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Ultracold Quantum Fields

Springer

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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 abovementioned 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.

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Utrecht, May 2008

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Koos Gubbels
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Contents

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 ^{4}He 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

$$T_{\mathrm{c}} = \frac{2\pi}{\zeta(3/2)^{2/3}} \frac{\hbar^2 n^{2/3}}{m k_{\mathrm{B}}} , \tag{1.1}$$

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 gas either in situ or after expansion. In particular, the trapping of atoms and cooling by means of evaporation turned out to be crucial. The reason for this is hidden in the prediction of (1.1) that for the relevant low densities of $10^{12} - 10^{15}$ atoms per cubic centimeter, extremely low temperatures of $1 - 100$ nK are required to reach Bose-Einstein condensation. These are impossible to achieve if the gas is in contact with material walls. Once the atomic gas is magnetically or optically trapped, evaporative cooling can be relatively easily implemented by lowering the trap depth, so that only the most energetic atoms can escape from the trap and the remaining gas cools after re-thermalization. Because of their complete isolation these ultracold gases are, unlike solid-state systems, very clean in the sense that there are essentially no impurities unless deliberately added. Moreover, due to the low densities, interaction effects can be sufficiently small as to be treated with perturbation theory. As a result, it is possible to obtain an accurate microscopic description of these ultracold atomic quantum gases using advanced field-theoretical methods. This is one of the main goals of this book. Furthermore, these systems have also turned out to be very flexible, as the external trapping potential and the interatomic interaction are under complete experimental control. This allows for a systematic study of an enormous variety of interesting many-body systems, ranging from weakly interacting to strongly interacting, from one dimensional to three dimensional, from homogeneous to periodic, where the microscopic parameters are always precisely known and tunable.

Shortly after the achievement of Bose-Einstein condensation, it was predicted that the superfluid regime could also be reached in a dilute gas of fermionic atoms [16]. However, the realization of this intriguing possibility turned out to be even more difficult than reaching BEC. This comes about because the previously mentioned BCS theory for the condensation of fermion pairs predicts that the critical temperature is exponentially dependent on the inverse of the (negative) scattering length a, which describes the strength of the attractive interactions between the fermions. Namely, we have that

$$T_{\mathrm{c}} = \frac{4(9\pi)^{1/3}}{\mathrm{e}^{2-\gamma}} \frac{\hbar^2 n^{2/3}}{m k_{\mathrm{B}}} \exp\left\{ -\frac{\pi}{2k_{\mathrm{F}}|a|} \right\} , \tag{1.2}$$

where $\gamma \simeq 0.5772$ is Euler's constant and $k_{\mathrm{F}} = (3\pi^2 n)^{1/3}$ is the Fermi wavevector. This in general shifts the required temperature beyond the reach of experiments with ultracold gases, which are dilute and therefore usually characterized by $k_{\mathrm{F}}|a| \ll 1$. Also, it turns out that it is more difficult to obtain an experimental signature for the onset of the superfluid phase in the Fermi system than in the case of bosons. The use of Feshbach resonances, which were theoretically discovered in the alkalis by Eite Tiesinga, Boudewijn Verhaar and Henk Stoof [17], has fortunately solved both of these problems.

In a Feshbach-resonant atomic collision, two atoms collide and virtually form a long-lived molecule with a different spin configuration than the incoming two atoms, where the molecule ultimately decays into two atoms again. The scattering properties of the colliding atoms depend very sensitively on the energy difference of the molecular state with respect to the threshold of the two-atom continuum. This energy difference is known as the detuning and can be changed with an applied magnetic field, because the different spin states of the incoming atoms and the molecule lead to a different Zeeman shift. In particular, the Feshbach resonance allows for a precise tuning of the scattering length a, which opens up the exciting possibility of reaching the superfluid regime for fermionic atoms. Namely, the interactions can be made strongly attractive, i.e. $k_{\mathrm{F}}|a| \gg 1$, which leads to a critical temperature comparable to that of an atomic Bose gas. This objective was ultimately achieved in a series of ground-breaking experiments by the group of Debbie Jin using ^{40}K [18] and the groups of Wolfgang Ketterle, John Thomas, Rudi Grimm, Christophe Salomon, and Randy Hulet using ^{6}Li [19, 20, 21, 22, 23]. A number of these experiments exploit the Feshbach resonance to its fullest by also using it to actually observe the Bose-Einstein condensate of Cooper pairs.

To understand the latter better, we realize that there is an intimate connection between the Bose-Einstein condensation of bosons and the Bose-Einstein condensation of loosely-bound fermionic Cooper pairs. Note that the first is responsible for the superfluidity of weakly-interacting Bose gases, while the latter is responsible for both the superfluidity of weakly-interacting Fermi gases and the superconductivity of metals. The connection between the two condensates might have already been anticipated from the fact that the critical temperatures in (1.1) and (1.2) are very similar in the strongly-interacting limit $k_{\mathrm{F}}|a| \gg 1$. Moreover, the atomic Bose-Einstein condensation experiments make use of alkali atoms, which are hydrogen-like composite bosons that can be seen as an outer electron bond to an inner core consisting of the fermionic nucleus and a surrounding electron cloud with an even number of electrons. As a result, a condensate of bosonic atoms can also be seen as a Bose-Einstein condensate of tightly-bound fermion pairs. We may thus conclude that fermionic superconductivity and bosonic superfluidity are in fact two sides of the same coin, differing only in the strength of the attraction between the fermions. If the attraction is weak, the Cooper pairs are very weakly bound and their size is much larger than the average interparticle distance $n^{-1/3}$, which is also called the superconductivity or BCS limit. However, in the superfluidity or BEC limit, the attraction is strong and the pairs are much smaller than the average interparticle distance, such that they act as composite bosons.

With an atomic Fermi gas near a Feshbach resonance, we can now for the first time experimentally explore both sides of the coin in one and the same system, i.e. study the full physics of the BEC-BCS crossover as first envisaged by David Eagles and Tony Leggett [24, 25]. By changing the magnetic field we can go from a large positive detuning above the Feshbach resonance, in which case we have no stable molecular state and a weakly-attractive interaction, to a large negative detuning below the Feshbach resonance, in which case there exists a deeply bound molecular state. In this manner, we thus evolve from a condensate of loosely bound Cooper pairs to a condensate of tightly bound molecules. The evolution between these two extremes turns out to be a smooth crossover, such that the transition between diatomic molecules and Cooper pairs is continuous. As mentioned above, this feature has been used to detect the Bose-Einstein condensate of Cooper pairs, by conveniently converting it into a Bose-Einstein condensate of tightly bound bosonic molecules with the use of an adiabatic magnetic-field sweep across the Feshbach resonance. The reason why it is so easy to observe a condensate of ideal bosons can be readily understood from their macroscopic occupation of the same one-particle ground state, which has a minimal kinetic energy. As a result, the atoms or diatomic molecules hardly spread out upon releasing the condensate from the trap, which leads to a very distinct peak in the velocity distribution at low velocities. The first atomic Bose-Einstein condensate was observed [10] in exactly the same manner.

Presently, there are many exciting directions that are being explored with ultracold atomic gases. First of all, we remark that the fermionic atoms that form the pairs in the BEC-BCS crossover must have two different spin states due to the Pauli principle. As a result, this crossover physics is usually studied in a balanced Fermi mixture with an equal number of atoms in each of the two different spin states. At the moment, a hot topic is to explore what precisely happens to the gas when the Fermi mixture becomes imbalanced, so that it is impossible for all the atoms to pair up simultaneously. Understanding this problem may also shed light on the physics in the core of a neutron star, where an imbalanced mixture of free quarks with attractive interactions can exist. These quarks may then form what is known as a color superconductor [26].

Another important direction is associated with the possibility of creating an intense standing wave of light with counter-propagating laser beams. This gives rise to a periodic potential for the atoms due to the Stark effect, which is also known as an optical lattice [27]. These optical lattices are very interesting for various reasons. An important one is that they can be used to simulate ionic lattices, which offers the opportunity to explore various aspects of solid-state physics in the very controlled environment of ultracold atoms. A particularly exciting possibility in this respect is to study systematically the microscopic models that have been proposed to govern high-temperature superconductors. Moreover, optical lattices can also be used to create low-dimensional atomic gases. In particular, with a very deep two-dimensional optical lattice we can make a two-dimensional array of one-dimensional gases, whereas a one-dimensional optical lattice creates a one-dimensional stack of two-dimensional systems. Low-dimensional quantum gases are interesting, because they often give rise to intriguing strongly-correlated behavior that is very different from the three-dimensional case. In various cases, low-dimensional many-body systems even allow for exact theoretical solutions.

Also of much interest in current research is the use of Feshbach resonances between two different atomic species to create ultracold heteronuclear molecules. These kind of molecules can have a large electronic dipole moment, which leads to a strong anisotropic dipole-dipole interaction. Since this interaction has a long-range nature it can possibly be used in combination with an optical lattice to create a new kind of superfluid, first proposed by Geoffrey Chester in 1970 [28], called a supersolid. This unusual new state of matter, which shares the properties of both a solid and a superfluid, has recently drawn a lot of attention in the context of solid ^{4}He. However, these experiments appear to be inconclusive at present [29], such that ultracold atomic gases may be a better system to explore this intriguing possibility [30]. To conclude, we remark that many other directions are being explored at present, leading us to believe that ultracold atomic quantum gases will remain an exciting area of physics for many years to come.

1.2 Outline

To facilitate the use of this book, we end this introduction by presenting a short overview of its contents. The book is divided into three parts that to a large extent can be read independently of each other. Part I contains the introductory material that is necessary for understanding the formulation of the functional-integral approach to quantum many-body physics, which is the method of choice for most condensed-matter theorists active in research today. Part II is then the core of the book, where the functional formalism is constructed, developed and used to discuss the canonical topics of superfluidity in interacting Bose and Fermi gases. In Part III, we discuss various more recent applications of the many-body techniques that are developed in Part II in order to explain important experiments that have recently been performed in the field of ultracold quantum gases.

1.2.1 Part One

Part I consists of Chaps. 2 to 6. We start in Chap. 2 with the mathematical foundations that are needed to follow the calculations in the rest of the book. A consequence of using the functional-integral approach to quantum field theory is that we very often have to perform integrations over infinitely many variables. Most frequently used is the Gaussian integral, because it is one of the few functional integrals that we can solve exactly. In Chap. 2 we therefore discuss Gaussian integration over an arbitrary number of variables, where we not only consider real variables, but also complex variables and Grassmann variables. These last kind of variables change sign upon permutation, which is very convenient when describing indistinguishable fermions, whose antisymmetric behavior leads to precisely the same property. In Chap. 3, we briefly review the basics of quantum mechanics that are relevant to our purposes. In particular, we discuss the exact solution to the harmonic oscillator problem, which is important for two reasons. First of all, in order to perform experiments on ultracold atomic gases these gases are always trapped in space, and the trapping potential is typically well approximated by a harmonic potential. Second, the interacting many-body system described with quantum field theory turns out to be equivalent to an infinite number of interacting harmonic oscillators. As a result, we can already introduce various important concepts in the familiar setting of a single harmonic oscillator, where later these concepts are generalized to the more abstract language of quantum field theory. Examples are the coherent states and the use of perturbation theory, whose generalization is a way to describe interaction effects in many-body systems. Finally, we also consider some aspects of scattering theory, because for ultracold atomic gases it turns out that we can calculate many-body interaction effects from first principles if we know the two-atom scattering properties at low kinetic energy.

Chap. 4 is devoted to statistical physics. Since interacting quantum gases typically consist of at least millions of particles, an exact treatment of all microscopic degrees of freedom is unfeasible. However, we are usually only interested in the averaged macroscopic quantities, whose description actually becomes more convenient as the number of particles increases. This is the domain of statistical physics, which also tells us how to deal with the effects of thermal fluctuations. Since experiments with ultracold atomic gases are never performed at exactly zero temperature, it is usually not sufficient to consider only the many-body ground state. We then find from statistical physics that all macroscopic quantities can be directly obtained from the partition function of the gas, such that the main challenge of a many-body theoretical physicist is to determine this quantity in a sufficiently accurate approximation. For the ideal Bose and Fermi gases, this quantity can be computed exactly, and we find that these two systems behave very differently at low temperatures. In particular, the ideal Bose gas undergoes a phase transition to a new state of matter called a Bose-Einstein condensate, as was already mentioned in the discussion of (1.1). The precise knowledge of the noninteracting quantum gases is then a good starting point to discuss the effects of interactions, which is treated in the second part of the book.

In Chap. 5, we discuss quantum mechanics using Feynman's path-integral approach, which is rather different from the more familiar operator formalism of Chap. 3. Path integrals turn out to be very well suited for a generalization to quantum field theory, such that a thorough knowledge of them is very useful to fully understand all the calculations in the later chapters. Many subtleties of the functional-integral formalism already show up in this chapter, where we also immediately show how to deal with them. In particular, we derive the path-integral expression for the partition function of a single trapped atom. To also be able to derive the functional integral for the partition function of an interacting many-body system, we need to reformulate the quantum mechanics of a many-body system in a somewhat more convenient way. This is achieved in Chap. 6 via a procedure which is known as second quantization. In the second-quantized approach to many-body quantum theory, the particles are represented by creation and annihilation operators, which are conveniently constructed such that they automatically incorporate the quantum statistics of the particles. The eigenstates of these annihilation operators are called coherent states, and are the final ingredient needed to derive the functional formulation of quantum field theory.

1.2.2 Part Two

This is then achieved in Part II of the book, which consists of Chaps. 7 to 14. Part II forms the core of the book, in which we develop all the functional tools in quantum field theory that are needed to understand the equilibrium properties of ultracold atomic quantum gases. In fact, the introduced methods have a much wider range of applicability, such that they can actually be used as a starting point to tackle any quantum condensed-matter problem. However, in order to keep the book coherent, most applications we discuss are from the field of ultracold atoms. A reader with a good undergraduate education in quantum mechanics and statistical physics can most likely enter the discussion here, after a quick study of Gaussian integrals and Grassmann variables in Chap. 2 and the second-quantization formalism in Chap. 6. Part II starts off with Chap. 7, in which we derive the functional integral for the partition function of an interacting many-body system. We also reconsider the ideal quantum gases, for which the partition function reduces to a Gaussian functional integral such that it can be calculated exactly. We perform this calculation in three different ways to familiarize ourselves with functional integration, and to introduce various concepts that come back time after time throughout the rest of the book.

In Chap. 8 we discuss the effects of interactions between the particles, which in general leave the partition function unsolvable, such that we have to resort to appropriate approximation methods. A first way to systematically study interaction effects is by performing a perturbative expansion in the interaction. The general structure of the resulting perturbation theory is then very conveniently visualized with the use of Feynman diagrams. We also explain several features of the expansion that are valid up to any order in the interaction strength, and that are therefore especially useful for arriving at accurate approximations. In particular, we discuss the famous Hartree-Fock approximation, which is a selfconsistent approximation that sums an infinite number of Feynman diagrams and is used very often in condensed-matter physics to obtain a first understanding of the importance of interaction effects. We derive the Hartree-Fock theory by using a variational approach and by using a Hubbard-Stratonovich transformation. This exact transformation turns out to be a very versatile and powerful tool which comes back in many different guises throughout the book.

In Chap. 9 we discuss the Landau theory of phase transitions, where an important concept is the order parameter. This is the observable that distinguishes the two phases involved in the phase transition by quantifying the occurrence of order in the system. We then show that a nonzero value of the order parameter is often associated with a spontaneous breakdown of symmetry, which means that an equilibrium state of the system has less symmetry then the underlying microscopic Hamiltonian. The usefulness of the Hubbard-Stratonovich transformation introduced in the previous chapter becomes particularly obvious in the context of phase transitions, because it can be used to bring the order parameter exactly into the many-body theory. Moreover, we show that fluctuations of the order parameter field can become crucial close to the phase transition, such that they can even cause a breakdown of Landau theory. To go beyond Landau theory turns out to be an exceedingly difficult task and requires advanced field-theoretical methods to which we return in Chap. 14. In order to reach our goal of obtaining an ab initio microscopic description for the phase transition to the superfluid state in interacting atomic Bose and Fermi gases, we still need to understand some specific properties of the alkali atoms that are involved in the actual experiments. In particular, the spin structure of the atoms is important, because it affects the scattering properties of two atoms, where the resulting interaction strength is an input parameter for the quantum field theory of the trapped atomic quantum gas. Chap. 10 deals in more detail with both the spin structure and the scattering of atoms.

In Chap. 11 we apply the developed field-theorical machinery to discuss the famous Bogoliubov and Popov theories of Bose-Einstein condensation, leading, amongst others, to the equally famous Gross-Pitaevskii equation for the condensate wavefunction. The Bogoliubov theory is only valid for temperatures close to zero Kelvin, while the range of validity for the Popov theory is larger, because it takes into account fluctuation effects in a similar manner to the Hartree-Fock theory discussed in Chap. 8. The historically most important success of the Bogoliubov theory was the correct prediction for the vibrational eigenfrequencies of a fully Bose-Einstein condensed atomic cloud. In view of this success, we discuss these collective modes in some detail using a hydrodynamic-like approach. We also briefly discuss what happens when we try to bring the Bose-Einstein condensed gas into rotation, which leads to interesting properties due to the superfluid nature of the gas. Finally, we show that a condensate with effectively attractive interatomic interactions is metastable and ultimately collapses into a Bosenova. In Chap. 12, the Bose-Einstein condensation of Cooper pairs in an ultracold Fermi gas is discussed. In particular, we show how a Hubbard-Stratonovich transformation introduces the appropriate order parameter of the phase transition into the theory. This order parameter describes the condensate of Cooper pairs, which means that the superfluity of an atomic Fermi gas has the same physical origin as the superconductivity of metals. We also derive the critical temperature for the transition in mean-field theory, the result already announced in (1.2). Finally, we also give a more detailed discussion of the BEC-BCS crossover taking place in an atomic gas near a Feshbach resonance.

After having discussed these two explicit examples of phase transitions, we are ready for a more general discussion of the consequences of symmetries and symmetry breaking in quantum field theory. This is the topic of Chap. 13, which has a somewhat more formal nature than the two earlier chapters. However, its results are of much importance to practical calculations. We remember that in order to compare theory with experiments, we usually have to make approximations, because interacting quantum field theories are often too difficult to solve exactly. Obviously, we want to arrive at approximations that do not violate the underlying symmetries of the theory, which is particularly important in the discussion of phase transitions. This is because we need the corresponding symmetry breaking to occur spontaneously and not by the approximation that we make. It turns out that it is possible to derive identities, known as the Ward identities, that check if our approximations still preserve the underlying symmetries. We give a few explicit examples of these Ward identities, and discuss how they can be used in the calculation of certain directly measurable quantities in experiments. Another fundamental issue that we touch upon is the fact that spontaneous symmetry breaking can formally only occur for systems with an infinite number of particles, while realistic experiments always deal with a finite number of particles. We discuss how these two facts can be reconciled with each other for the specific case of superfluid atomic Bose and Fermi gases by discussing the phenomenon of phase diffusion.

In Chap. 14, we go beyond the Landau theory of phase transitions. This is necessary when critical fluctuations extend over the whole many-body system, giving rise to critical phenomena. Since the critical fluctuations now dominate at each length scale, the system is actually scale invariant, which we can use to describe it recursively at increasing wavelengths. This leads to the renormalization group theory of critical many-body systems which, amongst other results, provides the explanation for universality, i.e. the remarkable observation that very different microscopic systems have identical critical properties. We also apply the renormalization group approach to the imbalanced Fermi gas in the strongly-interacting regime, where we can compare the resulting homogeneous phase diagram with beautiful experimental results that were obtained recently.

1.2.3 Part Three

The last three chapters, 15 to 17, form Part III of the book, in which the functional formalism is applied to various recent topics in ultracold atomic gases. In Chap. 15 we discuss low-dimensional, i.e. one and two-dimensional, atomic Bose gases. An important challenge in this chapter is caused by the breakdown of Popov theory due to the enhanced importance of fluctuations in low dimensions. It is then explained in detail how the Popov theory can be modified in order to resolve these problems and, in particular, to describe the famous Kosterlitz-Thouless phase transition in two dimensions. The low-dimensional atomic gases are experimentally realizable with the use of optical lattices, which are the topic of Chap. 16. These lattices also give rise to interesting new physics in three dimensions, because they can be used to simulate solid-state-like periodic potentials, where the depth of the periodic potential is now tunable by varying the laser intensity. As a result, if a shallow optical lattice is loaded with a Bose-Einstein condensate of bosonic atoms, the superfluidity can be destroyed by increasing the lattice depth, which then leads to the Mott-insulator state with precisely one trapped atom at each lattice site. This phase transition happens at zero temperature, and is thus an example of a quantum phase transition, which was observed by Greiner et al. in 2002 [31]. The same experiment can also be performed with an ultracold Fermi mixture, which leads to the possibility of observing the Néel state, and hopefully eventually to new insights into high-temperature superconductors. Finally, we end the book in Chap. 17 with the theory for Feshbach resonances, which now have many important applications in ultracold atomic physics experiments. We start with the two-body atomic physics that causes the resonance, after which we also explain how this two-body physics can be accurately captured in a quantum field theory of atoms and molecules. As an application, we finally consider the coherent Josephson oscillations between a Bose-Einstein condensate of atoms and a Bose-Einstein condensate of molecules, where we also compare the results with some beautiful quantum-mechanical interference experiments that are the ultracold atomic analog of the neutrino oscillations known from high-energy physics.

Part I

Chapter 2
Gaussian Integrals

We must admit with humility that, while number is purely a product of our minds, space has a reality outside our minds, so that we cannot completely prescribe its properties a priori.
– Carl Friedrich Gauss.

In this chapter, we lay the mathematical foundations for the functional-integral formalism that we develop in later chapters. We start with introducing the Gaussian probability distribution together with the corresponding integrals over this distribution, called Gaussian integrals. These concepts are then generalized to higher dimensions, to the complex plane, and to what are called Grassmann variables. The multi-dimensional Gaussian integral is of great importance for the rest of this book. In Chap. 7, we show that it leads to an exact solution of noninteracting quantum gases, which then also forms the basis for a perturbative description of interacting quantum gases. The goal of this chapter is to highlight the practical use of several important mathematical results that are needed to understand the rest of the book. The chapter is not intended to be a full mathematical account of all the above-mentioned topics, meaning that proofs will often be omitted or replaced by illustrative examples. The more experienced reader who is already familiar with Gaussian integrals, complex analysis, and Grassmann algebras, can use this chapter for reference.

2.1 The Gaussian Integral over Real Variables

The Gaussian or normal probability distribution is the most common distribution in statistical physics. The main reason for this is that the probability distribution for the sum of N independent random variables, each with a finite variance, converges for large N to the Gaussian distribution. This is called the central limit theorem of probability theory. Famous physical examples of Gaussian distributions are the Maxwell distribution for the velocities of the atoms in a classical ideal gas, or the spatial distribution for an atom in the quantum-mechanical ground state of a harmonic trap. The Gaussian probability distribution is given by

$$P(x) = \sqrt{\frac{\alpha}{\pi}} \exp\left\{-\alpha x^2\right\}, \tag{2.1}$$

such that it is properly normalized to 1. This follows from

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{e}^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}, \tag{2.2}$$

which is left as an exercise to the reader. The probability distribution of (2.1) has a maximum at $x = 0$, whereas in general the maximum could be at any arbitrary value x_0. Then, we have

$$P(x) = \sqrt{\frac{\alpha}{\pi}} \exp\left\{-\alpha(x-x_0)^2\right\}, \tag{2.3}$$

which corresponds, for example, to the probability distribution of the velocities in a thermal beam of atoms which is travelling at an average velocity x_0. The latter distribution has the property that the expectation value of the quantity x is equal to x_0, that is

$$\langle x \rangle \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\, x\, P(x) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x\, x\, \exp\left\{-\alpha(x-x_0)^2\right\} = x_0, \tag{2.4}$$

which is easily proven by performing the shift $x \rightarrow x + x_0$.

For our purposes, it is convenient to write the parameter α as $-G^{-1}/2 = -1/2G$, with $G < 0$. In the first instance, this looks overly complicated. However, it establishes a direct link with the notation used in later chapters for the Green's function in the functional-integral formalism. From now on, we also no longer explicitly denote the lower and upper limit of the integration when these are given by $-\infty$ and $+\infty$, respectively. With these changes, the Gaussian integral can be written as

$$\int \mathrm{d}x\, \exp\left\{\frac{1}{2}G^{-1}x^2\right\} = \sqrt{-2\pi G} = \sqrt{2\pi} \exp\left\{-\frac{1}{2}\log\left(-G^{-1}\right)\right\}. \tag{2.5}$$

2.1.1 Generating Function

By including a linear term Jx in the exponent, we introduce the generating function $Z(J)$ of the probability distribution. This is very useful because it allows us to calculate the expectation value of all the higher moments, i.e. the expectation values of x^n, by simply differentiating with respect to the current J. Specifically, we have for the Gaussian distribution

$$\begin{aligned} Z(J) &= \int \frac{\mathrm{d}x}{\sqrt{2\pi}} \exp\left\{\frac{1}{2}G^{-1}(x-x_0)^2 + Jx\right\} \\ &= \int \frac{\mathrm{d}x}{\sqrt{2\pi}} \exp\left\{\frac{1}{2}G^{-1}(x+GJ)^2 - \frac{1}{2}GJ^2 + Jx_0\right\} \\ &= \exp\left\{-\frac{1}{2}GJ^2 + Jx_0 - \frac{1}{2}\log\left(-G^{-1}\right)\right\}, \end{aligned} \tag{2.6}$$

where in the first step we performed the shift $x \to x + x_0$ before completing the square. Note that the additional factor $1/\sqrt{2\pi}$ conveniently cancels the factor $\sqrt{2\pi}$ coming from the Gaussian integral. The expectation value of x is now readily calculated from

$$\langle x \rangle = \frac{1}{Z(J)} \frac{\mathrm{d}}{\mathrm{d}J} Z(J) \bigg|_{J=0} = x_0, \tag{2.7}$$

and for $\langle x^2 \rangle$, we obtain

$$\langle x^2 \rangle = \frac{1}{Z(J)} \frac{\mathrm{d}^2}{\mathrm{d}J^2} Z(J) \bigg|_{J=0} = -G + x_0^2 = -G + \langle x \rangle^2. \tag{2.8}$$

Since we can always perform initially the shift $x \to x + x_0$, we consider from now on without loss of generality the case with $x_0 = 0$. A useful observation is that this leads to

$$\langle x^{2m+1} \rangle = 0, \tag{2.9}$$

where m is an integer. This is because the integrand of the integral

$$\int \mathrm{d}x \, x^{2m+1} \exp\left\{ \frac{1}{2} G^{-1} x^2 \right\}$$

is odd and the integral vanishes consequently. By repeatedly applying the derivative $\mathrm{d}/\mathrm{d}J$ an even number of times to the first line of (2.6) with $x_0 = 0$, we find that

$$\langle x^{2m} \rangle = \frac{1}{Z(J)} \frac{\mathrm{d}^{2m}}{\mathrm{d}J^{2m}} Z(J) \bigg|_{J=0}. \tag{2.10}$$

Explicitly calculating the right-hand side of (2.10), using the expression in the last line of (2.6), generates a large number of terms that vanish when we eventually take the limit $J \to 0$. To simplify the calculation, it is therefore convenient to realize that if we expand $Z(J)$ in powers of J only the terms proportional to J^{2m} contribute. In this manner, we find for $x_0 = 0$ that

$$\begin{aligned} \frac{1}{Z(J)} \frac{\mathrm{d}^{2m}}{\mathrm{d}J^{2m}} Z(J) \bigg|_{J=0} &= \frac{Z(0)}{Z(J)} \frac{\mathrm{d}^{2m}}{\mathrm{d}J^{2m}} \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{1}{2} G J^2 \right)^n \bigg|_{J=0} \\ &= \frac{(2m)!}{2^m m!} (-G)^m = (2m-1)!!(-G)^m, \end{aligned} \tag{2.11}$$

where $(2m-1)!! = (2m-1)(2m-3)(2m-5)\dots 1$. Hence, we conclude that

$$\langle x^{2m} \rangle = (2m-1)!!(-G)^m. \tag{2.12}$$

It is important to realize that $(2m-1)!!$ is exactly the number of ways in which $2m$ numbers can be divided into m pairs. Thus, we have found that the expectation value of x^{2m} is equal to the sum of all possible ways in which $\langle x^{2m} \rangle$ can be factorized as

$\langle x^2 \rangle^m$. This last statement is the essence of the famous Wick's theorem that will turn out to be of great importance in later chapters.

2.1.2 Multi-Dimensional Gaussian Integral

The previous results can be immediately generalized to higher-dimensional integrals. Consider a diagonal $n \times n$ matrix $\mathbf{G}$,

$$\mathbf{G} = \begin{bmatrix} G_{11} & & & \\ & G_{22} & & \\ & & G_{33} & \\ & & & \ddots \end{bmatrix}, \tag{2.13}$$

with again $G_{jj} < 0$. Then, the inverse $\mathbf{G}^{-1}$ of $\mathbf{G}$ is clearly given by

$$\mathbf{G}^{-1} = \begin{bmatrix} \frac{1}{G_{11}} & & & \\ & \frac{1}{G_{22}} & & \\ & & \frac{1}{G_{33}} & \\ & & & \ddots \end{bmatrix}. \tag{2.14}$$

We want to evaluate the Gaussian integral

$$\int \left(\prod_{j=1}^{n} \mathrm{d}x_j \right) \exp\left\{ \frac{1}{2} \mathbf{x} \cdot \mathbf{G}^{-1} \cdot \mathbf{x} \right\} \equiv \int \mathrm{d}\mathbf{x} \, \exp\left\{ \frac{1}{2} \mathbf{x} \cdot \mathbf{G}^{-1} \cdot \mathbf{x} \right\}, \tag{2.15}$$

where $\mathbf{x}$ denotes the vector $(x_1, x_2, \ldots, x_n)$. Because the integral factorizes into a product of n one-dimensional integrals, we find that

$$\int \mathrm{d}\mathbf{x} \, \exp\left\{ \frac{1}{2} \mathbf{x} \cdot \mathbf{G}^{-1} \cdot \mathbf{x} \right\} = \frac{(2\pi)^{n/2}}{\sqrt{\prod_{j=1}^{n} (-G_{jj}^{-1})}} = \frac{(2\pi)^{n/2}}{\sqrt{\mathrm{Det}[-\mathbf{G}^{-1}]}}, \tag{2.16}$$

where $\mathrm{Det}[-\mathbf{G}^{-1}]$ denotes the determinant of the matrix $-\mathbf{G}^{-1}$. In the same way we find that (2.6) generalizes to

$$\begin{aligned} Z(\mathbf{J}) &= \int \frac{\mathrm{d}\mathbf{x}}{\sqrt{(2\pi)^n}} \exp\left\{ \frac{1}{2} \mathbf{x} \cdot \mathbf{G}^{-1} \cdot \mathbf{x} + \mathbf{J} \cdot \mathbf{x} \right\} \\ &= \exp\left\{ -\frac{1}{2} \mathbf{J} \cdot \mathbf{G} \cdot \mathbf{J} - \frac{1}{2} \mathrm{Tr}[\log\left(-\mathbf{G}^{-1}\right)] \right\}, \end{aligned} \tag{2.17}$$

where we have taken again without loss of generality $\mathbf{x}_0 = \mathbf{0}$. Here $\mathrm{Tr}[\ldots]$ denotes the trace of a matrix, which is the sum of all diagonal elements. The n-th order correlation function $\langle x_{j_1} x_{j_2} \dots x_{j_n} \rangle$, given by the expectation value of the product of n coordinates x_j, is now easily calculated from

$$\langle x_{j_1} \dots x_{j_n} \dots \rangle = \frac{1}{Z(\mathbf{J})} \frac{\partial^n}{\partial J_{j_1} \dots \partial J_{j_n}} Z(\mathbf{J}) \bigg|_{\mathbf{J}=0} . \tag{2.18}$$

Example 2.1. Because $Z(\mathbf{J})$ depends quadratically on $\mathbf{J}$, it immediately follows that

$$\langle x_i \rangle = \frac{1}{Z(\mathbf{J})} \frac{\partial}{\partial J_i} Z(\mathbf{J}) \bigg|_{\mathbf{J}=0} = 0. \tag{2.19}$$

For the expectation value $\langle x_i x_j \rangle$, we find

$$\langle x_i x_j \rangle = \frac{1}{Z(\mathbf{J})} \frac{\partial^2}{\partial J_i \partial J_j} Z(\mathbf{J}) \bigg|_{\mathbf{J}=0} = -G_{ij}. \tag{2.20}$$

The above results were obtained for the specific case of a diagonal matrix. However, (2.17) is valid for any positive definite, symmetric matrix $-\mathbf{G}^{-1}$, where positive definite means that the matrix has only positive eigenvalues. First, note that $-\mathbf{G}^{-1}$ can always be assumed to be symmetric, because any antisymmetric part would give a vanishing contribution to the term $-\mathbf{x} \cdot \mathbf{G}^{-1} \cdot \mathbf{x}$. Then, a symmetric matrix can always be brought into diagonal form by a similarity transformation $\mathbf{S}$, which means that $\mathbf{S} \cdot \mathbf{G}^{-1} \cdot \mathbf{S}^{-1}$ is diagonal and $\mathbf{S}$ is orthonormal. Orthonormality implies that

$$|\mathrm{Det}[\mathbf{S}]| = 1, \tag{2.21}$$

such that the Jacobian of the coordinate transformation $\mathbf{x} = \mathbf{S}^{-1} \cdot \mathbf{x}'$ is equal to one. Applying the above considerations to (2.17), we have

$$\begin{aligned} Z(\mathbf{J}) &= \int \frac{d\mathbf{x}'}{\sqrt{(2\pi)^n}} \exp\left\{ \frac{1}{2} \mathbf{x}' \cdot \mathbf{S} \cdot \mathbf{G}^{-1} \cdot \mathbf{S}^{-1} \cdot \mathbf{x}' + \mathbf{J} \cdot \mathbf{S}^{-1} \cdot \mathbf{x}' \right\} \\ &= \exp\left\{ -\frac{1}{2} \mathbf{J} \cdot \mathbf{S}^{-1} \cdot \mathbf{S} \cdot \mathbf{G} \cdot \mathbf{S}^{-1} \cdot \mathbf{S} \cdot \mathbf{J} \right\} \frac{1}{\sqrt{\mathrm{Det}[-\mathbf{S} \cdot \mathbf{G}^{-1} \cdot \mathbf{S}^{-1}]}} \\ &= \exp\left\{ -\frac{1}{2} \mathbf{J} \cdot \mathbf{G} \cdot \mathbf{J} \right\} \frac{1}{\sqrt{\mathrm{Det}[-\mathbf{G}^{-1}]}}, \end{aligned} \tag{2.22}$$

where we also used the property that for an orthogonal matrix the inverse matrix and the transposed matrix are the same. Thus, we find that (2.17) is valid for any positive definite matrix $-\mathbf{G}^{-1}$.

2.2 Complex Analysis

In the following, we generalize the results of the previous paragraph to Gaussian integrals over n complex variables z_j. Before doing so, we first review some concepts from elementary complex analysis. The complex plane is a two-dimensional linear space, meaning that any number in the complex plane can be written as $x+\mathrm{i}y$, where x and y are real. Instead of using x and y as the independent variables to parametrize the complex plane, it is more convenient for our purposes to make a coordinate transformation that maps x and y onto the independent variables z and z^* in the following way

$$z \ = x+\mathrm{i}y \qquad \text{and} \qquad z^* = x-\mathrm{i}y. \tag{2.23}$$

Here, $|z|^2 = z^*z = x^2+y^2$ gives the square of the modulus of z, while the real and imaginary parts of z are given by $\mathrm{Re}[z] = (z+z^*)/2$ and $\mathrm{Im}[z] = (z-z^*)/2\mathrm{i}$. Instead of using the Cartesian coordinates x and y, it is also possible to introduce polar coordinates. In that case, complex numbers are written as

$$z = r\mathrm{e}^{\mathrm{i}\varphi}, \tag{2.24}$$

where $r = \sqrt{z^*z}$ is the complex modulus and $\varphi = \mathrm{Arg}[z]$ is the complex argument.

2.2.1 Differentiation and Contour Integrals

A general complex function $f(x,y)$ is a map from the complex plane to the complex plane and in general depends explicitly on both z and z^*. We write $f(x,y) = u(x,y) + \mathrm{i}v(x,y)$, where $u(x,y) = \mathrm{Re}[f(x,y)]$ and $v(x,y) = \mathrm{Im}[f(x,y)]$. In practise we will be dealing mostly with analytic functions, which turn out to depend only explicitly on $z = x+\mathrm{i}y$. Because such a function $f(x+\mathrm{i}y)$ or $f(z)$ only depends on z, we must have that $\mathrm{d}f/\mathrm{d}z = \partial f/\partial x = -\mathrm{i}\partial f/\partial y$ for an analytic function. Since

$$\frac{\partial f(x,y)}{\partial x} = \frac{\partial u(x,y)}{\partial x} + \mathrm{i}\frac{\partial v(x,y)}{\partial x} \tag{2.25}$$

and

$$-\mathrm{i}\frac{\partial f(x,y)}{\partial y} = -\mathrm{i}\frac{\partial u(x,y)}{\partial y} + \frac{\partial v(x,y)}{\partial y}, \tag{2.26}$$

we have that the functions u and v are not independent, but rather satisfy the following set of equations

$$\frac{\partial u(x,y)}{\partial x} = \frac{\partial v(x,y)}{\partial y} \qquad \text{and} \qquad \frac{\partial u(x,y)}{\partial y} = -\frac{\partial v(x,y)}{\partial x}. \tag{2.27}$$