STATISTICAL FIELD THEORY

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Contents

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Abstract

In this course we give a selfcontained introduction to the quantum field theory for many-particle systems, using functional methods throughout. We focus in general on the behavior of so-called quantum fluids, i.e., quantum gases and liquids, but use as an explicit example always the trapped atomic gases that have recently become accesible experimentally. We consider both equilibrium and nonequilibrium phenomena. In the equilibrium case, we first derive the appropriate Hartree-Fock theory for the properties of a quantum fluid in the normal phase. We then turn our attention to the properties in the superfluid phase, and present a microscopic derivation of the Bogoliubov theory of Bose-Einstein condensation and the Bardeen-Cooper-Schrieffer theory of superconductivity. The former is applicable to trapped bosonic gases such as rubidium, lithium, sodium and hydrogen, and the latter in particular to the fermionic isotope of atomic lithium. In the nonequilibrium case, we discuss a few topics for which a field-theoretical approach is especially suited. Examples are the macroscopic quantum tunneling of a Bose-Einstein condensate, the phase dynamics of bosonic and fermionic superfluids, and their collisionless collective modes.

1 Introduction

An important trend in the condensed matter physics of the last two decades, has been the use of advanced field-theoretical methods to discuss various subtle and fundamental properties of interacting many-particle systems at low temperatures. There are several reasons for this trend. The first reason is of course, that a traditional topic in statistical and condensed matter physics is the study of phase transitions and critical phenomena, for which the universal properties are independent of the microscopic details of the system and can therefore be determined by a field theory describing only the large-scale properties of the system of interest. Since the latter are usually solely determined by symmetry considerations, this has led to the important concept of spontaneous symmetry breaking, which has turned out to be not only highly successful in condensed matter physics, but also in high-energy physics and in particular in the Standard Model of elementary particles [1].

A second reason is that soon after the development of the renormalization group methods for critical phenomena [2], it was realized that the same methods can in fact be used to describe the large-scale properties of many-particle systems at any temperature and not only near the critical one. Moreover, application of the renormalization group ideas does not only lead to an understanding of the static behaviour but also of the dynamical properties [3]. As a result quantum field theories can be used to conveniently determine the dynamics of many-particle systems close to equilibrium, i.e., for example the linear hydrodynamical equations of motion. In addition, it can even be used in highly nonequilibrium situations where in general also nonlinearities play an important role. This feature, that also the dynamics of the system can be captured by a quantum field theory, has for instance led in recent years to the study of so-called quantum phase transitions [4].

Finally, the importance of field-theoretical methods in condensed matter physics is associated with the observation that also the effects of imperfections, i.e., disorder, can be treated in this way [5]. Apart from the technological importance of disorder, for example for superconducting magnets, disorder leads also to fundamentally new physics such as the phenomenon of localization [6]. In quantum Hall systems, a combination of disorder and interaction effects give rise to the realization of various peculiar quantum fluids with fractionally charged excitations [7]. The application of field theories has proven to be highly successful in this case and has led to a theory of the quantum Hall effect in terms of edge states that form a chiral Luttinger liquid [8]. In mesoscopic physics, the study of disorder in small electronic structures has resulted in the so-called random matrix theory [9], which has also been of much use in the study of the quantization of classically chaotic systems.

In this course we apply the methods of field theory to quantum fluids, and in particular use it to obtain a detailed understanding of the equilibrium and nonequilibrium properties of trapped atomic gases. After the first observations of Bose-Einstein condensation in 1995 [10–12], degenerate atomic gases have received again a great deal of attention and are presently the main subject of study of a large number of experimental and theoretical groups around the world. The reason for all this excitement is, first of all, that Bose-Einstein condensation has never before been observed experimentally in a clear-cut manner, even though this phenomenon was already predicted by Einstein in 1925 [13]. Second, it is of fundamental interest because it is the only phase transition that occurs also in the absense of interactions and is, therefore, the textbook example for the use of statistical-physics methods. Finally, the goal of achieving Bose-Einstein condensation turned out to be much more difficult than anticipated at first. Just before the breakthrough in 1995, it had even acquired the nature of a 'quest for the holy grail', since the pioneering experiments were already performed in 1980 [14].

From a theoretical point of view, a quantitative understanding of the experiments with cold atomic gases requires that we take into account the following two effects. First, the gas is magnetically trapped in an, usually axially symmetric, harmonic oscillator potential. This is necessary because, in order to obtain the required record low temperatures of $1 - 100$ nK, the gas cannot be allowed to have any contact with material walls. Second, the atoms of the gas interact with each other, which in general dramatically affects the behaviour of the condensed gas, even at the relevant low densities of $10^{12} - 10^{14}$ cm^{-3}. An accurate description of these degenerate gases thus requires the solution of a highly inhomogeneous many-body problem. The theoretical challenge posed by these new quantum systems lies therein that the density of the gas is sufficiently small that it should be possible to accurately solve this many-body problem from first principles and to compare the outcome of the theory directly with experiment, i.e., without any adjustable parameters. In our opinion, quantum field theory is the most simple way in which we are able to meet this challenge.

2 Equilibrium field theory

We start our development of the quantum field theory of gases and liquids by considering first the equilibrium properties of these fluids. We consider both Bose and Fermi fluids, and the ultimate aim of this section is to arrive, for both cases, at an accurate description of the normal and superfluid phases of the system. Although Bose and Fermi mixtures are also of great interest, we do not consider them explicitly here, because they can be treated by a straightforward generalization of the theory. We then turn to some nonequilibrium properties, which are perhaps the most interesting and certainly the least understood at present. The reason for organizing the course in this way, is that the development of the equilibrium theory gives us an opportunity to introduce all the necessary tools that are required for a treatment of the more complicated nonequilibrium case. In particular, we present in detail the way in which we can make use of functional methods. To make also a connection with the more familiar operator language, however, we first briefly summarize the outcome of the second quantization formalism.

2.1 Second quantization

The atoms of interest to us lateron have internal degrees of freedom due to the electron and nuclear spins. In principle this is very important, because it gives the atom a magnetic moment, which is for example used to trap the atoms in a magnetic field minumum. During this course, however, we restrict ourselves to atomic gases that are a mixture of at most two hyperfine states. Without loss of generality, we can then suppose to have N identical atoms with mass m and effective spin $\mathbf{s}$ in an external potential $V^{\text{ex}}(\mathbf{x})$. As a result, the time-dependent Schrödinger equation we have to solve is

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle \ , \tag{2.1}$$

where the hamiltonian is

$$\hat{H} = \sum_{i=1}^{N}\left\{\frac{\hat{\mathbf{p}}_i^2}{2m} + V^{\text{ex}}(\hat{\mathbf{x}}_i) - \gamma\hat{\mathbf{s}}_i \cdot \mathbf{B}\right\} + \frac{1}{2}\sum_{i\neq j=1}^{N} V(\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j) \ , \tag{2.2}$$

$[\hat{\mathbf{x}}_j, \hat{\mathbf{p}}_j]_- = i\hbar$, and all other commutators of the positions and momenta vanish. The first term in the right-hand side is the sum of the one-particle hamiltonians, which includes an effective Zeeman interaction that accounts for a possible difference in the hyperfine energies. The second term represents the interactions. For simplicity, we have assumed that the interaction $V(\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j)$ is independent of the hyperfine states of the atoms i and j. This is in general not justified for realistic atomic gases, but is valid for the specific applications that we have in mind. Moreover, in section 2.6 we also discuss the general case. Finally, we have also neglected possible three-body forces. This is a result of the fact that we are especially interested in dilute quantum gases, for which it is highly improbable for three atoms to simultaneously interact with each other.

Although we have motivated the above hamiltonian by atomic physics, it is in fact much more general. In particular, it is also the hamiltonian describing the electron gas in metals and semiconductors. The external potential represents then the periodic potential provided by the ionic cristal and the interaction $V(\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j)$ is due to the Coulomb repulsion between the electrons. The efffect of an external magnetic field is, however, not fully correctly incorporated in this case, because for charged particles the magnetic field does not only couple to the spin of the particles but also to their momenta. To arrive at the correct hamiltonian for an electron gas in a magnetic field we, therefore, need to perform the usual minimal coupling substitution $\hat{\mathbf{p}}_i \rightarrow \hat{\mathbf{p}}_i + e\mathbf{A}(\hat{\mathbf{x}}_i)$, with $-e$ the electron charge and $\mathbf{A}(\mathbf{x})$ the vector potential that is related to the magnetic field by $\mathbf{B}(\mathbf{x}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{x})$. For simplicity, we come back to these orbital effects of a strong magnetic field only much later in the course and for the moment assume that they can be neglected in first instance.

Without interactions the eigenstates of the hamiltonian in equation (2.2) are, of course, given by the states $\{|\mathbf{n}_1, \alpha_1\rangle_1 \otimes |\mathbf{n}_2, \alpha_2\rangle_2 \otimes \ldots \otimes |\mathbf{n}_N, \alpha_N\rangle_N\}$, where the specific quantum state for each particle is exactly known. Here $\mathbf{n} = (n_x, n_y, n_z)$ and the nonnegative integers n_x, n_y, and n_z denote the three quantum numbers that are required to specify the one-particle eigenstates in the external potential. The wave functions and energies of these eigenstates are $\chi_{\mathbf{n}}(\mathbf{x}) \equiv \langle \mathbf{x}|\mathbf{n}\rangle$ and $\epsilon_{\mathbf{n}}$, respectively, and are found from the time-independent Schrödinger equation

$$\left\{-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) - \epsilon_{\mathbf{n}}\right\} \chi_{\mathbf{n}}(\mathbf{x}) = 0 \ . \tag{2.3}$$

In addition, the internal state $|\alpha\rangle$ is a shorthand notation for $|s, m_s\rangle$. The many-body wave function $|\Psi(t)\rangle$, however, has to be symmetric or antisymmetric under permutations of bosonic or fermionic particles, respectively. Therefore it is more convenient to use a properly (anti)symmetrized version of the above basis, i.e., the states $|\{N_{\mathbf{n},\alpha}\}\rangle$ with the occupation numbers $N_{\mathbf{n},\alpha} = 0, 1, 2, \ldots, \infty$ for bosons and $N_{\mathbf{n},\alpha} = 0, 1$ for fermions. The Hilbert space of all these states, without the constraint $N = \sum_{\mathbf{n},\alpha} N_{\mathbf{n},\alpha}$, is known as the Fock space.

Clearly, the many-body wave function $|\Psi(t)\rangle$ can be expanded in this basis as

$$|\Psi(t)\rangle = \sum_{\{N_{\mathbf{n},\alpha}\}} \Psi(\{N_{\mathbf{n},\alpha}\}, t) |\{N_{\mathbf{n},\alpha}\}\rangle \ , \tag{2.4}$$

where $\Psi(\{N_{\mathbf{n},\alpha}\}, t)$ is the amplitude for the fluid to be in state $|\{N_{\mathbf{n},\alpha}\}\rangle$ at time t. In this basis the Schrödinger equation becomes

$$i\hbar \frac{\partial}{\partial t} \Psi(\{N_{\mathbf{n},\alpha}\}, t) = \sum_{\{N'_{\mathbf{n},\alpha}\}} \langle \{N_{\mathbf{n},\alpha}\}|\hat{H}|\{N'_{\mathbf{n},\alpha}\}\rangle \Psi(\{N'_{\mathbf{n},\alpha}\}, t) \ , \tag{2.5}$$

which shows that we need the matrix elements of the hamiltonian between different states in the Fock space. To calculate these most easily we make use of a procedure that is well-known from the quantum theory of the harmonic oscillator and introduce so-called annihilation operators $\hat{\psi}_{\mathbf{n},\alpha}$ by

$$\hat{\psi}_{\mathbf{n},\alpha} | \ldots, N_{\mathbf{n},\alpha}, \ldots\rangle = (\pm 1)^{M_{\mathbf{n},\alpha}} \sqrt{N_{\mathbf{n},\alpha}} | \ldots, N_{\mathbf{n},\alpha} - 1, \ldots\rangle \ , \tag{2.6}$$

where $M_{\mathbf{n},\alpha}$ counts the total number of particles that are in states which are located according to an arbitrary but fixed convention left of the state $|\mathbf{n}, \alpha\rangle$. From this definition it follows that the creation operators $\hat{\psi}^{\dagger}_{\mathbf{n},\alpha}$ obey

$$\hat{\psi}^{\dagger}_{\mathbf{n},\alpha} | \ldots, N_{\mathbf{n},\alpha}, \ldots\rangle = (\pm 1)^{M_{\mathbf{n},\alpha}} \sqrt{1 \pm N_{\mathbf{n},\alpha}} | \ldots, N_{\mathbf{n},\alpha} + 1, \ldots\rangle \ . \tag{2.7}$$

As a result, we see that the operator $\hat{\psi}^{\dagger}_{\mathbf{n},\alpha}\hat{\psi}_{\mathbf{n},\alpha}$ counts the number of particles in the state $|\mathbf{n}, \alpha\rangle$, i.e.,

$$\hat{\psi}^{\dagger}_{\mathbf{n},\alpha}\hat{\psi}_{\mathbf{n},\alpha} | \ldots, N_{\mathbf{n},\alpha}, \ldots\rangle = N_{\mathbf{n},\alpha} | \ldots, N_{\mathbf{n},\alpha}, \ldots\rangle \ . \tag{2.8}$$

We have also that $[\hat{\psi}_{\mathbf{n},\alpha}, \hat{\psi}_{\mathbf{n}',\alpha'}]_{\mp} = [\hat{\psi}^{\dagger}_{\mathbf{n},\alpha}, \hat{\psi}^{\dagger}_{\mathbf{n}',\alpha'}]_{\mp} = 0$ and most importantly that

$$[\hat{\psi}_{\mathbf{n},\alpha}, \hat{\psi}^{\dagger}_{\mathbf{n}',\alpha'}]_{\mp} = \delta_{\mathbf{n},\mathbf{n}'}\delta_{\alpha,\alpha'} \ . \tag{2.9}$$

In equations (2.6), (2.7) and (2.9) the upper sign refers to bosons and the lower to fermions. This will be true throughout the course.

Exercise 2.1: Show that equation (2.7) follows from equation (2.6).

Exercise 2.2: Prove the various (anti)commutation relations between the creation and annihilation operators $\hat{\psi}^{\dagger}_{\mathbf{n},\alpha}$ and $\hat{\psi}_{\mathbf{n},\alpha}$, respectively.

From these results we can now easily show, first of all, that the basis in the Fock space is given by

$$|\{N_{\mathbf{n},\alpha}\}\rangle = \prod_{\mathbf{n},\alpha} \frac{(\hat{\psi}^{\dagger}_{\mathbf{n},\alpha})^{N_{\mathbf{n},\alpha}}}{\sqrt{N_{\mathbf{n},\alpha}!}}|0\rangle \ , \tag{2.10}$$

with $|0\rangle$ the vacuum state containing no particles. Second, the hamiltonian is

$$\begin{aligned}\hat{H} &= \sum_{\mathbf{n},\alpha} \epsilon_{\mathbf{n},\alpha}\hat{\psi}^{\dagger}_{\mathbf{n},\alpha}\hat{\psi}_{\mathbf{n},\alpha} \\ &+ \frac{1}{2}\sum_{\alpha,\alpha'}\sum_{\mathbf{n},\mathbf{n}',\mathbf{m},\mathbf{m}'} V_{\mathbf{n},\mathbf{n}';\mathbf{m},\mathbf{m}'}\hat{\psi}^{\dagger}_{\mathbf{n},\alpha}\hat{\psi}^{\dagger}_{\mathbf{n}',\alpha'}\hat{\psi}_{\mathbf{m}',\alpha'}\hat{\psi}_{\mathbf{m},\alpha} \ ,\end{aligned} \tag{2.11}$$

with $\epsilon_{\mathbf{n},\alpha} = \epsilon_{\mathbf{n}} - \gamma m_s B \equiv \epsilon_{\mathbf{n}} + \epsilon_{\alpha}$ the one-particle energies. Furthermore,

$$V_{\mathbf{n},\mathbf{n}';\mathbf{m},\mathbf{m}'} = \int d\mathbf{x} \int d\mathbf{x}' \ \chi^{*}_{\mathbf{n}}(\mathbf{x})\chi^{*}_{\mathbf{n}'}(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\chi_{\mathbf{m}}(\mathbf{x})\chi_{\mathbf{m}'}(\mathbf{x}') \tag{2.12}$$

is the amplitude for a collision which scatters two particles out of the states $|\mathbf{m},\alpha\rangle$ and $|\mathbf{m}',\alpha'\rangle$ into the states $|\mathbf{n},\alpha\rangle$ and $|\mathbf{n}',\alpha'\rangle$, as schematically shown in figure 1(a).

Exercise 2.3: Show that the basis of the Fock space given in equation (2.10) is orthonormal.

Exercise 2.4: Show that the factor 1/2 in front of the interaction term in the right-hand side of equation (2.11) is correct. Do this by considering the matrix elements of $V(\mathbf{x}-\mathbf{x}')$ in properly (anti)symmetrized and normalized two-particle states, and comparing these to the same matrix elements in the language of second quantization.

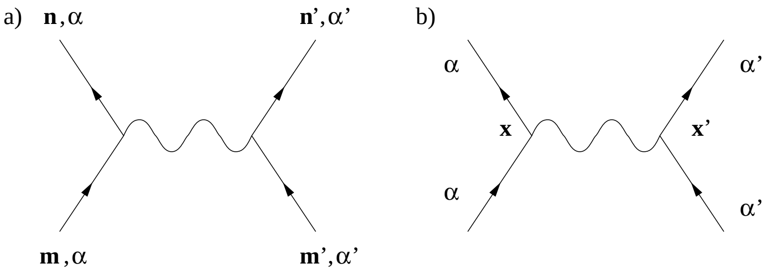

Fig. 1. Diagrammatic representation of the interaction terms in a) equation (2.11) and b) equation (2.13).

Introducing the field operators $\hat{\psi}_\alpha(\mathbf{x}) = \sum_\mathbf{n} \hat{\psi}_{\mathbf{n},\alpha}\chi_\mathbf{n}(\mathbf{x})$ and $\hat{\psi}^\dagger_\alpha(\mathbf{x}) = \sum_\mathbf{n} \hat{\psi}^\dagger_{\mathbf{n},\alpha}\chi^*_\mathbf{n}(\mathbf{x})$, that annihilate and create particles in the spin state $|\alpha\rangle$ at position $\mathbf{x}$ respectively, we can rewrite this result into

$$\begin{aligned}\hat{H} = \sum_\alpha \int d\mathbf{x}\ \hat{\psi}^\dagger_\alpha(\mathbf{x}) \left\{ -\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) + \epsilon_\alpha \right\} \hat{\psi}_\alpha(\mathbf{x}) \qquad (2.13)\\ +\frac{1}{2}\sum_{\alpha,\alpha'} \int d\mathbf{x} \int d\mathbf{x}'\ \hat{\psi}^\dagger_\alpha(\mathbf{x})\hat{\psi}^\dagger_{\alpha'}(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\hat{\psi}_{\alpha'}(\mathbf{x}')\hat{\psi}_\alpha(\mathbf{x})\ .\end{aligned}$$

Note that, due to the (anti)commutation relations of the creation and annihilation operators and the completeness of the wave functions $\chi_\mathbf{n}(\mathbf{x})$, the field operators obey $[\hat{\psi}_\alpha(\mathbf{x}), \hat{\psi}_{\alpha'}(\mathbf{x}')]_\mp = [\hat{\psi}^\dagger_\alpha(\mathbf{x}), \hat{\psi}^\dagger_{\alpha'}(\mathbf{x}')]_\mp = 0$ and $[\hat{\psi}_\alpha(\mathbf{x}), \hat{\psi}^\dagger_{\alpha'}(\mathbf{x}')]_\mp = \delta(\mathbf{x}-\mathbf{x}')\delta_{\alpha,\alpha'}$. Moreover, it is also important for the following to note that the number operator is

$$\hat{N} = \sum_{\mathbf{n},\alpha} \hat{\psi}^\dagger_{\mathbf{n},\alpha}\hat{\psi}_{\mathbf{n},\alpha} = \sum_\alpha \int d\mathbf{x}\ \hat{\psi}^\dagger_\alpha(\mathbf{x})\hat{\psi}_\alpha(\mathbf{x}) \qquad (2.14)$$

and, similarly, that the effective total spin operator is

$$\hat{\mathbf{S}} = \sum_{\mathbf{n},\alpha,\alpha'} \hat{\psi}^\dagger_{\mathbf{n},\alpha}\langle\alpha|\hat{\mathbf{s}}|\alpha'\rangle\hat{\psi}_{\mathbf{n},\alpha'} = \sum_{\alpha,\alpha'} \int d\mathbf{x}\ \hat{\psi}^\dagger_\alpha(\mathbf{x})\langle\alpha|\hat{\mathbf{s}}|\alpha'\rangle\hat{\psi}_{\alpha'}(\mathbf{x})\ . \qquad (2.15)$$

The density of particles in the state $|\alpha\rangle$ is thus simply $\hat{n}_\alpha(\mathbf{x}) = \hat{\psi}^\dagger_\alpha(\mathbf{x})\hat{\psi}_\alpha(\mathbf{x})$.

Exercise 2.5: Prove the various (anti)commutation relations between the field operators $\hat{\psi}_\alpha(\mathbf{x})$ and $\hat{\psi}^\dagger_\alpha(\mathbf{x})$.

This completes our brief discussion of the second quantization formalism. In principle, we could now proceed to develop an operator formulation of the quantum field theory of interest to us. Since the experimentally most important observables can be expressed as appropriate products of the field operators, as we have just seen, this would essentially amount to the study of the (imaginary) time evolution of the Heisenberg operator $\hat{\psi}(\mathbf{x},\tau) = e^{(\hat{H}-\mu\hat{N})\tau/\hbar}\hat{\psi}_\alpha(\mathbf{x})e^{-(\hat{H}-\mu\hat{N})\tau/\hbar}$ at a fixed chemical potential μ [15]. Put differently, the desired quantum field theory would be defined by the Heisenberg equation of motion

$$\hbar\frac{\partial}{\partial\tau}\hat{\psi}_\alpha(\mathbf{x},\tau) = [\hat{H}-\mu\hat{N},\hat{\psi}_\alpha(\mathbf{x},\tau)]_- \ , \tag{2.16}$$

and we would need to solve this equation in a sufficiently accurate approximation. As mentioned previously, however, we here want to develop Feynman's 'path-integral' formulation of the problem, which will turn out to be much more convenient for our purposes. To do so in a manner that is the same for both bosonic and fermionic quantum fluids, we first need to introduce some mathematical background.

Exercise 2.6: Give first the Heisenberg equation of motion for the field operators $\hat{\psi}_\alpha(\mathbf{x},\tau)$ and $\hat{\psi}^\dagger_\alpha(\mathbf{x},\tau)$ in the case of an ideal quantum gas with no interactions. Then solve these equations of motion in terms of the Schrödinger operators $\hat{\psi}^\dagger_{\mathbf{n},\alpha}$ and $\hat{\psi}_{\mathbf{n},\alpha}$.

2.2 Grassmann variables and coherent states

We have seen that in the case of fermions, we need to make use of anticommuting creation and annihilation operators. This automatically builds in the Pauli principle in the theory, because it implies that $(\hat{\psi}^\dagger_{\mathbf{n},\alpha})^2|0\rangle = 0$ and thus that the occupation numbers $N_{\mathbf{n},\alpha}$ are restricted to be either 0 or 1. For reasons that will become clear in a moment, it is in that case also convenient to introduce anticommuting complex numbers or Grassmann variables. The simplest example is to have two such Grassmann variables, say ϕ and ϕ^*. The set $\{1,\phi,\phi^*,\phi^*\phi\}$, and linear combinations thereof with complex coefficients, form then a so-called Grassmann algebra.

Exercise 2.7: Find a matrix representation of the above Grassmann algebra. Note that we need at least 4 × 4 matrices.

By definition we have $[\phi,\phi]_+ = [\phi,\phi^*]_+ = [\phi^*,\phi^*]_+ = 0$ and thus in particular $\phi^2 = {\phi^*}^2 = 0$. Therefore, the above set is indeed complete. The complex conjugation in this algebra is defined by $(\phi)^* = \phi^*$, $(\phi^*)^* = \phi$, and $(\phi^*\phi)^* = (\phi)^*(\phi^*)^* = \phi^*\phi$. Moreover, we can also define an analytic function on this algebra by

$$A(\phi^*,\phi) = a_{11} + a_{12}\phi + a_{21}\phi^* + a_{22}\phi^*\phi \ . \tag{2.17}$$

As a result, it is natural to define also a differentiation by

$$\frac{\partial}{\partial \phi} A(\phi^*, \phi) = a_{12} - a_{22}\phi^* \ . \tag{2.18}$$

To be more precise this is in fact a left differentiation and the minus sign occurs, because we need to permute ϕ^* and ϕ before we can differentiate with respect to ϕ. So, similarly, we have

$$\frac{\partial}{\partial \phi^*} A(\phi^*, \phi) = a_{21} + a_{22}\phi \tag{2.19}$$

and

$$\frac{\partial^2}{\partial \phi^* \partial \phi} A(\phi^*, \phi) = -\frac{\partial^2}{\partial \phi \partial \phi^*} A(\phi^*, \phi) = -a_{22} \ . \tag{2.20}$$

Next we also need integrations over these Grassmann variables. Note that since $\phi^2 = 0$ we have only two possible integrals, namely $\int d\phi \ 1$ and $\int d\phi \ \phi$. We define these by

$$\int d\phi \ 1 = 0 \tag{2.21}$$

and

$$\int d\phi \ \phi = 1 \ . \tag{2.22}$$

This means that integration is equivalent to differentation. The main reason for the above definition is that we want the integration to obey the usual rules of partial integration. In particular, this implies that

$$\int d\phi \ \frac{\partial F(\phi)}{\partial \phi} = 0 \ , \tag{2.23}$$

for any function $F(\phi) = f_1 + f_2\phi$. It is clear that this condition requires that $\int d\phi \ 1 = 0$. The result of $\int d\phi \ \phi$ is then solely a question of normalization. It turns out that we are primarily interested in integrals of the form

$$\int d\phi^* d\phi \ A(\phi^*, \phi) = \int d\phi^* d\phi \ (a_{11} + a_{12}\phi + a_{21}\phi^* + a_{22}\phi^*\phi) = -a_{22} \tag{2.24}$$

as we will see in section 2.3.

Clearly, we can now also consider the Grassmann algebra based on the variables ϕ_n and ϕ_n^* with $n = 1, 2, \ldots, \infty$. What we will need in the following are gaussian integrals over these variables. It is not difficult to show with the above definitions that

$$\int \left(\prod_n d\phi_n^* d\phi_n \right) \ \exp\left\{ -\sum_{n,n'} \phi_n^* A_{n,n'} \phi_{n'} \right\} = \mathrm{det} A = e^{\mathrm{Tr}[\ln A]} \ . \tag{2.25}$$

If the variables ϕ_n and ϕ_n^* were just ordinary complex numbers we would in contrast have the result

$$\int \left(\prod_n \frac{d\phi_n^* d\phi_n}{2\pi i} \right) \ \exp\left\{ -\sum_{n,n'} \phi_n^* A_{n,n'} \phi_{n'} \right\} = \frac{1}{\det A} = e^{-\mathrm{Tr}[\ln A]} \ . \quad (2.26)$$

These last two results will be used many times in the following.

Exercise 2.8: Indicate how we can go about to prove equations (2.25) and (2.26).

One immediate use of these Grassmann variables is that we can now consider eigenstates of the annihilation operator $\hat{\psi}_{\mathbf{n},\alpha}$, also when we are dealing with fermions. These eigenstates are called coherent states. Consider the state

$$|\phi_{\mathbf{n},\alpha}\rangle \equiv (1 - \phi_{\mathbf{n},\alpha}\hat{\psi}^\dagger_{\mathbf{n},\alpha})|0\rangle = \exp\left\{-\phi_{\mathbf{n},\alpha}\hat{\psi}^\dagger_{\mathbf{n},\alpha}\right\}|0\rangle \ , \quad (2.27)$$

where $\phi_{\mathbf{n},\alpha}$ is a Grassmann variable that also anticommutes with the creation and annihilation operators in our Fock space. Clearly we have that

$$\begin{aligned} \hat{\psi}_{\mathbf{n},\alpha}|\phi_{\mathbf{n},\alpha}\rangle &= \hat{\psi}_{\mathbf{n},\alpha}|0\rangle + \phi_{\mathbf{n},\alpha}\hat{\psi}_{\mathbf{n},\alpha}\hat{\psi}^\dagger_{\mathbf{n},\alpha}|0\rangle \quad (2.28) \\ &= \phi_{\mathbf{n},\alpha}|0\rangle = \phi_{\mathbf{n},\alpha}(1 - \phi_{\mathbf{n},\alpha}\hat{\psi}^\dagger_{\mathbf{n},\alpha})|0\rangle = \phi_{\mathbf{n},\alpha}|\phi_{\mathbf{n},\alpha}\rangle \ , \end{aligned}$$

so $|\phi_{\mathbf{n},\alpha}\rangle$ is indeed an eigenstate of $\hat{\psi}_{\mathbf{n},\alpha}$ with eigenvalue $\phi_{\mathbf{n},\alpha}$. In general we can now make the states

$$|\phi\rangle = \exp\left\{ -\sum_{\mathbf{n},\alpha} \phi_{\mathbf{n},\alpha}\hat{\psi}^\dagger_{\mathbf{n},\alpha} \right\}|0\rangle \quad (2.29)$$

that obey $\hat{\psi}_{\mathbf{n},\alpha}|\phi\rangle = \phi_{\mathbf{n},\alpha}|\phi\rangle$. Introducing the Grassmann-valued field $\phi_\alpha(\mathbf{x}) = \sum_{\mathbf{n}} \phi_{\mathbf{n},\alpha}\chi_{\mathbf{n}}(\mathbf{x})$, the latter two relations can be rewritten as

$$|\phi\rangle = \exp\left\{ -\sum_\alpha \int d\mathbf{x} \ \phi_\alpha(\mathbf{x})\hat{\psi}^\dagger_\alpha(\mathbf{x}) \right\}|0\rangle \quad (2.30)$$

and $\hat{\psi}_\alpha(\mathbf{x})|\phi\rangle = \phi_\alpha(\mathbf{x})|\phi\rangle$.

It is important to note that these coherent states are not orthonormal. In contrast, we find that

$$\begin{aligned} \langle\phi|\phi'\rangle &= \prod_{\mathbf{n},\alpha}\langle 0|(1 - \hat{\psi}_{\mathbf{n},\alpha}\phi^*_{\mathbf{n},\alpha})(1 - \phi'_{\mathbf{n},\alpha}\hat{\psi}^\dagger_{\mathbf{n},\alpha})|0\rangle \quad (2.31) \\ &= \prod_{\mathbf{n},\alpha}(1 + \phi^*_{\mathbf{n},\alpha}\phi'_{\mathbf{n},\alpha}) = \exp\left\{ \sum_{\mathbf{n},\alpha} \phi^*_{\mathbf{n},\alpha}\phi'_{\mathbf{n},\alpha} \right\} \\ &= \exp\left\{ \sum_\alpha \int d\mathbf{x} \ \phi^*_\alpha(\mathbf{x})\phi'_\alpha(\mathbf{x}) \right\} \equiv e^{(\phi|\phi')} \ . \end{aligned}$$

Nevertheless they obey a closure relation, as can be seen explicitly from

$$\begin{aligned}
&\int \left(\prod_{\mathbf{n},\alpha} d\phi^*_{\mathbf{n},\alpha} d\phi_{\mathbf{n},\alpha} \right) \ \exp\left\{ - \sum_{\mathbf{n},\alpha} \phi^*_{\mathbf{n},\alpha}\phi_{\mathbf{n},\alpha} \right\} |\phi\rangle\langle\phi| \\
&\quad = \prod_{\mathbf{n},\alpha} \int d\phi^*_{\mathbf{n},\alpha} d\phi_{\mathbf{n},\alpha} \ (1 - \phi^*_{\mathbf{n},\alpha}\phi_{\mathbf{n},\alpha})(1 - \phi_{\mathbf{n},\alpha}\hat{\psi}^\dagger_{\mathbf{n},\alpha})|0\rangle\langle 0|(1 - \hat{\psi}_{\mathbf{n},\alpha}\phi^*_{\mathbf{n},\alpha}) \\
&\quad = \prod_{\mathbf{n},\alpha} (|0\rangle\langle 0| + |1\rangle\langle 1|) = \hat{1} \ .
\end{aligned} \tag{2.32}$$

We write this from now on simply as

$$\int d[\phi^*]d[\phi] \ e^{-(\phi|\phi)}|\phi\rangle\langle\phi| = \hat{1} \ . \tag{2.33}$$

The interesting observation at this point is that essentially the same formulaes also hold for bosons [16,17]. We have only a minus sign difference in

$$|\phi\rangle = \exp\left\{ \sum_\alpha \int d\mathbf{x} \ \phi_\alpha(\mathbf{x})\hat{\psi}^\dagger_\alpha(\mathbf{x}) \right\} |0\rangle \ , \tag{2.34}$$

but then it can still be easily shown that $\hat{\psi}_\alpha(\mathbf{x})|\phi\rangle = \phi_\alpha(\mathbf{x})|\phi\rangle$. A convenient way to do so is, for instance, by noting that the commutation relation $[\hat{\psi}_\alpha(\mathbf{x}), \hat{\psi}^\dagger_{\alpha'}(\mathbf{x}')]_- = \delta(\mathbf{x} - \mathbf{x}')\delta_{\alpha,\alpha'}$ implies that $\hat{\psi}_\alpha(\mathbf{x})$ acts as $\delta/\delta\hat{\psi}^\dagger_\alpha(\mathbf{x})$ on these states. Furthermore, the same expressions hold for the overlap $\langle\phi|\phi'\rangle$ and the closure relation, if we define the integration measure by $\int d[\phi^*]d[\phi] \equiv \int \prod_{\mathbf{n},\alpha} d\phi^*_{\mathbf{n},\alpha} d\phi_{\mathbf{n},\alpha}/(2\pi i)$ in this case.

Exercise 2.9: Show that the coherent state in equation (2.34) is an eigenstate of the bosonic field operators $\hat{\psi}_\alpha(\mathbf{x})$. Do this by Taylor expanding the exponent and by explicitly calculating the effect of the annihilation operator on each term in the expansion.

Summarizing, we have thus found for bosons and fermions that

$$|\phi\rangle = \exp\left\{ \pm \sum_\alpha \int d\mathbf{x} \ \phi_\alpha(\mathbf{x})\hat{\psi}^\dagger_\alpha(\mathbf{x}) \right\} |0\rangle \ , \tag{2.35}$$

$$\langle\phi|\phi'\rangle = e^{(\phi|\phi')} \ , \tag{2.36}$$

and

$$\int d[\phi^*]d[\phi] \ e^{-(\phi|\phi)}|\phi\rangle\langle\phi| = \hat{1} \ . \tag{2.37}$$

The last ingredient we need is that in terms of these coherent states the trace of an operator $\hat{O}$ over the Fock space can be expressed as

$$\mathrm{Tr}[\hat{O}] = \int d[\phi^*]d[\phi]\ e^{-(\phi|\phi)}\langle \pm\phi|\hat{O}|\phi\rangle\ . \tag{2.38}$$

The minus sign in the fermionic case is easily understood from the fact that we then have $\langle\{N_{\mathbf{n},\alpha}\}|\phi\rangle\langle\phi|\{N_{\mathbf{n},\alpha}\}\rangle = \langle -\phi|\{N_{\mathbf{n},\alpha}\}\rangle\langle\{N_{\mathbf{n},\alpha}\}|\phi\rangle$, due to the anticommuting nature of the Grassmann variables. After this mathematical interlude we can now return to physics and to our goal of arriving at a unified treatment of bosonic and fermionic quantum fluids.

Exercise 2.10: Show that the minus sign in the right-hand side of equation (2.38) is indeed required for the fermionic case.

2.3 Functional integrals

We are interested in determining the equilibrium properties of a quantum fluid at some temperature T. From statistical physics we know that all these properties can be obtained from the grand-canonical partition function

$$Z = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]\ , \tag{2.39}$$

where $\beta = 1/k_BT$ and μ the chemical potential. We thus need to evaluate this quantity. As mentioned previously, we want to do so by making use of quantum field theory and, in addition, of Feynman's path-integral approach to quantum mechanics. We thus want to write the partition function as a functional integral over time-dependent fields $\phi_\alpha(\mathbf{x},\tau)$, just like the partition function of a single particle in an external potential can be written as a functional integral over all time-dependent paths $\mathbf{x}(\tau)$. This can indeed be achieved with the coherent states that we have introduced in the previous section.

We start with using our formula (2.38) for the trace of an operator,

$$Z = \int d[\phi^*]d[\phi]\ e^{-(\phi|\phi)}\langle \pm\phi|e^{-\beta(\hat{H}-\mu\hat{N})}|\phi\rangle\ , \tag{2.40}$$

and observe that we are thus faced with the task of calculating the matrix elements $\langle\phi_M|e^{-\beta(\hat{H}-\mu\hat{N})}|\phi_0\rangle$ with $\phi_0(\mathbf{x}) = \phi(\mathbf{x})$ and $\phi^*_M(\mathbf{x}) = \pm\phi^*(\mathbf{x})$. This is difficult in general but can be simplified in the following way. We first realize that the operator $e^{-\beta(\hat{H}-\mu\hat{N})}$ is identical to the quantum mechanical evolution operator $U(t,0) = e^{-i(\hat{H}-\mu\hat{N})t/\hbar}$ evaluated at $t = -i\hbar\beta$. Put differently, we thus want to calculate the matrix elements of the imaginary-time evolution operator $U(-i\tau,0)$ for $\tau = \hbar\beta$. To do so, we next split the

Fig. 2. Illustration of the slicing of the imaginary time interval $[0, \hbar\beta]$ needed for Feynman's path-integral formulation of the partition function.

time interval $[0, \hbar\beta]$ into M pieces, with $\tau_m = m\hbar\beta/M$ and $m = 0, 1, \ldots, M$. So $\Delta\tau = \hbar\beta/M$. The procedure is summarized in figure 2.

At each intermediate time τ_m we then apply a closure relation of the coherent states. This gives

$$\begin{aligned}&\langle\phi_M|e^{-\beta(\hat{H}-\mu\hat{N})}|\phi_0\rangle \\ &\quad = \int \left(\prod_{m=1}^{M-1} d[\phi_m^*]d[\phi_m]\ e^{-(\phi_m|\phi_m)}\right) \prod_{m=1}^{M} \langle\phi_m|e^{-\Delta\tau(\hat{H}-\mu\hat{N})/\hbar}|\phi_{m-1}\rangle\ .\end{aligned} \tag{2.41}$$

Now we can use that in the limit $M \to \infty$ we only need to know the latter matrix elements up to order $\Delta\tau$, because terms of order $(\Delta\tau)^2$ lead to corrections of order $M(\Delta\tau)^2 \propto 1/M$, which vanish in that limit. Hence

$$\begin{aligned}\langle\phi_m|e^{-\Delta\tau(\hat{H}-\mu\hat{N})/\hbar}|\phi_{m-1}\rangle &\simeq \langle\phi_m|1 - \Delta\tau(\hat{H} - \mu\hat{N})/\hbar|\phi_{m-1}\rangle \\ &\equiv \langle\phi_m|\phi_{m-1}\rangle(1 - \Delta\tau H[\phi_m^*, \phi_{m-1}]/\hbar)\ ,\end{aligned} \tag{2.42}$$

with the grand-canonical hamiltonian functional resulting from equations (2.13) and (2.14) equal to

$$\begin{aligned}H[\phi^*, \phi] &= \sum_\alpha \int d\mathbf{x}\ \phi_\alpha^*(\mathbf{x}) \left\{-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) + \epsilon_\alpha - \mu\right\} \phi_\alpha(\mathbf{x}) \\ &+ \frac{1}{2}\sum_{\alpha,\alpha'} \int d\mathbf{x} \int d\mathbf{x}'\ \phi_\alpha^*(\mathbf{x})\phi_{\alpha'}^*(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')\phi_{\alpha'}(\mathbf{x}')\phi_\alpha(\mathbf{x})\ ,\end{aligned} \tag{2.43}$$

since $\psi_\alpha(\mathbf{x})|\phi\rangle = \phi_\alpha(\mathbf{x})|\phi\rangle$ and $\langle\phi|\psi_\alpha^\dagger(\mathbf{x}) = \langle\phi|\phi_\alpha^*(\mathbf{x})$.

Thus, neglecting terms of order $(\Delta\tau)^2$, we can again exponentiate the right-hand side of equation (2.42), which leads in first instance to

$$\langle\phi_m|e^{-\Delta\tau(\hat{H}-\mu\hat{N})/\hbar}|\phi_{m-1}\rangle = e^{(\phi_m|\phi_{m-1}) - \Delta\tau H[\phi_m^*, \phi_{m-1}]/\hbar}\ , \tag{2.44}$$

and therefore for the desired matrix element of the imaginary-time evolution operator to

$$\begin{aligned}\langle\phi_M|e^{-\beta(\hat{H}-\mu\hat{N})}|\phi_0\rangle &= \int\left(\prod_{m=1}^{M-1} d[\phi_m^*]d[\phi_m]\ e^{-(\phi_m|\phi_m)}\right) \qquad (2.45)\\ &\times\exp\left\{\sum_{m=1}^{M}((\phi_m|\phi_{m-1})-\Delta\tau H[\phi_m^*,\phi_{m-1}]/\hbar)\right\}\ .\end{aligned}$$

This can then be manipulated into the suggestive form

$$\begin{aligned}\langle\phi_M|e^{-\beta(\hat{H}-\mu\hat{N})}|\phi_0\rangle &= e^{(\phi_M|\phi_M)}\int\left(\prod_{m=1}^{M-1} d[\phi_m^*]d[\phi_m]\right) \qquad (2.46)\\ &\times\exp\left\{-\frac{1}{\hbar}\sum_{m=1}^{M}\Delta\tau\left(\hbar\frac{(\phi_m|\phi_m)-(\phi_m|\phi_{m-1})}{\Delta\tau}+H[\phi_m^*,\phi_{m-1}]\right)\right\}\ .\end{aligned}$$

Taking now the continuum limit $M\to\infty$ and putting $\phi_m\equiv\phi(\tau_m)$, we find that

$$\begin{aligned}&\langle\phi_M|e^{-\beta(\hat{H}-\mu\hat{N})}|\phi_0\rangle \qquad (2.47)\\ &\quad= e^{(\phi(\hbar\beta)|\phi(\hbar\beta))}\int_{\phi(0)=\phi_0}^{\phi^*(\hbar\beta)=\phi_M^*} d[\phi^*]d[\phi]\ e^{-S[\phi^*,\phi]/\hbar}\ ,\end{aligned}$$

where the so-called Euclidean action is

$$\begin{aligned}&S[\phi^*,\phi] \qquad (2.48)\\ &\quad=\int_0^{\hbar\beta}d\tau\ \left\{\sum_\alpha\int d\mathbf{x}\ \phi_\alpha^*(\mathbf{x},\tau)\hbar\frac{\partial}{\partial\tau}\phi_\alpha(\mathbf{x},\tau)+H[\phi^*(\tau),\phi(\tau)]\right\}\ .\end{aligned}$$

This is essentially the desired functional integral over the complex fields $\phi_\alpha(\mathbf{x},\tau)$ with the boundary conditions $\phi_\alpha(\mathbf{x},0)=\phi_{0;\alpha}(\mathbf{x})$ and $\phi_\alpha^*(\mathbf{x},\hbar\beta)=\phi_{M;\alpha}^*(\mathbf{x})$. It is precisely the field theory analogue of the Feynman path integral. To obtain the partition function we only need to put $\phi_0(\mathbf{x})$ equal to $\pm\phi_M(\mathbf{x})$ and perform a last integration over $\phi_M(\mathbf{x})$ and $\phi_M^*(\mathbf{x})$. It then finally becomes

$$Z=\int d[\phi^*]d[\phi]\ e^{-S[\phi^*,\phi]/\hbar} \qquad (2.49)$$

with the boundary conditions $\phi_\alpha(\mathbf{x},\hbar\beta)=\pm\phi_\alpha(\mathbf{x},0)$, i.e., the fields are periodic in $[0,\hbar\beta]$ for bosons and antiperiodic for fermions. Note that in equation (2.47) we have used the same notation for the integration measure as in equation (2.49), although there is in principle one more integration in the expression for the partition function. The difference is in the continuum limit accounted for in the boundary conditions, which are in practice usually left implicite. Having arrived at an exact identity between the partition function and a functional integral, we are now going to familiarize ourselves with this identity, and with how to perform functional integrals in general, by considering the ideal quantum gases.

Exercise 2.11: Consider a single atom moving in an external potential $V^{\rm ex}(\mathbf{x}) = \alpha\mathbf{x}^2 + \beta\mathbf{x}^4/2$. Give the path-integral expression for the matrix element $\langle\mathbf{x}|e^{-i\hat{H}t/\hbar}|\mathbf{x}\rangle$. Derive from this the path-integral expression for the partition function of the atom, by performing an analytic continuation to imaginary time. What are the boundary conditions of this path-integral? Compare your result with equations (2.48) and (2.49). Take finally the classical limit $\hbar\beta \downarrow 0$. Show that you have obtained the correct classical partition function for the atom.

2.4 Ideal quantum gases

Since the partition functions Z_0 of the ideal quantum gases are known exactly, they are ideal test cases for our field-theoretical methods. Moreover, a thorough knowledge of the ideal quantum gases is also an important first step in understanding experiments with trapped atomic gases, because the effects of the interatomic interaction can essentially be included perturbatively. How this perturbation theory is performed is discussed in detail in section 2.5, but before we can do that we need to understand the noninteracting gases first. In that case, we have

$$S_0[\phi^*,\phi] = \sum_\alpha \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \times \phi^*_\alpha(\mathbf{x},\tau)\left\{\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\rm ex}(\mathbf{x}) + \epsilon_\alpha - \mu\right\}\phi_\alpha(\mathbf{x},\tau) \tag{2.50}$$

and the partition function is a gaussian integral, which explains why we were interested in gaussian integrals in section 2.2. It will be illustrative to evaluate this partition function in three different ways.

Exercise 2.12: Determine the partition function of the ideal quantum gases, by first expanding the fields $\phi_m(\mathbf{x})$ into the eigenstates of the external potential and then making use of equations (2.25), (2.26) and (2.46) to calculate the partition function for a finite value of M. Take finally the limit $M \to \infty$. For the latter use the result $\lim_{M\to\infty}(1 - x/M)^M = e^{-x}$.

2.4.1 Semiclassical method

In the first way, we perform the evaluation of the trace involved in the definition of the partition function at the end of the calculation, and start by considering the matrix element $\langle \pm\phi | e^{-\beta(\hat{H}-\mu\hat{N})} | \phi \rangle$ as the functional integral

$$\int_{\phi(0)=\phi}^{\phi^*(\hbar\beta)=\pm\phi^*} \left(\prod_{\mathbf{n},\alpha} d[\phi^*_{\mathbf{n},\alpha}] d[\phi_{\mathbf{n},\alpha}] \right) \ \exp\left\{ \sum_{\mathbf{n},\alpha} \phi^*_{\mathbf{n},\alpha}(\hbar\beta)\phi_{\mathbf{n},\alpha}(\hbar\beta) \right\} \\ \times \exp\left\{ -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \sum_{\mathbf{n},\alpha} \phi^*_{\mathbf{n},\alpha}(\tau) \left(\hbar\frac{\partial}{\partial\tau} + \epsilon_{\mathbf{n},\alpha} - \mu \right) \phi_{\mathbf{n},\alpha}(\tau) \right\} \ ,$$

which is the product for each $\mathbf{n}$ and α of the path integral

$$\int d[\phi^*]d[\phi] \ \exp\left\{ \phi^*(\hbar\beta)\phi(\hbar\beta) - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \ \phi^*(\tau) \left(\hbar\frac{\partial}{\partial\tau} + \epsilon - \mu \right) \phi(\tau) \right\}$$

with the boundary conditions $\phi(0) = \phi$ and $\phi^*(\hbar\beta) = \pm\phi^*$. It clearly corresponds to the matrix element $\langle \pm\phi | e^{-\beta(\epsilon-\mu)\hat{\psi}^\dagger\hat{\psi}} | \phi \rangle$ for one particular value of $\mathbf{n}$ and α. We calculate this matrix element by performing a shift in the integration variables, i.e., $\phi(\tau) = \phi_{\rm cl}(\tau) + \xi(\tau)$ and $\phi^*(\tau) = \phi^*_{\rm cl}(\tau) + \xi^*(\tau)$, where $\phi_{\rm cl}(\tau)$ obeys the 'classical' equations of motion

$$\left.\frac{\delta S_0[\phi^*,\phi]}{\delta\phi^*(\tau)}\right|_{\phi=\phi_{\rm cl}} = \left(\hbar\frac{\partial}{\partial\tau} + \epsilon - \mu \right) \phi_{\rm cl}(\tau) = 0 \tag{2.51}$$

and similarly for $\phi^*_{\rm cl}(\tau)$. The solutions with the correct boundary solutions are $\phi_{\rm cl}(\tau) = \phi e^{-(\epsilon-\mu)\tau/\hbar}$ and $\phi^*_{\rm cl}(\tau) = \pm\phi^* e^{(\epsilon-\mu)(\tau-\hbar\beta)/\hbar}$, leading to the path integral

$$\exp\left\{ \pm e^{-\beta(\epsilon-\mu)}\phi^*\phi \right\} \\ \times \int d[\xi^*]d[\xi] \ \exp\left\{ -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \ \xi^*(\tau) \left(\hbar\frac{\partial}{\partial\tau} + \epsilon - \mu \right) \xi(\tau) \right\}$$

with the boundary conditions $\xi^*(\hbar\beta) = \xi(0) = 0$. This means that the last path integral is just equal to $\langle 0 | e^{-\beta(\epsilon-\mu)\hat{\psi}^\dagger\hat{\psi}} | 0 \rangle = 1$ and that the desired result is just the prefactor.

Substituting this for each value of $\mathbf{n}$ and α, we apparently have

$$\langle \pm\phi | e^{-\beta(\hat{H}-\mu\hat{N})} | \phi \rangle = \exp\left\{ \pm \sum_{\mathbf{n},\alpha} e^{-\beta(\epsilon_{\mathbf{n},\alpha}-\mu)} \phi^*_{\mathbf{n},\alpha}\phi_{\mathbf{n},\alpha} \right\} \tag{2.52}$$

and the partition function becomes the product

$$Z_0 = \prod_{\mathbf{n},\alpha} \int \frac{d\phi^*_{\mathbf{k},\alpha} d\phi_{\mathbf{k},\alpha}}{(2\pi i)^{(1\pm1)/2}} \ \exp\left\{-(1 \mp e^{-\beta(\epsilon_{\mathbf{n},\alpha}-\mu)})\phi^*_{\mathbf{n},\alpha}\phi_{\mathbf{n},\alpha}\right\} \qquad (2.53)$$

$$= \prod_{\mathbf{n},\alpha} (1 \mp e^{-\beta(\epsilon_{\mathbf{n},\alpha}-\mu)})^{\mp 1} = \exp\left\{\mp \sum_{\mathbf{n},\alpha} \ln(1 \mp e^{-\beta(\epsilon_{\mathbf{n},\alpha}-\mu)})\right\} \ .$$

This is the correct result, because from the usual thermodynamic identity $\langle \hat{N} \rangle = \partial \ln Z_0 / \partial(\beta\mu)$ we find

$$\langle \hat{N} \rangle = \sum_{\mathbf{n},\alpha} \frac{1}{e^{\beta(\epsilon_{\mathbf{n},\alpha}-\mu)} \mp 1} \ , \qquad (2.54)$$

as desired.

2.4.2 Matsubara expansion

The second way is easier and more common in practice. We immediately start with

$$Z_0 = \int d[\phi^*] d[\phi] \ e^{-S_0[\phi^*,\phi]/\hbar} \qquad (2.55)$$

and incorporate the boundary conditions by expanding the fields as

$$\phi_\alpha(\mathbf{x},\tau) = \sum_{\mathbf{n},n} \phi_{\mathbf{n},n,\alpha} \chi_{\mathbf{n}}(\mathbf{x}) \frac{e^{-i\omega_n \tau}}{\sqrt{\hbar\beta}} \qquad (2.56)$$

where $\omega_n = \pi(2n)/\hbar\beta$ for bosons and $\omega_n = \pi(2n+1)/\hbar\beta$ for fermions. These are known as the even and odd Matsubara frequencies, respectively. Using this expansion we have

$$Z_0 = \int \left(\prod_{\mathbf{n},n,\alpha} \frac{d\phi^*_{\mathbf{n},n,\alpha} d\phi_{\mathbf{n},n,\alpha}}{(2\pi i)^{(1\pm1)/2}} \frac{1}{(\hbar\beta)^{\pm 1}} \right) \qquad (2.57)$$

$$\times \exp\left\{ -\frac{1}{\hbar} \sum_{\mathbf{n},n,\alpha} \phi^*_{\mathbf{n},n,\alpha} (-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu) \phi_{\mathbf{n},n,\alpha} \right\} \ ,$$

if we also take account of the jacobian involved in the change of integration variables. Note that the difference between the jacobians in the bosonic and fermionic case, is a consequence of the fact that for Grassmann variables we have that $\int d\phi f_2 \phi = f_2 = \int d(f_2\phi) f_2 (f_2\phi)$ instead of the result $\int d(f_2\phi)(1/f_2)(f_2\phi)$ that we expect on the basis of ordinary complex integration. Note also that these are all again gaussian integrals, so we find in first instance

$$Z_0 = \prod_{\mathbf{n},n,\alpha} (\beta(-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu))^{\mp 1} \tag{2.58}$$
$$= \exp\left\{ \mp \sum_{\mathbf{n},n,\alpha} \ln(\beta(-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu)) \right\} .$$

To evaluate the sum over Matsubara frequencies we need to add a convergence factor $e^{i\omega_n \eta}$ and finally take the limit $\eta \downarrow 0$. The precise reason for this particular procedure cannot be fully understood at this point but is explained in section 2.5. However, doing so we indeed find that

$$\lim_{\eta\downarrow 0} \sum_n \ln(\beta(-i\hbar\omega_n + \epsilon - \mu)) e^{i\omega_n \eta} = \ln(1 \mp e^{-\beta(\epsilon-\mu)}) . \tag{2.59}$$

To see that this is correct, we differentiate the latter equation with respect to $\beta\mu$. This gives us

$$\lim_{\eta\downarrow 0} \frac{1}{\hbar\beta} \sum_n \frac{e^{i\omega_n \eta}}{i\omega_n - (\epsilon-\mu)/\hbar} = \mp \frac{1}{e^{\beta(\epsilon-\mu)} \mp 1} , \tag{2.60}$$

which can be proved by contour integration in the following way. The function $\hbar\beta/(e^{\hbar\beta z} \mp 1)$ has poles at the even and odd Matsubara frequencies with residu ± 1. Hence, by Cauchy's theorem the left-hand side is equal to

$$\lim_{\eta\downarrow 0} \frac{1}{2\pi i} \int_C dz \, \frac{e^{\eta z}}{z - (\epsilon-\mu)/\hbar} \, \frac{\pm 1}{e^{\hbar\beta z} \mp 1}$$

with C a contour that fully encloses the imaginary axis in the direction shown in figure 3. Adding to the contour C the contour C', which gives no contribution to the integral, we can again apply Cauchy's theorem to obtain the desired result. Why does the integration over the contour C' vanish? The reason for this is that the integrant behaves as $\pm e^{-(\hbar\beta-\eta)\mathrm{Re}(z)}/|z|$ for $\mathrm{Re}(z) \to \infty$ and as $-e^{\eta \mathrm{Re}(z)}/|z|$ for $\mathrm{Re}(z) \to -\infty$. The integrant thus always vanishes much faster than $1/|z|$ on the contour C' for any $0 < \eta < \hbar\beta$.

Exercise 2.13: Show by contour integration, in the same way as before, that

$$\lim_{\eta\downarrow 0} \frac{1}{\hbar\beta} \sum_n \frac{e^{i\omega_n \eta}}{-i\omega_n - (\epsilon-\mu)/\hbar} = \mp \frac{1}{e^{\beta(\epsilon-\mu)} \mp 1} - 1 .$$

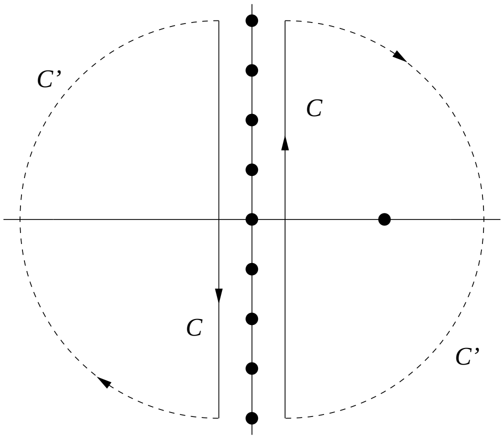

Fig. 3. Illustration of the contour integration that is required to perform the summation over the Matsubara frequencies. The black dots indicate the position of the poles in the integrant.

2.4.3 Green's function method

The third and last method is simplest and, therefore, most common in practice. We first rewrite the partition function as

$$Z_0 = \int d[\phi^*]d[\phi]\ \exp\left\{\sum_\alpha \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \right. \tag{2.61}$$
$$\left. \times \sum_{\alpha'} \int_0^{\hbar\beta} d\tau' \int d\mathbf{x}'\ \phi^*_\alpha(\mathbf{x},\tau) G^{-1}_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau')\phi_{\alpha'}(\mathbf{x}',\tau')\right\}$$

and see G^{-1} as a 'matrix' both in spin space as in coordinate space. We then know that this gaussian integral is just

$$Z_0 = [\det(-G^{-1})]^{\mp 1} = \exp\left\{\mp \mathrm{Tr}[\ln(-G^{-1})]\right\}\ . \tag{2.62}$$

Clearly, we have from the action $S_0[\phi^*,\phi]$ that

$$G^{-1}_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau') \tag{2.63}$$
$$= -\frac{1}{\hbar}\left\{\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) + \epsilon_\alpha - \mu\right\}\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')\delta_{\alpha,\alpha'}$$

or equivalently that

$$\left\{\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) + \epsilon_\alpha - \mu\right\} G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau') \tag{2.64}$$
$$= -\hbar\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')\delta_{\alpha,\alpha'}\ ,$$

which means that $G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau')$ is a Green's function. We come back to its physical meaning shortly. For now we only need to see that the last equation is solved by

$$\begin{aligned} &G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau') \\ &\quad = \delta_{\alpha,\alpha'} \sum_{\mathbf{n},n} \frac{-\hbar}{-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu} \chi_{\mathbf{n}}(\mathbf{x}) \chi^*_{\mathbf{n}}(\mathbf{x}') \frac{e^{-i\omega_n(\tau-\tau')}}{\hbar\beta} \end{aligned} \tag{2.65}$$

thus again

$$\begin{aligned} Z_0 &= \exp\left\{ \mp \sum_{\mathbf{n},n,\alpha} \ln(\beta(-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu)) \right\} \\ &= \exp\left\{ \mp \sum_{\mathbf{n},\alpha} \ln(1 \mp e^{-\beta(\epsilon_{\mathbf{n},\alpha}-\mu)}) \right\} \ . \end{aligned} \tag{2.66}$$

In principle, we have slightly cheated in the last step of this derivation, because equation (2.65) shows that

$$G_{\mathbf{n},n,\alpha;\mathbf{n}',n',\alpha'} = \delta_{\mathbf{n},\mathbf{n}'} \delta_{n,n'} \delta_{\alpha,\alpha'} \frac{-\hbar}{-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu} \ . \tag{2.67}$$

The problem with this last way of calculating the functional integral is that it does not correctly account for the jacobian involved in the change of variables from imaginary time τ to the Matsubara frequencies ω_n. However, this problem can be avoided by calculating never a single determinant, but always the ratio of two determinants. In this manner the effect of the jacobian is exactly cancelled. We will see some examples of how this works in sections 2.6 and 2.8.3.

We now return to the physical meaning of the above Green's function. To see its meaning, we first consider the time-ordered expectation value

$$\begin{aligned} &\langle T[\hat{\psi}_\alpha(\mathbf{x},\tau)\hat{\psi}^\dagger_{\alpha'}(\mathbf{x}',\tau')]\rangle \\ &\quad \equiv \theta(\tau-\tau')\langle\hat{\psi}_\alpha(\mathbf{x},\tau)\hat{\psi}^\dagger_{\alpha'}(\mathbf{x}',\tau')\rangle \pm \theta(\tau'-\tau)\langle\hat{\psi}^\dagger_{\alpha'}(\mathbf{x}',\tau')\hat{\psi}_\alpha(\mathbf{x},\tau)\rangle \ . \end{aligned} \tag{2.68}$$

Here the expectation value is taken in the grand-canonical ensemble and $\hat{\psi}_\alpha(\mathbf{x},\tau)$ is the imaginary time Heisenberg operator, which is defined by $e^{(\hat{H}-\mu\hat{N})\tau/\hbar}\hat{\psi}_\alpha(\mathbf{x})e^{-(\hat{H}-\mu\hat{N})\tau/\hbar}$ and therefore obeys the Heisenberg equation of motion $\hbar\partial_\tau\hat{\psi}_\alpha(\mathbf{x},\tau) = [\hat{H}-\mu\hat{N},\hat{\psi}_\alpha(\mathbf{x},\tau)]_-$. For the noninteracting case it reads

$$\hbar\frac{\partial}{\partial\tau}\hat{\psi}_\alpha(\mathbf{x},\tau) = \left(\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} - V^{\mathrm{ex}}(\mathbf{x}) - \epsilon_\alpha + \mu\right)\hat{\psi}_\alpha(\mathbf{x},\tau) \ . \tag{2.69}$$

As a result

$$\hbar\frac{\partial}{\partial\tau}\langle T[\hat{\psi}_\alpha(\mathbf{x},\tau)\hat{\psi}^\dagger_{\alpha'}(\mathbf{x}',\tau')]\rangle = \hbar\delta(\tau-\tau')\langle[\hat{\psi}_\alpha(\mathbf{x},\tau),\hat{\psi}^\dagger_{\alpha'}(\mathbf{x}',\tau')]_\mp\rangle \\ + \left(\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} - V^{\mathrm{ex}}(\mathbf{x}) - \epsilon_\alpha + \mu\right)\langle T[\hat{\psi}_\alpha(\mathbf{x},\tau)\hat{\psi}^\dagger_{\alpha'}(\mathbf{x}',\tau')]\rangle \ . \tag{2.70}$$

Substituting the equal-time relations that we derived in section 2.1, i.e., $[\hat{\psi}_\alpha(\mathbf{x},\tau),\hat{\psi}^\dagger_{\alpha'}(\mathbf{x}',\tau)]_\mp = \delta(\mathbf{x}-\mathbf{x}')\delta_{\alpha,\alpha'}$, thus suggests that

$$G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau') = -\langle T[\hat{\psi}_\alpha(\mathbf{x},\tau)\hat{\psi}^\dagger_{\alpha'}(\mathbf{x}',\tau')]\rangle \ . \tag{2.71}$$

We can actually also prove this important relation, that bridges the gap between the functional formulation of quantum field theory used here and the more familiar operator formalism. First of all, it is clear from the slicing procedure used in our derivation of the functional integral in section 2.3, that it automatically leads to time-ordered expectation values. We should, therefore, only be able to prove that

$$-G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau') = \langle\phi_\alpha(\mathbf{x},\tau)\phi^*_{\alpha'}(\mathbf{x}',\tau')\rangle \\ \equiv \frac{1}{Z_0}\int d[\phi^*]d[\phi]\ \phi_\alpha(\mathbf{x},\tau)\phi^*_{\alpha'}(\mathbf{x}',\tau')e^{-S_0[\phi^*,\phi]/\hbar} \ . \tag{2.72}$$

This is most easily achieved in the following way. We introduce a partition function in the presence of external currents $J_\alpha(\mathbf{x},\tau)$ and $J^*_\alpha(\mathbf{x},\tau)$, where in the fermionic case these currents are also Grassmann variables. The partition function is taken to be

$$Z_0[J,J^*] = \int d[\phi^*]d[\phi]\ \exp\left\{-\frac{1}{\hbar}S_0[\phi^*,\phi] \right. \\ \left. + \sum_\alpha\int_0^{\hbar\beta}d\tau\int d\mathbf{x}\ (\phi^*_\alpha(\mathbf{x},\tau)J_\alpha(\mathbf{x},\tau) + J^*_\alpha(\mathbf{x},\tau)\phi_\alpha(\mathbf{x},\tau))\right\} \ , \tag{2.73}$$

since then we must simply prove that

$$-G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau') = \frac{\pm 1}{Z_0}\left.\frac{\delta^2 Z_0}{\delta J^*_\alpha(\mathbf{x},\tau)\delta J_{\alpha'}(\mathbf{x}',\tau')}\right|_{J,J^*=0} \ . \tag{2.74}$$

Using a short-hand notation we have

$$Z_0[J,J^*] = \int d[\phi^*]d[\phi]\ \exp\left\{(\phi|G^{-1}|\phi) + (\phi|J) + (J|\phi)\right\} \ . \tag{2.75}$$

The terms in the exponent can be rewritten as $(\phi + JG|G^{-1}|\phi + GJ) - (J|G|J)$, which is usually called completing the square. Performing a shift in the integration variables, we then easily see that

$$Z_0[J,J^*] = Z_0[0,0]e^{-(J|G|J)} = Z_0[0,0]\exp\left\{-\sum_{\alpha}\int_0^{\hbar\beta}d\tau\int d\mathbf{x}\right. \tag{2.76}$$
$$\left.\times\sum_{\alpha'}\int_0^{\hbar\beta}d\tau'\int d\mathbf{x}'\; J^*_\alpha(\mathbf{x},\tau)G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau')J_{\alpha'}(\mathbf{x}',\tau')\right\}\ ,$$

which after differentiation indeed leads to the desired result. We can now in fact calculate the expectation value of the time-ordered product of any number of operators. With the above expression for $Z_0[J,J^*]$ one can easily prove that this results in the sum of all possible products of time-ordered expectation values of two operators. For instance

$$\begin{aligned}&\langle\phi^*_\alpha(\mathbf{x},\tau)\phi^*_{\alpha'}(\mathbf{x}',\tau')\phi_{\alpha''}(\mathbf{x}'',\tau'')\phi_{\alpha'''}(\mathbf{x}''',\tau''')\rangle \\ &\quad=\langle\phi^*_\alpha(\mathbf{x},\tau)\phi_{\alpha'''}(\mathbf{x}''',\tau''')\rangle\langle\phi^*_{\alpha'}(\mathbf{x}',\tau')\phi_{\alpha''}(\mathbf{x}'',\tau'')\rangle \\ &\quad\pm\langle\phi^*_\alpha(\mathbf{x},\tau)\phi_{\alpha''}(\mathbf{x}'',\tau'')\rangle\langle\phi^*_{\alpha'}(\mathbf{x}',\tau')\phi_{\alpha'''}(\mathbf{x}''',\tau''')\rangle\ .\end{aligned}\tag{2.77}$$

This is the famous Wick's theorem, which plays a crucial role in the next section where we start to discuss the profound effects that interactions can have on the results obtained thusfar.

Exercise 2.14: Prove equation (2.77) by an appropriate differentiation of $Z_0[J,J^*]$.

2.5 Interactions and Feynmann diagrams

The Green's function, or one-particle propagator, $G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau')$ is one of the most important quantities that we want to determine theoretically, because it gives us the possibility to calculate in principle the expectation value of any one-particle observable. It also gives us the elementary excitations of our system of interest. For example, the average density of the spin state $|\alpha\rangle$ is in an ideal gas given by

$$\begin{aligned}&\langle\hat{\psi}^\dagger_\alpha(\mathbf{x},\tau)\hat{\psi}_\alpha(\mathbf{x},\tau)\rangle = \mp G_{\alpha,\alpha}(\mathbf{x},\tau;\mathbf{x},\tau^+) \\ &=\lim_{\eta\downarrow 0}\sum_{\mathbf{n},n}\frac{\pm e^{i\omega_n\eta}}{\beta(-i\hbar\omega_n+\epsilon_{\mathbf{n},\alpha}-\mu)}|\chi_{\mathbf{n}}(\mathbf{x})|^2 = \sum_{\mathbf{n}}\frac{1}{e^{\beta(\epsilon_{\mathbf{n},\alpha}-\mu)}\mp 1}|\chi_{\mathbf{n}}(\mathbf{x})|^2\ ,\end{aligned}\tag{2.78}$$

where we introduced the notation τ^+ for the limit $\eta\downarrow 0$ of $\tau+\eta$. Note that this procedure is necessary due to the time-ordening involved in the definition of the Green's function and the fact that the field operators do not commute at equal times. It also gives a natural explanation for our previous use of the convergence factor $e^{i\omega_n\eta}$. Moreover, from the argument of the

Bose or Fermi distribution function, we see that the elementary excitations have an energy of $\epsilon_{\mathbf{n},\alpha} - \mu$. If we replace in the Fourier transform of the Green's function, i.e., in

$$G_{\alpha,\alpha'}(\mathbf{x},\mathbf{x}';i\omega_n) = -\hbar\delta_{\alpha,\alpha'}\sum_{\mathbf{n}} \frac{1}{-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu}\chi_{\mathbf{n}}(\mathbf{x})\chi^*_{\mathbf{n}}(\mathbf{x}') \ , \tag{2.79}$$

$i\omega_n$ by ω we also see that $G_{\alpha,\alpha'}(\mathbf{x},\mathbf{x}';\omega)$ has a pole at $\hbar\omega = \epsilon_{\mathbf{n},\alpha} - \mu$. This is a general result: Poles in $G_{\alpha,\alpha'}(\mathbf{x},\mathbf{x}';\omega)$ correspond to the energies of the elementary excitations. These energies in general can also have a negative imaginary components, which then correspond to the lifetime of the excitation. The question that arises, therefore, is how to determine also the Green's function for an interacting system.

Exercise 2.15: Calculate also $\langle\hat{\psi}_\alpha(\mathbf{x},\tau)\hat{\psi}^\dagger_\alpha(\mathbf{x},\tau)\rangle = -G_{\alpha,\alpha}(\mathbf{x},\tau^+;\mathbf{x},\tau)$, by making use of exercise 2.13. Do you now physically understand the additional term -1 in the outcome of that exercise?

This can be done in perturbation theory, as follows. We want to calculate the expectation value

$$\begin{aligned} &-\langle\phi_\alpha(\mathbf{x},\tau)\phi^*_{\alpha'}(\mathbf{x}',\tau')\rangle \\ &\qquad = -\frac{1}{Z}\int d[\phi^*]d[\phi]\ \phi_\alpha(\mathbf{x},\tau)\phi^*_{\alpha'}(\mathbf{x}',\tau')e^{-S[\phi^*,\phi]/\hbar} \end{aligned} \tag{2.80}$$

with the action $S[\phi^*,\phi] = S_0[\phi^*,\phi] + S_{\text{int}}[\phi^*,\phi]$. We now expand both the numerator and the denominator in powers of S_{int}. Up to first order we find for the partition function

$$\begin{aligned} Z &= \int d[\phi^*]d[\phi]\ e^{-S_0[\phi^*,\phi]/\hbar}\left(1 - \frac{S_{\text{int}}[\phi^*,\phi]}{\hbar}\right) \\ &\equiv Z_0\left(1 - \frac{1}{\hbar}\langle S_{\text{int}}[\phi^*,\phi]\rangle_0\right) \ . \end{aligned} \tag{2.81}$$

Using Wick's theorem, we thus have

$$\begin{aligned} -\frac{1}{\hbar}\langle S_{\text{int}}[\phi^*,\phi]\rangle_0 = &\frac{1}{2}\sum_{\alpha,\alpha'}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\int d\mathbf{x}'\ G_{0;\alpha,\alpha}(\mathbf{x},\tau;\mathbf{x},\tau^+) \\ &\qquad\qquad \times \frac{-V(\mathbf{x}-\mathbf{x}')}{\hbar}G_{0;\alpha',\alpha'}(\mathbf{x}',\tau;\mathbf{x}',\tau^+) \\ &\pm\frac{1}{2}\sum_{\alpha}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\int d\mathbf{x}'\ G_{0;\alpha,\alpha}(\mathbf{x}',\tau;\mathbf{x},\tau^+) \\ &\qquad\qquad \times \frac{-V(\mathbf{x}-\mathbf{x}')}{\hbar}G_{0;\alpha,\alpha}(\mathbf{x},\tau;\mathbf{x}',\tau^+) \ . \end{aligned} \tag{2.82}$$

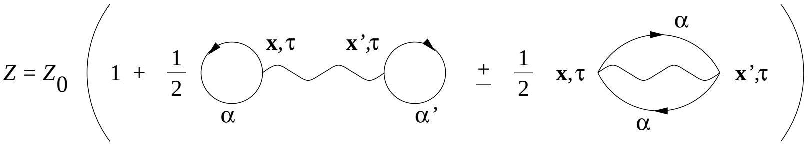

Fig. 4. Diagrammatic representation of the partition function up to first order in the interaction.

To understand the general structure of the perturbation expansion, it is very convenient to represent equations (2.81) and (2.82) in terms of Feynman diagrams. The final result is shown in figure 4, where a wiggly line corresponds to the factor $-V(\mathbf{x}-\mathbf{x}')/\hbar$ and a thin arrowed line pointing from $(\mathbf{x}',\tau')$ to $(\mathbf{x},\tau)$ represents the noninteracting Green's function $G_{0;\alpha,\alpha}(\mathbf{x},\tau;\mathbf{x}',\tau')$. In figure 4 we have, for clarity sake, also explicitly indicated the various coordinates and spin degrees of freedom that we have to either integrate or sum over, respectively. It is, however, much more common in practice to suppress in Feynman diagrams those degrees of freedom that have to be integrated or summed over, and denote only the degrees of freedom on which the quantity of interest depends explicitly. For example, for the numerator of equation (2.80) we obtain

$$\begin{aligned} &-\int d[\phi^*]d[\phi]\;\phi_\alpha(\mathbf{x},\tau)\phi^*_{\alpha'}(\mathbf{x}',\tau')e^{-S_0[\phi^*,\phi]/\hbar}\left(1-\frac{S_{\rm int}[\phi^*,\phi]}{\hbar}\right) \qquad (2.83)\\ &\quad = Z_0\left(-\langle\phi_\alpha(\mathbf{x},\tau)\phi^*_{\alpha'}(\mathbf{x}',\tau')\rangle_0+\frac{1}{\hbar}\langle\phi_\alpha(\mathbf{x},\tau)\phi^*_{\alpha'}(\mathbf{x}',\tau')S_{\rm int}[\phi^*,\phi]\rangle_0\right), \end{aligned}$$

whose diagrammatic equivalent is then given in figure 5. Up to first order the interacting Green's function, which is represented by a thick arrowed line,

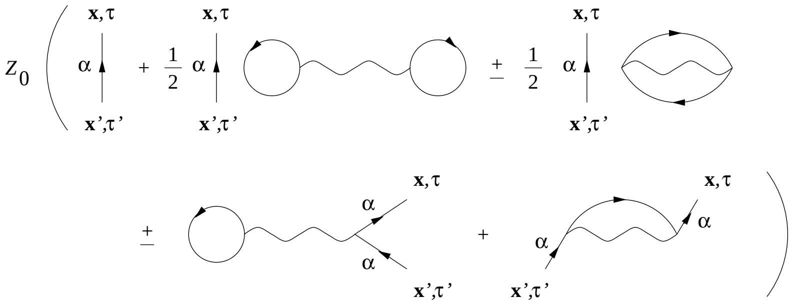

Fig. 5. Diagrammatic representation of the numerator of equation (2.80) up to first order in the interaction.

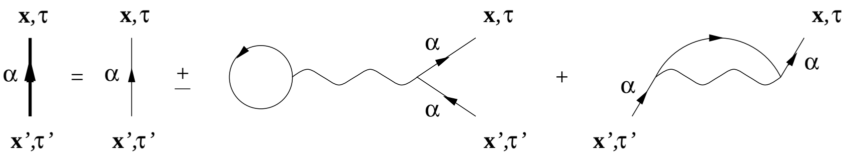

Fig. 6. Interacting Green's function up to first order in the interaction.

obeys the equation shown in figure 6. Note that the so-called disconnected diagrams have exactly cancelled. This is a general feature that happens for any expectation value, i.e., the disconnected diagrams that occur in the numerator are always exactly cancelled by the denominator [18, 19].

Exercise 2.16: Show diagrammatically that also up to second order the interacting Green's function contains no disconnected diagrams.

One can also show that the general structure of the perturbation expansion of the Green's function is as in figure 7, in which only one-particle irreducible diagrams contribute to the selfenergy $\hbar\Sigma$. These one-particle irreducible diagrams can be distinguished from the fact that they do not become disconnected if we cut a single thin arrowed line. This is Dyson's equation [20]. It is particularly insightful for homogeneous systems and for an inhomogeneous system in the so-called weak-coupling limit, in which the typical strength of the interaction is small compared to the energy splitting of the states in the external potential. In both cases the one-particle states $\chi_{\mathbf{n}}(\mathbf{x})$ are, either exactly or in a good approximation, not affected by the interactions and the interacting one-particle propagator can be written as

$$G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau') = \sum_{\mathbf{n},n} G_{\alpha,\alpha'}(\mathbf{n}, i\omega_n)\chi_{\mathbf{n}}(\mathbf{x})\chi^*_{\mathbf{n}}(\mathbf{x}')\frac{e^{-i\omega_n(\tau-\tau')}}{\hbar\beta} \ . \tag{2.84}$$

Note that for realistic trapped atomic gases this weak-coupling limit is essentially always realized in the normal phase of the gas. It is, therefore, also of some experimental interest to consider that limit in more detail first.

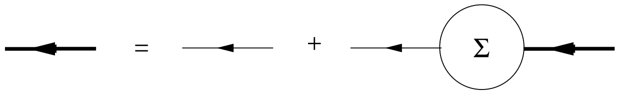

Fig. 7. Exact Dyson equation for the interacting Green's function.

One then finds that the Dyson equation in first instance becomes

$$\begin{aligned} G_{\alpha,\alpha'}(\mathbf{n},i\omega_n) &= G_{0;\alpha,\alpha'}(\mathbf{n},i\omega_n) \\ &\quad + \sum_{\alpha'',\alpha'''} G_{0;\alpha,\alpha''}(\mathbf{n},i\omega_n)\Sigma_{\alpha'',\alpha'''}(\mathbf{n},i\omega_n)G_{\alpha''',\alpha'}(\mathbf{n},i\omega_n)\ . \end{aligned} \tag{2.85}$$

Because $G_{0;\alpha,\alpha'}(\mathbf{n},i\omega_n) = G_{0;\alpha}(\mathbf{n},i\omega_n)\delta_{\alpha,\alpha'}$ and because we have assumed the interactions to be spin independent, we can easily convince ourselves that in perturbation theory it is always true that the selfenergy obeys $\Sigma_{\alpha'',\alpha'''}(\mathbf{n},i\omega_n) = \Sigma_{\alpha''}(\mathbf{n},i\omega_n)\delta_{\alpha'',\alpha'''}$ and as a result also that up to all orders in the interaction $G_{\alpha,\alpha'}(\mathbf{n},i\omega_n) = G_{\alpha}(\mathbf{n},i\omega_n)\delta_{\alpha,\alpha'}$. As we will see in section 2.6, however, nonperturbative effect can change this result due to the phenomena of spontaneous broken symmetry. Ignoring the latter for the moment, we find for each spin state the uncoupled equation

$$G_{\alpha}(\mathbf{n},i\omega_n) = G_{0;\alpha}(\mathbf{n},i\omega_n) + G_{0;\alpha}(\mathbf{n},i\omega_n)\Sigma_{\alpha}(\mathbf{n},i\omega_n)G_{\alpha}(\mathbf{n},i\omega_n)\ , \tag{2.86}$$

or

$$\begin{aligned} \frac{1}{G_{\alpha}(\mathbf{n},i\omega_n)} &= \frac{1}{G_{0;\alpha}(\mathbf{n},i\omega_n)} - \Sigma_{\alpha}(\mathbf{n},i\omega_n) \\ &= -\frac{1}{\hbar}(-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu) - \Sigma_{\alpha}(\mathbf{n},i\omega_n)\ . \end{aligned} \tag{2.87}$$

Hence

$$G_{\alpha}(\mathbf{n},i\omega_n) = \frac{-\hbar}{-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} + \hbar\Sigma_{\alpha}(\mathbf{n},i\omega_n) - \mu}\ , \tag{2.88}$$

which shows that the poles in the Green's function are indeed shifted by the interactions.

In our lowest order calculation we have found for the selfenergy the diagrammatic result shown in figure 8. This is the most simple approximation we can think of. In the weak-coupling limit it is mathematically equal to

$$\begin{aligned} \hbar\Sigma_{\alpha}(\mathbf{n},i\omega_n) &= \sum_{\mathbf{n}',\alpha'} V_{\mathbf{n},\mathbf{n}';\mathbf{n},\mathbf{n}'}\frac{1}{e^{\beta(\epsilon_{\mathbf{n}',\alpha'}-\mu)} \mp 1} \\ &\qquad\qquad \pm \sum_{\mathbf{n}'} V_{\mathbf{n}',\mathbf{n};\mathbf{n},\mathbf{n}'}\frac{1}{e^{\beta(\epsilon_{\mathbf{n}',\alpha}-\mu)} \mp 1} \\ &= \sum_{\mathbf{n}',\alpha'} (V_{\mathbf{n},\mathbf{n}';\mathbf{n},\mathbf{n}'} \pm V_{\mathbf{n}',\mathbf{n};\mathbf{n},\mathbf{n}'}\delta_{\alpha,\alpha'})\frac{1}{e^{\beta(\epsilon_{\mathbf{n}',\alpha'}-\mu)} \mp 1}\ . \end{aligned} \tag{2.89}$$

The first term is known as the direct or Hartree, and the second term as the exchange or Fock contribution to the selfenergy. From equation (2.89) we conclude that the matrix elements of the interaction enter only in the combination $V_{\mathbf{n},\mathbf{n}';\mathbf{n},\mathbf{n}'} \pm V_{\mathbf{n}',\mathbf{n};\mathbf{n},\mathbf{n}'}\delta_{\alpha,\alpha'}$. Clearly, this is a refection of the

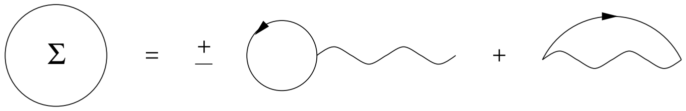

Fig. 8. Selfenergy up to first order in the interaction.

Pauli principle, which forces the effective interaction between two fermionic atoms in the same state $|\mathbf{n},\alpha\rangle$ to vanish.

Exercise 2.17: To understand the Hartree-Fock approximation physically, we are going to derive the zero-temperature limit of the Hartree-Fock selfenergy by means of a variational calculation. We consider only the fermion case. To do so, assume that the groundstate of the system is a single Slater determinant of one-particle states $\chi'_{\mathbf{n},\alpha}$ with energies $\epsilon'_{\mathbf{n},\alpha}$, which we both want to determine variationally. Put differently, in the many-body groundstate $|\Psi_g\rangle$ all the states $\chi'_{\mathbf{n},\alpha}$ that have an energy $\epsilon'_{\mathbf{n},\alpha}$ below the chemical potential μ are assumed to be occupied. Calculate now the average energy $\langle\Psi_g|\hat{H}|\Psi_g\rangle$ of this groundstate, where $\hat{H}$ is the hamiltonian from equation (2.13). Then minimize the average energy, by introducing the Lagrange multipliers $\epsilon'_{\mathbf{n},\alpha}$ that take into account the fact that the states $\chi'_{\mathbf{n},\alpha}$ should be properly normalized. In this manner you arrive at a Schrödinger-like equation that determines the one-particle states and energies. In the weak-coupling limit you can immediately read of the Hartree-Fock selfenergies. Do you also know how to proceed in the strong-coupling limit?

To make the theory selfconsistent we should use in the expression for the selfenergy not the noninteracting propegators, but precisely those that follow from the Dyson equation. This is the Hartree-Fock approximation, which is diagrammatically given in figure 9. It leads in the weak-coupling limit to the new dispersion relation $\hbar\omega_{\mathbf{n},\alpha} = \epsilon_{\mathbf{n},\alpha} + \hbar\Sigma^{HF}_{\alpha}(\mathbf{n},0) - \mu$ for the 'dressed' particles or quasiparticles of the gas, where the selfenergy is essentially also found from equation (2.89). We only have to replace in the

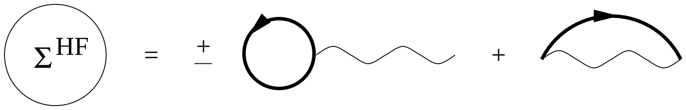

Fig. 9. Hartree-Fock approximation for the selfenergy.

right-hand side $\epsilon_{\mathbf{n}',\alpha'} - \mu$ by $\epsilon_{\mathbf{n}',\alpha'} + \hbar\Sigma^{HF}_{\alpha'}(\mathbf{n}', 0) - \mu$. In this manner we have thus obtained an approximation to the interacting Green's function that is nonperturbative in the interaction and effectively sums an infinite number of Feynman diagrams. Of course, the Hartree-Fock approximation can also be used in the strong-coupling limit. In that case it diagrammatically still corresponds to the solution of the Dyson equation of figure 7, with a selfenergy as shown in figure 9. However, we are then no longer allowed to assume that the exact Green's function is diagonal in the eigenstates $\chi_{\mathbf{n}}(\mathbf{x})$ of the external trapping potential. To see more explicitly what this means physically, it is convenient to rederive the Hartree-Fock theory without making use of perturbation theory.

Exercise 2.18: Calculate the Hartree-Fock selfenergy for spin-less particles with a point-like interaction $V(\mathbf{x}-\mathbf{x}') = V_0\delta(\mathbf{x}-\mathbf{x}')$. Express your answer in terms of the average particle density $n(\mathbf{x})$. Do you understand why the selfenergy vanishes for the fermion case?

2.6 Hartree-Fock theory for an atomic Fermi gas

Because the Hartree-Fock theory is very useful in a large number of circumstances, and because we want to illustrate a very useful technique which is nowadays often used in the literature, we are now going to reproduce the above results without making use of a diagramatic expansion. We consider for simplicity a fermionic mixture with an equal number of atoms in two hyperfine states and start by splitting our spin-independent interaction $V(\mathbf{x} - \mathbf{x}')$ into two spin-dependent parts such that one contributes only to the Hartree diagram and the other only to the Fock diagram. Denoting a spin-dependent interaction by $V_{\alpha',\beta';\alpha,\beta}(\mathbf{x} - \mathbf{x}')$ we thus want that

$$V(\mathbf{x} - \mathbf{x}')\delta_{\alpha,\alpha'}\delta_{\beta,\beta'} = V^H_{\alpha',\beta';\alpha,\beta}(\mathbf{x} - \mathbf{x}') + V^F_{\alpha',\beta';\alpha,\beta}(\mathbf{x} - \mathbf{x}') \qquad (2.90)$$

with $\sum_\beta V^H_{\beta,\alpha;\alpha,\beta}(\mathbf{x} - \mathbf{x}') = \sum_\beta V^F_{\alpha,\beta;\alpha,\beta}(\mathbf{x} - \mathbf{x}') = 0$. Using operators in spin space, a possible solution to these equations is

$$\hat{V}^H = \frac{2}{3}(2 - \hat{P}_{12})V(\mathbf{x} - \mathbf{x}') \qquad (2.91)$$

and

$$\hat{V}^F = \frac{1}{3}(2\hat{P}_{12} - 1)V(\mathbf{x} - \mathbf{x}') \; , \qquad (2.92)$$

where $\hat{P}_{12} = (1 + \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2)/2$ is the exchange operator of the spins of atoms 1 and 2, and $\boldsymbol{\sigma}_{\alpha,\alpha'}$ are the usual Pauli matrices. Note that we are describing the atoms as having effectively a spin one half. Clearly, we now have

$$\begin{aligned} S_{\rm int}[\phi^*,\phi] &= \frac{1}{2}\sum_{\alpha,\alpha';\beta,\beta'}\int_0^{\hbar\beta} d\tau \int d\mathbf{x} \int d\mathbf{x}' \\ &\times \Big\{ \phi^*_{\alpha'}(\mathbf{x},\tau)\phi_\alpha(\mathbf{x},\tau)V^H_{\alpha',\beta';\alpha,\beta}(\mathbf{x}-\mathbf{x}')\phi^*_{\beta'}(\mathbf{x}',\tau)\phi_\beta(\mathbf{x}',\tau) \\ &\quad - \phi^*_{\alpha'}(\mathbf{x},\tau)\phi_\beta(\mathbf{x}',\tau)V^F_{\alpha',\beta';\alpha,\beta}(\mathbf{x}-\mathbf{x}')\phi^*_{\beta'}(\mathbf{x}',\tau)\phi_\alpha(\mathbf{x},\tau)\Big\}\ , \end{aligned} \tag{2.93}$$

which we write as

$$S_{\rm int}[\phi^*,\phi] \equiv \frac{1}{2}(\phi^*\phi|V^H|\phi^*\phi) - \frac{1}{2}(\phi^*\phi||V^F||\phi^*\phi)\ . \tag{2.94}$$

We next apply a so-called Hubbard-Stratonovich transformation [21,22] to both the Hartree and the Fock parts of the interaction. First the Hartree part.

We note that $e^{-S^H_{\rm int}[\phi^*,\phi]}$ can be written as a functional integral over the four real fields contained in $\kappa_{\alpha,\alpha'}(\mathbf{x},\tau) \equiv \kappa_0(\mathbf{x},\tau)\delta_{\alpha,\alpha'} + \boldsymbol{\kappa}(\mathbf{x},\tau)\cdot\boldsymbol{\sigma}_{\alpha,\alpha'}$ as

$$\begin{aligned} &\exp\left\{-\frac{1}{2\hbar}(\phi^*\phi|V^H|\phi^*\phi)\right\} \\ &= \int d[\kappa]\ \exp\left\{\frac{1}{2\hbar}(\kappa|V^{H^{-1}}|\kappa) - \frac{1}{2\hbar}(\kappa|\phi^*\phi) - \frac{1}{2\hbar}(\phi^*\phi|\kappa)\right\}\ . \end{aligned} \tag{2.95}$$

If we put $S^F_{\rm int}[\phi^*,\phi]=0$ for a moment, we can substitute this equality in the partition function to obtain $Z = \int d[\kappa]d[\phi^*]d[\phi]e^{-S[\kappa,\phi^*,\phi]/\hbar}$ with the action

$$\begin{aligned} S[\kappa,\phi^*,\phi] &= -\frac{1}{2}(\kappa|V^{H^{-1}}|\kappa) + \sum_{\alpha,\alpha'}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \phi^*_\alpha(\mathbf{x},\tau)\Big\{\Big(\hbar\frac{\partial}{\partial\tau} \\ &-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\rm ex}(\mathbf{x}) + \epsilon_\alpha - \mu\Big)\delta_{\alpha,\alpha'} + \kappa_{\alpha,\alpha'}(\mathbf{x},\tau)\Big\}\phi_{\alpha'}(\mathbf{x},\tau)\ . \end{aligned} \tag{2.96}$$

We see that in this manner the action for the fermions has become quadratic with a selfenergy $\hbar\Sigma_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau') = \kappa_{\alpha,\alpha'}(\mathbf{x},\tau)\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')$. Hence, we can now integrate out the fermion fields to obtain $Z = \int d[\kappa]e^{-S^{\rm eff}[\kappa]/\hbar}$ and

$$S^{\rm eff}[\kappa] = -\frac{1}{2}(\kappa|V^{H^{-1}}|\kappa) - \hbar{\rm Tr}[\ln(-G^{-1})]\ , \tag{2.97}$$

with $G^{-1} = G_0^{-1} - \Sigma$ also a functional of $\kappa_{\alpha,\alpha'}(\mathbf{x},\tau)$. Up to now we have not made any approximations and have only performed an exact rewriting of the partition function. However, the action $S^{\rm eff}[\kappa]$ contains all powers of the fields $\kappa_{\alpha,\alpha'}(\mathbf{x},\tau)$ and is thus quite complicated. It may therefore appear that we have not made any progress.

This is not the case, because the partition function will be largest for configurations that minimize the action $S^{\rm eff}[\kappa]$. To make use of this observation, we expand the action around its minimum, i.e., we put $\kappa_{\alpha,\alpha'}(\mathbf{x},\tau) = \langle\kappa_{\alpha,\alpha'}(\mathbf{x})\rangle + \delta\kappa_{\alpha,\alpha'}(\mathbf{x},\tau)$ and require that $\delta S^{\rm eff}[\kappa]/\delta\kappa_{\alpha,\alpha'}(\mathbf{x},\tau)|_{\kappa=\langle\kappa\rangle} = 0$. If we neglect the fluctuations, we find that $Z \simeq e^{-S^{\rm eff}[\langle\kappa\rangle]/\hbar}$. This will turn out to be the Hartree approximation, as we will show now. First of all we have

$$G^{-1} = G_0^{-1} - \langle\kappa\rangle/\hbar - \delta\kappa/\hbar \equiv {G^H}^{-1} - \delta\kappa/\hbar = {G^H}^{-1}(1 - G^H\delta\kappa/\hbar) \ . \quad (2.98)$$

Substituting this in equation (2.97) gives us for the terms linear in the fluctuations

$$-\hbar{\rm Tr}[-G^H\delta\kappa/\hbar] - (\delta\kappa|{V^H}^{-1}|\langle\kappa\rangle) \ .$$

If $\langle\kappa_{\alpha,\alpha'}(\mathbf{x})\rangle$ is indeed a minimum of the action $S^{\rm eff}[\kappa]$, these linear terms have to vanish, which implies that

$$\langle\kappa_{\alpha',\alpha}(\mathbf{x})\rangle = \sum_{\beta,\beta'}\int d\mathbf{x}\ V^H_{\alpha',\beta';\alpha,\beta}(\mathbf{x}-\mathbf{x}')G^H_{\beta,\beta'}(\mathbf{x}',\tau;\mathbf{x}',\tau^+) \ . \quad (2.99)$$

As promised, this is precisely the most general mathematical expression for the Hartree contribution to the selfenergy in figure 9. Taking again $\langle\kappa_{\alpha',\alpha}(\mathbf{x})\rangle = \kappa(\mathbf{x})\delta_{\alpha',\alpha}$, we also have that the Hartree approximation to the one-particle propagator obeys $G^H_{\beta,\beta'}(\mathbf{x}',\tau;\mathbf{x}',\tau^+) = n(\mathbf{x}')\delta_{\beta,\beta'}/2$, with $n(\mathbf{x}')$ the average total atomic density, and we obtain the usual Hartree selfenergy

$$\kappa(\mathbf{x}) = \sum_{\beta}\int d\mathbf{x}'\ V^H_{\alpha,\beta;\alpha,\beta}(\mathbf{x}-\mathbf{x}')\frac{n(\mathbf{x}')}{2} = \int d\mathbf{x}'\ V(\mathbf{x}-\mathbf{x}')n(\mathbf{x}') \ . \quad (2.100)$$

Exercise 2.19: Consider the quadratic terms in $\delta\kappa$ and determine from these diagrammatically the propagator of these fields. Argue from equation (2.96) that this propagator corresponds physically to the screened interaction between the atom.

Now we again want to include the Fock part of the interaction and treat this also by a Hubbard-Stratonovich transformation. This requires introducing four real fields that depend on two spatial coordinates. They are denoted by $\lambda_{\alpha,\alpha'}(\mathbf{x},\mathbf{x}',\tau)$. Schematically we then use

$$\begin{aligned} &\exp\left\{\frac{1}{2\hbar}(\phi^*\phi||V^F||\phi^*\phi)\right\} \quad (2.101)\\ &= \int d[\lambda]\ \exp\left\{-\frac{1}{2\hbar}(\lambda||{V^F}^{-1}||\lambda) + \frac{1}{2\hbar}(\lambda||\phi^*\phi) + \frac{1}{2\hbar}(\phi^*\phi||\lambda)\right\} \ , \end{aligned}$$

which leads to the total selfenergy

$$\hbar\Sigma_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau') = [\kappa_{\alpha,\alpha'}(\mathbf{x},\tau)\delta(\mathbf{x}-\mathbf{x}') - \lambda_{\alpha,\alpha'}(\mathbf{x},\mathbf{x}',\tau)]\delta(\tau-\tau') \quad (2.102)$$

and after integration over the fermion fields to the effective action

$$S^{\mathrm{eff}}[\kappa,\lambda] = -\frac{1}{2}(\kappa|V^{H^{-1}}|\kappa) + \frac{1}{2}(\lambda||V^{F^{-1}}||\lambda) - \hbar\mathrm{Tr}[\ln(-G^{-1})] \ . \quad (2.103)$$

Requiring now that also $\delta S^{\mathrm{eff}}[\kappa,\lambda]/\delta\lambda_{\alpha,\alpha'}(\mathbf{x},\mathbf{x}',\tau)|_{\lambda=\langle\lambda\rangle} = 0$, then leads to the expected Fock selfenergy

$$\langle\lambda_{\alpha',\alpha}(\mathbf{x}',\mathbf{x})\rangle = \sum_{\beta,\beta'} V^F_{\beta',\alpha';\alpha,\beta}(\mathbf{x}-\mathbf{x}')G^{HF}_{\beta',\beta}(\mathbf{x}',\tau;\mathbf{x},\tau^+) \ . \quad (2.104)$$

In the symmetric case it simply becomes $\langle\lambda_{\alpha',\alpha}(\mathbf{x}',\mathbf{x})\rangle = \lambda(\mathbf{x}',\mathbf{x})\delta_{\alpha',\alpha}$ with

$$\lambda(\mathbf{x}',\mathbf{x}) = V(\mathbf{x}-\mathbf{x}')n(\mathbf{x}',\mathbf{x}) \quad (2.105)$$

and $n(\mathbf{x}',\mathbf{x}) = \sum_\beta G^{HF}_{\beta,\beta}(\mathbf{x}',\tau;\mathbf{x},\tau^+)/2 = \sum_\beta\langle\psi^\dagger_\beta(\mathbf{x},\tau)\psi_\beta(\mathbf{x}',\tau)\rangle/2$ exactly the Hartree-Fock approximation to the off-diagonal part of the one-particle density matrix.

Note that to actually perform the Hartree-Fock calculation in the latter case, we need to be able to determine the Green's function $G^{HF}_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau')$. The easiest way to do so, is by realizing that it is the Green's function of the operator in the fermionic piece of the action $S[\kappa,\lambda,\phi^*,\phi]$ obtained after the Hubbard-Stratonovich transformations. If we diagonalize this operator by solving the eigenvalue problem

$$\left\{-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) + \kappa(\mathbf{x}) - \epsilon'_{\mathbf{n}}\right\}\chi'_{\mathbf{n}}(\mathbf{x}) - \int d\mathbf{x}' \ \lambda(\mathbf{x},\mathbf{x}')\chi'_{\mathbf{n}}(\mathbf{x}') = 0 \ , \quad (2.106)$$

the desired one-particle propagator aquires the ideal gas form

$$G^{HF}_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x}',\tau') = \delta_{\alpha,\alpha'}\sum_{\mathbf{n},n}\frac{-\hbar}{-i\hbar\omega_n + \epsilon'_{\mathbf{n},\alpha} - \mu}\chi'_{\mathbf{n}}(\mathbf{x})\chi'^*_{\mathbf{n}}(\mathbf{x}')\frac{e^{-i\omega_n(\tau-\tau')}}{\hbar\beta} \ , \quad (2.107)$$

with new one-particle energies $\epsilon'_{\mathbf{n},\alpha} = \epsilon'_{\mathbf{n}} + \epsilon_\alpha$ and eigenstates $\chi'_{\mathbf{n}}(\mathbf{x})$ that incorporate the average effect of the interactions of an atom with all the other atoms in the gas. Clearly, in the cases that the eigenstates are not affected by these so-called mean-field effects, we recover the weak-coupling results of the previous section.

Exercise 2.20: Consider an electron gas in the presence of a homogeneous and positively charged background with the same density as the average density $n_{\rm e}$ of the electron gas. This corresponds to the so-called jellium model for electrons in a metal. The equation of motion for the total density $n(\mathbf{x},t)$ is determined by the continuity equation $\partial n/\partial t+\boldsymbol{\nabla}\cdot\mathbf{J}=0$, and Newton's law for the particle-current density $\mathbf{J}(\mathbf{x},t)$ that reads in this case $m\partial\mathbf{J}/\partial t+\boldsymbol{\nabla}p=-en\mathbf{E}$. Here, m is the electron mass, $p(\mathbf{x},t)$ is the local pressure, $-e$ is the electron charge and $\mathbf{E}(\mathbf{x},t)$ is the electric field in the gas, which is determined by Gauss' law $\boldsymbol{\nabla}\cdot\mathbf{E}=-e(n-n_{\rm e})/\epsilon_0$. Linearize these equations around equilibrium to obtain a single equation for the density fluctuations $\delta n(\mathbf{x},t)=n(\mathbf{x},t)-n_{\rm e}$. Show then that the dispersion relation for these density fluctuations obeys

$$\omega(\mathbf{k})=\sqrt{\frac{1}{m}\left(\left.\frac{\partial p}{\partial n}\right|_{n_{\rm e}}\right)\mathbf{k}^2+\omega_{\rm p}^2}\ ,$$

with the plasma frequency given by $\omega_{\rm p}=(e^2n_{\rm e}/m\epsilon_0)^{1/2}$. What would be the result if the electrons were neutral particles? Determine in that case also $\left.\partial p/\partial n\right|_{n_{\rm e}}$ for temperatures far below the Fermi temperature.

Exercise 2.21: We are now going to reproduce these results in two steps using field-theoretical methods. We thus take the interaction potential equal to the Coulomb potential, i.e.,

$$V(\mathbf{x}-\mathbf{x}')=\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{x}-\mathbf{x}'|}\ .$$

We then first perform a Hubbard-Stratonovich transformation by introducing a single field $\kappa(\mathbf{x},\tau)$ that on average is related to the total density of the electron gas by means of $\int d\mathbf{x}'\ V(\mathbf{x}-\mathbf{x}')n(\mathbf{x}',\tau)$. Show by expanding the effective action $S^{\rm eff}[\kappa]$ up to quadratic terms in the fluctuations $\delta\kappa$ and by performing a Fourier analysis, that the Green's function for these fluctuations is in lowest order given by

$$G_\kappa(\mathbf{k},i\omega_n)=-\frac{1}{V^{-1}(\mathbf{k})-\pi(\mathbf{k},i\omega_n)}\ ,$$

where $V^{-1}(\mathbf{k})=\epsilon_0\mathbf{k}^2/e^2$,

$$\pi(\mathbf{k},i\omega_n)=2\int\frac{d\mathbf{p}}{(2\pi)^3}\ \frac{N(\mathbf{k}+\mathbf{p})-N(\mathbf{p})}{\epsilon(\mathbf{k}+\mathbf{p})-\epsilon(\mathbf{p})-i\hbar\omega_n}\ ,$$

$N(\mathbf{k})$ is the Fermi distribution and $\epsilon(\mathbf{k})=\hbar^2\mathbf{k}^2/2m$.

Exercise 2.22: Secondly, we want to examine the poles of $G_\kappa(\mathbf{k},\omega)$, which should in this case give us the dispersion of the density fluctuations. Show that $\pi(\mathbf{k},\omega) \simeq n_{\mathrm{e}}\mathbf{k}^2/m\omega^2$ for $k/\omega \to 0$, so that for long wavelengths we indeed have a pole at the plasma frequency ω_{p}. What would have been the result if we had considered neutral particles with an interaction obeying $V^{-1}(\mathbf{0}) > 0$?

Exercise 2.23: As mentioned in exercise 2.19, the Fourier transform of the (static) screened interaction between the electrons is given by the expression $V^{\mathrm{sc}}(\mathbf{k}) = -G_\kappa(\mathbf{k},0)$. Consider the long-wavelength behaviour of this screened interaction and show from this that the so-called Thomas-Fermi screening length λ_{TF} of the electron gas is at low temperatures equal to $(2\epsilon_0\epsilon_{\mathrm{F}}/3n_{\mathrm{e}}e^2)^{1/2}$, with ϵ_{F} the Fermi energy. This screening length is defined by the fact that

$$V^{\mathrm{sc}}(\mathbf{x}-\mathbf{x}') \simeq \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{x}-\mathbf{x}'|}\, e^{-|\mathbf{x}-\mathbf{x}'|/\lambda_{\mathrm{TF}}}$$

for large distances $|\mathbf{x}-\mathbf{x}'|$.

Although we have thus precisely reproduced our diagrammatic result, there are two important advantages in using the Hubbard-Stratonovich transformation. First, it is in principle exact, and allows us to also calculate corrections to the Hartree-Fock approximation. For example, if we expand $S^{\mathrm{eff}}[\kappa,\lambda]$ up to quadratic order in $\delta\kappa$ and $\delta\lambda$, and neglect all higher orders, we find the so-called Generalized Random Phase Approximation. The latter approach actually gives us also the opportunity to study the density fluctuations and therefore the collective excitations of the gas. Second, it allows for a beautiful way to describe phase transitions. As mentioned previously, in perturbation theory we always find for a homogeneous gas that $G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x},\tau^+) = n\delta_{\alpha,\alpha'}/2$ due to the same feature of $G_{0;\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x},\tau^+)$. From a fundamental point of view this is a result of the translational invariance of the gas and of the rotational symmetry in spin space. However, we can imagine that in principle we can also find selfconsistent solutions that do not have this property. We then have a spontaneous breaking of symmetry and therefore a phase transition in our system. For example, if below a certain temperature $G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x},\tau^+) = n(\mathbf{x})\delta_{\alpha,\alpha'}/2$, we are dealing with a transition to a charge density wave or (Wigner) crystal. If on the other hand $G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x},\tau^+) = n\delta_{\alpha,\alpha'}/2 + \mathbf{m}\cdot\boldsymbol{\sigma}_{\alpha,\alpha'}$ the gas is in a ferromagnetic phase. For a spin-density wave we even have that $G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x},\tau^+) = n\delta_{\alpha,\alpha'}/2 + \mathbf{m}(\mathbf{x})\cdot\boldsymbol{\sigma}_{\alpha,\alpha'}$. In all these cases the Hubbard-Stratonovich approach used above leads in a natural way to the appropriate Landau theory of the phase transition. Since the Landau theory is also

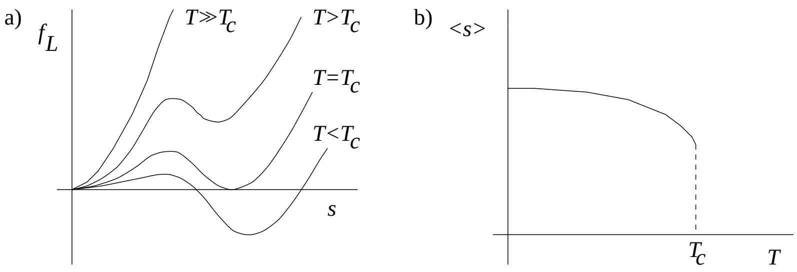

Fig. 10. Qualitative behaviour of a) the Landau free energy and b) the order parameter for a discontinuous phase transition.

very useful for the understanding of superfluidity in atomic gases, which is clearly the primary goal of the present course, we use the next section to give a short introduction into this subject.

2.7 Landau theory of phase transitions

In this summary of the Landau theory of phase transitions, we restrict ourselves in first instance to the homogeneous case because this makes the discussion more transparent. However, at the end of the section we also briefly mention how the inhomogeneity enters the theory. We have seen, for example in the Hartree-Fock theory discussed above, that the Green's function $G_{\alpha,\alpha'}(\mathbf{x},\tau;\mathbf{x},\tau^+) = n\delta_{\alpha,\alpha'}/2 + \langle \mathbf{s} \rangle \cdot \boldsymbol{\sigma}_{\alpha,\alpha'}$ can have a nonzero value of the average spin density $\langle \mathbf{s} \rangle = \langle \hat{\psi}^\dagger_\alpha(\mathbf{x},\tau) \boldsymbol{\sigma}_{\alpha,\alpha'} \hat{\psi}_{\alpha'}(\mathbf{x},\tau) \rangle/2$, which is usually called the magnetization $\mathbf{m}$ in this context. This signals a phase transition to a ferromagnetic phase and the magnetization is called the order parameter of this transition. In the previous section we have also seen how we can, in principle exactly, obtain an expression for the partition function as a functional integral over the field $\mathbf{s}(\mathbf{x},\tau)$, i.e.,

$$Z = \int d[\mathbf{s}]\ e^{-S^{\text{eff}}[\mathbf{s}]/\hbar}\ . \tag{2.108}$$

We just have to integrate out the fields κ_0 and $\lambda_{\alpha,\alpha'}$. For space and time independent values of the magnetization $\mathbf{s}$ the action $S^{\text{eff}}[\mathbf{s}]$ is $\hbar\beta V f_L(\mathbf{s})$, where $f_L(\mathbf{s})$ is the Landau free-energy density and V is the total volume of system. Because of the symmetry of $S[\phi^*,\phi]$ under rotations of the spin, this free-energy density must also be rotationally invariant and can therefore only depend on the magnitude of $\mathbf{s}$, which we denote by s. If a phase transition occurs the behaviour of $f_L(s)$ can essentially fall only into two categories.

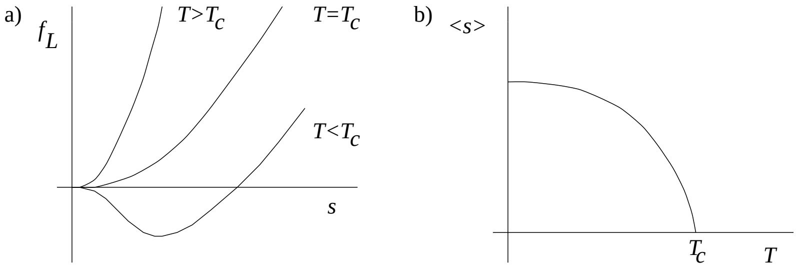

Fig. 11. Qualitative behaviour of a) the Landau free energy and b) the order parameter for a continuous phase transition.

At temperatures very high compared to the critical temperature T_c, the system is fully disorded and the free energy $f_L(s)$ must have a single minimum at $s = 0$ to make sure that the order parameter $\langle s\rangle$ is zero. Bringing the temperature closer to T_c, however, the free energy can develop a second local minimum. As long as the free energy in this second local minimum is higher than the minimum at $s = 0$, the equilibrium value of $\langle s\rangle$ will still be zero and no phase transition has occured. Lowering the temperature further, the value of the free energy in the second minimum decrease until, precisely at the critical temperature T_c, it is equal to the free energy at $s = 0$. For temperatures below this critical one the second minimum has actually become the global minimum of the free energy, which implies that $\langle s\rangle \neq 0$ and we are in the ordered phase. In this scenario the order parameter has always a discontinuity at the critical temperature. As a result, this corresponds to a discontinuous, or first-order, phase transition. The behaviour of the free energy and the order parameter is illustarted in figure 10. This should be compared with the behaviour of the free energy and the order parameter for a continuous, i.e., second or higher order, phase transition, which is quite different and depicted in figure 11. Now the Landau free energy $f_L(s)$ has always a single minimum, which for temperatures above T_c is at $s = 0$ but at temperatures below the critical temperature shifts to a nonzero value of s. In particular, the order parameter thus shows no discontinuity at T_c.

In the case of a second-order phase transition, we conclude that near the critical temperature $\langle s\rangle$ is very small. As a result we can then expand the Landau free-energy density in powers of s. Because the free energy must also be symmetric under $s \to -s$, we have

$$f_L(\mathbf{s}) = \alpha(T)|\mathbf{s}|^2 + \frac{\beta}{2}|\mathbf{s}|^4 \ , \tag{2.109}$$

with $\beta > 0$ and $\alpha(T) = \alpha_0(T/T_c - 1)$. Thus if $T > T_c$ we have $\alpha(T) > 0$

and $\langle s \rangle = 0$. But for $T < T_c$, $\alpha(T)$ becomes negative and we have

$$\langle s \rangle = \sqrt{\frac{\alpha_0}{\beta}\left(1 - \frac{T}{T_c}\right)} . \tag{2.110}$$

Note that the free-energy density in this minimum is $-\alpha_0^2(1-T/T_c)^2/2\beta < 0$ and has a discontinuity in its second derivative with respect to the temperature. Historically, this is the reason why the corresponding phase transition was named to be of second order.

In fact, the Landau theory of second-order phase transitions is slightly more involved, because it also considers slow spatial fluctuations in $\mathbf{s}$. Since a uniform rotation of $\mathbf{s}$ costs no energy, we must have that the free energy is

$$F_L[\mathbf{s}] = \int d\mathbf{x} \ \left(\gamma(\boldsymbol{\nabla}\mathbf{s}(\mathbf{x}))^2 + \alpha(T)|\mathbf{s}(\mathbf{x})|^2 + \frac{\beta}{2}|\mathbf{s}(\mathbf{x})|^4\right) \tag{2.111}$$

and $Z \simeq \int d[\mathbf{s}]\ e^{-\beta F_L[\mathbf{s}]}$. Landau theory now esentially corresponds to minimizing $F_L[\mathbf{s}]$ and taking only quadratic fluctuations into account. Taking also higher order fluctuations into account turns out to be very difficult. It requires Renormalization Group methods, which we are only going to discuss briefly lateron and that can be found in much more detail in the literature [18]. The effects of these fluctuation corrections to Landau theory are generally known as critical phenomena. Interestingly, they do not occur in first-order phase transitions. The physical reason for this is that for second-order phase transitions the typical length scale ξ on which the magnetization is correlated diverges in the Landau theory as

$$\xi^{-1} = \sqrt{\frac{\alpha_0}{\gamma}\left(1 - \frac{T}{T_c}\right)} , \tag{2.112}$$

whereas for first-order phase transitions it remains finite. More importantly for our purposes is, however, that for atomic gases the fluctuations are only important in a small temperature interval around the critical temperature. For many applications it is, therefore, possible to neglect them. What usually cannot be negected is the effect of the inhomogeneity of the gas. In the context of Landau theory that implies that the coefficients $\alpha(T)$, β and γ in equation (2.111) become also dependend on the spatial position in the trapping potential. We will see several examples of this feature in the following.

2.8 Superfluidity and superconductivity

We finally want to consider two important second-order phase transitions, that are purely due to quantum effects and can be conveniently treated with the methods that we have developed sofar. Moreover, they occur very often in nature, for example in metals, in liquid helium and recently of course also in atomic gases of rubidium [10], lithium [11], sodium [12] and hydrogen [23].

2.8.1 Superfluidity

Let us first consider the last case, which is associated with a gas of spin-less bosons. For the low temperatures of interest the action is

$$\begin{aligned} &S[\phi^*, \phi] \\ &\quad = \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \phi^*(\mathbf{x},\tau) \left\{ \hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) - \mu \right\} \phi(\mathbf{x},\tau) \\ &\quad + \frac{1}{2}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ V_{\mathbf{0}}\phi^*(\mathbf{x},\tau)\phi^*(\mathbf{x},\tau)\phi(\mathbf{x},\tau)\phi(\mathbf{x},\tau)\ , \end{aligned} \tag{2.113}$$

where $V(\mathbf{x}-\mathbf{x}')$ is taken to be equal to $V_{\mathbf{0}}\delta(\mathbf{x}-\mathbf{x}')$. The justification for this simplificaties is, roughly speaking, that the thermal de Broglie wavelength $\Lambda_{\mathrm{th}} = (2\pi\hbar^2/mk_BT)^{1/2}$ of the atoms is much larger than the range of the interatomic interaction. In this system the phase transition of interest is Bose-Einstein condensation. The associated order parameter is $\langle\phi(\mathbf{x},\tau)\rangle$, since for time independent $\phi(\mathbf{x},\tau)$ the above action has presicely the form of a Landau theory with a 'free-energy' of

$$\begin{aligned} &F_L[\phi^*, \phi] \\ &\quad = \int d\mathbf{x}\ \left(\frac{\hbar^2}{2m}|\boldsymbol{\nabla}\phi(\mathbf{x})|^2 + (V^{\mathrm{ex}}(\mathbf{x}) - \mu)|\phi(\mathbf{x})|^2 + \frac{V_{\mathbf{0}}}{2}|\phi(\mathbf{x})|^4 \right)\ . \end{aligned} \tag{2.114}$$

We conclude that in lowest order the critical temperature is determined by $\mu(T_c) = \epsilon_{\mathbf{0}}$, because then the configurations $\phi(\mathbf{x}) \propto \chi_{\mathbf{0}}(\mathbf{x})$ precisely make a vanishing contribution to the quadratic part of the 'free energy'. This condition makes sense, because it is exactly the condition that we have a Bose-Einstein condensation in the ideal case: In the ideal Bose gas the number of particles in the one-particle ground state is $N_{\mathbf{0}} = 1/(e^{\beta(\epsilon_{\mathbf{0}}-\mu)}-1)$, which indeed diverges for $\mu = \epsilon_{\mathbf{0}}$.

To determine the corrections to this result we now explicitly substitute $\phi(\mathbf{x},\tau) = \phi_{\mathbf{0}}(\mathbf{x}) + \phi'(\mathbf{x},\tau)$ into our functional integral. It is for lateron important to realize that to consistently define the fluctuations $\phi'(\mathbf{x},\tau)$ in this manner, we also have to require that

$$\int d\mathbf{x}\ \phi^*_{\mathbf{0}}(\mathbf{x})\phi'(\mathbf{x},\tau) + \int d\mathbf{x}\ \phi_{\mathbf{0}}(\mathbf{x})\phi'^*(\mathbf{x},\tau) = 0\ . \tag{2.115}$$

The physical reason behind this condition is that $\phi'(\mathbf{x},\tau)$ should contain all the configurations that are orthogonal to $\phi_{\mathbf{0}}(\mathbf{x})$. In principle, therefore, it should also contain configurations that in effect only multiply $\phi_{\mathbf{0}}(\mathbf{x})$ by a global phase. Such fluctuations lead to the phenomena of phase 'diffusion' and are discussed in section 2.10. In full detail we find after the above substitution that

$$S[\phi'^*,\phi'] = \hbar\beta F_L[\phi^*_{\mathbf{0}},\phi_{\mathbf{0}}] + S_0[\phi'^*,\phi'] + S_{\text{int}}[\phi'^*,\phi'] \ , \tag{2.116}$$

where the linear and quadratic terms are given by

$$\begin{aligned} &S_0[\phi'^*,\phi'] \\ &= \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \phi'^*(\mathbf{x},\tau)\left\{-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu + V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2\right\}\phi_{\mathbf{0}}(\mathbf{x}) \\ &+ \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \phi'(\mathbf{x},\tau)\left\{-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu + V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2\right\}\phi^*_{\mathbf{0}}(\mathbf{x}) \\ &+ \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \phi'^*(\mathbf{x},\tau) \\ &\qquad \times\left\{\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu + 2V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2\right\}\phi'(\mathbf{x},\tau) \\ &+\frac{1}{2}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ V_{\mathbf{0}}(\phi_{\mathbf{0}}(\mathbf{x}))^2\phi'^*(\mathbf{x},\tau)\phi'^*(\mathbf{x},\tau) \\ &+\frac{1}{2}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ V_{\mathbf{0}}(\phi^*_{\mathbf{0}}(\mathbf{x}))^2\phi'(\mathbf{x},\tau)\phi'(\mathbf{x},\tau) \ , \end{aligned} \tag{2.117}$$

and the cubic and quartic terms by

$$\begin{aligned} S_{\text{int}}[\phi'^*,\phi'] &= \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ V_{\mathbf{0}}\phi_{\mathbf{0}}(\mathbf{x})\phi'^*(\mathbf{x},\tau)\phi'^*(\mathbf{x},\tau)\phi'(\mathbf{x},\tau) \\ &+ \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ V_{\mathbf{0}}\phi^*_{\mathbf{0}}(\mathbf{x})\phi'^*(\mathbf{x},\tau)\phi'(\mathbf{x},\tau)\phi'(\mathbf{x},\tau) \\ &+\frac{1}{2}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ V_{\mathbf{0}}\phi'^*(\mathbf{x},\tau)\phi'^*(\mathbf{x},\tau)\phi'(\mathbf{x},\tau)\phi'(\mathbf{x},\tau) \ , \end{aligned} \tag{2.118}$$

respectively.

In the Bogoliubov approximation we neglect the last three interaction terms [24]. Furthermore, to make sure that $\langle\phi(\mathbf{x},\tau)\rangle = \phi_{\mathbf{0}}(\mathbf{x})$ and therefore that $\langle\phi'(\mathbf{x},\tau)\rangle = 0$, we need to require that the terms linear in ϕ' and ϕ'^* drop out of the action $S_0[\phi'^*,\phi']$. Clearly, this implies that

$$\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\text{ex}}(\mathbf{x}) + V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2\right)\phi_{\mathbf{0}}(\mathbf{x}) = \mu\phi_{\mathbf{0}}(\mathbf{x}) \ , \tag{2.119}$$

which is the same result as obtained from minimizing the Landau 'free-energy' $F_L[\phi^*,\phi]$. In the context of trapped atomic gases, this equation is known as the Gross-Pitaevskii equation [25]. It determines the macroscopic wave function of the condensate. The reason for calling $\phi_{\mathbf{0}}(\mathbf{x})$ the macroscopic wave function follows from the fact that the total density of the gas now obeys

$$n(\mathbf{x}) = \langle \phi(\mathbf{x},\tau)\phi^*(\mathbf{x},\tau^+)\rangle = |\phi_{\mathbf{0}}(\mathbf{x})|^2 + \langle \phi'(\mathbf{x},\tau)\phi'^*(\mathbf{x},\tau^+)\rangle \ . \qquad (2.120)$$

The total number of condensate atoms thus equals $N_{\mathbf{0}} = \int d\mathbf{x}\ |\phi_{\mathbf{0}}(\mathbf{x})|^2$. As equation (2.120) shows, it is in general always smaller that the total number of atoms in the gas due to the effect of the fluctuations. Note that in our present formulation the average $\langle \phi'(\mathbf{x},\tau)\phi'^*(\mathbf{x},\tau^+)\rangle$ physically describes not only the depletion of the condensate due to the usual thermal fluctuations known from the ideal Bose gas, but also due to the interactions, i.e., purely due to quantum fluctuations.

Exercise 2.24: The Gross-Pitaevskii equation turns out to be equivalent to the Hartree approximation. This can be seen as follows. We assume that the ground state wave function of the system is a product of a single one-particle state $\chi'_{\mathbf{0}}$ with an energy $\epsilon'_{\mathbf{0}}$, which we both want to determine variationally. Put differently, in the many-body groundstate $|\Psi_g\rangle$ all the atoms are in the same state $\chi'_{\mathbf{0}}$ that has an energy $\epsilon'_{\mathbf{0}}$. Calculate now the average energy $\langle \Psi_g|\hat{H}|\Psi_g\rangle$ of this groundstate, where $\hat{H}$ is the hamiltonian from equation (2.13). Then minimize the average energy, by introducing the Lagrange multiplier $\epsilon'_{\mathbf{0}}$ that takes into account the fact that the state $\chi'_{\mathbf{0}}$ should be properly normalized. In this manner you arrive at a Schrödinger-like equation that determines the one-particle state and energie. If you introduce $\phi_{\mathbf{0}} = \sqrt{N_{\mathbf{0}}}\chi'_{\mathbf{0}}$ and use $V(\mathbf{x}-\mathbf{x}') = V_{\mathbf{0}}\delta(\mathbf{x}-\mathbf{x}')$ it reduces to the Gross-Pitaevskii equation. Do you understand why $\epsilon'_{\mathbf{0}}$ should be interpreted as the chemical potential?

Assuming that we have solved for the Gross-Pitaevskii equation, the fluctuation corrections are in the Bogoliubov theory determined by a quadratic action of the form

$$\begin{aligned} &S_B[\phi'^*,\phi'] &(2.121)\\ &\quad = -\frac{\hbar}{2}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \left[\phi'^*(\mathbf{x},\tau),\phi'(\mathbf{x},\tau)\right]\cdot \mathbf{G}^{-1}\cdot \left[\begin{array}{c}\phi'(\mathbf{x},\tau)\\ \phi'^*(\mathbf{x},\tau)\end{array}\right] \ , \end{aligned}$$

where the associated Green's function $\mathbf{G}$ has now a matrix structure because not only the normal average $\langle \phi'(\mathbf{x},\tau)\phi'^*(\mathbf{x}',\tau')\rangle$ but also the anomalous average $\langle \phi'(\mathbf{x},\tau)\phi'(\mathbf{x}',\tau')\rangle$ is now unequal to zero. We thus have that

$$-\mathbf{G}(\mathbf{x},\tau;\mathbf{x}',\tau') = \left\langle \left[\begin{array}{c}\phi'(\mathbf{x},\tau)\\ \phi'^*(\mathbf{x},\tau)\end{array}\right]\cdot \left[\phi'^*(\mathbf{x}',\tau'),\phi'(\mathbf{x}',\tau')\right]\right\rangle \ . \qquad (2.122)$$

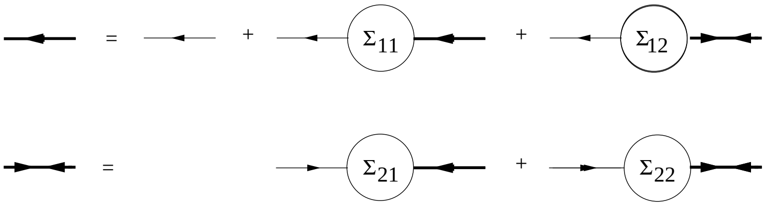

Fig. 12. Exact Dyson equation for the interacting normal and anomalous Green's functions.

From equation (2.117) we in fact find that in the Bogoliubov approximation

$$\mathbf{G}^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') = \mathbf{G}_0^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') \\ -\frac{1}{\hbar}\left[\begin{array}{cc} 2V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2 & V_{\mathbf{0}}(\phi_{\mathbf{0}}(\mathbf{x}))^2 \\ V_{\mathbf{0}}(\phi^*_{\mathbf{0}}(\mathbf{x}))^2 & 2V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2 \end{array}\right]\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')\ . \tag{2.123}$$

with the noninteracting Green's function $\mathbf{G}_0$ defined by

$$\mathbf{G}_0^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') = \left[\begin{array}{cc} G_0^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') & 0 \\ 0 & G_0^{-1}(\mathbf{x}',\tau';\mathbf{x},\tau) \end{array}\right] \tag{2.124}$$

and, of course,

$$G_0^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') \\ = -\frac{1}{\hbar}\left\{\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\rm ex}(\mathbf{x}) - \mu\right\}\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')\ . \tag{2.125}$$

This is clearly only the lowest order result for the Green's function, because a perturbative treatment of $S_{\rm int}[\phi'^*,\phi']$ leads, in the same way as in section 2.5, to higher order corrections. In general, the Dyson equation is, however, always of the form

$$\left[\begin{array}{cc} G_{11} & G_{12} \\ G_{21} & G_{22} \end{array}\right]^{-1} = \left[\begin{array}{cc} G_0^{-1} & 0 \\ 0 & G_0^{-1} \end{array}\right] - \left[\begin{array}{cc} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{array}\right]\ . \tag{2.126}$$

The off-diagonal elements are again called anomalous, since they vanish in the normal phase of the gas. Diagrammatically the Dyson equations for G_{11} and G_{21} are shown in figure 12.

The selfenergy in the Bogoliubov approximation is

$$\hbar\boldsymbol{\Sigma}(\mathbf{x},\tau;\mathbf{x}',\tau') \\ = \left[\begin{array}{cc} 2V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2 & V_{\mathbf{0}}(\phi_{\mathbf{0}}(\mathbf{x}))^2 \\ V_{\mathbf{0}}(\phi^*_{\mathbf{0}}(\mathbf{x}))^2 & 2V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2 \end{array}\right]\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')\ . \tag{2.127}$$

Because we have completely negelected the cubic and quartic terms in the action to obtain this selfenergy, the Bogoliubov approach is only valid if the fluctuations are sufficiently small. Physically, this impies that the deplection of the condensate must be small. It can, therefore, not be applied to liquid helium, but is expected to be valid for a weakly-interacting atomic gas at such low temperature that it essentially only consists of a condensate. Under these conditions the Bogoliubov theory not only predicts the condensate density profile $n_{\mathbf{0}}(\mathbf{x}) = |\phi_{\mathbf{0}}(\mathbf{x})|^2$ but also the collective modes of the condensate. Both these predictions have been accurately verified in recent experiments [26–28]. Theoretically, the eigenfrequencies of the collective modes are again determined by the poles in the one-particle Green's function. To understand more clearly how these can be determined, we first consider a homogeneous Bose gas.

In a box with volume $V = L^3$ the one-particle states are most easily characterized by the wavevector $\mathbf{k} = (2\pi/L)\mathbf{n}$ and equal to $e^{i\mathbf{k}\cdot\mathbf{x}}/\sqrt{V}$. The one-particle energies are thus $\epsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$. Moreover, the Gross-Pitaevskii equation reduces to $\mu = V_{\mathbf{0}}|\phi_{\mathbf{0}}|^2$ in that case, because the Landau 'free-energy' is minimized for a macroscopic wave function that is independent of the position in the box. Making use of this fact, equation (2.123) can immediately be solved by a Fourier transformation. The result is

$$\begin{aligned}
&-\hbar\mathbf{G}^{-1}(\mathbf{k}, i\omega_n) \qquad (2.128)\\
&= \left[\begin{array}{cc} -i\hbar\omega_n + \epsilon_{\mathbf{k}} + V_{\mathbf{0}}|\phi_{\mathbf{0}}|^2 & V_{\mathbf{0}}\phi_{\mathbf{0}}^2 \\ V_{\mathbf{0}}\phi_{\mathbf{0}}^{*2} & i\hbar\omega_n + \epsilon_{\mathbf{k}} + V_{\mathbf{0}}|\phi_{\mathbf{0}}|^2 \end{array}\right] .
\end{aligned}$$

Clearly there are poles in $G(\mathbf{k}, \omega)$ if the determinant of the right-hand side is zero or if

$$\hbar\omega = \hbar\omega_{\mathbf{k}} \equiv \sqrt{\epsilon_{\mathbf{k}}^2 + 2V_{\mathbf{0}}|\phi_{\mathbf{0}}|^2\epsilon_{\mathbf{k}}} = \sqrt{\epsilon_{\mathbf{k}}^2 + 2V_{\mathbf{0}}n_{\mathbf{0}}\epsilon_{\mathbf{k}}} \,. \qquad (2.129)$$

This is the famous Bogoliubov dispersion of the collective excitations. Note that to finish the calculation we still have to obtain the condensate density $n_{\mathbf{0}} = |\phi_{\mathbf{0}}|^2$. This is determined by the total density of the gas, which obeys

$$n = |\phi_{\mathbf{0}}|^2 - G_{11}(\mathbf{x}, \tau; \mathbf{x}, \tau^+) = n_{\mathbf{0}} + n' \,, \qquad (2.130)$$

with n' the density of the 'above' condensate particles. By inverting the right-hand side of equation (2.128), we find that the noncondensate density is equal to

$$\begin{aligned}
n' &= \lim_{\eta\downarrow 0} \frac{\hbar}{V\hbar\beta} \sum_{\mathbf{k}\neq\mathbf{0},n} e^{i\omega_n\eta} \frac{i\hbar\omega_n + \epsilon_{\mathbf{k}} + V_{\mathbf{0}}n_{\mathbf{0}}}{(\hbar\omega_n)^2 + (\hbar\omega_{\mathbf{k}})^2} \qquad (2.131)\\
&= \frac{1}{V}\sum_{\mathbf{k}\neq\mathbf{0}} \left(\frac{\epsilon_{\mathbf{k}} + V_{\mathbf{0}}n_{\mathbf{0}}}{\hbar\omega_{\mathbf{k}}} \frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} + \frac{\epsilon_{\mathbf{k}} + V_{\mathbf{0}}n_{\mathbf{0}} - \hbar\omega_{\mathbf{k}}}{2\hbar\omega_{\mathbf{k}}} \right) .
\end{aligned}$$

For a given density and temperature, the last two equations thus fully determine the condensate density. Note that equation (2.131) explicitly shows that the condensate is indeed depleted both by thermal as well as quantum effects.

Exercise 2.25: Show that the exact normal and anomalous Green's functions for a homogeneous Bose-Einstein condensed gas obey $G_{22}(\mathbf{k}, i\omega_n) = G_{11}(-\mathbf{k}, -i\omega_n)$ and $G_{12}(\mathbf{k}, i\omega_n) = G^*_{21}(-\mathbf{k}, -i\omega_n)$. What do these relations imply for the exact normal and anomalous selfenergies?

Exercise 2.26: It can also be shown that the exact normal and anomalous selfenergies obey $\mu = \hbar\Sigma_{22}(\mathbf{0}, 0) - |\hbar\Sigma_{12}(\mathbf{0}, 0)|$. Check that this is true for the Bogoliubov theory and prove from this relationship that the dispersion of the collective excitations must be gapless.

The generalization to the inhomogeneous case is straightforward. First we again have to solve the Gross-Pitaevskii equation at a fixed chemical potential. Given the condensate wave function, we can then calculate the collective mode frequencies by finding the poles of $\mathbf{G}$, or equivalently but more conveniently, the zero's of $\mathbf{G}^{-1}$. Clearly, the latter are located at $\hbar\omega = \hbar\omega_{\mathbf{n}}$, where $\hbar\omega_{\mathbf{n}}$ is found from the eigenvalue problem

$$\begin{aligned} &\begin{bmatrix} \hat{K} + 2V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2 & V_{\mathbf{0}}(\phi_{\mathbf{0}}(\mathbf{x}))^2 \\ V_{\mathbf{0}}(\phi^*_{\mathbf{0}}(\mathbf{x}))^2 & \hat{K} + 2V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2 \end{bmatrix} \cdot \begin{bmatrix} u_{\mathbf{n}}(\mathbf{x}) \\ v_{\mathbf{n}}(\mathbf{x}) \end{bmatrix} \\ &\qquad = \hbar\omega_{\mathbf{n}} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} u_{\mathbf{n}}(\mathbf{x}) \\ v_{\mathbf{n}}(\mathbf{x}) \end{bmatrix} \end{aligned} \tag{2.132}$$

and we introduced the operator $\hat{K} = -\hbar^2\mathbf{\nabla}^2/2m + V^{\mathrm{ex}}(\mathbf{x}) - \mu$. This is de Bogoliubov-de Gennes equation that has recently been applied with great succes to the collective modes of a Bose condensed rubidium and sodium gas [29, 30]. Note that a special solution with $\hbar\omega_{\mathbf{0}} = 0$ is given by $[u_{\mathbf{0}}(\mathbf{x}), v_{\mathbf{0}}(\mathbf{x})] = [\phi_{\mathbf{0}}(\mathbf{x}), -\phi^*_{\mathbf{0}}(\mathbf{x})]$. As a result we can, by making use of the fact that the left-hand side of the Bogoliubov-de Gennes equation involves a hermitian operator, easily prove that all the solutions obey

$$\int d\mathbf{x}\ \phi^*_{\mathbf{0}}(\mathbf{x}) u_{\mathbf{n}}(\mathbf{x}) + \int d\mathbf{x}\ \phi_{\mathbf{0}}(\mathbf{x}) v_{\mathbf{n}}(\mathbf{x}) = 0\ , \tag{2.133}$$

as required by the condition in equation (2.115). Moreover, we can similary show that the solutions with $\hbar\omega_{\mathbf{n}} > 0$ can always be normalized as [31]

$$\int d\mathbf{x}\ (|u_{\mathbf{n}}(\mathbf{x})|^2 - |v_{\mathbf{n}}(\mathbf{x})|^2) = 1\ . \tag{2.134}$$

Physically, the zero frequency solution $\mathbf{n} = \mathbf{0}$ describes the dynamics of the global phase of the condensate [32]. Because of the so-called $U(1)$ symmetry of the action, i.e., its invariance under the simultaneous phase changes $\phi(\mathbf{x},\tau) \to e^{i\vartheta}\phi(\mathbf{x},\tau)$ and $\phi^*(\mathbf{x},\tau) \to e^{-i\vartheta}\phi^*(\mathbf{x},\tau)$, this solution is essentially of no importance to the thermodynamic properties of a macroscopic gas sample and is therefore usually neglected. Nevertheless, it has from a fundamental point of view some interesting consequences, as we will see in section 2.10. Knowing all the eigenstates of $\mathbf{G}^{-1}$ we can then easily perform the inversion and finally again determine the density profile of the noncondensed atoms. Keeping the physical significance of the zero frequency mode in mind, we ultimately find,

$$n'(\mathbf{x}) = \sum_{\mathbf{n}\neq\mathbf{0}} \left((|u_{\mathbf{n}}(\mathbf{x})|^2 + |v_{\mathbf{n}}(\mathbf{x})|^2) \frac{1}{e^{\beta\hbar\omega_{\mathbf{n}}} - 1} + |v_{\mathbf{n}}(\mathbf{x})|^2 \right) \ , \tag{2.135}$$

which may be compared with equation (2.131).

At temperatures near absolute zero, we have as a good approximation that $n'(\mathbf{x}) = 0$ and the Bogoliubov theory applies. However at nonzero temperatures we thermally excite particles and $n'(\mathbf{x})$ becomes nonzero. If we treat the effect of the noncondensate part of the gas in the Hartree-Fock approximation, we find that $S_{\text{int}}[\phi'^*, \phi']$ on average adds

$$\begin{aligned} S^{\text{HF}}_{\text{int}}[\phi'^*, \phi'] = {} & 2\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ V_{\mathbf{0}} n'(\mathbf{x}) \phi'^*(\mathbf{x},\tau)\phi_{\mathbf{0}}(\mathbf{x}) \\ & +2\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ V_{\mathbf{0}} n'(\mathbf{x}) \phi'(\mathbf{x},\tau)\phi^*_{\mathbf{0}}(\mathbf{x}) \\ & +2\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ V_{\mathbf{0}} n'(\mathbf{x}) \phi'^*(\mathbf{x},\tau)\phi'(\mathbf{x},\tau) \ , \end{aligned} \tag{2.136}$$

to the action $S_0[\phi'^*, \phi']$. In figure 13 we indicate how this can be understood diagramatically. Performing the same analysis as before, we conclude that the Gross-Pitaevskii equation is modified to

$$\left(-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + V^{\text{ex}}(\mathbf{x}) + 2V_{\mathbf{0}} n'(\mathbf{x}) + V_{\mathbf{0}} |\phi_{\mathbf{0}}(\mathbf{x})|^2 \right) \phi_{\mathbf{0}}(\mathbf{x}) = \mu \phi_{\mathbf{0}}(\mathbf{x}) \ , \tag{2.137}$$

and the normal selfenergies are changed into $2V_{\mathbf{0}}|\phi_{\mathbf{0}}(\mathbf{x})|^2 + 2V_{\mathbf{0}} n'(\mathbf{x}) = 2V_{\mathbf{0}} n(\mathbf{x})$. The Bogoliubov-de Gennes equation for the elementary excitations is, therefore, now given by

$$\begin{aligned} & \left[\begin{array}{cc} \hat{K} + 2V_{\mathbf{0}} n(\mathbf{x}) & V_{\mathbf{0}}(\phi_{\mathbf{0}}(\mathbf{x}))^2 \\ V_{\mathbf{0}}(\phi^*_{\mathbf{0}}(\mathbf{x}))^2 & \hat{K} + 2V_{\mathbf{0}} n(\mathbf{x}) \end{array} \right] \cdot \left[\begin{array}{c} u_{\mathbf{n}}(\mathbf{x}) \\ v_{\mathbf{n}}(\mathbf{x}) \end{array} \right] \\ & \qquad = \hbar\omega_{\mathbf{n}} \left[\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right] \cdot \left[\begin{array}{c} u_{\mathbf{n}}(\mathbf{x}) \\ v_{\mathbf{n}}(\mathbf{x}) \end{array} \right] \ . \end{aligned} \tag{2.138}$$

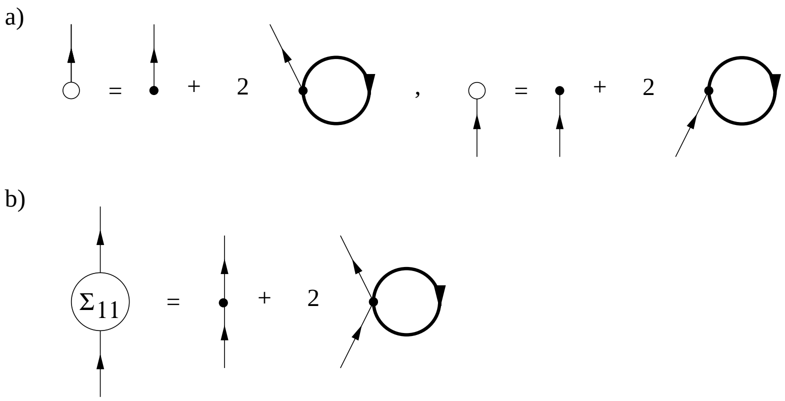

Fig. 13. Hartree-Fock corrections to a) the linear and b) the quadratic interaction terms of the Bogoliubov theory. This represents the Popov theory.

These last two equations in combination with equation (2.135) are known as the Popov theory in the recent literature [33]. It is much studied at present in the context of Bose-Einstein condensation in atomic gases, and has been applied with succes to the equilibrium density profile of the gas below the critical temperature [34]. It has also been used to determine the collective mode frequencies of the gas at nonzero temperatures, however, with much less success [35,36]. The reason for the failure of the Popov theory in this case is that the Bogoliubov-de Gennes equation in equation (2.138) describes physically only the motion of the condensate in the presence of a static noncondensed cloud and not the dynamics of the noncondensed cloud itself. Now we briefly want to make a connection to the interaction parameter $V_{\mathbf{0}}$ used in the Bogoliubov and Popov theories and the specific two-body scattering properties of the atomic gas of interest in a particular experiment.

Exercise 2.27: Determine the dispersion relation $\hbar\omega_{\mathbf{k}}$ for the collective excitations in the Popov theory for the homogeneous Bose gas. Is it gapless?

2.8.2 Some atomic physics

In the previous section we mentioned that the Bogoliubov theory, and to a certain extent also the Popov theory, agree very well with experiment. It is clear, however, that to apply these theories to an actual experiment we need to know the interaction parameter $V_{\mathbf{0}}$. In the case of atomic gases it is indeed possible to perform an *ab initio* calculation of this quantity,

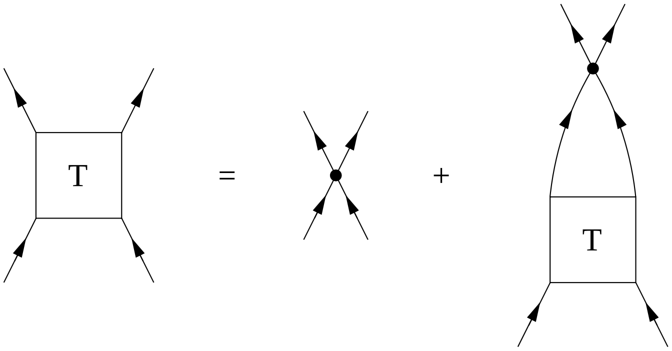

Fig. 14. T-matrix equation for the effective interatomic interaction.

something which for instance cannot be done for liquid helium. The reason why $V_{\mathbf{0}}$ can be determined for atomic gases, is that under the experimental conditions of interest the densities are always so low that we only need to consider all two-body processes taking place in the gas and we can neglect three-body and higher-body processes. This implies physically that we only have to calculate and add the quantum mechanical amplitudes for two atoms to scatter of each other an arbitrary number of times. Diagrammatically the procedure can essentially be summarized by the T-matrix equation in figure 14, because by iteration of this equation we easily see that we are indeed summing all two-body interacion processes.

Denoting the total momentum of the two incoming particles by $\hbar\mathbf{K}$ and the sum of the two Matsubara frequencies by Ω_n, the T-matrix equation in figure 14 can, with our knowledge of how to perform the Matsubara sum in the right-hand side, easily be shown to be mathematically equivalent to

$$\begin{aligned} T(\mathbf{K}, i\Omega_n) = V_{\mathbf{0}} + \frac{V_{\mathbf{0}}}{V} \sum_{\mathbf{k}} & \frac{1}{i\hbar\Omega_n - \epsilon_{\mathbf{K}/2+\mathbf{k}} - \epsilon_{\mathbf{K}/2-\mathbf{k}} + 2\mu} \\ & \times \left(1 + \frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2+\mathbf{k}} - \mu)} - 1} + \frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2-\mathbf{k}} - \mu)} - 1} \right) T(\mathbf{K}, i\Omega_n) \ . \end{aligned} \tag{2.139}$$

It is immediately solved by

$$\begin{aligned} \frac{1}{T(\mathbf{K}, i\Omega_n)} = \frac{1}{V_{\mathbf{0}}} - \frac{1}{V} \sum_{\mathbf{k}} & \frac{1}{i\hbar\Omega_n - \epsilon_{\mathbf{K}/2+\mathbf{k}} - \epsilon_{\mathbf{K}/2-\mathbf{k}} + 2\mu} \\ & \times \left(1 + \frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2+\mathbf{k}} - \mu)} - 1} + \frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2-\mathbf{k}} - \mu)} - 1} \right) \ . \end{aligned} \tag{2.140}$$

Note that this is a somewhat formal result, because the momentum sum in the right-hand side has an ultra-violet divergence, which from a field-theoretical point of view requires a renormalization procedure.

Exercise 2.28: Derive equation (2.139) from its diagrammatic representation presented in figure 14.

The physical reason for the divergence is that we have used the approximate potential $V_{\mathbf{0}}\delta(\mathbf{x}-\mathbf{x}')$ instead of the actual interactomic potential $V(\mathbf{x}-\mathbf{x}')$. The argument for using the δ-function approximation was that the thermal de Broglie wavelength of the atoms is for the ultra-low temperatures of interest always much larger than the typical range of the interaction. We now see that this argument is not fully correct, because if we calculate corrections in perturbation theory, we have to deal with momentum sums which are not always restricted to momenta of order $\hbar/\Lambda_{\text{th}}$ and are therefore sensitive to the precise details of the interaction potential.

To cure this disease we note that if we put in equation (2.139) the Bose occupation numbers equal to zero, we precisely get the T-matrix or Lippmann-Schwinger equation [37] for two atoms interacting with the potential $V_{\mathbf{0}}\delta(\mathbf{x}-\mathbf{x}')$. Furthermore, if the atoms interact with the potential $V(\mathbf{x}-\mathbf{x}')$ the solution of the corresponding Lippmann-Schwinger equation is known from elementary scattering theory to be equal to $4\pi a\hbar^2/m$ for small incoming momenta and energies, where a is the s-wave scattering length. We thus conclude that we must interpret

$$\frac{1}{V_{\mathbf{0}}}-\frac{1}{V}\sum_{\mathbf{k}}\frac{1}{i\hbar\Omega_n-\epsilon_{\mathbf{K}/2+\mathbf{k}}-\epsilon_{\mathbf{K}/2-\mathbf{k}}+2\mu}$$

as being equal to $m/4\pi a\hbar^2$ and, therefore, that the desired T-matrix in principle obeys

$$\begin{aligned}\frac{1}{T(\mathbf{K},i\Omega_n)}=\frac{m}{4\pi a\hbar^2}-\frac{1}{V}\sum_{\mathbf{k}}&\frac{1}{i\hbar\Omega_n-\epsilon_{\mathbf{K}/2+\mathbf{k}}-\epsilon_{\mathbf{K}/2-\mathbf{k}}+2\mu}\\ &\times\left(\frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2+\mathbf{k}}-\mu)}-1}+\frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2-\mathbf{k}}-\mu)}-1}\right)\ .\end{aligned} \tag{2.141}$$

To obtain an accurate theory for a trapped atomic Bose gas that includes the effect of all two-body processes, we should now use instead of $V_{\mathbf{0}}$ the above T-matrix in the Bogoliubov or Popov theories. Of course, in the normal phase the same is true for the Hartree-Fock theory. If the temperature is not too close to the critical temperature for Bose-Einstein condensation, it turns out that $T(\mathbf{K},i\Omega_n)\simeq 4\pi a\hbar^2/m$ and we arrive at the conclusion that for an application to realistic atomic gases we must replace everywhere in section 2.8.1 the interaction parameter $V_{\mathbf{0}}$ by $4\pi a\hbar^2/m$. For temperatures close to the critical temperature, this is however no longer true and the Bose distribution functions have a nonnegligible effect of the T-matrix [38, 39]. The theory that, by using 'dressed' one-particle propagators in figure 14, selfconsistently includes these effects of the medium on the scattering properties of the atoms is known as the many-body T-matrix theory.

2.8.3 Superconductivity

Finally, we want to briefly discuss the Bardeen-Cooper-Schrieffer or BCS theory of superconductivity [40], which has received considerable attention recently in connection with ongoing experiments with the fermionic isotope of lithium. The reasons for this will become clear shortly. We are in that case dealing with effective spin 1/2 fermions and the action is taken to be

$$\begin{aligned} &S[\phi^*, \phi] \qquad\qquad (2.142) \\ &\quad = \sum_{\alpha=\uparrow,\downarrow} \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \phi^*_\alpha(\mathbf{x},\tau) \left\{ \hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\boldsymbol{\nabla}^2}{2m} - \mu \right\} \phi_\alpha(\mathbf{x},\tau) \\ &\quad + \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ V_{\mathbf{0}} \phi^*_\uparrow(\mathbf{x},\tau)\phi^*_\downarrow(\mathbf{x},\tau)\phi_\downarrow(\mathbf{x},\tau)\phi_\uparrow(\mathbf{x},\tau)\ . \end{aligned}$$

Note that the use of a single chemical potential implies that we only consider the optimal case of an equal density in each hyperfine state. This situation is optimal in the sense that, for unequal densities in each hyperfine state, it is no longer possible to pair up all the atoms in the gas. As a result the critical temperature of the gas drops dramatically, and in general becomes experimentally inaccessible. The effect is to a large extent analogous to putting superfluid ^{3}He in an homogeneous magnetic field. Furthermore, we in first instance consider the homogeneous case, because we want to illustrate in this section the local-density approximation to include the effect of the external trapping potential. Physically, this approximation treats the gas as consisting of a large number of independent gases that are in diffusive equilibrium with each other. Such an approach only works if the correlation length of the gas is much smaller than the typical length scale associated with changes of the external potential. Fortunately, this is almost always the case for realistic trapped atomic gases and for that reason the local-density approximation is often used in practice.

The BCS theory is the theory of Bose-Einstein condensation of so-called Cooper pairs. This means that the order parameter is $\langle\phi_\downarrow(\mathbf{x},\tau)\phi_\uparrow(\mathbf{x},\tau)\rangle$, in analogy with the order parameter $\langle\phi(\mathbf{x},\tau)\rangle$ for the Bose case just discussed. Furthermore, it requires that the interaction parameter $V_{\mathbf{0}}$ is negative, since otherwise the formation of pairs would not be energetically favorable. From now on we assume, therefore, that this is the case. The condensate of Cooper pairs can also be nicely treated with a Hubbard-Stratonovich transformation. We now introduce a complex field $\Delta(\mathbf{x},\tau)$ and use

$$\begin{aligned}
&\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\; V_{\mathbf{0}}\phi^*_\uparrow(\mathbf{x},\tau)\phi^*_\downarrow(\mathbf{x},\tau)\phi_\downarrow(\mathbf{x},\tau)\phi_\uparrow(\mathbf{x},\tau)\right\} \qquad (2.143)\\
&\quad = \int d[\Delta^*]d[\Delta]\;\exp\left\{\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\;\left(\frac{|\Delta(\mathbf{x},\tau)|^2}{V_{\mathbf{0}}}\right.\right.\\
&\quad \left.\left. +\;\Delta^*(\mathbf{x},\tau)\phi_\downarrow(\mathbf{x},\tau)\phi_\uparrow(\mathbf{x},\tau) + \phi^*_\uparrow(\mathbf{x},\tau)\phi^*_\downarrow(\mathbf{x},\tau)\Delta(\mathbf{x},\tau)\right)\right\}\;.
\end{aligned}$$

This leads to a partition function with the action

$$\begin{aligned}
S[\Delta^*,\Delta,\phi^*,\phi] = &-\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\;\frac{|\Delta(\mathbf{x},\tau)|^2}{V_{\mathbf{0}}} \qquad (2.144)\\
&-\frac{\hbar}{2}\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\;\left[\phi^*_\downarrow(\mathbf{x},\tau),\phi_\uparrow(\mathbf{x},\tau)\right]\cdot\mathbf{G}^{-1}\cdot\left[\begin{array}{c}\phi_\downarrow(\mathbf{x},\tau)\\ \phi^*_\uparrow(\mathbf{x},\tau)\end{array}\right]\;,
\end{aligned}$$

where

$$\begin{aligned}
\mathbf{G}^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') = &\;\mathbf{G}_0^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') \qquad (2.145)\\
&-\frac{1}{\hbar}\left[\begin{array}{cc}0 & \Delta(\mathbf{x},\tau)\\ \Delta^*(\mathbf{x},\tau) & 0\end{array}\right]\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')\;,
\end{aligned}$$

and the noninteracting Green's function $\mathbf{G}_0$ is defined by

$$\mathbf{G}_0^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') = \left[\begin{array}{cc}G_0^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') & 0\\ 0 & -G_0^{-1}(\mathbf{x}',\tau';\mathbf{x},\tau)\end{array}\right] \qquad (2.146)$$

and

$$G_0^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') = -\frac{1}{\hbar}\left\{\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2\boldsymbol{\nabla}^2}{2m} - \mu\right\}\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')\;. \qquad (2.147)$$

We thus see that the fermionic part has exactly the same matrix structure as in the case of a condensed Bose gas, only the selfenergy is now

$$\left[\begin{array}{cc}\Sigma_{11} & \Sigma_{12}\\ \Sigma_{21} & \Sigma_{22}\end{array}\right] = \frac{1}{\hbar}\left[\begin{array}{cc}0 & \Delta(\mathbf{x},\tau)\\ \Delta^*(\mathbf{x},\tau) & 0\end{array}\right]\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')\;. \qquad (2.148)$$

If we again integrate out the fermion fields, we get the effective action

$$S^{\text{eff}}[\Delta^*,\Delta] = -\int_0^{\hbar\beta} d\tau \int d\mathbf{x}\;\frac{|\Delta(\mathbf{x},\tau)|^2}{V_{\mathbf{0}}} - \hbar\mathrm{Tr}[\ln(-\mathbf{G}^{-1})]\;, \qquad (2.149)$$

which we can expand in powers of Δ by using $\mathbf{G}^{-1} = \mathbf{G}_0^{-1} - \mathbf{\Sigma} = \mathbf{G}_0^{-1}(1 - \mathbf{G}_0\mathbf{\Sigma})$ and therefore

$$-\hbar \mathrm{Tr}[\ln(-\mathbf{G}^{-1})] = -\hbar \mathrm{Tr}[\ln(-\mathbf{G}_0^{-1})] + \hbar \sum_{m=1}^{\infty} \frac{1}{m} \mathrm{Tr}[(\mathbf{G}_0\mathbf{\Sigma})^m] \ . \tag{2.150}$$

Explicite calculation [41] shows that for space and time independent Δ we obtain near the critical temperature a ‘free-energy’ density of the form of the Landau-theory of second-order phase transitions, i.e.,

$$f_L(|\Delta|) = \alpha(T)|\Delta|^2 + N(0)\frac{7\zeta(3)}{16(\pi k_B T_c)^2}|\Delta|^4 \ , \tag{2.151}$$

with as expected

$$\begin{aligned} \alpha(T) &= -\frac{1}{V_{\mathbf{0}}} + \frac{1}{V}\sum_{\mathbf{k}} \frac{1}{2(\epsilon_{\mathbf{k}} - \mu)} \left(1 - \frac{2}{e^{\beta(\epsilon_{\mathbf{k}}-\mu)} + 1}\right) \\ &\equiv N(0) \ln\left(\frac{T}{T_c}\right) \simeq N(0)\left(\frac{T}{T_c} - 1\right) \ . \end{aligned} \tag{2.152}$$

Here $N(0) = mk_F/(2\pi^2\hbar^2)$ is the density of states of a single spin state at the Fermi energy $\epsilon_F \equiv \hbar^2 k_F^2/2m$ and the critical temperature is given by

$$T_c = \frac{8e^{\gamma-2}}{\pi}\frac{\epsilon_F}{k_B} \exp\left\{-\frac{\pi}{2k_F|a|}\right\} \ , \tag{2.153}$$

if we use the same renormalization procedure as in section 2.8.2 to eliminate the interaction parameter $V_{\mathbf{0}}$ in favor of the negative s-wave scattering length a.

Exercise 2.29: Prove the validity of equation (2.151). For the calculation of the $|\Delta|^4$-term you can make use of the identity

$$\sum_{\omega_n} \frac{1}{|\hbar\omega_n|^3} = \frac{7\zeta(3)}{4}\frac{1}{(\pi k_B T)^3} \ ,$$

where ω_n are the fermionic Matsubara frequencies and $\zeta(3) \simeq 1.202$.

Below T_c we thus have a nonzero average $\langle\Delta(\mathbf{x},\tau)\rangle \equiv \Delta_0$. Using this in the Green’s function for the fermions and neglecting fluctations, we find in momentum space that

$$-\hbar\mathbf{G}^{-1}(\mathbf{k}, i\omega_n) = \begin{bmatrix} -i\hbar\omega_n + \epsilon_{\mathbf{k}} - \mu & \Delta_0 \\ \Delta_0^* & -(i\hbar\omega_n + \epsilon_{\mathbf{k}} - \mu) \end{bmatrix} \tag{2.154}$$

and therefore poles in $\mathbf{G}(\mathbf{k},\omega)$ if

$$\hbar\omega_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}}-\mu)^2+|\Delta_0|^2}\ . \tag{2.155}$$

This disperion relation has clearly a gap of magnitude $|\Delta_0|$ at the Fermi surface. As a consequence $|\Delta_0|$ is known as the BCS gap parameter. Note that the critical temperature below which the gap becomes nonzero depends exponentally on the parameter $\pi/2k_F|a|$. For typical atomic gases this is a quantity which is much larger than one, and the BCS transition is experimentally inaccesible. The only exception at the moment appears to be ^{6}Li, with its anomalously large and negative triplet scattering length of $-2160\ a_0$ [42]. This explains the present interest in spin-polarized atomic lithium.

Exercise 2.30: The many-body wave function $|\Psi_{\rm BCS}\rangle$ for the BCS theory can be found from the fact that $\langle\Psi_{\rm BCS}|\hat\psi_\downarrow(\mathbf{x})\hat\psi_\uparrow(\mathbf{x})|\Psi_{\rm BCS}\rangle$ must be nonzero and equal to the Cooper pair wave function $\phi_{\downarrow\uparrow}(\mathbf{x}-\mathbf{x}')$. Put differently, the BCS ground state is an eigenstate of the operator $\hat\psi_\downarrow(\mathbf{x})\hat\psi_\uparrow(\mathbf{x})$ with the eigenvalue $\phi_{\downarrow\uparrow}(\mathbf{x}-\mathbf{x}')$. Show now that this implies that

$$|\Psi_{\rm BCS}\rangle \propto \prod_{\mathbf{k}}\left(u_{\mathbf{k}}+v_{\mathbf{k}}\hat\psi^\dagger_{\mathbf{k},\downarrow}\hat\psi^\dagger_{-\mathbf{k},\uparrow}\right)|0\rangle\ .$$

Determine in the same way also the many-body wave function $|\Psi_{\rm BEC}\rangle$ of a Bose-Einstein condensate. What is the difference with excercise 2.24?

Exercise 2.31: In principle a BCS transition could also occur in a Bose gas with attractive interactions, i.e., $V_{\mathbf{0}} < 0$. Show that the dispersion relation of the single-particle excitations is

$$\hbar\omega_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}}-\mu)^2-|\Delta_0|^2}$$

in that case. What happens is $\mu = |\Delta_0|$?

In view of this exciting possibility, we have recently studied the equilibrium properties of atomic lithium is a harmonic oscillator potential $V^{\rm ex}(\mathbf{x}) = m\omega^2\mathbf{x}^2/2$, with a trapping frequency of $\omega/2\pi = 144$ Hz [43]. To incorporate the effect of the external potential we have, as mentioned above, applied the local-density approximation. The result is shown in figure 15. Note that the use of the local-density approximation implies that we perform the above outlined homogeneous calculation for each point in space with a chemical potential that is equal to

$$\mu(\mathbf{x}) = \mu - \frac{1}{2}m\omega^2\mathbf{x}^2 - \frac{4\pi a\hbar^2}{m}\frac{n(\mathbf{x})}{2}\ . \tag{2.156}$$

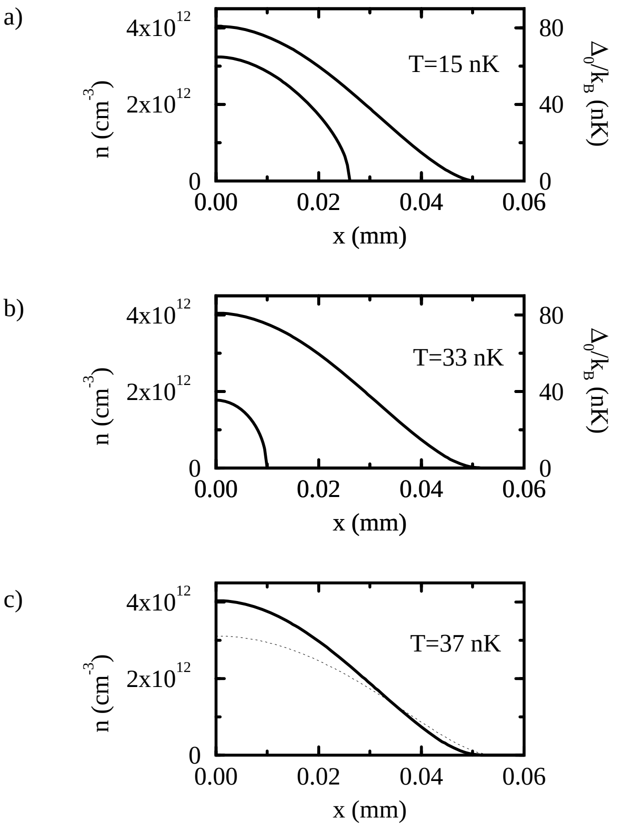

Fig. 15. Density distribution $n(\mathbf{x})$ and energy gap $\Delta_0(\mathbf{x})$ for a ^{6}Li atomic gas consisting of 2.865×10^5 atoms in each spin state a) at $T = 15$ nK, b) at $T = 33$ nK, slightly below T_c, and c) at $T = T_c = 37$ nK. The left scale of each plot refers to the density and the right scale to the energy gap. The dotted line in c) shows the density distribution for an ideal Fermi gas with the same number of particles and at the same temperature.

The third term in the right-hand side represents the mean-field effect of the Hartree contribution to the selfenergy of the fermions. Since our Hubbard-Stratonovich procedure is in principle exact, it is not immediately clear why such a term must be included in the theory. It can, however, be shown that it arises from the fluctuations of the BCS gap parameter. With this remark we essentially end our development of the equilibrium field theory. Next we discuss two applications.

2.9 Macroscopic quantum tunneling of a condensate

As we have already seen several times, the equlibrium field theory gives us also information on dynamical properties of the gas by means of the substitution $\omega_n \to -i\omega$ or equivalently $\tau \to it$. However, the Popov theory of Bose-Einstein condensation has shown us that we have to be very careful with this procedure, because we may not always end up with the correct physics needed for a discription of a particular experiment. It is for these cases that a truly nonequilibrium field theory is required. However, we can consider two important dynamical problems where the equilibrium theory does give us all the answers.

In a Bose gas with effectively attractive interactions, i.e., with a negative scattering length a, a condensate will always have the tendency to collapse to a high density state due to the gain in energy that can be obtained in this way [44]. The most important question in this context is, therefore, if a condensate can exist sufficiently long to be experimentally observed. Neglecting the variation of the noncondensate density on the size of the condensate [45, 46], we know from the Popov theory that the dynamics of the collapse is, apart from an unimportant shift in the chemical potential, determined by the Gross-Pitaevskii equation [25]

$$\begin{aligned} & i\hbar\frac{\partial}{\partial t}\langle\phi(\mathbf{x},t)\rangle \\ & \quad = \left\{-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu + \frac{4\pi a\hbar^2}{m}|\langle\phi(\mathbf{x},t)\rangle|^2\right\}\langle\phi(\mathbf{x},t)\rangle \ . \end{aligned} \tag{2.157}$$

More precisely, this determines only the semiclassical dynamics. If we also want to study the quantum fluctuations, which is necessary if we are also interested in how the condensate tunnels through the macroscopic energy barrier, it is most convenient to calculate the grand canonical partition function of the condensate [47]. Quantizing the Gross-Pitaevskii equation we obtain for this partition function the functional integral

$$Z(\mu) = \int d[\phi^*]d[\phi] \ \exp\left\{-\frac{1}{\hbar}S[\phi^*,\phi]\right\} \ , \tag{2.158}$$

over the complex field $\phi(\mathbf{x},\tau)$ and with the Euclidian action

$$\begin{aligned} S[\phi^*,\phi] = \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \ \phi^*(\mathbf{x},\tau)\left(\hbar\frac{\partial}{\partial\tau} + \frac{\hbar^2\boldsymbol{\nabla}^2}{2m}\right. \\ \left. + V^{\text{ex}}(\mathbf{x}) - \mu + \frac{2\pi a\hbar^2}{m}|\phi(\mathbf{x},\tau)|^2\right)\phi(\mathbf{x},\tau) \ . \end{aligned} \tag{2.159}$$

As always for Bose systems, the integration is only over fields that are periodic on the imaginary time axis.

Although it has recently been shown by Freire and Arovas that the tunneling process can also be studied in terms of the complex field $\phi(\mathbf{x},\tau)$ [48], we believe that it leads to somewhat more physical insight if we use instead the fields $\rho(\mathbf{x},\tau)$ and $\theta(\mathbf{x},\tau)$ that correspond to the density and phase fluctuations of the condensate, respectively. They are introduced by performing the canonical variable transformation [33]

$$\phi(\mathbf{x},\tau) = \sqrt{\rho(\mathbf{x},\tau)}e^{i\theta(\mathbf{x},\tau)}$$

in the functional integral for the partition function. As a result we find

$$Z(\mu) = \int d[\rho]d[\theta]\ \exp\left\{-\frac{1}{\hbar}S[\rho,\theta;\mu]\right\}\ , \tag{2.160}$$

with

$$\begin{aligned} S[\rho,\theta;\mu] = \int_0^{\hbar\beta} d\tau \int d\mathbf{x}\ \Bigg(& i\hbar\rho(\mathbf{x},\tau)\frac{\partial\theta(\mathbf{x},\tau)}{\partial\tau} \\ & + \frac{\hbar^2\rho(\mathbf{x},\tau)}{2m}(\boldsymbol{\nabla}\theta(\mathbf{x},\tau))^2 + \frac{\hbar^2}{8m\rho(\mathbf{x},\tau)}(\boldsymbol{\nabla}\rho(\mathbf{x},\tau))^2 \\ & + V^{\mathrm{ex}}(\mathbf{x})\rho(\mathbf{x},\tau) - \mu\rho(\mathbf{x},\tau) + \frac{2\pi a\hbar^2}{m}\rho^2(\mathbf{x},\tau)\Bigg)\ . \end{aligned} \tag{2.161}$$

Next, we notice that this action is only quadratic in the phase fluctuations. The field $\theta(\mathbf{x},\tau)$ can therefore be integrated over exactly, because it only involves the evaluation of a gaussian integral.

Compared to ordinary gaussian integrals there is, however, one slight complication which is associated with the fact that $\theta(\mathbf{x},\tau)$ are phase variables. This implies that the periodicity of the original field $\phi(\mathbf{x},\tau)$ only constraints the phase field $\theta(\mathbf{x},\tau)$ to be periodic up to a multiple of 2π. To evaluate the grand canonical partition function in equation (2.160) we must therefore first integrate over all fields $\theta(\mathbf{x},\tau)$ that obey the boundary condition $\theta(\mathbf{x},\hbar\beta) = \theta(\mathbf{x},0) + 2\pi j$ and subsequently sum over all possible integers j. Because these different boundary conditions only affect the zero-momentum part of $\theta(\mathbf{x},\tau)$ we first have to evaluate the sum

$$\sum_j \int^{\theta_{\mathbf{0}}(\hbar\beta)=\theta_{\mathbf{0}}(0)+2\pi j} d[\theta_{\mathbf{0}}]\ \exp\left\{-i\int_0^{\hbar\beta} d\tau\ N_{\mathbf{0}}(\tau)\frac{\partial\theta_{\mathbf{0}}(\tau)}{\partial\tau}\right\}\ ,$$

with $N_{\mathbf{0}}(\tau) = \int d\mathbf{x}\ \rho(\mathbf{x},\tau)$ the number of condensate particles. After performing a partial integration on the integral in the exponent, we can carry out the path integration over $\theta_{\mathbf{0}}(\tau)$ to obtain

$$\sum_j e^{2\pi i N_{\mathbf{0}} j}\delta\left[\frac{\partial N_{\mathbf{0}}(\tau)}{\partial\tau}\right]\ .$$

As expected, the integration over the global phase of the condensate leads to the constraint of a constant number of condensate particles, i.e., $N_{\mathbf{0}}(\tau) = N_{\mathbf{0}}$. Moreover, we have $\sum_j e^{2\pi i N_{\mathbf{0}} j} = \sum_j \delta(N_{\mathbf{0}} - j)$, which restricts the number of condensate particles to an integer. Putting all these results together, we see that the integration over the zero-momentum part of $\rho(\mathbf{x},\tau)$ is only a sum over the number of condensate particles and we have that

$$Z(\mu) = \sum_{N_{\mathbf{0}}} e^{\beta\mu N_{\mathbf{0}}} Z_{N_{\mathbf{0}}} \ . \tag{2.162}$$

Here we introduced the canonical partition function of the condensate, which is apparently equal to the functional integral

$$Z_{N_{\mathbf{0}}} = \int d[\rho]d[\theta] \ \exp\left\{-\frac{1}{\hbar}S[\rho,\theta;0]\right\} \tag{2.163}$$

over all the nonzero momentum components of the density and phase fields.

The integration over the nonzero momentum components of the phase field $\theta(\mathbf{x},\tau)$ is easily performed, because it now involves an ordinary gaussian integral. Introducing the Green's function for the phase fluctuations $G(\mathbf{x},\mathbf{x}';\rho)$ by

$$\frac{\hbar}{m}\left((\boldsymbol{\nabla}\rho)\cdot\boldsymbol{\nabla} + \rho\boldsymbol{\nabla}^2\right) G(\mathbf{x},\mathbf{x}';\rho) = \delta(\mathbf{x}-\mathbf{x}') \ , \tag{2.164}$$

we immediately obtain the desired effective action for the density field

$$\begin{aligned} S^{\text{eff}}[\rho] = & \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \int d\mathbf{x}' \ \left(-\frac{\hbar}{2}\frac{\partial\rho(\mathbf{x},\tau)}{\partial\tau} G(\mathbf{x},\mathbf{x}';\rho)\frac{\partial\rho(\mathbf{x}',\tau)}{\partial\tau}\right) \\ & + \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \ \left(\frac{\hbar^2}{8m\rho(\mathbf{x},\tau)}(\boldsymbol{\nabla}\rho(\mathbf{x},\tau))^2 + V^{\text{ex}}(\mathbf{x})\rho(\mathbf{x},\tau)\right. \\ & \qquad\qquad\qquad\qquad \left. + \frac{2\pi a\hbar^2}{m}\rho^2(\mathbf{x},\tau)\right) \ . \end{aligned} \tag{2.165}$$

Being an action for the density fluctuations of the condensate, $S^{\text{eff}}[\rho]$ also describes all the collisionless modes of the condensate. This is important for our purposes, because the mode which becomes unstable first, determines precisely how the condensate collapses. Moreover, it determines the probability with which the collapse is going to take place, both for quantum and thermal fluctuations, since the energy barrier is smallest in that direction of the configuration space. It should be noted that as long as we can neglect the interaction between the condensate and the thermal cloud, the action $S^{\text{eff}}[\rho]$ describes also the collective modes of a gas with positive scattering length. For various other theoretical approaches that have been applied under these conditions see, for example, Refs. [29, 30, 49–55]. The actual measurements of the collective mode frequencies have been performed by Jin *et al.* [26] and Mewes *et al.* [27] and are at sufficiently low temperatures indeed in good agreement with the theoretical predictions [35, 36]. We expect the same to be true for a gas with effectively attractive interactions and, therefore, the action $S^{\text{eff}}[\rho]$ to be a good starting point for the following discussion.

To obtain the collisionless modes explicitly we consider first the case of an ideal Bose gas by putting $a = 0$. For the ideal Bose gas we expect the gaussian profile

$$\rho(\mathbf{x}; q(\tau)) = N_{\mathbf{0}} \left(\frac{1}{\pi q^2(\tau)} \right)^{3/2} \exp\left(-\frac{\mathbf{x}^2}{q^2(\tau)} \right) \qquad (2.166)$$

to describe an exact mode of the condensate. The reason is that in the noninteracting case we can make a density fluctuation by taking one particle from the condensate and putting that in one of the excited states of the external potential. The corresponding density fluctuation obeys

$$\delta\rho(\mathbf{x}, t) \propto e^{-i(\epsilon_{\mathbf{n}} - \epsilon_{\mathbf{0}})t/\hbar} \chi^*_{\mathbf{n}}(\mathbf{x}) \chi_{\mathbf{0}}(\mathbf{x}) \ .$$

For the experimentally relevant case of an isotropic harmonic oscillator [11] it is more convenient to use instead of the cartesian quantum numbers $\mathbf{n}$, the two angular momentum quantum numbers ℓ and m and the quantum number n that counts the number of nodes in the radial wave function $\chi_{n\ell}(x)$. The density fluctuation then becomes

$$\delta\rho(\mathbf{x}, t) \propto e^{-i(2n+\ell)\omega t} \chi_{n\ell}(x) Y^*_{\ell m}(\hat{\mathbf{x}}) \frac{e^{-x^2/2l^2}}{(\pi l^2)^{3/4}} \ ,$$

with $\epsilon_{n\ell m} - \epsilon_{000} = (2n + \ell)\hbar\omega$ the excitation energy and $l = (\hbar/m\omega)^{1/2}$ the size of the condensate wave function. Comparing this now with the expansion of the gaussian profile in equation (2.166) around the groundstate density profile, which is obtained by substituting $q(\tau) = l + \delta q(\tau)$, we find that

$$\delta\rho(\mathbf{x}, \tau) = -\sqrt{6} N_{\mathbf{0}} \frac{\delta q(\tau)}{l} \chi_{10}(x) Y^*_{00}(\hat{\mathbf{x}}) \frac{e^{-x^2/2l^2}}{(\pi l^2)^{3/4}} \qquad (2.167)$$

has precisely the same form as a density fluctuation in which one particle is taken from the condensate and put into the harmonic oscillator state with quantum numbers $(n\ell m) = (100)$. The frequency of this so-called 'breathing' mode described by the gaussian density profile must therefore be equal to 2ω.

To prove that this is indeed correct, we need to evaluate the effective action $S^{\text{eff}}[\rho]$, and hence the Green's function $G(\mathbf{x}, \mathbf{x}'; \rho)$, for a gaussian density profile. Substituting such a profile in equation (2.164) immediately leads to $G(\mathbf{x},\mathbf{x}';\rho) = G(\mathbf{x},\mathbf{x}';q)/\rho(\mathbf{x}';q)$, with

$$\frac{\hbar}{m}\left(-\frac{2}{q^2}\mathbf{x}\cdot\boldsymbol{\nabla}+\boldsymbol{\nabla}^2\right)G(\mathbf{x},\mathbf{x}';q) = \delta(\mathbf{x}-\mathbf{x}')\ . \tag{2.168}$$

The latter equation can be solved, if we can solve the eigenvalue problem

$$\left(\boldsymbol{\nabla}^2 - \frac{2x}{q^2}\frac{\partial}{\partial x}\right)\xi(\mathbf{x}) = \lambda\xi(\mathbf{x})\ . \tag{2.169}$$

This turns out to be an easy task, because substituting

$$\xi_{n\ell m}(\mathbf{x}) = \xi_{n\ell}(x)\frac{e^{x^2/2q^2}}{x}Y_{\ell m}(\hat{\mathbf{x}}) \tag{2.170}$$

gives essentially the radial Schrödinger equation for an isotropic harmonic oscillator with frequency $\omega_q = \hbar/mq^2$, i.e.,

$$\begin{aligned} -\frac{2m}{\hbar^2}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}m\omega_q^2x^2+\frac{\hbar^2\ell(\ell+1)}{2mx^2}-\frac{3}{2}\hbar\omega_q\right)\xi_{n\ell}(x) \\ = \lambda_{n\ell}\xi_{n\ell}(x)\ . \end{aligned} \tag{2.171}$$

The desired eigenfunctions are therefore $\xi_{n\ell m}(\mathbf{x};q) = \varphi_{n\ell m}(\mathbf{x})e^{x^2/2q^2}$, with $\varphi_{n\ell m}(\mathbf{x})$ the properly normalized harmonic oscillator states with the energies $(2n+\ell+3/2)\hbar\omega_q$, and the corresponding eigenvalues are $\lambda_{n\ell}(q) = -2(2n+\ell)/q^2$. Introducing finally the 'dual' eigenfunctions $\bar{\xi}_{n\ell m}(\mathbf{x};q) \equiv \varphi^*_{n\ell m}(\mathbf{x})e^{-x^2/2q^2}$, the Green's function $G(\mathbf{x},\mathbf{x}';q)$ is given by

$$G(\mathbf{x},\mathbf{x}';q) = {\sum_{n\ell m}}' \xi_{n\ell m}(\mathbf{x};q)\frac{m}{\hbar\lambda_{n\ell}(q)}\bar{\xi}_{n\ell m}(\mathbf{x}';q)\ . \tag{2.172}$$

Note that prime on the summation sign indicates that the sum is over all quantum numbers except $(n\ell m) = (000)$. The latter is excluded because the associated eigenfunction $\xi_{000}(\mathbf{x};q)$ is just a constant and thus does not contribute to $G(\mathbf{x},\mathbf{x}';\rho)$, which is defined as the Green's function for all phase fluctuations with nonvanishing momenta.

Putting all these results together, we see that the dynamics of the collective variable $q(\tau)$ is determined by the action

$$\begin{aligned} S^{\text{eff}}[q] &= \int_0^{\hbar\beta} d\tau\ \left\{\frac{3mN_{\mathbf{0}}}{4}\left(\frac{dq}{d\tau}\right)^2 + N_{\mathbf{0}}\left(\frac{3\hbar^2}{4mq^2}+\frac{3}{4}m\omega^2q^2\right)\right\} \\ &\equiv \int_0^{\hbar\beta} d\tau\ \left\{\frac{1}{2}m^*\left(\frac{dq}{d\tau}\right)^2 + V(q)\right\}\ , \end{aligned} \tag{2.173}$$

that is equivalent to the action of a particle with effective mass $m^* = 3mN_{\mathbf{0}}/2$ in a potential $V(q) = N_{\mathbf{0}}(3\hbar^2/4mq^2 + 3m\omega^2q^2/4)$. As expected from our previous remarks, this potential has a minimum for $q = l$ and can be expanded near its minimum as

$$V(q) \simeq \frac{3}{2}N_{\mathbf{0}}\hbar\omega + \frac{1}{2}m^*(2\omega)^2(\delta q)^2 \ . \tag{2.174}$$

It thus comfirms that the gaussian profile describes a breathing mode with frequency 2ω around an equilibrium density profile that is given by $\rho(\mathbf{x}; l) = N_{\mathbf{0}}|\chi_{000}(\mathbf{x})|^2$.

Our next task is to investigate how interactions affect this result. Considering again only gaussian density profiles, the action $S^{\mathrm{eff}}[q]$ is again that of a particle with effective mass $m^* = 3mN_{\mathbf{0}}/2$ but now in the potential [56]

$$V(q) = N_{\mathbf{0}}\left(\frac{3\hbar^2}{4mq^2} + \frac{3}{4}m\omega^2q^2 - \frac{N_{\mathbf{0}}}{\sqrt{2\pi}}\frac{\hbar^2|a|}{mq^3}\right) \ . \tag{2.175}$$

The physically most important feature of this potential is that it is unbounded from below, since $V(q) \to -\infty$ if $q \downarrow 0$. Hence, the condensate indeed always has the tendency to collapse to the high-density state $\lim_{q\downarrow 0}\rho(\mathbf{x}; q) = N_{\mathbf{0}}\delta(\mathbf{x})$. However, if the number of condensate particles is sufficiently small, or more precisely if [57]

$$N_{\mathbf{0}} < \frac{2\sqrt{2\pi}}{5^{5/4}}\frac{l}{|a|} \simeq 0.68\frac{l}{|a|} \ , \tag{2.176}$$

the condensate has to overcome a macroscopic energy barrier before it can collapse. Under these conditions the condensate is therefore really metastable and can in principle be observed experimentally. The most important question in this respect is of course: How metastable is the condensate? Within the gaussian approximation this question is easily answered, because then the dynamics of the condensate is equivalent to the dynamics of a particle in an unstable potential, as we have just seen. We therefore only need to evaluate the WKB-expression for the tunnneling rate [58] and compare this to the rate of decay due to thermal fluctuations by calculating also the height of the energy barrier. The outcome of this comparison for the conditions of the experiment with atomic ^{7}Li is presented in reference [59] and shows that, for the relatively high temperatures $T \gg \hbar\omega/k_B$ that have been obtained thusfar [11], the decay by means of thermal fluctuations over the energy barrier is the dominant decay mechanism of the condensate.

More important for our purposes, however, is that sufficiently close to the maximum number of condensate particles N_{max} the collective decay of the condensate discussed above is always much more probable than the decay due to two and three-body collisions that lead to a spin-flip or the

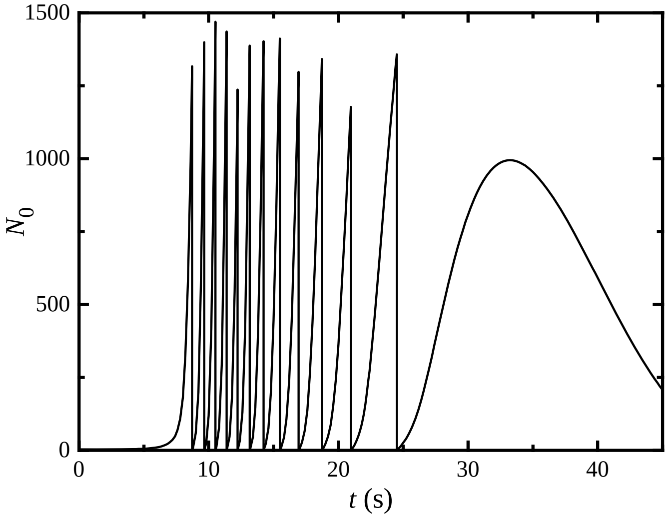

Fig. 16. Typical evolution of condensate number N_0 in response to evaporative cooling. The long-time decay of the condensate is due to two and three-body inelastic collisions.

formation of ^{7}Li molecules, respectively. As a result the collapse of the condensate should be observable within the finite lifetime of the gas. In fact, on the basis of this separation of time scales we expect the condensate to go through a number of growth and collapse cycles [59, 60]. Physically this picture arises as follows. Starting from a gas with a number of atoms $N \gg N_{\max}$, the condensate will initially grow as a response to evaporative cooling. However, if the number of condensate atoms starts to come close to $N_{\max}$, the condensate fluctuates over the energy barrier and collapses in a very short time of $\mathcal{O}(1/\omega)$ [61]. During the collapse the condensate density increases rapidly and two and three-body inelastic processes quickly remove almost all the atoms from the condensate. After this has occurred the condensate grows again from the noncondensed part of the gas and a new growth and collapse cycle begins. It is only after many of these cycles that enough atoms are removed for the gas to relax to an equilibrium with a number of condensate particles that is less than $N_{\max}$. This is shows quantitatively in figure 16 for the experimental conditions of interest.

A final issue which needs to be addressed at this point is the actual dynamics of the collapse and, in particular, how we must include the effect of the inelastic growth and decay processes on this dynamics. Unfortunately, the inclusion of these effects is rather complicated. It is, however, of some interest because Sackett *et al.* have recently observed that after a single collapse there remains a remnant of the condensate with about 10% of the initial number of atoms [62]. At present, it is an important open problem to theoretically understand the magnitude of this remnant.

2.10 Phase diffusion

As we have just seen explicitly, a particularly interesting consequence of the finite size of the gas is that quantum fluctuations play a much more important role. Although this is especially true for the case of attractive interactions that we considered in section 2.9, it is also true for a Bose gas with repulsive interactions. A striking example in this respect is the phenomenon of phase 'diffusion', which was recently discussed by Lewenstein and You [32]. We rederive their results for a trapped Bose gas in a moment, but first consider also the same phenomenon for a neutral and homogeneous superconductor. In this manner it is possible to bring out the physics involved more clearly.

Using the approach of section 2.8.3, it can be shown that at zero temperature the dynamics of the superconducting order parameter, i.e., the BCS gap parameter $\Delta(\mathbf{x}, t)$ that is proportional to the wave function of the condensate of Cooper pairs, is in a good approximation determined by a time-dependent Ginzburg-Landau theory [41, 63, 64] with the action

$$S^{\text{eff}}[\Delta^*, \Delta] = \frac{N(0)}{4} \int dt \int d\mathbf{x} \left\{ \frac{\hbar^2}{|\Delta_0|^2} \left| \frac{\partial \Delta}{\partial t} \right|^2 \right. \tag{2.177}$$
$$\left. - \frac{\hbar^2 v_F^2}{3|\Delta_0|^2} |\boldsymbol{\nabla}\Delta|^2 + 2|\Delta|^2 \left(1 - \frac{|\Delta|^2}{2|\Delta_0|^2} \right) \right\} ,$$

where $N(0)$ is the density of states for one spin projection at the Fermi energy $\epsilon_F = m v_F^2/2$ and Δ_0 is the equilibrium value of the order parameter [65]. Writing the complex order parameter in terms of an amplitude and a phase, we immediately observe that the amplitude fluctuations are gapped [66] and can, therefore, be safely neglected at large length scales. The long-wavelength dynamics of the superconductor is thus dominated by the phase fluctuations, according to the action

$$S^{\text{eff}}[\theta] = \frac{N(0)\hbar^2}{4} \int dt \int d\mathbf{x} \left\{ \left(\frac{\partial \theta}{\partial t} \right)^2 - \frac{v_F^2}{3} \left(\boldsymbol{\nabla}\theta \right)^2 \right\} . \tag{2.178}$$

This also implies that the global phase $\theta_{\mathbf{0}}(t) = \int d\mathbf{x}\ \theta(\mathbf{x}, t)/V$ of the superconductor has a dynamics that is governed by

$$S^{\mathrm{eff}}[\theta_{\mathbf{0}}] = \frac{N(0)N\hbar^2}{4n} \int dt \, \left(\frac{d\theta_{\mathbf{0}}}{dt} \right)^2 \ , \tag{2.179}$$

using the fact that the total volume V of the system is given by N/n.

Up to now our discussion has again been semiclassical. To consider also the quantum fluctuations, we have to quantize this theory by applying the usual rules of quantum mechanics. Doing so, we find that the wave function of the overall phase obeys a Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(\theta_{\mathbf{0}}; t) = -\frac{n}{N(0)N} \, \frac{\partial^2}{\partial \theta_{\mathbf{0}}^2} \Psi(\theta_{\mathbf{0}}; t) \ , \tag{2.180}$$

with a 'diffusion' constant that can easily be shown to be equal to the quantity $(2/\hbar)\partial\epsilon_F/\partial N$ [67] and is, most importantly for our purposes, proportional to $1/N$. In the thermodynamic limit $N \to \infty$ a state with a well defined stationary phase is clearly a solution and we are then dealing with a system having a spontaneously broken $U(1)$ symmetry. However, for a finite (and fixed) number of particles the global phase cannot be well defined at all times and always has to 'diffuse' in accordance with the above Schrödinger equation. Note also that in the groundstate the phase is fully undetermined and $|\Psi(\theta_{\mathbf{0}}; t)|^2 = 1/2\pi$. Maybe surprisingly, the same calculation is somewhat more complicated for a Bose gas because the amplitude fluctuations of the order parameter cannot be neglected even at the largest length scales. However, taking these amplitude fluctuations into account properly, we nevertheless arrive at an action that is equivalent to equation (2.179) and hence again leads to the phenomenon of phase 'diffusion'.

We start again from the action $S[\rho, \theta; \mu]$ for the condensate. The difference with the previous subsection is, however, that now we are not so much interested in the dynamics of the density but in the phase dynamics instead. Therefore we now want to integrate over the density field $\rho(\mathbf{x}, \tau)$. This cannot be done exactly and we therefore here consider only the strong-coupling limit, which was also treated by Lewenstein and You [32]. In that limit we are allowed to neglect the gradient of the average density profile [68] and the action $S[\rho, \theta; \mu]$ is for the longest wavelengths well approximated by

$$\begin{aligned} S[\rho, \theta; \mu] = \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \, \Bigg(& i\hbar\rho(\mathbf{x}, \tau) \frac{\partial \theta(\mathbf{x}, \tau)}{\partial \tau} \\ & + V^{\mathrm{ex}}(\mathbf{x})\rho(\mathbf{x}, \tau) - \mu\rho(\mathbf{x}, \tau) + \frac{2\pi a \hbar^2}{m} \rho^2(\mathbf{x}, \tau) \Bigg) \ . \end{aligned} \tag{2.181}$$

In equilibrium the average density profile of the condensate thus obeys

$$\langle \rho(\mathbf{x}) \rangle = \frac{m}{4\pi a \hbar^2} \left(\mu - V^{\mathrm{ex}}(\mathbf{x}) \right) \Theta(\mu - V^{\mathrm{ex}}(\mathbf{x})) \ . \tag{2.182}$$

Performing now the shift $\rho(\mathbf{x},\tau) = \langle\rho(\mathbf{x})\rangle + \delta\rho(\mathbf{x},\tau)$, we find for the zero-momentum part of the action [69]

$$S[\delta N_{\mathbf{0}},\theta_{\mathbf{0}};\mu] = \hbar\beta E_{\mathbf{0}}(\mu) + \int_0^{\hbar\beta} d\tau \left(i\hbar\delta N_{\mathbf{0}} \frac{d\theta_{\mathbf{0}}}{d\tau} + \frac{2\pi a\hbar^2}{mV_{\mathbf{0}}(\mu)} (\delta N_{\mathbf{0}})^2 \right) \ , \tag{2.183}$$

where $E_{\mathbf{0}}(\mu)$ and $V_{\mathbf{0}}(\mu)$ correspond, respectively, to the energy and the volume of the condensate in the so-called Thomas-Fermi approximation [70]. Moreover, $\delta N_{\mathbf{0}}(\tau) = \int d\mathbf{x}\ \delta\rho(\mathbf{x},\tau)$ represents the fluctuations in the total number of condensate particles in that same approximation, implying that the density fluctuations $\delta\rho(\mathbf{x},\tau)$ are only nonzero in that region of space where the condensate density does not vanish.

Performing now the integration over the number fluctuations $\delta N_{\mathbf{0}}(\tau)$ and the usual Wick rotation to real times $\tau \to it$, we immediately see that the effective action for the global phase of the condensate has precisely the same form as in equation (2.179), i.e.,

$$S^{\text{eff}}[\theta_{\mathbf{0}};\mu] = \frac{mV_{\mathbf{0}}(\mu)}{8\pi a} \int dt \left(\frac{d\theta_{\mathbf{0}}}{dt} \right)^2 \ . \tag{2.184}$$

The appropriate ‘diffusion’ constant is therefore equal to $2\pi a\hbar/mV_{\mathbf{0}}(\mu)$, which can easily be shown to be equal to $(1/2\hbar)\partial\mu/\partial N_{\mathbf{0}}$ if we make use of the fact that in the Thomas-Fermi approximation the chemical potential obeys $\mu = m\omega^2 R_{TF}^2/2$ and the radius of the condensate is given by $R_{TF} = (15a\hbar^2 N_{\mathbf{0}}/m^2\omega^2)^{1/5}$ [56]. Hence, the ‘diffusion’ constant is proportional to $1/N_{\mathbf{0}}^{3/5}$. Note that if the condensate where contained in a box the ‘diffusion’ constant would be proportional to $1/N_{\mathbf{0}}$ instead. It is important to note also that, in contrast to the case of a fermionic superfluid, we have to integrate over the amplitude fluctuations of the order parameter to arrive at a quadratic action for the phase fluctuations. This leads to the important conclusion that for a bosonic superfluid it is impossible to be in a state with only phase fluctuations and no density fluctuations, even at the largest length scales.

Exercise 2.32: The effective action $S^{\text{eff}}[\theta_{\mathbf{0}};\mu]$ in principle also contains the topological term $i\hbar N_{\mathbf{0}}(\mu)\int dt\ d\theta_{\mathbf{0}}/dt$, with $N_{\mathbf{0}}(\mu) = \int d\mathbf{x}\ \langle\rho(\mathbf{x})\rangle$ the average number of condensate atoms. Add this topological term to the effective action in equation (3.28) and rederive the Schrödinger equation for the wave function $\Psi(\theta_{\mathbf{0}};t)$. What is the wave function of the ground state?

3 Outlook

With the latter remark we end this course on the use of field-theoretical methods for the study of the equilibrium and nonequilibrium properties of trapped atomic gases. Although we have in principle illustrated all the necessary tools for an *ab initio* treatment of these new quantum systems, many interesting topics still need to be considered in detail. We already mentioned such topics as Fermi-Bose mixtures, the dynamics of condensate collapse, the strong-coupling theory for the formation of a condensate in either atomic Bose of Fermi gases, and the hydrodynamics of single or multicomponent atomic gases. Several other important areas of research, which can also be easily addressed within the context of quantum field theory, are atom lasers, the damping of collective modes, the behaviour of spinor condensates, the dynamics of topological excitations such as kinks, vortices and skyrmions, quantum critical phenomena, the optical properties of superfluid gases, and two-dimensional phase transitions. In view of these and many other possibilities that are now experimentally feasible, it appears certain that the physics of degenerate atomic gases will remain very exciting for years to come.

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