplied specifically for the purpose of being entered and executed on a computer system, for exclusive use by the purchaser of the work.

Preface

On June 19th 1999, the European Ministers of Education signed the Bologna Declaration, with which they agreed that the European university education should be uniformized throughout Europe and based on the two-cycle bachelor-master's system. The Institute for Theoretical Physics at Utrecht University quickly responded to this new challenge and created an international master's programme in Theoretical Physics which started running in the summer of 2000. At present, the master's programme is a so-called prestige master at Utrecht University, and it aims at training motivated students to become sophisticated researchers in theoretical physics. The programme is built on the philosophy that modern theoretical physics is guided by universal principles that can be applied to any subfield of physics. As a result, the basis of the master's programme consists of the obligatory courses Statistical Field Theory and Quantum Field Theory. These focus in particular on the general concepts of quantum field theory, rather than on the wide variety of possible applications. These applications are left to optional courses that build upon the firm conceptual basis given in the obligatory courses. The subjects of these optional courses include, for instance, Strongly-Correlated Electrons, Spintronics, Bose-Einstein Condensation, The Standard Model, Cosmology, and String Theory. The master's programme in Theoretical Physics is preceded by a summer school that is organized in the last two weeks of August to help prospective students prepare for the intensive master's courses. Short courses are offered in quantum mechanics, electrodynamics, statistical physics and computational methods, and are aimed at overcoming possible deficiencies in any of these subjects.

The idea of writing this book came about during the period of 2000-2005, when one of us was teaching the course on Statistical Field Theory for the above-mentioned master's programme in Theoretical Physics. The lecture notes used for this course were an extended version of the lecture notes for the Les Houches summer school on *Coherent Atomic Matter Waves* that took place in 1999. Although these lecture notes, in combination with the lectures and tutorials, were supposed to be self-contained, in practice students often expressed a desire for more calculational details, applications and background material.

It was also during this period that the research field of ultracold atomic gases, pushed in particular by the impressive experimental progress since the first observation of Bose-Einstein condensation in 1995, made rapid developments that helped shape the field as we know it today. Nowadays, many experimental groups around the world can routinely prepare quantum degenerate gases of bosons, fermions, and various mixtures thereof. Moreover, the microscopic details of these atomic gases are well known and can be controlled very accurately, leading to the exciting possibility of addressing fundamental questions about interacting quantum systems in unprecedented detail. Because of this, it is also possible to perform *ab initio* theoretical calculations that allow for a quantitative comparison with experiments, such that the connection between theory and experiment is particularly close in this field of physics. There are various ways to perform these calculations, but most research topics can be dealt with in a unified manner by using quantum field theoretical methods. Although there are several textbooks available on quantum field theory, to date there does not exist a textbook that applies advanced quantum field theory, and in particular its functional formulation, to ultracold atomic quantum gases.

The level of this textbook is geared to students beginning with their master's and to graduate students already working in the field of ultracold atoms. To overcome the differences in educational background between the various students, the book has been divided into three parts which can in principle be read independently of each other. The first part briefly introduces elementary concepts from mathematics, statistical physics, and quantum mechanics which are indispensable for a full understanding of the rest of the book. Various important concepts that return later in the language of quantum field theory are introduced here in a more familiar setting. At the end of each chapter, there are references to various excellent textbooks that provide more background on each of the discussed topics. This part of the book is particularly aimed at the Utrecht Summer School in Theoretical Physics and provides the participants with the appropriate background material for the obligatory field theory courses that form the basis of the master's programme in Theoretical Physics. The second part of the book is devoted to laying the conceptual basis of the functional formulation of quantum field theory from a condensed-matter point of view. This part forms the core of the above mentioned Statistical Field Theory course, in which also the canonical topics of superfluidity and superconductivity of interacting Bose and Fermi gases are treated. The third part of the book is then largely aimed at applications of the developed theoretical techniques to various aspects of ultracold quantum gases that are currently being explored, such that the chosen topics give an idea of the present status of the field. It is our hope that, after having read this part, students will be well prepared to enter this exciting field of physics and be able to start contributing themselves to the rapid developments that are taking place today.

The knowledge presented in this book has been acquired through many collaborations and interactions with our colleagues over the last two decades. Here, we would like to sincerely thank everybody involved for that. It is unfortunately impossible to give everybody the proper credit for their contribution. As a result, both in this short word of thanks, as well as in citing references throughout the book,

subjective choices are made and important contributions left out. Our main aim in citing has been to provide students with interesting additional reading material, and not to give an exhaustive overview of the enormous amount of literature in the field of ultracold atoms. We hope to be forgiven for that. With this in mind, we thank the following persons together with the members of their groups, namely Immanuel Bloch, Georg Bruun, Keith Burnett, Eric Cornell, Peter Denteneer, Steve Girvin, Randy Hulet, Allan MacDonald, Cristiane Morais Smith, Guthrie Partridge, Chris Pethick, Subir Sachdev, Cass Sackett, Jörg Schmiedmayer, Kevin Strecker, Peter van der Straten, Stefan Vandoren, and Eugene Zaremba for the collaborations that have led to joint publications. We also thank the postdoctoral researchers Usama Al Khawaja, Jens Andersen, Behnam Farid, Masud Haque, Jani Martikainen, Pietro Massignan, and Nick Proukakis, and the graduate students Michel Bijlsma, Marianne Houbiers, Michiel Bijlsma, Rembert Duine, Dries van Oosten, Gianmaria Falco, Lih-King Lim, Mathijs Romans, Michiel Snoek, Arnaud Koetsier, and Jeroen Diederix of the Utrecht Quantum Fluids and Solids Group. In particular, we mention Usama Al Khawaja, Rembert Duine, Dries van Oosten, and Nick Proukakis for their direct contributions to the recent applications that are discussed in the third part of the book. We also thank our experimental colleagues Immanuel Bloch, Eric Cornell, Randy Hulet, Wolfgang Ketterle, and Wenhui Li, for kindly providing us with the experimental data that has allowed us to compare the theory to experiment in this book. We thank Rembert Duine for providing several exercises and for many helpful comments on the manuscript. Furthermore we express our gratitude to Tom Spicer from Canopus Publishing for all his effort in bringing forth this book. We are especially grateful to Randy Hulet for more than 15 years of friendship and fruitful collaboration, from which we benefitted greatly, both personally and professionally.

Finally, we wish to thank Jolanda, Maurice, Inèz, Joke, Harry, Winy, Theo, Roos, Hein, Paulien, Ryoko, Miguel, and the rest of our families and friends for all their unconditional support and for sharing the joy of life.

Utrecht, May 2008

Henk Stoof
Koos Gubbels
Dennis Dickerscheid

Contents

1	Introduction	1
1.1	Ultracold Atomic Quantum Gases	2
1.2	Outline	6
1.2.1	Part One	6
1.2.2	Part Two	8
1.2.3	Part Three	10
2	Gaussian Integrals	15
2.1	The Gaussian Integral over Real Variables	15
2.1.1	Generating Function	16
2.1.2	Multi-Dimensional Gaussian Integral	18
2.2	Complex Analysis	20
2.2.1	Differentiation and Contour Integrals	20
2.2.2	Laurent Series and the Residue Theorem	22
2.3	Gaussian Integrals over Complex Variables	25
2.4	Grassmann Variables	26
2.5	Problems	28
3	Quantum Mechanics	33
3.1	Hilbert Spaces	34
3.2	Observables	35
3.3	Schrödinger vs. Heisenberg Picture	39
3.4	Bosonic Harmonic Oscillator	41
3.5	Creation and Annihilation Operators	42
3.6	Three-Dimensional Harmonic Oscillator	43
3.7	Coherent States	45
3.8	Fermionic Harmonic Oscillator	47
3.9	Spin	49
3.10	Perturbation Theory	52
3.11	Scattering Theory	53
3.12	Many-particle Quantum Mechanics	57

3.13	Problems	57
4	Statistical physics	59
4.1	Legendre Transformations	59
4.2	Statistical Physics	61
4.2.1	Spin Chain	61
4.2.2	Canonical Ensemble	64
4.2.3	Grand-Canonical Ensemble	65
4.3	Ideal Gases	67
4.3.1	Ideal Maxwell-Boltzmann Gas	68
4.3.2	Ideal Bose Gas: Bose-Einstein Condensation	72
4.3.3	Ideal Fermi Gas	77
4.4	Density Matrix	80
4.5	Problems	83
5	Path Integrals	85
5.1	Functionals and Functional Derivatives	85
5.2	Principle of Least Action	87
5.3	Phase-Space Representation	89
5.4	The Feynman Path Integral	90
5.4.1	Continuum Limit and Fluctuation Expansion	93
5.4.2	Gel'fand-Yaglom Method	95
5.5	Matrix Elements and Time Ordering	99
5.6	Quantum-Mechanical Partition Function	103
5.7	Expectation Values	104
5.8	Hubbard-Stratonovich Transformation	105
5.9	Problems	106
6	Second Quantization	109
6.1	Many-Body Hamiltonian	110
6.2	Fock Space	111
6.3	Creation and Annihilation Operators	114
6.3.1	Second-Quantized Hamiltonian	116
6.3.2	Field Operators	117
6.4	Equivalence of First and Second Quantization	119
6.5	Coherent States	122
6.6	Problems	125
7	Functional Integrals	131
7.1	Grand-Canonical Partition Function	131
7.2	Ideal Quantum Gases	134
7.2.1	Semiclassical Method	135
7.2.2	Matsubara Expansion	137
7.2.3	Green's Function Method	142
7.3	Wick's Theorem	146
7.4	Problems	149

8	Interactions and Feynman Diagrams	151
8.1	Quasiparticles	152
8.1.1	The Lehmann Representation	153
8.1.2	The Spectral-Weight Function	156
8.1.3	Collective Excitations	158
8.2	Perturbation Theory	159
8.3	Dyson's Equation	164
8.4	Hartree-Fock Approximation	167
8.5	Variational Approach	168
8.6	Hubbard-Stratonovich Transformation	171
8.6.1	Hartree Theory	172
8.6.2	Fock Theory	176
8.6.3	Hartree-Fock Theory for an Atomic Fermi Gas	178
8.7	The Jellium Model	182
8.7.1	Field-Theory Approach	184
8.7.2	Effective Action	185
8.7.3	Dispersion and Screened Coulomb Interaction	188
8.8	Problems	190
9	Landau Theory of Phase Transitions	193
9.1	Ising Model in d Dimensions	194
9.2	Landau Approach	199
9.3	Hubbard-Stratonovich Transformation	203
9.4	Gaussian Fluctuations	205
9.5	Spontaneous Symmetry Breaking	208
9.6	Problems	211
10	Atomic Physics	213
10.1	Atomic Structure	214
10.1.1	Fine Structure	215
10.1.2	Hyperfine Structure	216
10.2	Zeeman Effect	217
10.3	Two-body Scattering in Vacuum	219
10.3.1	Two-Body Transition Matrix	220
10.3.2	Partial-Wave Expansion	222
10.3.3	Scattering from a Square-Well Potential	224
10.4	Two-Body Scattering in a Medium	227
10.5	Physical Regimes	230
10.6	Problems	232
11	Bose-Einstein Condensation	235
11.1	Definitions for a Bose-Einstein Condensate	236
11.2	Superfluidity	238
11.2.1	Landau Criterion	239
11.2.2	Superfluid Density	240

11.3	Field-Theory Approach	241
11.3.1	Bogoliubov Theory and the Gross-Pitaevskii Equation	243
11.3.2	Dyson Equation	245
11.3.3	Quasiparticle Dispersion	246
11.4	Thermodynamic Potential for Bosons	248
11.5	Bogoliubov-de Gennes Equation	251
11.6	Popov Theory	253
11.7	Hydrodynamic-Like Approach	255
11.7.1	Time-Dependent Gross-Pitaevskii Equation	255
11.7.2	Collective Modes	257
11.8	Rotating Bose-Einstein Condensates	259
11.9	Attractive Interactions	262
11.9.1	Effective Action	263
11.9.2	Breathing Mode	265
11.9.3	Metastability of the Condensate	268
11.10	Problems	269
12	Condensation of Fermionic Pairs	273
12.1	Introduction	273
12.2	Thouless Criterion	274
12.3	Hubbard-Stratonovich Transformation	276
12.4	Bardeen-Cooper-Schrieffer Theory	278
12.5	Critical Temperature	280
12.6	Gap Equation	283
12.7	Thermodynamic Potential for Fermions	286
12.8	The BEC-BCS Crossover	288
12.8.1	Theoretical Results	289
12.8.2	Comparison with Experiment	292
12.9	Problems	294
13	Symmetries and Symmetry Breaking	299
13.1	Effective Actions	300
13.2	Noether's Theorem	303
13.3	Ward Identities	305
13.3.1	Hugenholtz-Pines Theorem	309
13.3.2	Bragg Scattering	310
13.4	RF Spectroscopy	313
13.4.1	Second-Order Perturbation Theory	317
13.4.2	Ladder Summations	319
13.4.3	Absence of Clock Shift	320
13.4.4	Absence of Vertex Corrections	324
13.5	Phase Diffusion	325
13.6	Problems	328

14 Renormalization Group Theory	329
14.1 The Renormalization-Group Transformation	330
14.1.1 Scaling	333
14.1.2 Interactions	335
14.2 Quantum Effects	340
14.2.1 Interactions	343
14.2.2 Nonuniversal Quantities	346
14.3 Renormalization Group for Fermions	347
14.3.1 Renormalization-Group Equations	348
14.3.2 Extremely-Imbalanced Case	350
14.3.3 Homogeneous Phase Diagram	352
14.4 Problems	354
15 Low-Dimensional Systems	359
15.1 Modified Popov Theory	360
15.1.1 Phase Fluctuations	360
15.1.2 Many-Body T Matrix	362
15.1.3 Long-Wavelength Physics	363
15.2 Comparison with Popov Theory	364
15.2.1 One Dimension	364
15.2.2 Two Dimensions	366
15.2.3 Three Dimensions	370
15.3 Vortices in Two Dimensions	371
15.4 Kosterlitz-Thouless Phase Transition	373
15.5 Trapped Bose Gases	377
15.5.1 Density Profiles	379
15.5.2 Phase Fluctuations	381
15.5.3 Comparison with Exact Results	385
15.6 Problems	389
16 Optical Lattices	391
16.1 Introduction	392
16.2 Coupling between Atoms and Light	393
16.2.1 Two-Level Approximation	393
16.2.2 Fine Structure	395
16.3 Band Structure	397
16.4 Hubbard Models	397
16.5 Superfluid-Mott Insulator Transition	400
16.5.1 Bogoliubov Approximation	402
16.5.2 Decoupling Approximation	406
16.5.3 Hubbard-Stratonovich Transformation	413
16.6 Fluctuations	418
16.6.1 Mott Insulator	420
16.6.2 Superfluid Phase	421
16.7 Bragg Spectroscopy	423

16.8 Problems	428
17 Feshbach Resonances	431
17.1 Example of a Feshbach Resonance	432
17.2 Bare Atom-Molecule Theory	439
17.3 Ladder Summations	447
17.4 Effective Atom-Molecule theory	453
17.4.1 Scattering Properties	454
17.4.2 Bound-State Energy	455
17.4.3 Molecular Density of States	456
17.5 Bogoliubov Theory for the Bose-Einstein Condensed Phase	458
17.6 Experiments	462
17.7 Josephson Frequency	466
17.8 Problems	471
References	475
Index	481

Chapter 1

Introduction

The field of many-body quantum physics has a long history of fundamental discoveries, many of which have gone far beyond our wildest imagination. These include the study of novel states of matter, the observation of previously unseen phase transitions, and the discovery of new macroscopic quantum effects which arise when the intriguing rules of quantum mechanics are no longer restricted to the subatomic world, but rather determine the collective behavior of systems that are observable with the naked eye. In the past, it has often been proven difficult to obtain the underlying theory that yields an accurate description of the collective quantum phenomenon on the microscopic level. A good example is the discovery of superfluidity in liquid ^4He by Pyotr Kapitsa, John Allen and Don Misener in 1938 [1, 2], where superfluidity refers to the fact that the liquid can flow without experiencing resistance, which leads for example to the spectacular fountain effect [3]. Since the atoms interact very strongly, the precise internal state of liquid helium is notoriously difficult to determine.

An exception to this rule, however, is the question of what happens to a noninteracting gas of bosons when it is cooled down to zero temperature. This question was already theoretically answered long before the discovery of superfluid helium. In fact, the answer was already obtained before the final formulation of quantum mechanics and before a good understanding of phase transitions was achieved. The question found its origin in the early 1920s, when Satyendra Bose introduced a different way of counting microstates than was usual in classical statistical mechanics [4]. In this way, he was able to rederive Planck's law for the energy spectrum of black-body radiation. Albert Einstein generalized this result in 1924 to the case of indistinguishable noninteracting massive bosons by including the effect of particle-number conservation, which led to the famous Bose-Einstein distribution [5]. Einstein also realized that a remarkable consequence of this Bose-Einstein distribution is that below a certain critical temperature

$$T_c = \frac{2\pi}{\zeta(3/2)^{2/3}} \frac{\hbar^2 n^{2/3}}{mk_B}, \quad (1.1)$$

it predicts that a macroscopic fraction of the bosons occupies the same one-particle quantum state. Here \hbar is Dirac's constant, i.e. Planck's constant h divided by 2π , m is the mass of the particles, k_B is Boltzmann's constant, n is the particle density of the gas, and $\zeta(3/2) \simeq 2.612$. This promotes the wavefunction of that particular one-particle quantum state to the macroscopic level and gives rise to a new state of matter that is known as a Bose-Einstein condensate or BEC. It is believed that Bose-Einstein condensation is also the mechanism behind the superfluid behavior of liquid helium. However, in liquid helium the density is high and the interaction between the helium atoms is very strong, such that it is far from an ideal Bose gas. As a result, Einstein's theory needs to be modified considerably, and so far the properties of liquid helium have been impossible to determine analytically. Furthermore, the presence of a macroscopic occupation of a one-particle quantum state has never been directly observed in this system.

The microscopic theory for the phenomenon of superconductivity, which was discovered experimentally in 1911 by Heike Kamerlingh Onnes [6], also turned out to be an extremely challenging task. After superconductivity had been found it was studied experimentally in a wide variety of metals, leading to many important discoveries. A crucial example, known as the Meissner effect [7], reveals that a superconductor is a perfect diamagnet because any applied magnetic field is completely expelled from its interior. It took almost fifty years before John Bardeen, Leon Cooper, and Robert Schrieffer [8] finally realized that superconductivity is actually caused by a Bose-Einstein condensation of loosely bound fermion pairs. The Bardeen-Cooper-Schrieffer or BCS theory of superconductivity is based on the description of the electrons in a metal as a gas, where the electrons need an effectively attractive interaction to form stable Cooper pairs. Physically, this attractive interaction is the result of the rather subtle effect that the electrons can deform the positively charged ionic lattice that is present in the metal. It is perhaps ironic that if the theory was invented before the experimental discovery of Kamerlingh Onnes, physicists would probably have never started looking for superconductivity in metals, because electrons do not usually form pairs due to their strongly repulsive Coulomb interaction. In 1986, high-temperature superconductors were discovered in ceramic materials [9]. However, the precise microscopic mechanism governing these cuprates is still not clear today.

1.1 Ultracold Atomic Quantum Gases

From the moment that Bose-Einstein condensation was finally achieved in trapped dilute gases of bosonic alkali atoms in 1995 by the groups of Eric Cornell and Carl Wieman, Randy Hulet, and Wolfgang Ketterle [10, 11, 12], a completely new category of systems became available for studying macroscopic quantum effects. The most important ingredients for this accomplishment were the precooling of the atoms using laser cooling [13], the trapping of the atoms in a magnetic trap [14], the final cooling of the atoms using evaporative cooling [15], and the imaging of the