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Nonequilibrium Bose–Einstein condensates

Bose–Einstein condensation was predicted in 1925 [Ein24, Ein25] but, except for its indirect manifestation in the superfluidity of He^4 [Lon38, Kap38, AllMis38], it remained a purely theoretical construct until 1995, when condensation in alkali gases was achieved in the laboratory [CorWie02, Ket02]. Since then, a great deal of the theoretical work in the previous 70 years has been put to the experimental test, while new avenues have been opening up, such as the superfluid–insulator or Mott transition [FWGF89, GMEHB02, CaHuRe06], the BEC-BCS cross-over [Leg06, Reg04] and the Tonks gas regime [Gir60, Par04]. Because of the great experimental control over the relevant parameters and the deep understanding of the fundamental physics, BECs have become a field of choice to perform experiments of interest not just in atomic and molecular physics, but also in quantum optics, condensed matter physics, quantum critical dynamics, even field theory, gravitation, cosmology and black hole physics [CoEnWi99, PetSmi02, Sou02, BonSen04, ParZha93, ParZha95, UnrSch07, BaLiVi05]. Moreover, cold Bose gases on optical lattices have been proposed as a possible implementation of a quantum information processing (QIP) device [JakZol04], boosting new interest in these systems.

As introductions and reviews on this fast evolving subject abound, it is perhaps more fitting for us to focus on certain aspects of the nonequilibrium field theory of BEC, specifically [And04] the application of quantum field theoretic methods described in this book to the description of nonequilibrium evolution of condensed gases in magneto-optical traps [ChCoPh95].[1]

Of course NEqQFT is not the only possible description. Reflecting on the characteristics of this field as a current attractor of different subdisciplines listed above, the literature presents an almost bewildering array of possibilities. However, there are a few basic criteria that any successful description must meet: it must be faithful to the presence of gapless excitations above the condensate [HohMar65, Gri96, ShiGri98], and must respect the basic conservation laws of particle number and energy–momentum [Kra60, BayKad61, Bay62]. These requirements are sealed at the roots of a quantum field theoretical formulation

[1] This means we would have to sacrifice the description of important topics like the physics of cold atoms in optical lattices, which has a rapidly expanding literature [ChCoPh95], and vortices in BECs and their associated phenomena [ElKrVo06], purely from space limitation considerations.

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and, as such, provide a benchmark and standard against which other approximations may be compared. It also provides a systematic way to develop a perturbative expansion to arbitrary order [PRSC02, SPRS02, BFGR01, BaFrRa02, Boy02].

Realistically, once one gets to the point of actually writing down a nonrelativistic field-theoretic action to describe the second-quantized atomic gas, the functional approach developed earlier in this book in the context of relativistic scalar field theories works well in every detail we have considered so far. This is one of the strengths of this approach. For this reason we will concentrate on the first stage, namely, how to get from the physical model of the trapped gas to a nonrelativistic field theory. In the process, we shall attempt to give a model-independent characterization of the two requirements mentioned above, and to discuss how they enter into the functional method.

Current experimental work on BECs presents a variety of nonequilibrium problems, including the dynamics of condensation itself and the response of the BEC to changes in its environment (temperature and trapping fields) and particle interactions [KaSuSh96, KaSuSh97]. Probably the most extreme demonstration of far-from-equilibrium behavior is the so-called Bose–Nova experiment [Don01, Cla03a, Cla03b, CoThWi06, SaiUed03, SanShl02, BajaMa04, Adh04, GaFrTo01, SaRoHo03, WuHoSa05, Yur02, CalHu03, WDBDBH07], where a sudden sign change in the interatomic interaction triggers the implosion of the condensate. The possible use of cold gases in optical lattices in QIP poses, among others, two specific challenges for a nonequilibrium theory: the detailed description of the initialization of the device [Rey04, Bre05, Pup04, ReBlCl03], and an accurate estimation of static and dynamic decoherence times [SaOHTh97, Oos02, PuWiPr06, Rei05].

The plan for this chapter is as follows: starting from the second-quantized version of the weakly interacting Bose gas Hamiltonian in a closed time path (CTP) framework, we shall present the basic (symmetry-breaking) formulation in a model-independent way. We shall give a precise formulation to the requirements of a gapless spectrum (the so-called Hugenholtz–Pines theorem) and particle number conservation in the mean. In the process, we shall introduce the class of $\mathbf{\Phi}$-derivable theories as a broad framework for viable models of BEC dynamics.

Then we shall introduce the 1PI and 2PI effective action descriptions of the BEC, as described in Chapter 6 [LutWar60, DomMar64a, DomMar64b, CoJaTo74, LunRam02]. This means that we opt to follow the evolution of the condensate through the unfolding of correlation functions, as opposed, for example, to obtaining a time-dependent wavefunction for the many-body system [KohBur02, PrBuSt98, GKGB04]. We shall show that, *in principle,* the 2PIEA leads to a $\mathbf{\Phi}$-derivable theory which is both gapless and conserving. However, the appearance of many models derived from truncations of the 2PIEA in different degrees may tell a different story. We shall show how the familiar theories arise from such truncations and examine them in detail. They are the

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Gross–Pitaevskii (GP), Bogoliubov, one-loop, Hartree–Fock–Bogoliubov (HFB), Popov and two-loop approximations. We shall show that the two-loop approximation yields a minimal theory which is both gapless (to the required order in perturbation theory) and conserving. We shall not discuss other approximation schemes, like the $1/N$ approximation because they can be analyzed in terms similar to those introduced in Chapter 6 [TemGas06, GBSS07].

Our next goal will be to discuss two specific predictions of the two-loop theory, namely, that the evolution of condensate fluctuations is dissipative and stochastic. This is in accord with the fluctuation–dissipation theorem discussed earlier in the book. In particular, to discuss fluctuations we shall adopt a coarse-grained effective action scheme where high-energy "noncondensate" modes act as an environment for the low-energy "condensate band" modes, where condensation takes place. We shall concentrate on the derivation of the noise terms coupled to the Gross–Pitaevskii equation, yielding a stochastic GP equation. Of course, in so doing the initial conditions for the condensate can also become stochastic, which is an important consideration in actual applications.

In the regime where modes above the condensate are highly populated – not macroscopically, of course – relaxation is efficient enough that a kinetic theory description becomes possible, leading eventually to a two-fluid hydrodynamic. Since we have discussed quantum kinetic theory in detail earlier in the book, we shall focus here only on those features which are characteristic of the BEC environment.

Finally, we shall close the chapter with a brief description of the so-called *particle number conserving* formalism. The symmetry breaking approach described so far has the drawback that strictly speaking it cannot be applied to a system with a finite number of particles. The particle number conserving formalism overcomes this difficulty. In particular, we shall discuss a functional implementation of this formalism, which makes it as flexible as the better known symmetry breaking approach.

13.1 The closed time path integral approach to BECs

In this section we put together the basic formulae for the coherent state representation [NegOrl98] of the causal or CTP path integral method (introduced in Chapters 3, 5 and 6) to compute the expectation values of physical observables. Let ρ_i be the density matrix describing the initial state of the system at $t = t_i$. Then expectation values with respect to ρ_i may be obtained from the CTP generating functional (cf. Chapter 6)

$$e^{iW} = \mathrm{Tr}\left\{U_2^{-1}\left(t_f, t_i\right) U_1\left(t_f, t_i\right) \rho\left(t_i\right)\right\} \tag{13.1}$$

where

$$U_{1,2}\left(t_f, t_i\right) = T\left[e^{-i\int_{t_i}^{t_f} dt\; H^{1,2}(t)}\right] \tag{13.2}$$

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We shall use the well-known coherent state representation [NegOrl98] in the construction of a path integral representation of the generating functional in the next subsection. The CTP boundary conditions will be introduced in the following subsection.

13.1.1 The coherent state representation

For simplicity, we consider a single one-particle state. There is a basis made of occupation number eigenstates $|n\rangle$

$$N\,|n\rangle = n\,|n\rangle \tag{13.3}$$

where N is the number operator (in particular, $n = 0$ is the vacuum state $|0\rangle$). These states are orthonormal and complete

$$\langle m\,|n\rangle = \delta_{mn} \tag{13.4}$$

$$\sum |n\rangle\,\langle n| = 1 \tag{13.5}$$

The destruction and creation operators relate states of different occupation numbers

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle\,; \qquad \hat{a}^{\dagger}\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{13.6}$$

Therefore

$$\hat{a}^{\dagger}\hat{a} = N; \qquad [\hat{a},\hat{a}^{\dagger}] = \mathbf{1} \tag{13.7}$$

A coherent state $|a\rangle$ is an eigenstate of the destruction operator

$$\hat{a}\,|a\rangle = a\,|a\rangle \tag{13.8}$$

It follows that

$$\langle n\,|a\rangle = \frac{1}{\sqrt{n}}\,\langle n-1|\,\hat{a}\,|a\rangle = \frac{a}{\sqrt{n}}\,\langle n-1\,|a\rangle \tag{13.9}$$

Adopting the normalization

$$\langle 0\,|a\rangle = 1 \tag{13.10}$$

one gets

$$\langle n\,|a\rangle = \frac{a^n}{\sqrt{n!}} \tag{13.11}$$

Or else,

$$|a\rangle = \sum \frac{a^n}{\sqrt{n!}}\,|n\rangle = \sum \frac{a^n\hat{a}^{\dagger n}}{n!}\,|0\rangle = \exp\left\{a\hat{a}^{\dagger}\right\}|0\rangle \tag{13.12}$$

Observe that

$$\hat{a}^{\dagger}\,|a\rangle = \frac{\partial}{\partial a}\,|a\rangle \tag{13.13}$$

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Let $|b\rangle$ be a second coherent state; then

$$b\langle a\,|b\rangle = \langle a|\,\hat{a}\,|b\rangle = \frac{\partial}{\partial a^*}\langle a\,|b\rangle \tag{13.14}$$

and

$$\langle a\,|b\rangle = \exp\{a^* b\} \tag{13.15}$$

The constant is determined by recognizing that the vacuum is the coherent state with $a = 0$. From this point on, we shall omit the hats on operators whenever there is no risk of confusion.

While not orthogonal, the coherent states are complete, in the following sense

$$\int \frac{da^* da}{2\pi i} \exp\{-a^* a\}\,|a\rangle\,\langle a| = \mathbf{1} \tag{13.16}$$

We may use the completeness relationship to write down the trace of an operator A

$$\mathrm{Tr}A = \sum \langle n|\,A\,|n\rangle = \int \frac{da^* da}{2\pi i} \exp\{-a^* a\}\,\langle a|\,A\,|a\rangle \tag{13.17}$$

Now consider the transition amplitude between the state $|a_i\rangle$ at time $t_i = 0$ and the state $|\bar{a}_f\rangle$ at time t_f. We have (setting $\hbar = 1$)

$$|\bar{a}_f\rangle = e^{iHt_f}\,|\bar{a}\rangle \tag{13.18}$$

and

$$\langle \bar{a}_f\,|a_i\rangle = \langle \bar{a}|\,e^{-iHt_f}\,|a_i\rangle \tag{13.19}$$

Note that $|\bar{a}_f\rangle$ is *not* a solution of the Schrödinger equation, but an eigenstate of the Heisenberg operator $a\,(t_f)$ with proper value $\bar{a}$. Since $a\,(t_f) = e^{iHt_f} a e^{-iHt_f}$, we have $a\,(t_f)\,|\bar{a}_f\rangle = \bar{a}\,|\bar{a}_f\rangle$.

Let N be some large number and $\varepsilon = t_f/N$. Write $a_i = a_0$, $\bar{a} = a_N$. Then, inserting $N-1$ identity operators, we have

$$\langle \bar{a}_f\,|a_i\rangle = \int \left\{ \prod_{n=1}^{N-1} \frac{da_n^* da_n}{2\pi i} \exp\{-a_n^* a_n\}\,\langle a_{n+1}|\,e^{-iH\varepsilon}\,|a_n\rangle \right\} \langle a_1|\,e^{-iH\varepsilon}\,|a_0\rangle \tag{13.20}$$

which may be written as (assuming the Hamiltonian $H = H(a^\dagger, a)$ is in a normal form)

$$\langle a_N\,|a_0\rangle = \int [Da]_{N-1}\,\exp\{iS_N\,[a^*, a]\}\,e^{a_N^* a_N} \tag{13.21}$$

where

$$[Da]_{N-1} = \prod_{n=1}^{N-1} \frac{da_n^* da_n}{2\pi i} \tag{13.22}$$

$$S_N\,[a^*, a] = \sum_{n=1}^{N} \{ia_n^*\,(a_n - a_{n-1}) - \varepsilon H\,(a_n^*, a_{n-1})\} \tag{13.23}$$

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Going to the continuum limit, where $a_n - a_{n-1} \sim \varepsilon \partial a/\partial t$, we get

$$\langle \bar{a}_f \, | a \rangle = \int [Da] \, \exp \{ iS [a^*, a] \} \, e^{a^* a(t_f)} \tag{13.24}$$

$$S [a^*, a] = \int dt \, \left\{ ia^* \frac{\partial a}{\partial t} - H (a^*, a) \right\} \tag{13.25}$$

The integration is over paths which interpolate between $a(0) = a$ and $a^*(t_f) = \bar{a}^*$.

13.1.2 The closed time path boundary conditions

We now have all the necessary elements to evaluate the CTP generating functional (13.1). The idea is that the initial density matrix ρ is propagated forwards in time with some Hamiltonian H^1 and then backwards with a Hamiltonian H^2. Insert three identity operators in (13.1) to obtain

$$\begin{aligned} e^{iW} = & \int \frac{da_N^* da_N}{2\pi i} \frac{da_0^{1*} da_0^1}{2\pi i} \frac{da_0^{2*} da_0^2}{2\pi i} \exp \left\{ - \left(a_N^* a_N + a_0^{1*} a_0^1 + a_0^{2*} a_0^2 \right) \right\} \\ & \times \langle a_N | \, U_2 (t_f, t_i) \left| a_0^2 \right\rangle^* \langle a_N | \, U_1 (t_f, t_i) \left| a_0^1 \right\rangle \left\langle a_0^1 \right| \rho (t_i) \left| a_0^2 \right\rangle \end{aligned} \tag{13.26}$$

Now use the corresponding path integral representations

$$\begin{aligned} e^{iW} = & \int \frac{da_N^* da_N}{2\pi i} \frac{da_0^{1*} da_0^1}{2\pi i} \frac{da_0^{2*} da_0^2}{2\pi i} \exp \left\{ a_N^* a_N - a_0^{1*} a_0^1 - a_0^{2*} a_0^2 \right\} \left\langle a_0^1 \right| \rho (t_i) \left| a_0^2 \right\rangle \\ & \times \int \left[Da^2 \right]_{N-1}^* \, \exp \left\{ -iS_N^2 \left[a^{2*}, a^2 \right]^* \right\} \int \left[Da^1 \right]_{N-1} \, \exp \left\{ iS_N^1 \left[a^{1*}, a^1 \right] \right\} \end{aligned} \tag{13.27}$$

The configuration on the forward branch has $a^1(0) = a_0^1$ and $a^{1*}(t_f) = a_N^*$. On the backward branch, we have $a^{2*}(0) = a_0^{2*}$ and $a^2(t_f) = a_N$. Once W is known, causal expectation values may be computed by differentiation. Equation (13.27) is the main result of this section.

13.2 The symmetry-breaking approach to BECs

For a field-theoretic description of BECs we begin with a second-quantized field operator $\Psi(\mathbf{x}, t)$ which removes an atom at the location $\mathbf{x}$ at times t. It obeys the canonical commutation relations

$$[\Psi (\mathbf{x}, t) \, , \Psi (\mathbf{y}, t)] = 0 \tag{13.28}$$

$$\left[\Psi (\mathbf{x}, t) \, , \Psi^\dagger (\mathbf{y}, t) \right] = \delta (x - \mathbf{y}) \tag{13.29}$$

The dynamics of this field is given by the Heisenberg equations of motion

$$-i\hbar \frac{\partial}{\partial t} \Psi = [\mathbf{H}, \Psi] \tag{13.30}$$

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where $\mathbf{H}$ is the Hamiltonian. The theory is invariant under a global phase change of the field operator

$$\Psi \rightarrow e^{i\theta}\Psi, \qquad \Psi^\dagger \rightarrow e^{-i\theta}\Psi^\dagger \tag{13.31}$$

The constant of motion associated with this invariance through Noether's theorem is the total particle number.

To motivate the symmetry-breaking approach to BECs we observe that there is a special one-particle state, with wavefunction ϕ_0, which, upon condensation, acquires a macroscopic occupation number N_0, comparable to the total number of particles N. We call this state the "condensate." We regard ϕ_0 as the first element of a complete basis of one-particle states, and expand $\Psi = a_0\phi_0 + \ldots$ The operator a_0 is the destruction operator for the condensate.

Let $|N, N_0\rangle$ be the state of the gas with N particles, N_0 of which are in the condensate. Then

$$a_0\,|N, N_0\rangle = \sqrt{N_0}\,|N-1, N_0-1\rangle \tag{13.32}$$

If N and N_0 are both very large, then the state does not change much. We see that the condensed state is very close to a coherent state for a_0. Taking the actual state for a coherent state is an excellent approximation when both N and N_0 are macroscopic (but an approximation nonetheless). We shall return to this point below, in Section 13.3.

Under the approximation

$$a_0\,|N, N_0\rangle \approx \sqrt{N_0}\,|N, N_0\rangle \tag{13.33}$$

the expectation value of the field operator is no longer zero

$$\langle\Psi\rangle \equiv \Phi \approx \sqrt{N_0}\phi_0 \tag{13.34}$$

Because the field operator develops an expectation value, the symmetry (13.31) is spontaneously broken. (Beware that the actual relationship between the expectation value and the wavefunction of the condensate is more complex than a simple proportionality, see Section 13.3.)

In the symmetry-breaking approach to BEC dynamics, one relegates this motivation to the background and views the condensation as a resultant of the spontaneous breakdown of symmetry (13.31). Upon symmetry breaking Ψ develops a nonzero expectation value Φ (c-number). We introduce a background field decomposition for Ψ

$$\Psi = \Phi + \psi \tag{13.35}$$

where ψ (q-number) is the field operator corresponding to quantum fluctuations with zero mean $\langle\psi\rangle$. Various approaches differ on how to handle the dynamics of these two constituents.

To progress further, we need a specific model for the atom–atom interactions. In principle, we should specify the atom–atom interaction potential. However,

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in many applications it is enough to know the cross-section σ for low-energy spherically symmetric scattering of two identical bosons. We introduce the scattering length a through $\sigma \equiv 8\pi a^2$, where the factor 8π involves both integration over all scattering angles and Bose enhancement factors. We shall adopt as a model atom–atom interaction a contact potential $U\delta(\mathbf{x})$. To reproduce the right scattering length we need $U = 4\pi\hbar^2 a/M$, where M is the mass of the atoms. A positive value of a means a repulsive interaction; we adopt the convention that an attractive interaction is described by a negative value of a.

We observe that from the expectation value Φ and the scattering length a it is possible to build a new characteristic length, the healing length ξ, as $\xi^{-2} \equiv a\Phi^2$. Physically, suppose we introduce a condition such as a boundary into the condensate forcing $\Phi = 0$ there. Then ξ is the distance from the boundary where Φ grows back to its asymptotic value. The healing length also plays an important role in the spectrum of fluctuations above the condensate, as we shall show below.

Assuming a contact atom–atom potential we get then the Hamiltonian

$$\mathbf{H} = \int d^d\mathbf{x}\, \left\{ \Psi^\dagger H\Psi + \frac{U}{2}\Psi^{\dagger 2}\Psi^2 \right\} \tag{13.36}$$

The single-particle Hamiltonian H is given by

$$H\Psi = -\frac{\hbar^2}{2M}\nabla^2\Psi + V_{\mathrm{trap}}(\mathbf{x})\,\Psi \tag{13.37}$$

where $V_{\mathrm{trap}}(\mathbf{x})$ denotes a confining trap potential. Then the Heisenberg equation of motion

$$i\hbar\frac{\partial}{\partial t}\Psi = H\Psi + U\Psi^\dagger\Psi^2 \tag{13.38}$$

is also the classical equation of motion derived from the action

$$S = \int d^{d+1}x\; i\hbar\Psi^*\frac{\partial}{\partial t}\Psi - \int dt\;\mathbf{H} \tag{13.39}$$

For later use, it is convenient to introduce a single field doublet $\Psi^A = \left(\Psi, \Psi^\dagger\right)$. Recall the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{13.40}$$

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{13.41}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{13.42}$$

We also include spatial and temporal position in the A indices (repeated indices are added over discrete indices and integrated over spacetime). The classical action reads (we also set $\hbar = 1$)

$$S = \frac{1}{2}\sigma_{2AB}\Psi^A\frac{\partial}{\partial t}\Psi^B - \frac{1}{2}\sigma_{1AB}\Psi^A H\Psi^B - \frac{U_{ABCD}}{24}\Psi^A\Psi^B\Psi^C\Psi^D \tag{13.43}$$

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where

$$\sigma_{iAB} \to \sigma_{iAB}\delta\left(\mathbf{x}_A - \mathbf{x}_B\right)\delta\left(t_A - t_B\right) \tag{13.44}$$

$$\begin{aligned} U_{ABCD} \to U & \left[\sigma_{1AB}\sigma_{1CD} + \sigma_{1AC}\sigma_{1DB} + \sigma_{1AD}\sigma_{1BC}\right] \\ & \delta\left(\mathbf{x}_A - \mathbf{x}_B\right)\delta\left(\mathbf{x}_A - \mathbf{x}_C\right)\delta\left(\mathbf{x}_A - \mathbf{x}_D\right) \\ & \delta\left(t_A - t_B\right)\delta\left(t_A - t_C\right)\delta\left(t_A - t_D\right) \end{aligned} \tag{13.45}$$

is totally symmetric. $U_{ABCD} = 2U$ if $(ABCD)$ is a permutation of (2211), and zero otherwise. The Heisenberg equations become

$$\sigma_{2AB}\frac{\partial}{\partial t}\Psi^B - \sigma_{1AB}H\Psi^B - \frac{U_{ABCD}}{6}\Psi^B\Psi^C\Psi^D = 0 \tag{13.46}$$

From the expectation value of the Heisenberg equations we find the mean field equation

$$\sigma_{2AB}\frac{\partial}{\partial t}\Phi^B - \sigma_{1AB}H\Phi^B - \eta_A = 0 \tag{13.47}$$

where we parameterize

$$\eta_A = \frac{U_{ABCD}}{6}\left\langle \Psi^C\Psi^D\Psi^B\right\rangle \tag{13.48}$$

We adopt the convention that whenever different operators evaluated at the same time appear within an expectation value, they must be normal ordered. Therefore, in expanded notation

$$\eta_2 = \eta_1^\dagger = U\left\langle \Psi^\dagger\Psi^2\right\rangle \tag{13.49}$$

In Section 13.2.9 we will relate η to the chemical potential.

The fluctuations around the mean field will be described through the correlation functions

$$\left\langle T\left[\Psi^A\left(t,\mathbf{x}\right)\Psi^B\left(t',\mathbf{y}\right)\right]\right\rangle \equiv \Phi^A\left(t,\mathbf{x}\right)\Phi^B\left(t',\mathbf{y}\right) + G^{AB}\left(\left(t,\mathbf{x}\right),\left(t',\mathbf{y}\right)\right) \tag{13.50}$$

$$G^{AB} = \left\langle T\left[\psi^A\left(t,\mathbf{x}\right)\psi^B\left(t',\mathbf{y}\right)\right]\right\rangle \tag{13.51}$$

These include the so-called normal and anomalous densities

$$\tilde{n}\left(t,\mathbf{x}\right) = \left\langle \psi^\dagger\psi\right\rangle\left(t,\mathbf{x}\right) = G^{21}\left(\left(t,\mathbf{x}\right),\left(t,\mathbf{x}\right)\right) \tag{13.52}$$

$$\tilde{m}\left(t,\mathbf{x}\right) = \left\langle \psi^2\right\rangle\left(t,\mathbf{x}\right) = G^{11}\left(\left(t,\mathbf{x}\right),\left(t,\mathbf{x}\right)\right) \tag{13.53}$$

The fluctuation field ψ inherits the ETCR

$$\left[\psi^A\left(\mathbf{x},t\right),\psi^B\left(\mathbf{y},t\right)\right] = i\sigma_2^{AB}\delta\left(\mathbf{x}-\mathbf{y}\right) \tag{13.54}$$

From the usual formulae

$$\begin{aligned} \left\langle T\left[\psi^A\left(t,\mathbf{x}\right)\psi^B\left(t',\mathbf{y}\right)\right]\right\rangle = & \,\theta\left(t-t'\right)\left\langle \psi^A\left(t,\mathbf{x}\right)\psi^B\left(t',\mathbf{y}\right)\right\rangle \\ & + \theta\left(t'-t\right)\left\langle \psi^B\left(t',\mathbf{y}\right)\psi^A\left(t,\mathbf{x}\right)\right\rangle \end{aligned} \tag{13.55}$$

and the equation of motion for the fluctuations (which is obtained by subtracting the mean field from the Heisenberg equations)

$$\sigma_{2AB}\frac{\partial}{\partial t}\psi^B - \sigma_{1AB}H\psi^B - \frac{U_{ABCD}}{6}\Psi^B\Psi^C\Psi^D + \eta_A = 0 \tag{13.56}$$

the equations of motion for the propagators read

$$0 = \sigma_{2AB}\frac{\partial}{\partial t}G^{\mathrm{BE}} - \sigma_{1AB}HG^{\mathrm{BE}} - \frac{U_{ABCD}}{6}\left\langle T\left(\Psi^C\Psi^D\Psi^B\psi^E\right)\right\rangle - i\delta_A^E \tag{13.57}$$

which we parameterize as

$$0 = \sigma_{2AB}\frac{\partial}{\partial t}G^{\mathrm{BE}} - \sigma_{1AB}HG^{\mathrm{BE}} - \Sigma_{AB}G^{\mathrm{BE}} - i\delta_A^E \tag{13.58}$$

$$\Sigma_{AB}G^{\mathrm{BE}} = \frac{U_{ABCD}}{6}\left\langle T\left(\Psi^C\Psi^D\Psi^B\psi^E\right)\right\rangle \tag{13.59}$$

Let us define the “free” propagators D^{BE} as the solutions to

$$0 = \sigma_{2AB}\frac{\partial}{\partial t}D^{\mathrm{BE}} - \sigma_{1AB}HD^{\mathrm{BE}} - i\delta_A^E \tag{13.60}$$

Observe that

$$D_{AB}^{-1} = -i\left.\frac{\delta^2 S}{\delta\Phi^A\delta\Phi^B}\right|_{\Phi=0} \tag{13.61}$$

or, more explicitly,

$$D_{AB}^{-1} = (-i)\begin{pmatrix} 0 & D^{-1*} \\ D^{-1} & 0 \end{pmatrix} \tag{13.62}$$

$$D^{-1} = i\hbar\partial_t + \frac{\hbar^2}{2M}\nabla^2 - V(\mathbf{x}) \tag{13.63}$$

We may then write this equation as

$$G_{AB}^{-1} = D_{AB}^{-1} + i\Sigma_{AB} \tag{13.64}$$

Of course we cannot compute η_A and Σ_{AB} in closed form. Different theories arise from different ansatz for these unknowns as functionals of the mean fields and propagators, thus closing the system.

13.2.1 A relationship between η_A and Σ_{AB}

Observe that all of the above remains valid if we consider fields defined on a closed time path. If we need to differentiate among the branches of the time path, we shall make them explicit in the time argument. We shall write t for a generic point on the time path, or else t^a, where $a = 1$ denotes a point on the first (forward) branch, and $a = 2$ a point on the second (backward) one.

One way of generating a vacuum expectation value for the field is coupling it to an external source. The mean field is obtained from the derivatives of a

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generating functional

$$\Phi^A = \frac{\delta W\,[J]}{\delta J_A} \tag{13.65}$$

$$e^{iW} = \left\langle e^{i\int J_A \Psi^A} \right\rangle \tag{13.66}$$

In the presence of the sources, the Heisenberg equations now read

$$\sigma_{2AB}\frac{\partial}{\partial t}\Psi^B - \sigma_{1AB}H\Psi^B - \frac{U_{ABCD}}{6}\Psi^B\Psi^C\Psi^D = -J_A \tag{13.67}$$

so taking the expectation value we obtain

$$\sigma_{2AB}\frac{\partial}{\partial t}\Phi^B - \sigma_{1AB}H\Phi^B - \eta_A = -J_A \tag{13.68}$$

Since we have not committed ourselves as to the nature of η_A, this statement is totally general.

We now have the linear response theory result

$$\frac{\delta\Phi^A}{\delta J_E} = iG^{AE} \tag{13.69}$$

whereby

$$i\delta_A^E = \sigma_{2AB}\frac{\partial}{\partial t}G^{\mathrm{BE}} - \sigma_{1AB}HG^{BE} - \frac{d\eta_A}{d\Phi^{\mathrm{B}}}G^{BE} \tag{13.70}$$

We use d for the variational derivative of η_A in the last term to emphasize that we mean the $full$ derivative. We shall return to this point below. Comparing with (13.58) we see that in the *exact* theory there is a connection

$$\Sigma_{AB} = \frac{d\eta_A}{d\Phi^B} \tag{13.71}$$

Any approximation which does not respect this will get into trouble at some point.

13.2.2 Gaplessness and phase invariance

It is a property of the Heisenberg equations that if $\Psi^A = \left(\Psi, \Psi^\dagger\right)$ is a solution, then

$$\exp\left(i\sigma_{3AB}\theta\right)\Psi^B = \left(e^{i\theta}\Psi, e^{-i\theta}\Psi^\dagger\right) \tag{13.72}$$

where θ is a constant, is also a solution. In the exact theory, this property is inherited by the mean field equations, and so the small fluctuations equations must always admit a solution $\delta\Phi^A = \sigma_{3AB}\Phi^B$. This means that the fundamental solutions $-iG^{AB}$ must have a pole.

In equilibrium, time-translation invariance means that Φ^A must have the form

$$\Phi^A = e^{-i\sigma_{3AB}\mu t}\Phi_0^B = \left(e^{-i\mu t}\Phi_0^1, e^{i\mu t}\Phi_0^2\right) \tag{13.73}$$

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where Φ_0^B is constant and may be chosen as real, $\Phi_0^1 = \Phi_0^2$. Now recall the mean field equations and write

$$\eta_A = e^{i\sigma_{3AB}\mu t}\eta_{A0} = \left(e^{i\mu t}\eta_{10}, e^{-i\mu t}\eta_{20}\right) \tag{13.74}$$

Then

$$\eta_{10} = \eta_{20} = (\mu - H)\,\Phi_0^1 \tag{13.75}$$

For a homogeneous trap $V(\mathbf{x}) = 0$, Φ_0^1 is a constant and $H\Phi_0^1 = 0$.

The linearized equations are

$$\left[\sigma_{2AB}\frac{\partial}{\partial t} - \sigma_{1AB}H - \Sigma_{AB}\right]\delta\Phi^B = 0 \tag{13.76}$$

The requirement that these equations must admit a solution where $\delta\Phi_A$ is a constant times a simple harmonic factor means that the operator in brackets has a zero, but this is the same as saying that the two-point functions G^{AB} have a pole. Therefore, provided the relationship above between the self-energy Σ_{AB} and the "force" η_A holds, the theory must be gapless.

Actually, substituting $\delta\Phi_A = \sigma_{3AC}e^{-i\sigma_{3CB}\mu t}\Phi_0^B = \left(e^{-i\mu t}\Phi_0, -e^{i\mu t}\Phi_0\right)$ and

$$\Sigma_{AB} = \begin{pmatrix} \Sigma_{11}^0 e^{i\mu(t+t')} & \Sigma_{12}^0 e^{i\mu(t-t')} \\ \Sigma_{21}^0 e^{-i\mu(t-t')} & \Sigma_{22}^0 e^{-i\mu(t+t')} \end{pmatrix} \tag{13.77}$$

implies

$$(\mu - H)\,\Phi_0(\mathbf{x}) - \int dt' d^3\mathbf{y}\ \left[\Sigma_{21}^0 - \Sigma_{22}^0\right]((t,\mathbf{x}),(t',\mathbf{y}))\,\Phi_0(\mathbf{y}) = 0 \tag{13.78}$$

If $V(\mathbf{x}) = 0$, the constant Φ_0 cancels out and we obtain a connection between μ and the Σ_{AB}. This is the Hugenholtz–Pines theorem [HugPin59, Gold61]

$$\mu = \int dt' d^3\mathbf{y}\ \left[\Sigma_{21}^0 - \Sigma_{22}^0\right]((t,\mathbf{x}),(t',\mathbf{y})) \tag{13.79}$$

13.2.3 Conserving and $\mathbf{\Phi}$-derivable theories

A theory is called conserving if particle number is conserved in the mean. The theory is called $\mathbf{\Phi}$-derivable if there is a functional $\mathbf{\Phi}$ of Φ^A and G^{AB} such that

$$\eta_A = \frac{\delta\mathbf{\Phi}}{\delta\Phi^A} \tag{13.80}$$

$$\Sigma_{AB} = 2\frac{\delta\mathbf{\Phi}}{\delta G^{AB}} \tag{13.81}$$

We shall now show that a $\mathbf{\Phi}$-derivable theory is necessarily conserving provided the $\mathbf{\Phi}$ functional is invariant under *time-dependent* phase changes

$$\Phi^A \to \exp\left[i\sigma_{3AB}\theta(t_A)\right]\Phi^B \tag{13.82}$$

$$G^{AB} \to \exp\left[i\sigma_{3AC}\theta(t_A)\right]\exp\left[i\sigma_{3BD}\theta(t_B)\right]G^{CD} \tag{13.83}$$

This is a more demanding requirement than the global phase invariance of the classical action. To see this, introduce a tensor

$$c_{ABC} = \frac{1}{2}\delta\left(t_A - t_B\right)\sigma_{1BC} \tag{13.84}$$

The particle number operator is

$$N_A = c_{ABC}\Psi^B\Psi^C \tag{13.85}$$

Global particle number conservation means that

$$\frac{\partial}{\partial t}\left\langle N_A\right\rangle = 0 \tag{13.86}$$

But

$$\frac{\partial}{\partial t}\left\langle N_A\right\rangle = c_{ABC}\left[2\Phi^C\frac{\partial\Phi^B}{\partial t_B} + \frac{\partial}{\partial t_B}G^{BC} + \frac{\partial}{\partial t_C}G^{BC}\right] \tag{13.87}$$

By symmetry in the $SU(2)$ indices and a spatial integration by parts the mean field equations imply

$$2c_{ABC}\Phi^C\frac{\partial\Phi^B}{\partial t_B} = i\delta\left(t_A - t_B\right)\sigma_{3BC}\Phi^C\eta_B \tag{13.88}$$

Analogously

$$0 = \frac{\partial}{\partial t_B}G^{BC} + i\sigma_3^{BD}H_D G^{DC} - \sigma_2^{BD}\Sigma_{DE}G^{EC} - i\sigma_2^{BC} \tag{13.89}$$

$$0 = \frac{\partial}{\partial t_C}G^{BC} + i\sigma_3^{DC}H_D G^{BD} + \sigma_2^{EC}\Sigma_{DE}G^{BD} + i\sigma_2^{BC} \tag{13.90}$$

Therefore, a conserving theory must obey

$$0 = i\delta\left(t_A - t_C\right)\left\{\sigma_{3BC}\Phi^C\eta_B + \left[\sigma_3^{DC}G^{EC} + \sigma_3^{EC}G^{CD}\right]\frac{\Sigma_{DE}}{2}\right\} \tag{13.91}$$

which for a $\mathbf{\Phi}$-derivable theory is just the invariance statement above.

By extending the symmetry properties of the $\mathbf{\Phi}$ functional it is possible to enforce energy and momentum conservation as well. The discussion is similar to the general proof of energy–momentum conservation in the mean in relativistic theories, and we shall not repeat it here.

We emphasize that in the exact theory, particle number is strongly conserved, not only in the mean. Strong particle number conservation implies an infinite chain of identities which several correlation functions must obey; in a $\mathbf{\Phi}$-derivable theory, they cannot all be satisfied.

Gapless, conserving and $\mathbf{\Phi}$-derivable theories

To summarize, $\mathbf{\Phi}$-derivable theories are always conserving if the $\mathbf{\Phi}$ functional is invariant under time-dependent simultaneous phase changes of the mean fields

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and propagators. They are also gapless if

$$\Sigma_{AB} = 2\frac{\delta\mathbf{\Phi}}{\delta G^{AB}} = \frac{d\eta_A}{d\Phi^B} = \frac{\delta^2\mathbf{\Phi}}{\delta\Phi^A\delta\Phi^B} + \frac{1}{2}\frac{\delta\Sigma_{CD}}{\delta\Phi^A}\frac{dG^{CD}}{d\Phi^B} \tag{13.92}$$

In the last term, the propagators are regarded as functionals of the mean fields through their equation of motion, namely

$$G^{-1}_{AB} = D^{-1}_{AB} + i\Sigma_{AB} \tag{13.93}$$

implies

$$\left[G^{-1}_{EG}G^{-1}_{HF} + i\frac{\delta\Sigma_{EF}}{\delta G^{GH}}\right]\frac{dG^{GH}}{d\Phi^B} = (-i)\,\frac{\delta\Sigma_{EF}}{\delta\Phi^B}, \tag{13.94}$$

so the condition for a gapless theory becomes

$$\Sigma_{AB} = 2\frac{\delta\mathbf{\Phi}}{\delta G^{AB}} = \frac{\delta^2\mathbf{\Phi}}{\delta\Phi^A\delta\Phi^B} - \frac{i}{2}\frac{\delta\Sigma_{GH}}{\delta\Phi^A}\left[G^{-1}_{EG}G^{-1}_{HF} + i\frac{\delta\Sigma_{EF}}{\delta G^{GH}}\right]^{-1}\frac{\delta\Sigma_{EF}}{\delta\Phi^B} \tag{13.95}$$

Observe that in general the term in brackets is nonlocal, so either

$$\frac{\delta\Sigma_{GH}}{\delta\Phi^A} = 0 \tag{13.96}$$

or else the self-energy Σ_{AB} must contain a nonlocal part. This observation will be crucial below.

13.2.4 The full 2PI effective action as a Φ-derivable approach

In this subsection, we shall discuss the 2PIEA as a Φ-derivable approach, assuming one knows the full effective action.

As shown in Chapter 6, the 2PIEA is given by [RHCRC04]

$$\Gamma_2\left[\Phi^A, G^{AB}\right] = S\left[\Phi^A\right] + \frac{1}{2}S_{,AB}G^{AB} - \frac{1}{2}i\hbar\mathrm{Tr}\,\ln G + \Gamma_Q \tag{13.97}$$

where Γ_Q is the sum of all 2PI vacuum bubbles for a theory with propagators G^{AB} and vertices

$$\frac{U_{ABCD}}{24}\psi^A\psi^B\psi^C\psi^D \qquad \text{and} \qquad \frac{U_{ABCD}}{6}\Phi^A\psi^B\psi^C\psi^D \tag{13.98}$$

The equations of motion are

$$S_{,A} + \frac{1}{2}S_{,ABC}G^{BC} + \frac{\delta\Gamma_Q}{\delta\Phi^A} = 0 \tag{13.99}$$

$$-iS_{,AB} - 2i\frac{\delta\Gamma_Q}{\delta G^{AB}} = \left[G^{-1}\right]_{AB} \tag{13.100}$$

Therefore

$$\eta_A = \frac{U_{ABCD}}{6}\Phi^B\Phi^C\Phi^D + \frac{U_{ABCD}}{2}\Phi^B G^{CD} - \frac{\delta\Gamma_Q}{\delta\Phi^A} \tag{13.101}$$

$$\Sigma_{AB} = \frac{U_{ABCD}}{2}\Phi^C\Phi^D - 2\frac{\delta\Gamma_Q}{\delta G^{AB}} \tag{13.102}$$

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which follow from the functional

$$\mathbf{\Phi} = \frac{U_{ABCD}}{24}\Phi^A\Phi^B\Phi^C\Phi^D + \frac{U_{ABCD}}{4}\Phi^A\Phi^B G^{CD} - \Gamma_Q \tag{13.103}$$

Conservation follows from the fact that Γ_Q is made out of graphs where the same number of 1 and 2 fields enter at each vertex.

Since we are assuming Γ_Q contains all graphs, the theory must be gapless. Nevertheless, it is interesting to seek a direct proof. We must verify the identity (13.95). To do this, let us put back the external sources in the equations of motion

$$iD^{-1}_{AB}\Phi^B - \eta_A = -J_A - K_{AB}\Phi^B \tag{13.104}$$

$$iD^{-1}_{AB} - i\left[G^{-1}\right]_{AB} - \Sigma_{AB} = -K_{AB} \tag{13.105}$$

Taking variations we get

$$iD^{-1}_{AB}\frac{\delta\Phi^B}{\delta J_C} - \frac{\delta\eta_A}{\delta\Phi^B}\frac{\delta\Phi^B}{\delta J_C} - \frac{\delta\eta_A}{\delta G^{BD}}\frac{\delta G^{BD}}{\delta J_C} = -\delta^C_A \tag{13.106}$$

$$i\left[\left[G^{-1}\right]_{AD}\left[G^{-1}\right]_{EB} + i\frac{\delta\Sigma_{AB}}{\delta G^{DE}}\right]\frac{\delta G^{DE}}{\delta J_C} - \frac{\delta\Sigma_{AB}}{\delta\Phi^D}\frac{\delta\Phi^D}{\delta J_C} = 0 \tag{13.107}$$

In any $\mathbf{\Phi}$-derivable approach,

$$\frac{\delta\eta_A}{\delta G^{BD}} = \frac{1}{2}\frac{\delta\Sigma_{BD}}{\delta\Phi^A} \tag{13.108}$$

and we still have the LRT result (13.69), from which we get

$$\frac{\delta G^{DE}}{\delta J_C} = \left[\left[G^{-1}\right]_{AD}\left[G^{-1}\right]_{EB} + i\frac{\delta\Sigma_{AB}}{\delta G^{DE}}\right]^{-1}\frac{\delta\Sigma_{AB}}{\delta\Phi^F}G^{FC} \tag{13.109}$$

so the first equation (13.106) becomes

$$\begin{aligned}\left[G^{-1}\right]_{AB} = D^{-1}_{AB} &+ i\frac{\delta\eta_A}{\delta\Phi^B}\\ &+\frac{1}{2}\frac{\delta\Sigma_{FD}}{\delta\Phi^A}\left[\left[G^{-1}\right]_{GD}\left[G^{-1}\right]_{EF} + i\frac{\delta\Sigma_{GE}}{\delta G^{DF}}\right]^{-1}\frac{\delta\Sigma_{GE}}{\delta\Phi^B}\end{aligned} \tag{13.110}$$

QED

This shows that, *in principle*, the 2PIEA yields a theory which is *both* gapless and conserving. In reality, though, one does not known the full effective action, and truncations may spoil either of these features, or both.

13.2.5 Varieties of theories from truncations of the 2PI effective action

Let us expand on this last statement by looking at some common approaches to nonequilibrium BECs as truncations of the 2PIEA. For simplicity, in this section we assume $V(\mathbf{x}) = 0$.

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(1) The simplest, and surprisingly useful, approach is the **Gross–Pitaevskii** (GP) one: just write the classical equations of motion for Φ, and forget about G. However, this approach is incomplete, because it says nothing about fluctuations.

(2) The next simplest approach is **Bogoliubov**'s, which is based on the identifications

$$\eta_A^{\text{Bog}} = \frac{U_{ABCD}}{6} \Phi^B \Phi^C \Phi^D \tag{13.111}$$

$$\Sigma_{AB}^{\text{Bog}} = \frac{U_{ABCD}}{2} \Phi^C \Phi^D \tag{13.112}$$

or, in expanded notation

$$\eta_2^{0\text{Bog}} = U \Phi_0^3 \tag{13.113}$$

$$\Sigma_{21}^{0\text{Bog}} = 2\Sigma_{22}^{0\text{Bog}} = 2U\Phi_0^2 \delta\left(t - t'\right) \delta\left(\mathbf{x} - \mathbf{y}\right) \tag{13.114}$$

Here, the mean fields obey the Gross–Pitaevskii equation

$$i\frac{\partial}{\partial t}\Phi = H\Phi + U\Phi^\dagger \Phi^2 \tag{13.115}$$

and the fluctuations the linearized equation

$$i\frac{\partial}{\partial t}\psi = H\psi + U\psi^\dagger \Phi^2 + 2U\Phi^\dagger \Phi\psi \tag{13.116}$$

Write $\Phi = e^{-i\mu t}\Phi_0$, $\psi = e^{-i\mu t}\psi_{\text{phys}}$ to get

$$\mu = U\Phi_0^2 \tag{13.117}$$

$$i\frac{\partial}{\partial t}\psi_{\text{phys}} = H\psi_{\text{phys}} + U\Phi_0^2 \left[\psi_{\text{phys}}^\dagger + \psi_{\text{phys}}\right] \tag{13.118}$$

Bogoliubov's approach is not $\boldsymbol{\Phi}$-derivable; however, it is gapless, because the equation for the propagators is defined to be identical to the first variation of the equation for the mean fields, and this is phase invariant. Equivalently, we see that the Bogoliubov approach is consistent with the Hugenholtz–Pines theorem.

The Bogoliubov approach is not conserving. This may be seen from the analysis above, but it is probably simplest to give a direct proof. Since the equation for the mean field is just the classical equation, its contribution to particle number is conserved, so the only question is about the number of particles in the fluctuation field. From the equations above we find

$$\frac{d\left\langle N\right\rangle}{dt} = (-i)\, U\Phi_0^2 \int d^d\mathbf{x}\, \left[\left\langle \psi_{\text{phys}}^{\dagger 2}\right\rangle - \left\langle \psi_{\text{phys}}^2\right\rangle\right] \tag{13.119}$$

which does not vanish identically.

The simplest $\mathbf{\Phi}$-derivable extension of the Bogoliubov approach is the one-loop theory, where $\Gamma_Q = 0$

$$\mathbf{\Phi}^{1\,\text{loop}} = \frac{U_{ABCD}}{24}\Phi^A\Phi^B\Phi^C\Phi^D + \frac{U_{ABCD}}{4}\Phi^A\Phi^B G^{CD} \tag{13.120}$$

From the above analysis, one loop is obviously conserving, but it is not gapless. This can be seen from the fact that Σ_{AB} is purely local, while to satisfy the gapless condition it must also include nonlocal terms.

Alternatively, we can check that the one-loop approximation violates the Hugenholtz–Pines theorem. The one-loop self-energies are the same as in the Bogoliubov approach, but the forces are different

$$\eta_2^{01\text{loop}} = \left[U\Phi_0^2 + U\left(2\tilde{n} + \tilde{m}\right)\right]\Phi_0 \tag{13.121}$$

leading to

$$\mu = U\Phi_0^2 + U\left(2\tilde{n} + \tilde{m}\right) \tag{13.122}$$

(3) The so-called **Hartree–Fock–Bogoliubov** approximation (HFB) is another local $\mathbf{\Phi}$-derivable approach, where Γ_Q is reduced to the double-bubble diagram

$$\mathbf{\Phi}^{\text{HFB}} = \mathbf{\Phi}^{1\,\text{loop}} + \frac{U_{ABCD}}{8}G^{AB}G^{CD} \tag{13.123}$$

HFB is conserving but not gapless, for the same reasons as the one-loop approach. The HFB forces are the same as in the one-loop approach, while the self-energies are

$$\Sigma_{22}^{0\text{HFB}} = U\left(\Phi_0^2 + \tilde{m}\right)\delta\left(t - t'\right)\delta\left(\mathbf{x} - \mathbf{y}\right) \tag{13.124}$$

$$\Sigma_{21}^{0\text{HFB}} = 2U\left(\Phi_0^2 + \tilde{n}\right)\delta\left(t - t'\right)\delta\left(\mathbf{x} - \mathbf{y}\right) \tag{13.125}$$

Observe that the Hugenholtz–Pines theorem is violated because of the $\tilde{m}$ term. This suggests a simple way to modify HFB so that it becomes gapless, though no longer conserving. In the HFB approach, the equations for the mean fields are

$$i\frac{\partial}{\partial t}\Phi = H\Phi + U\Phi^\dagger\Phi^2 + 2U\left\langle\psi^\dagger\psi\right\rangle\Phi + U\left\langle\psi^2\right\rangle\Phi^\dagger \tag{13.126}$$

and the fluctuations obey the linearized equation

$$i\frac{\partial}{\partial t}\psi = H\psi + U\psi^\dagger\left(\Phi^2 + \left\langle\psi^2\right\rangle\right) + 2U\left(\Phi^\dagger\Phi + \left\langle\psi^\dagger\psi\right\rangle\right)\psi \tag{13.127}$$

(4) In the so-called **Popov** approximation, one neglects the "anomalous" density in both equations (13.126), (13.127). Writing $\Phi = e^{-i\mu t}\Phi_0$, $\psi = e^{-i\mu t}\psi_{\text{phys}}$, we get

$$\mu = U\left[\Phi_0^2 + 2\left\langle\psi^\dagger\psi\right\rangle\right] \tag{13.128}$$

$$i\frac{\partial}{\partial t}\psi_{\text{phys}} = H\psi_{\text{phys}} + U\Phi_0^2\left[\psi_{\text{phys}}^\dagger + \psi_{\text{phys}}\right] \tag{13.129}$$

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which is easily verified to give a gapless spectrum (see the next subsection). The first equation is the Hugenholtz–Pines theorem reduced to this approximation.

The spectrum under the Popov approximation

We now investigate more closely the spectrum which results from the Popov approximation. To this end, let us reinstate $\hbar$ into the equation, and assume a homogeneous condensate in a three-dimensional normalizing box of volume V. Φ_0 is a constant, and ψ_{phys} may be expanded

$$\psi_{\text{phys}} = \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}x}}{\sqrt{V}} \psi_{\mathbf{k}}(t) \tag{13.130}$$

$$i\hbar\frac{\partial}{\partial t}\psi_{\mathbf{k}} = \frac{\hbar^2 k^2}{2M}\psi_{\mathbf{k}} + U\Phi_0^2\left[\psi^{\dagger}_{-\mathbf{k}} + \psi_{\mathbf{k}}\right] \tag{13.131}$$

We seek a solution

$$\psi_{\mathbf{k}} = \alpha_k A_{\mathbf{k}} e^{-i\omega_k t} - \beta_k A^{\dagger}_{-\mathbf{k}} e^{i\omega_k t} \tag{13.132}$$

where α_k and β_k are real and spherically symmetric, and $\alpha_k^2 - \beta_k^2 = 1$. Collecting positive and negative frequency terms we get

$$\left(\frac{\hbar^2 k^2}{2M} + U\Phi_0^2 - \hbar\omega_k\right)\alpha_k - U\Phi_0^2\beta_k = 0 \tag{13.133}$$

$$U\Phi_0^2\alpha_k - \left(\frac{\hbar^2 k^2}{2M} + U\Phi_0^2 + \hbar\omega_k\right)\beta_k = 0 \tag{13.134}$$

leading to the dispersion relation

$$\hbar^2\omega_{\mathbf{k}}^2 = \left(\frac{\hbar^2 k^2}{2M} + U\Phi_0^2\right)^2 - U^2\Phi_0^4 \tag{13.135}$$

and to a gapless spectrum, as expected. Let us write

$$\frac{\hbar^2 k^2}{2M} + U\Phi_0^2 = \hbar\omega_k \ \cosh 2\varphi \tag{13.136}$$

$$U\Phi_0^2 = \hbar\omega_k \ \sinh 2\varphi \tag{13.137}$$

Then

$$\alpha_k = \cosh\varphi, \qquad \beta_k = \sinh\varphi \tag{13.138}$$

It follows that

$$\tanh\varphi = \frac{U\Phi_0^2}{\left(\frac{\hbar^2 k^2}{2M} + U\Phi_0^2 + \hbar\omega_k\right)} \tag{13.139}$$

and so

$$\beta_k = \frac{U\Phi_0^2}{\left[\left(\frac{\hbar^2 k^2}{2M} + U\Phi_0^2 + \hbar\omega_k\right)^2 - U^2\Phi_0^4\right]^{1/2}} \tag{13.140}$$

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Let us introduce the scattering length a through $U \sim \hbar^2 a/M$ and the healing length ξ through $a\Phi_0^2 = \xi^{-2}$. Then the dispersion relation reads

$$\omega_k = c_{\mathrm{s}} k \sqrt{1 + \frac{1}{4}(\xi k)^2} \tag{13.141}$$

where the speed of sound is

$$c_{\mathrm{s}} = \frac{\hbar}{M\xi} \tag{13.142}$$

We see that there are roughly two set of modes, *hard* modes with $k > \xi^{-1}$ which remain mostly undisturbed by the condensate, and soft modes $k < \xi^{-1}$ which lose their particle-like character and become phonon-like.

The above analysis does not apply to the homogeneous mode, which by construction has zero frequency. Therefore the amplitude of the zero mode will grow linearly in time, and eventually it will invalidate perturbation theory. The point is that within the symmetry-breaking approach this is unavoidable. Of course the zero mode is physically different from other modes, being closer to a collective variable [Raj87] than to a true physical degree of freedom. Therefore it is justified to treat it in a different way than other modes [MCBE98, SiCaWi06]. But when we do so we move beyond the symmetry-breaking approach. A possible strategy is the particle conserving formulation, to be discussed later in this chapter.

The equation obtained from the Popov approximation may be used to clarify one important point, namely, what the physical small parameter in the loop expansion is. As a measure of the size of the higher corrections, let us compare the density of noncondensate particles $\tilde{n} = \left\langle \psi^\dagger_{\mathrm{phys}} \psi_{\mathrm{phys}} \right\rangle$ against the condensate density Φ_0^2. In the continuous approximation

$$\tilde{n} = \int d^3\mathbf{k}\, \beta_{\mathbf{k}}^2 = 4\pi \int_0^\infty dk\, k^2 \beta_{\mathbf{k}}^2 \tag{13.143}$$

The integral converges at both limits. For small k, $\omega_{\mathbf{k}} \sim k\left[U\Phi_0^2/M\right]^{1/2}$ and

$$\beta_{\mathbf{k}}^2 \sim \left(MU\Phi_0^2\right)^{1/2}/\hbar k \tag{13.144}$$

Replacing $U \sim \hbar^2 a/M$ we get $k^2\beta_{\mathbf{k}}^2 \sim a^{-2}(ka)\left(a^{3/2}\Phi_0\right)$. In the opposite limit of large k, we have $\hbar\omega_{\mathbf{k}} \sim \hbar^2 k^2/2M$ and $k^2\beta_{\mathbf{k}}^2 \sim a^{-2}(ka)^{-2}\left(a^{3/2}\Phi_0\right)^4$. The largest contribution comes from the cross-over region where $k \sim a^{-1}\left(a^{3/2}\Phi_0\right)$.

The resulting estimate yields $\tilde{n} \sim \Phi_0^2\left(a^{3/2}\Phi_0\right)$. We see that the physical small parameter in the expansion is $\sqrt{N_a}$, where $N_a = a^3\Phi_0^2 \sim a^3 N/V$ is the number of particles within a scattering length of a given particle. The loop expansion is therefore a dilute gas approximation.

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13.2.6 Higher gapless approximations

We see from the previous discussion that, while the 2PIEA yields a theory which is truly both gapless and conserving, in practice truncations of the effective action lead to approaches where one or the other feature must be sacrificed. To prevent this, we must stick to approximations to the 2PIEA which satisfy the gapless condition

$$\begin{aligned}-2\frac{\delta\Gamma_Q}{\delta G^{AB}} &= \frac{U_{ABCD}}{2}G^{CD} - \frac{\delta\Gamma_Q}{\delta\Phi^A\delta\Phi^B} \\ &\quad -\frac{i}{2}\left[U_{GHAD}\Phi^D - 2\frac{\delta\Gamma_Q}{\delta G^{GH}\delta\Phi^A}\right]\left[G^{-1}_{EG}G^{-1}_{HF} - 2i\frac{\delta^2\Gamma_Q}{\delta G^{EF}\delta G^{GH}}\right]^{-1} \\ &\quad \times\left[U_{EFBJ}\Phi^J - 2\frac{\delta\Gamma_Q}{\delta G^{EF}\delta\Phi^B}\right] \end{aligned} \tag{13.145}$$

This nonlinear equation in functional derivatives of Γ_Q is too complex to admit a closed-form solution, but it can be solved iteratively: we start by replacing some value of $\Gamma_Q^{(n)}$ on the right-hand side, and find $\Gamma_Q^{(n+1)}$ by one integration with respect to G. We thereby generate a family of theories which are gapless within a prescribed accuracy.

Choosing as starting point the Bogoliubov approximation $\Gamma_Q^{(1)} = 0$, we obtain the first nontrivial approximation

$$\Gamma_Q^{(2)} = -\frac{U_{ABCD}}{8}G^{AB}G^{CD} + \frac{i}{12}U_{GHAD}\Phi^D G^{AB}G^{GE}G^{HF}U_{EFBJ}\Phi^J \tag{13.146}$$

which is the full two-loop approximation to the 2PIEA, including the double-bubble and setting sun graphs. This approximation was first explored by Beliaev [Bel58a, Bel58b].

We note that other approximation schemes have been explored in the literature, most notably the $1/N_f$ expansion in a theory with N_f "flavors" or equivalent Bose fields. If going over to a nonlocal approximation is considered too involved, another possibility is to depart from the 2PIEA approach, adding *ad hoc* terms, for example, to restore gaplessness in an otherwise conserving theory.

As we have discussed in detail in earlier chapters, the two-loop approximation leads to self-energies which are in general complex, signaling damping of the condensate fluctuations. At zero temperature, the leading damping mechanism is the decay of a condensate fluctuation into two noncondensate excitations. This so-called Beliaev damping [Bel58a, Bel58b] has been discussed in detail in Chapter 8, in the simpler context of a $g\phi^3$ scalar field theory. At finite temperature a new mechanism appears, the so-called Landau damping where a condensate fluctuation is absorbed by a noncondensate excitation, which transmutes into a higher energy excitation. The imaginary parts of the thermal self-energy have been discussed in Chapter 10, to which we refer the reader for details.

Finally, we observe that for cold gases in an optical lattice, gaplessness may actually become a problem, if one is interested in describing the Mott regime.

Let us return to $\Gamma_Q^{(2)} = \Gamma_Q^{\mathrm{HFB}} + \delta\Gamma_Q$. In a more natural notation,

$$\delta\Gamma_Q = \frac{iU^2}{2}\left\langle\left\{\int dtd^3\mathbf{x}\ \left[\Phi^*\psi^\dagger\psi^2 + \Phi\psi^{\dagger 2}\psi\right]\right\}^2\right\rangle \tag{13.147}$$

where the expectation value is computed under a Gaussian approximation and only 2PI terms are kept. Recall that the time integration runs over the closed time path, and that products of fields are path ordered, or normal ordered if the path ordering prescription is ambiguous. Expanding

$$\begin{aligned}\delta\Gamma_Q = \frac{iU^2}{2}&\int dtd^3\mathbf{x}\int dt'd^3\mathbf{y}\\ &\times\left\{\Phi^*(t,\mathbf{x})\,\Phi^*(t',\mathbf{y})\left[2\left\langle\psi^\dagger\psi^{\dagger\prime}\right\rangle\left\langle\psi\psi'\right\rangle^2 + 4\left\langle\psi^\dagger\psi'\right\rangle\left\langle\psi\psi^{\dagger\prime}\right\rangle\left\langle\psi\psi'\right\rangle\right]\right.\\ &+\Phi^*(t,\mathbf{x})\,\Phi(t',\mathbf{y})\left[4\left\langle\psi^\dagger\psi^{\dagger\prime}\right\rangle\left\langle\psi\psi'\right\rangle\left\langle\psi\psi^{\dagger\prime}\right\rangle + 2\left\langle\psi^\dagger\psi'\right\rangle\left\langle\psi\psi^{\dagger\prime}\right\rangle^2\right]\\ &+\Phi(t,\mathbf{x})\,\Phi^*(t',\mathbf{y})\left[2\left\langle\psi\psi^{\dagger\prime}\right\rangle\left\langle\psi^\dagger\psi'\right\rangle^2 + 4\left\langle\psi\psi'\right\rangle\left\langle\psi^\dagger\psi'\right\rangle\left\langle\psi^\dagger\psi^{\dagger\prime}\right\rangle\right]\\ &\left.+\Phi(t,\mathbf{x})\,\Phi(t',\mathbf{y})\left[2\left\langle\psi^\dagger\psi^{\dagger\prime}\right\rangle^2\left\langle\psi\psi'\right\rangle + 4\left\langle\psi^\dagger\psi'\right\rangle\left\langle\psi\psi^{\dagger\prime}\right\rangle\left\langle\psi^\dagger\psi^{\dagger\prime}\right\rangle\right]\right\}\end{aligned} \tag{13.148}$$

Although the model is built to be gapless to $O\left(U^2\right)$, it is interesting to give a direct check. We consider only the zero temperature case. Observe that

$$\eta_2 = \eta_2^{\mathrm{HFB}} + \delta\eta_2 \tag{13.149}$$

$$\begin{aligned}\delta\eta_2 = iU^2&\int dt'd^3\mathbf{y}\\ &\times\left\{\Phi^*(t',\mathbf{y})\left[2\left\langle\psi^\dagger\psi^{\dagger\prime}\right\rangle\left\langle\psi\psi'\right\rangle^2 + 4\left\langle\psi^\dagger\psi'\right\rangle\left\langle\psi\psi^{\dagger\prime}\right\rangle\left\langle\psi\psi'\right\rangle\right]\right.\\ &\left.+\Phi(t',\mathbf{y})\left[4\left\langle\psi^\dagger\psi^{\dagger\prime}\right\rangle\left\langle\psi\psi'\right\rangle\left\langle\psi\psi^{\dagger\prime}\right\rangle + 2\left\langle\psi^\dagger\psi'\right\rangle\left\langle\psi\psi^{\dagger\prime}\right\rangle^2\right]\right\}\end{aligned} \tag{13.150}$$

In equilibrium, and after extracting the phases, this leads to a chemical potential

$$\mu = \mu^{\mathrm{HFB}} + \delta\mu \tag{13.151}$$

with

$$\begin{aligned}\delta\mu = iU^2\int dt'd^3\mathbf{y}\ &\left[2\left\langle\psi^\dagger\psi^{\dagger\prime}\right\rangle\left\langle\psi\psi'\right\rangle^2 + 4\left\langle\psi^\dagger\psi'\right\rangle\left\langle\psi\psi^{\dagger\prime}\right\rangle\left\langle\psi\psi'\right\rangle\right.\\ &\left.+4\left\langle\psi^\dagger\psi^{\dagger\prime}\right\rangle\left\langle\psi\psi'\right\rangle\left\langle\psi\psi^{\dagger\prime}\right\rangle + 2\left\langle\psi^\dagger\psi'\right\rangle\left\langle\psi\psi^{\dagger\prime}\right\rangle^2\right]\end{aligned} \tag{13.152}$$

To $O(U^2)$ we may compute the expectation values as pertaining to a free field. At zero temperature $\delta\mu$ vanishes.

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Similarly we compute the self-energies

$$\Sigma_{AB} = \Sigma_{AB}^{\mathrm{HFB}} + \delta\Sigma_{AB} \tag{13.153}$$

$$\delta\Sigma_{21}^0 = -2iU^2\Phi_0^2 \left\langle \psi\psi^{\dagger\prime}\right\rangle^0 \left[2\left\langle \psi\psi'\right\rangle^0 + \left\langle \psi\psi^{\dagger\prime}\right\rangle^0 + 2\left\langle \psi^\dagger\psi'\right\rangle + 2\left\langle \psi^\dagger\psi^{\dagger\prime}\right\rangle^0\right] \tag{13.154}$$

$$\delta\Sigma_{22}^0 = -2iU^2\Phi_0^2 \left\langle \psi\psi'\right\rangle^0 \left[\left\langle \psi\psi'\right\rangle^0 + 2\left\langle \psi\psi^{\dagger\prime}\right\rangle^0 + 2\left\langle \psi^\dagger\psi'\right\rangle^0 + 2\left\langle \psi^\dagger\psi^{\dagger\prime}\right\rangle^0\right] \tag{13.155}$$

In equilibrium, $\delta\Sigma_{22}^0 = 0$ and

$$\delta\Sigma_{21}^0 = -2iU^2\Phi_0^2 \left(\left\langle \psi\psi^{\dagger\prime}\right\rangle^0\right)^2 \tag{13.156}$$

The gaplessness condition reads

$$2U\tilde{m} = \int dt'd^3\mathbf{y}\;\delta\Sigma_{21}^0 \tag{13.157}$$

to lowest order in U.

To compute the left-hand side we expand the destruction operators as

$$\psi^0 = \sum \frac{e^{i(\mathbf{kx}-\omega_k t)}}{\sqrt{V}} a_{\mathbf{k}} \tag{13.158}$$

where

$$\omega_k = \frac{\hbar k^2}{2M} \tag{13.159}$$

Therefore, after separating the contributions from both branches of the closed time path

$$\int dt'd^3\mathbf{y}\;\delta\Sigma_{21}^0 = -\frac{2U^2\Phi_0^2}{V}\sum_{\mathbf{p},\mathbf{q}}\frac{\delta_{\mathbf{p}+\mathbf{q}}}{\omega_p+\omega_q} = -\frac{U^2\Phi_0^2}{V}\sum_{\mathbf{p}}\frac{1}{\omega_p} \tag{13.160}$$

On the other hand, at zero temperature

$$\tilde{m} = \frac{-1}{V}\sum_{\mathbf{p}}\alpha_p\beta_p \tag{13.161}$$

To lowest order we have $\alpha_p = 1$

$$\beta_p = \frac{U\Phi_0^2}{2\hbar\omega_p} \tag{13.162}$$

QED

13.2.7 Damping

The fact that under the above approximation there are nonlocal terms in the equations of motion for both the mean field and propagators suggest that they already include damping effects. Indeed, this has been proved by Beliaev [Bel58a, Bel58b].

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Let us consider the evolution of a mean field fluctuation $e^{-i\mu t}\delta\Phi$. The linearized equation of motion is

$$i\frac{\partial}{\partial t}\delta\Phi = (H-\mu)\,\delta\Phi + U\Phi_0^2\left[\delta\Phi^\dagger + 2\delta\Phi\right] + 2U\left\langle\psi^\dagger\psi\right\rangle_0\delta\Phi + U\left\langle\psi^2\right\rangle_0\delta\Phi^\dagger$$
$$+U\Phi_0\left[2\delta\left\langle\psi^\dagger\psi\right\rangle + \delta\left\langle\psi^2\right\rangle\right] + \delta\eta_2\left[\delta\Phi\right] \tag{13.163}$$

We see that there are two types of nonlocal terms, the terms coming from the modification of the fluctuating field propagators, and terms from the second variation of the effective action. The former will be shown to be proportional to $U\Phi_0^2$ and therefore will dominate at low temperatures, where almost all particles are condensed. Conversely, we expect the direct variation terms to dominate immediately below the critical temperature. We consider only the former case.

Since the perturbed propagators appear already in $O(U)$ terms, we only need to compute them to $O(U)$ accuracy. At this level, it is enough to consider the Heisenberg equation

$$i\frac{\partial}{\partial t}\psi_{\text{phys}} = (H-\mu)\,\psi_{\text{phys}} + U\psi^\dagger_{\text{phys}}\left(\Phi_0^2 + 2\Phi_0\delta\Phi\right)$$
$$+2U\left(\Phi_0^2 + \Phi_0\left(\delta\Phi^\dagger + \delta\Phi\right) + \left\langle\psi^\dagger\psi\right\rangle_0\right)\psi_{\text{phys}} \tag{13.164}$$

To the desired order

$$\mu = U\left[\Phi_0^2 + 2\left\langle\psi^\dagger\psi\right\rangle\right] \tag{13.165}$$

and

$$i\frac{\partial}{\partial t}\psi_{\text{phys}} = H\psi_{\text{phys}} + U\psi^\dagger_{\text{phys}}\left(\Phi_0^2 + 2\Phi_0\delta\Phi\right)$$
$$+U\left(\Phi_0^2 + 2\Phi_0\left(\delta\Phi^\dagger + \delta\Phi\right)\right)\psi_{\text{phys}} \tag{13.166}$$

Let us write

$$\psi_{\text{phys}} = \psi^{\text{eq}}_{\text{phys}} + \delta\psi \tag{13.167}$$

where

$$\psi^{\text{eq}}_{\text{phys}} = \sum\frac{e^{i\mathbf{kx}}}{\sqrt{V}}\left[A_{\mathbf{k}}e^{-i\omega_k t} - \frac{U\Phi_0^2}{2\hbar\omega_p}A^\dagger_{-\mathbf{k}}e^{i\omega_k t}\right] \tag{13.168}$$

and expand

$$\delta\Phi = \int\frac{d\omega}{2\pi}\sum_k\frac{e^{i(\mathbf{kx}-\omega t)}}{\sqrt{V}}f_{\mathbf{k}}\left(\omega\right) \tag{13.169}$$

Keeping only up to $O(U)$ terms

$$i\frac{\partial}{\partial t}\delta\psi - H\delta\psi = 2\Phi_0 U\left[\psi^{\text{eq}\dagger}_{\text{phys}}\delta\Phi + \left(\delta\Phi^\dagger + \delta\Phi\right)\psi^{\text{eq}}_{\text{phys}}\right] \tag{13.170}$$

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and so

$$\delta\psi = 2\Phi_0 U \int \frac{d\omega}{2\pi} \sum_{\mathbf{p},\mathbf{q}} \frac{e^{i(\mathbf{p}+\mathbf{q})\mathbf{x}}}{V} \times \left\{ \frac{f_{\mathbf{p}}(\omega) A^{\dagger}_{-\mathbf{q}} e^{-i(\omega-\omega_q)t}}{\omega - \omega_q - \omega_{|\mathbf{p}+\mathbf{q}|} + i\varepsilon} + \frac{\left[f_{\mathbf{p}}(\omega) + f^{*}_{-\mathbf{p}}(-\omega)\right] A_{\mathbf{q}} e^{-i(\omega+\omega_q)t}}{\omega + \omega_q - \omega_{|\mathbf{p}+\mathbf{q}|} + i\varepsilon} \right\} \tag{13.171}$$

We may now compute

$$\delta\left\langle \psi^{\dagger}\psi\right\rangle = \left\langle \psi^{\mathrm{eq}\dagger}_{\mathrm{phys}} \delta\psi \right\rangle + \left\langle \delta\psi^{\dagger}\psi^{\mathrm{eq}}_{\mathrm{phys}} \right\rangle = O\left(U^2\right) \tag{13.172}$$

$$\delta\left\langle \psi^2\right\rangle = \left\langle \psi^{\mathrm{eq}}_{\mathrm{phys}} \delta\psi \right\rangle = 2\Phi_0 U \int \frac{d\omega}{2\pi} \sum_{\mathbf{p},\mathbf{q}} \frac{e^{i(\mathbf{p}\mathbf{x}-\omega t)}}{V^{3/2}} \frac{f_{\mathbf{p}}(\omega)}{\omega - \omega_q - \omega_{|\mathbf{p}+\mathbf{q}|} + i\varepsilon} \tag{13.173}$$

The equation for the fluctuation is then

$$i\frac{\partial}{\partial t}\delta\Phi = H\delta\Phi + U\Phi_0^2\left[\delta\Phi^{\dagger} + \delta\Phi\right] + U\left\langle \psi^2\right\rangle_0 \delta\Phi^{\dagger} + U\Phi_0\delta\left\langle \psi^2\right\rangle \tag{13.174}$$

or, after Fourier transformation,

$$\left[\omega - \omega_p - U\Phi_0^2 - \frac{2U^2\Phi_0^2}{V}\sum_{\mathbf{q}} \frac{1}{\left(\omega - \omega_q - \omega_{|\mathbf{p}+\mathbf{q}|} + i\varepsilon\right)}\right] f_{\mathbf{p}}(\omega) - U\left[\Phi_0^2 + \tilde{m}\right] f^{*}_{-\mathbf{p}}(-\omega) = 0 \tag{13.175}$$

Changing $\mathbf{p} \to -\mathbf{p}$, $\omega \to -\omega$ and conjugating we find the second equation

$$U\left[\Phi_0^2 + \tilde{m}\right] f_{\mathbf{p}}(\omega) + \left[\omega + \omega_p + U\Phi_0^2 - \frac{2U^2\Phi_0^2}{V}\sum_{\mathbf{q}} \frac{1}{\left(\omega + \omega_q + \omega_{|\mathbf{p}+\mathbf{q}|} + i\varepsilon\right)}\right] f^{*}_{-\mathbf{p}}(-\omega) = 0 \tag{13.176}$$

Up to $O(U^2)$ the secular equation is

$$0 = \omega^2 - \left(\omega_p + U\Phi_0^2\right)^2 - \frac{2U^2\Phi_0^2}{\hbar^2 V}\left(\omega - \omega_p\right)\sum_{\mathbf{q}} \frac{1}{\left(\omega + \omega_q + \omega_{|\mathbf{p}+\mathbf{q}|} + i\varepsilon\right)} - \frac{2U^2\Phi_0^2}{\hbar^2 V}\left(\omega + \omega_p\right)\sum_{\mathbf{q}} \frac{1}{\left(\omega - \omega_q - \omega_{|\mathbf{p}+\mathbf{q}|} + i\varepsilon\right)} + U^2\Phi_0^4 \tag{13.177}$$

We expect that the solution will be close to ω_p, but if there is a $\mathbf{q}$ such that $\omega_p \sim \omega_q + \omega_{\mathbf{p}+\mathbf{q}}$ then the $O(U^2)$ terms become large and perturbation theory breaks down. What is going on is that the free evolution of condensate fluctuations cannot be described as oscillations with a small number of fundamental

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frequencies. This is clearly seen in the continuum limit, where we may replace

$$\frac{1}{V}\sum_{\mathbf{q}} \to \int \frac{d^3\mathbf{q}}{(2\pi)^3} \tag{13.178}$$

The resulting integrals have an imaginary part and the frequencies for the free evolution of condensate fluctuations become complex, $\omega \sim \omega_p - i\Gamma$

$$\Gamma \sim \frac{U^2\Phi_0^2 M}{8\pi\hbar^3} p \sim \left(\frac{a}{\xi}\right) c_s p \tag{13.179}$$

The underlying mechanism is that the energy of a condensate fluctuation carrying momentum $\mathbf{p}$ is spent in exciting two particles out of the condensate, one of momentum $-\mathbf{q}$ and another of momentum $\mathbf{p}+\mathbf{q}$. Of course, this mechanism requires the presence of a condensate. The term $\delta\eta_2\,[\delta\Phi]$ contains additional channels describing the direct decay of the condensate fluctuation into three particles.

Also, we have assumed that the mode p was hard enough that it fell into the "particle-like" part of the spectrum. In practice, damping is very sensitive to the shape of the dispersion relation and to the number of spatial dimensions [TsuGri03, TsuGri05, Rob05, RHCC05]. A more detailed calculation shows, for example, that the mechanism we have described does not work in one dimension, because it is not possible to satisfy energy conservation. In such a case damping becomes a higher order effect.

13.2.8 The stochastic Gross–Pitaevskii equation

If the evolution of condensate fluctuations is damped, then from fluctuation–dissipation relation considerations we must expect it will also be stochastic. This is indeed the case. The resulting "stochastic Gross–Pitaevskii equation" has been investigated by Stoof [Sto99], Duine and Stoof [DuiSto01] and specially by Gardiner and collaborators [GaAnFu01, GarDav03, Jaigar04, BrBlGa05]. Our treatment is essentially a translation of the discussion by Gardiner, Anglin and Fudge [GaAnFu01] into the language of this book [CaHuVe07]. It is interesting to compare our treatment of this problem with [DaDzOn02, KKHOSK06] and [DomRit02].

The simplest way to identify the stochastic elements in the evolution of the condensate is to adopt a coarse-grained effective action scheme (cf. Chapter 5) where the single-particle modes are divided into a "condensate band" (system) of low-lying modes, where most of the condensation takes place, and a "noncondensate" band (environment) of higher modes which act as an environment for the system. In the open system treatment (see Chapters 5 and 8) the quantum fluctuations of the higher band can be represented as classical stochastic fluctuations in the lower band through the nonlinear coupling between the two bands.

A second source of stochasticity is in the random initial conditions appropriate to the condensate [Ste98, ScHuGa06, NobaGa05, NobaGa06].

Since the basic formalism and its physical content have been discussed in detail in the quoted chapters, we shall only review here the simplest scenario. We consider a bosonic gas confined to a box of volume V with periodic boundary conditions, and assume the condensate band to contain just the homogeneous mode, namely

$$\Psi\left(\mathbf{x},t\right)=\phi_{\mathrm{c}}\left(t\right)+\chi\left(\mathbf{x},t\right) \tag{13.180}$$

where ϕ_{c} is the condensate band field operator. Note the subscript "c" here denotes condensate, not classical, thus this is not quite the background field-quantum field split we have considered so far because ϕ_{c}, unlike the mean field Φ, is a q-number, and the noncondensate band operator χ, unlike the fluctuation field ψ, has no zero mode.

We compute the influence functional (equivalent to the coarse-grained closed time path effective action) for the ϕ field to order U^2, to which order the field χ is just a nonrelativistic free bosonic field. Let ${\phi_{\mathrm{c}}}^1$ and ${\phi_{\mathrm{c}}}^2$ be the fields in the first and second branch, respectively, and write $\left(\phi^n\right)_-=\left({\phi_{\mathrm{c}}}^1\right)^n-\left({\phi_{\mathrm{c}}}^2\right)^n$, $\left(\phi^n\right)_+=\left(\left({\phi_{\mathrm{c}}}^1\right)^n+\left({\phi_{\mathrm{c}}}^2\right)^n\right)/2$. Then

$$\begin{aligned}S_{\mathrm{IF}}\left[{\phi_{\mathrm{c}}}^1,{\phi_{\mathrm{c}}}^2\right]=S\left[{\phi_{\mathrm{c}}}^1\right]-S\left[{\phi_{\mathrm{c}}}^2\right]&\\ +\frac{iU^2}{2}\int dt\;dt'\Big\{&\left(\phi^{\dagger 2}\right)_-(t)\left(\phi^2\right)_+(t')\,\nu\left(t-t'\right)\theta\left(t-t'\right)\\ &-\left(\phi^2\right)_-(t)\left(\phi^{\dagger 2}\right)_+(t')\,\nu\left(t'-t\right)\theta\left(t-t'\right)\\ &+\frac{1}{2}\left(\phi^{\dagger 2}\right)_-(t)\left(\phi^2\right)_-(t')\,\nu\left(t-t'\right)\Big\}\end{aligned} \tag{13.181}$$

where

$$\nu\left(t-t'\right)=\sum_{\mathbf{p}}e^{-2i\omega_p\left(t-t'\right)},\quad \omega_p=\frac{\hbar p^2}{2M} \tag{13.182}$$

The last line in the influence functional may be traded for two stochastic sources

$$\begin{aligned}&\exp\left\{\frac{-U^2}{4\hbar}\int dt\;dt'\;\left(\phi^{\dagger 2}\right)_-(t)\left(\phi^2\right)_-(t')\,\nu\left(t-t'\right)\right\}\\ &\quad=\int D\xi D\xi^*\;P\left[\xi,\xi^*\right]\exp\left\{\frac{iU}{2\hbar}\int dt\;\left[\xi(t)\left(\phi^2\right)_-(t)+\xi^*(t)\left(\phi^{\dagger 2}\right)_-(t)\right]\right\}\end{aligned} \tag{13.183}$$

where P is a Gaussian measure defined by the correlations

$$\begin{aligned}\left\langle\xi(t)\right\rangle=\left\langle\xi(t)\,\xi(t')\right\rangle&=0\\ \left\langle\xi^*(t)\,\xi(t')\right\rangle&=\hbar\nu\left(t-t'\right)\end{aligned} \tag{13.184}$$

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Variation of the influence functional yields the stochastic GPE for the condensate field

$$i\hbar\phi_{c,t} - U{\phi_c}^{\dagger}{\phi_c}^2 + \frac{iU^2}{V}{\phi_c}^{\dagger}\int^{t} dt'\, \nu\,(t-t')\,{\phi_c}^2\,(t') = -\frac{U}{V}\xi^*\,(t)\,{\phi_c}^{\dagger}\,(t) \quad (13.185)$$

As a check, let us seek the equilibrium solution (neglecting the stochastic term). In equilibrium,

$$\phi_c = \sqrt{\frac{N}{V}}\,e^{-i\mu t/\hbar} \quad (13.186)$$

so the only unknown is the chemical potential

$$\mu = \frac{UN}{V} - \frac{U^2 N}{2V^2}\sum_p \frac{1}{\omega_p - \mu - i\varepsilon} \quad (13.187)$$

which is equivalent to the one-loop result.

We see that in general the condensate will undergo non-Markovian dynamics driven by multiplicative colored noise. The generalization of (13.185) for a trap of arbitrary shape is given in [CaHuVe07].

13.2.9 The hydrodynamic and quantum kinetic approach to BECs

So far we have described in some detail the equilibrium and linear response regimes of the condensate, but a nonequilibrium approach has not shown its worth unless it can tackle also the out-of-equilibrium evolution. Of course, the truly far from equilibrium case is as hard to handle as with all other quantum fields we have discussed in this book; see e.g. Chapter 12. However, there is one case where one should be able to make progress, namely, when both the condensate and noncondensate densities are high enough to enforce efficient local thermalization. Then a quantum kinetic theory approach along the lines of Chapter 11 ought to be viable.

The quantum kinetic theory approach to BECs was introduced by Kane and Kadanoff [KanKad65] and elaborated in two series of papers by Gardiner, Zoller and collaborators and Holland, Wachter, Walser and collaborators [GarZol97, JaGaZo97, GarZol98, JGGZ98, GarZol00a, WWCH99, WaCoHo00, WWCH01, WWCH02a, BhWaHo02, WWCH02b]. The derivation of quantum kinetic theory from the 2PIEA is discussed in [BaiSto04, RHCC05]. We follow the latter reference.

There are two basic differences between the quantum kinetic theory applied to BECs and to a generic scalar field theory as discussed in Chapter 11. First, there are two fundamental quantum fields (ψ and $\psi^{\dagger}$) and therefore the number of propagators is higher. This poses only formal difficulties and we will not discuss it in detail (similar problems arise in the application of the quantum kinetic theory approach to gauge theories, see Chapter 11).

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Second, the quantum kinetic theory approach assumes that all mean fields are slowly varying on the scale of the wavelength of the relevant quantum modes, so that an adiabatic expansion is feasible. In the case of BECs, this assumption can be made for the condensate density, but the condensate phase may show strong position dependence.

A solution to this problem is suggested by the long known fact that the evolution of the condensate as described by the GPE is equivalent to the evolution of an irrotational fluid. The idea is that the kinetic description will be valid when the hydrodynamic variables (rather than the condensate wavefunction itself) are slowly varying functions of position.

Let us begin by briefly reviewing the hydrodynamic formulation. Unlike the relativistic theories described in Chapter 12, the condensate is represented as a nonrelativistic (super) fluid. Since the superfluid carries no entropy, the energy density ϵ, pressure p, number density ρ, chemical potential μ, superfluid velocity $\mathbf{v}$ and momentum density π are linked through the relationship

$$\varepsilon + p - \rho\mu - \mathbf{v}\cdot\pi = 0 \tag{13.188}$$

This implies the Gibbs–Duhem relation

$$dp - \rho d\mu - \pi\cdot d\mathbf{v} = 0 \tag{13.189}$$

If we assume the usual relationship $\pi = M\rho\mathbf{v}$, this suggests

$$\mu = \mu_0 - \frac{1}{2}M\mathbf{v}^2 \tag{13.190}$$

where the relationship between μ_0 and p is the usual one for a fluid at rest

$$dp = \rho d\mu_0 \tag{13.191}$$

We have to make contact between this fluid description and the usual one in terms of a condensate wavefunction. Let us write the mean field as [Mad27, Hal81, Cas04]

$$\Phi = e^{i\Theta(\mathbf{x},t)}\sqrt{\rho\left(\mathbf{x},t\right)} \tag{13.192}$$

(observe the position dependence of the phase), whereby we have a microscopic interpretation of the density, and the propagators as

$$G^{AB}\left(\left(\mathbf{x},t\right),\left(\mathbf{y},t'\right)\right) = e^{i\sigma_{3AC}\Theta(\mathbf{x},t)}e^{i\sigma_{3BD}\Theta\left(\mathbf{y},t'\right)}\bar{G}^{CD}\left(\left(\mathbf{x},t\right),\left(\mathbf{y},t'\right)\right) \tag{13.193}$$

Observe that since Γ_Q is built out of Feynman graphs based on local interactions it has no explicit dependence on the phases $\Theta\left(\mathbf{x},t\right)$. Therefore the force η_2 will transform as

$$\eta_2\left[\Phi\right] = e^{i\Theta(\mathbf{x},t)}\bar{\eta}\left[\rho,\bar{G}^{AB}\right] \tag{13.194}$$

Now the mean field equation is given by

$$e^{-i\Theta(\mathbf{x},t)}\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2M}\nabla^2\right]\left\{e^{i\Theta(\mathbf{x},t)}\sqrt{\rho\left(\mathbf{x},t\right)}\right\} - V\left(\mathbf{x}\right)\sqrt{\rho} - \bar{\eta} = 0 \tag{13.195}$$

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Its imaginary part reads

$$\frac{\partial\rho}{\partial t}+\frac{\hbar}{M}\nabla\left[\rho\nabla\Theta\right]=2\sqrt{\rho}\mathrm{Im}\,\bar{\eta} \tag{13.196}$$

This allows us to identify

$$\mathbf{v}=\frac{\hbar}{M}\nabla\Theta \tag{13.197}$$

as the superfluid velocity, which is therefore (locally) irrotational by definition. There may be global rotation, if the volume occupied by the condensate is not simply connected.

The real part of the mean field equation reads

$$-\hbar\frac{\partial\Theta}{\partial t}=\frac{M}{2}\mathbf{v}^2+V\left(x\right)+\frac{\mathrm{Re}\,\bar{\eta}}{\sqrt{\rho}}-\frac{\hbar^2}{2M\sqrt{\rho}}\nabla^2\sqrt{\rho} \tag{13.198}$$

This leads to the evolution equation for the superfluid velocity

$$\frac{\partial v^i}{\partial t}+\left(v^j\nabla_j\right)v^i=\frac{-1}{M}\nabla^i\left[V\left(x\right)+\frac{\mathrm{Re}\,\bar{\eta}}{\sqrt{\rho}}-\frac{\hbar^2}{2M\sqrt{\rho}}\nabla^2\sqrt{\rho}\right] \tag{13.199}$$

where we have used the assumption that the superfluid velocity is irrotational. For the momentum density we get

$$\frac{\partial M\rho v^i}{\partial t}+\nabla_j\left[M\rho v^jv^i\right]+\rho\nabla^i\frac{\mathrm{Re}\,\bar{\eta}}{\sqrt{\rho}}=-\rho\nabla^i\left[V\left(x\right)-\frac{\hbar^2}{2M\sqrt{\rho}}\nabla^2\sqrt{\rho}\right]+2Mv^i\sqrt{\rho}\mathrm{Im}\,\bar{\eta} \tag{13.200}$$

The usual hydrodynamic equation would read

$$\frac{\partial M\rho v^i}{\partial t}+\nabla_jT^{ij}=F^i \tag{13.201}$$

where T^{ij} is the nonrelativistic momentum flux tensor

$$T^{ij}=M\rho v^jv^i+p\delta^{ij} \tag{13.202}$$

Comparing the hydrodynamic and the microscopic forms of the equation for the superfluid velocity we may identify the pressure. Assume $\mathrm{Re}\,\bar{\eta}$ is a function of ρ. Then

$$\frac{dp}{d\rho}=\rho\frac{d}{d\rho}\left[\frac{\mathrm{Re}\,\bar{\eta}}{\sqrt{\rho}}\right] \tag{13.203}$$

It is interesting to observe that also

$$\frac{dp}{d\rho}=Mc_{\mathrm{s}}^2 \tag{13.204}$$

defines the speed of sound in the condensate. Going back to the Gibbs–Duhem relation we find

$$\mu_0=\frac{\mathrm{Re}\,\bar{\eta}}{\sqrt{\rho}} \tag{13.205}$$

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and so the equation for the time dependence of the phase is

$$-\hbar\frac{\partial\Theta}{\partial t}=\frac{1}{2}M\mathbf{v}^2+V\left(x\right)+\mu_0-\frac{\hbar^2}{2M\sqrt{\rho}}\nabla^2\sqrt{\rho} \tag{13.206}$$

To close this system we need the equations for the propagators. From the decompositions

$$G^{-1}_{AB}\left(\left(\mathbf{x},t\right),\left(\mathbf{y},t'\right)\right)=e^{-i\sigma_{3AC}\Theta(\mathbf{x},t)}e^{-i\sigma_{3BD}\Theta\left(\mathbf{y},t'\right)}\bar{G}^{-1}_{CD}\left(\left(\mathbf{x},t\right),\left(\mathbf{y},t'\right)\right) \tag{13.207}$$

$$\Sigma_{AB}\left(\left(\mathbf{x},t\right),\left(\mathbf{y},t'\right)\right)=e^{-i\sigma_{3AC}\Theta(\mathbf{x},t)}e^{-i\sigma_{3BD}\Theta\left(\mathbf{y},t'\right)}\bar{\Sigma}_{CD}\left(\left(\mathbf{x},t\right),\left(\mathbf{y},t'\right)\right) \tag{13.208}$$

we get

$$\bar{G}^{-1}_{AB}=\bar{D}^{-1}_{AB}+i\bar{\Sigma}_{AB} \tag{13.209}$$

where

$$\bar{D}^{-1}_{AB}=e^{i\sigma_{3AC}\Theta(\mathbf{x},t)}D^{-1}_{CD}e^{i\sigma_{3BD}\Theta\left(\mathbf{y},t'\right)} \tag{13.210}$$

Concretely,

$$\bar{D}^{-1}_{AB}=(-i)\begin{pmatrix}0 & \bar{D}^{-1*}\\ \bar{D}^{-1} & 0\end{pmatrix} \tag{13.211}$$

$$\begin{aligned}\bar{D}^{-1}&=e^{-i\Theta}\left[i\hbar\partial_t+\frac{\hbar^2}{2M}\nabla^2-V\left(x\right)\right]e^{i\Theta}\\&=i\hbar\left(\partial_t+\mathbf{v}.\nabla+\frac{(\nabla.\mathbf{v})}{2}\right)+\frac{\hbar^2}{2M}\nabla^2+\mu_0-\frac{\hbar^2\left(\nabla^2\sqrt{\rho}\right)}{2M\sqrt{\rho}}\end{aligned} \tag{13.212}$$

From this point on, the derivation of the quantum kinetic equation for the noncondensate particles follows the lines of Chapter 11. For a discussion of nontrivial hydrodynamic behavior in BECs see [HACCES06].

13.3 The particle number conserving formalism

The symmetry-breaking approach described above has the disturbing feature that, strictly speaking, symmetry breaking only occurs in the thermodynamic limit. We therefore have a formalism that assumes the number of particles is essentially infinite. Most actual experiments deal with situations where particle number is bounded. Under this circumstance a condensate as described above simply cannot happen.

In this section we shall describe an alternative formulation which is designed to deal with gases with fixed particle numbers. We shall call this formulation the particle number conserving formalism, PNC for short. See [GirArn59, GirArn98, CasDum97, CasDum98, MorCas03, Gar97, GJDCZ00, Mor04, Mor99, Mor00, Idz05a, Dzi05b, GarMor07]. Let us begin by discussing how is it possible to speak of a BEC in a situation where there is no symmetry breaking.

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13.3.1 Problems with the symmetry-breaking approach

Recall in the symmetry-breaking (SB) approach to BEC, condensation is signaled by a spontaneous breakdown of phase invariance (13.31), whereby Ψ develops a nonzero expectation value Φ. We can therefore employ a background field decomposition [NegOrl98, PetSmi02] around Φ (c-number): $\Psi = \Phi + \psi$ where ψ (q-number) is the field operator describing quantum fluctuations (see equation (13.35)).

A common feature of these approaches is that the total particle number

$$\mathbf{N} = \int d^d\mathbf{x}\ \Psi^\dagger \Psi \tag{13.213}$$

is not fixed. For example, let us assume that the condensate is confined within a homogeneous box of volume V, condensation occurring in the lowest (translation-invariant) mode. Let $a_\mathbf{k}$ be the operator that destroys an atom in the $\mathbf{k}$ mode. Then we may approximate (see the more careful discussion below)

$$\psi(\mathbf{x}, t) = \sum_{\mathbf{k}\neq 0} \frac{e^{i\mathbf{kx}}}{\sqrt{V}} a_\mathbf{k} \tag{13.214}$$

Even if we treat ψ as a linear perturbation on the condensate, the Hamiltonian is not diagonal on the $a_\mathbf{k}$. To diagonalize it, we must introduce phonon destruction operators $A_\mathbf{k}$ and perform a Bogoliubov transformation

$$a_\mathbf{k} = \alpha_\mathbf{k} A_\mathbf{k} + \beta_\mathbf{k} A^\dagger_{-\mathbf{k}} \tag{13.215}$$

At zero temperature, the state is the phonon vacuum, $A_\mathbf{k}|0\rangle = 0$ for all $\mathbf{k} \neq 0$. We find

$$\langle \mathbf{N} \rangle = \int d^d\mathbf{x}\ \left\langle \Psi^\dagger \Psi \right\rangle = V \left[|\Phi|^2 + \tilde{n} \right] \tag{13.216}$$

where

$$\tilde{n} = \left\langle \psi^\dagger \psi \right\rangle = \frac{1}{V} \sum_{\mathbf{k}\neq 0} \left\langle a^\dagger_\mathbf{k} a_\mathbf{k} \right\rangle = \frac{1}{V} \sum_{\mathbf{k}\neq 0} |\beta_\mathbf{k}|^2 \tag{13.217}$$

but

$$\left\langle \mathbf{N}^2 \right\rangle = V^2 \left[\left(|\Phi|^2 \right)^2 + |\Phi|^2 \left(4\tilde{n} + \frac{1}{V} \right) + \Phi^{*2}\tilde{m} + \Phi^2 \tilde{m}^* + \ldots \right] \tag{13.218}$$

where

$$\tilde{m} = \left\langle \psi^2 \right\rangle = \frac{1}{V} \sum_{\mathbf{k}\neq 0} \langle a_{-\mathbf{k}} a_\mathbf{k} \rangle = \frac{1}{V} \sum_{\mathbf{k}\neq 0} \alpha_\mathbf{k} \beta_\mathbf{k} \tag{13.219}$$

The Bogoliubov coefficients $\alpha_\mathbf{k}$ and $\beta_\mathbf{k}$ cannot be equal, because the canonical (Bose) commutation relations imply $|\alpha_\mathbf{k}|^2 - |\beta_\mathbf{k}|^2 = 1$, and so also $\tilde{m} \neq \tilde{n}$. We conclude that necessarily $\left\langle \mathbf{N}^2 \right\rangle \neq \langle \mathbf{N} \rangle^2$ in the symmetry-breaking approach, signaling the presence of particle number fluctuations.

13.3.2 The one-body density matrix and long-range coherence

We consider as above a second-quantized Bose field Ψ. The state of the many-body system is an eigenstate of total particle number operator (13.213). There is no particle exchange with the environment.

In this case of a finite system, there is no symmetry breaking. The symmetry-broken state is essentially a coherent state and thus a coherent superposition of states with arbitrarily large total particle number. Nevertheless, there are situations where there is long-range coherence across the system, thus capturing the essential feature of the condensed states. Sometimes these situations are referred to as quasi-condensates, but we shall not make this distinction, just referring to them as the symmetry-broken siblings of BECs.

To characterize the BEC state, let us introduce the one-body density matrix [PenOns56]

$$\sigma(\mathbf{x}, \mathbf{y}, t) = \left\langle \Psi^{\dagger}(\mathbf{x}, t) \Psi(\mathbf{y}, t) \right\rangle \tag{13.220}$$

Long-range coherence appears when σ fails to decay as x and y are taken apart. Observe that σ is Hermitian and nonnegative, in the sense that for any function f

$$\int d^d\mathbf{x} d^d\mathbf{y}\ f^*(\mathbf{x}) \sigma(\mathbf{x}, \mathbf{y}, t) f(\mathbf{y}) \geq 0 \tag{13.221}$$

Therefore it admits a basis of eigenfunctions

$$\int d^d\mathbf{x}\ \sigma(\mathbf{x}, \mathbf{y}, t) \phi_\alpha(\mathbf{y}, t) = n_\alpha \phi_\alpha(\mathbf{x}, t) \tag{13.222}$$

where the eigenvalues n_α are real and nonnegative. We assume the ϕ_α are normalized

$$(\phi_\alpha, \phi_\beta) = \delta_{\alpha\beta} \tag{13.223}$$

$$(f, g) = \int d^d\mathbf{x}\ f^* g \tag{13.224}$$

and complete

$$\sum_\alpha \phi^*_\alpha(\mathbf{x}, t) \phi_\alpha(\mathbf{y}, t) = \delta(\mathbf{x} - \mathbf{y}) \tag{13.225}$$

The field operator may be expanded in this basis

$$\Psi(\mathbf{x}, t) = \sum_\alpha a_\alpha(t) \phi_\alpha(\mathbf{x}, t) \tag{13.226}$$

The Bose commutation relations imply

$$\left[a_\alpha(t), a^\dagger_\beta(t)\right] = \delta_{\alpha\beta} \tag{13.227}$$

The $a_\alpha(t)$ are operators which, at time t, destroy a particle in the one-particle state α whose wavefunction is $\phi_\alpha(\mathbf{x}, t)$. From the definition of σ we find

$$\left\langle a^\dagger_\alpha(t) a_\beta(t) \right\rangle = n_\alpha(t) \delta_{\alpha\beta} \tag{13.228}$$

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Therefore the eigenvalues $n_\alpha(t)$ are the mean number of particles in the one-body state α at time t. We also have the strong identity

$$N = \sum_\alpha a_\alpha^\dagger(t)\, a_\alpha(t) \tag{13.229}$$

Condensation occurs when one of the n_α, say $\alpha = 0$, becomes comparable with N itself. Then we have, for large separations

$$\sigma(\mathbf{x}, \mathbf{y}, t) \sim n_0 \phi_0^*(\mathbf{x}, t)\, \phi_0(\mathbf{y}, t) \tag{13.230}$$

which displays long-range coherence, as expected. Here $\phi_0(\mathbf{x}, t)$ is the condensate wavefunction. We stress that this is the fundamental definition; $\phi_0(\mathbf{x}, t)$ is not necessarily proportional to the mean field Φ introduced in the symmetry-breaking approach.

13.3.3 The particle number conserving approach

We shall now discuss the dynamics of the condensate wavefunction $\phi_0(\mathbf{x}, t)$ and the condensate occupation number N_0 (we switch to a capital N to emphasize its macroscopic character). We envisage a situation in which N is finite but large, and will seek equations of motion as an expansion in inverse powers of N. In preparation for this, it is convenient to scale the interaction term, writing $U = u/N$.

As we have seen above, in the symmetry-breaking approach the condensate state (for an interacting gas) is seen as a coherent superposition of particle pairs, each pair having zero total momentum. The basic insight of the PNC approach is that each particle above the condensate corresponds to a hole in the condensate, so we may speak of *particle–hole* (PH) pairs. Of course, introducing a PH into the system does not change the total number of particles.

Following Arnowitt and Girardeau, let us introduce the operator

$$\beta = \frac{1}{\sqrt{\hat{N}_0 + 1}} a_0 = a_0 \frac{1}{\sqrt{\hat{N}_0}} \tag{13.231}$$

where

$$\hat{N}_0 = N - \sum_{\alpha \neq 0} a_\alpha^\dagger a_\alpha \tag{13.232}$$

is the condensate number Heisenberg operator. Observe that for a number eigenstate $\beta\, |N_0\rangle = |N_0 - 1\rangle$ unless $N_0 = 0$, in which case $\beta\, |0\rangle = 0$. Therefore β preserves the norm for all states orthogonal to the state with no particles in the zeroth mode (which is much stronger than not having a condensate). If there is a condensate, any physically meaningful state will satisfy this requirement, and β may be considered a unitary operator, with inverse

$$\beta^\dagger = \frac{1}{\sqrt{\hat{N}_0}} a_0^\dagger = a_0^\dagger \frac{1}{\sqrt{\hat{N}_0 + 1}} \tag{13.233}$$

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We now introduce the destruction operator of a PH with the particle in mode α

$$\lambda_\alpha = \beta^\dagger a_\alpha \tag{13.234}$$

If we consider the β's as unitary, then the λ's satisfy bosonic canonical commutation relations. This relationship may be inverted:

$$a_\alpha = \beta \lambda_\alpha \tag{13.235}$$

The number of particles in a given mode is equal to the number of PH

$$a_\alpha^\dagger a_\alpha = \lambda_\alpha^\dagger \lambda_\alpha \tag{13.236}$$

We write the field operator restricted to the subspace with a well-defined total number of particles N as $\Psi = \sqrt{N}\beta\phi$

$$\phi = \phi_0\left(\mathbf{x}, t\right) + \frac{1}{\sqrt{N}}\lambda\left(\mathbf{x}, t\right) - \frac{1}{2N} f\left[\delta n\left(t\right)\right]\phi_0\left(\mathbf{x}, t\right) \tag{13.237}$$

where

$$\lambda\left(\mathbf{x}, t\right) = \sum_{\alpha \neq 0} \lambda_\alpha\left(t\right)\phi_\alpha\left(\mathbf{x}, t\right) \tag{13.238}$$

$$\delta n\left(t\right) = \int d^3\mathbf{x}\, \lambda^\dagger \lambda \tag{13.239}$$

$$f\left(x\right) = 2N\left[1 - \sqrt{1 - \frac{x}{N}}\right] \sim x + O\left(N^{-1}\right) \tag{13.240}$$

Within our approximations β commutes with ϕ. Finally we have the relationship

$$0 = \left\langle a_0^\dagger\left(t\right) a_\alpha\left(t\right)\right\rangle = \left\langle a_0^\dagger\left(t\right)\beta\lambda_\alpha\left(t\right)\right\rangle = \sqrt{N}\left\langle\left[\sqrt{1 - \frac{1}{N}\sum_{\gamma\neq 0}\lambda_\gamma^\dagger\lambda_\gamma}\right]\lambda_\alpha\left(t\right)\right\rangle \tag{13.241}$$

which implies

$$\langle\lambda\rangle = \frac{1}{2N}\left\langle f\left[\delta n\left(t\right)\right]\lambda\right\rangle \tag{13.242}$$

The idea is to seek a solution of the Heisenberg equations of motion for Ψ where β and the λ_α's have developments in inverse powers of N. Define a "q-number" chemical potential $\hat{\mu}$ from

$$\beta^\dagger \frac{d\beta}{dt} = \frac{-i\hat{\mu}}{\hbar} \tag{13.243}$$

We have

$$i\hbar\frac{\partial}{\partial t}\phi = \left(H - \hat{\mu}\right)\phi + u\phi^\dagger\phi^2 \tag{13.244}$$

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We then find

$$
\begin{aligned}
0 &= -i\hbar\phi_{0,t} + (H - \hat{\mu})\,\phi_0 + u\phi_0^3 \\
&\quad + \frac{1}{\sqrt{N}}\left[-i\hbar\lambda_{,t} + (H - \hat{\mu})\,\lambda + u\phi_0^2\left(2\lambda + \lambda^\dagger\right)\right] + O\left(N^{-1}\right)
\end{aligned} \tag{13.245}
$$

Taking the expectation value we find

$$
0 = -i\hbar\phi_{0,t} + (H - \langle\hat{\mu}\rangle)\,\phi_0 + u\phi_0^3 - \frac{1}{\sqrt{N}}\langle\hat{\mu}\lambda\rangle + O\left(N^{-1}\right) \tag{13.246}
$$

Recall that ϕ_0 is real (if the condensate is nondegenerate) and $\hat{\mu}$ is Hermitian. So we may decompose this equation into

$$
0 = (H - \langle\hat{\mu}\rangle)\,\phi_0 + u\phi_0^3 - \frac{1}{2\sqrt{N}}\left\langle\hat{\mu}\lambda + \lambda^\dagger\hat{\mu}\right\rangle + O\left(N^{-1}\right) \tag{13.247}
$$

and

$$
0 = -i\hbar\phi_{0,t} - \frac{1}{2\sqrt{N}}\left\langle\hat{\mu}\lambda - \lambda^\dagger\hat{\mu}\right\rangle + O\left(N^{-1}\right) \tag{13.248}
$$

This is consistent with the normalization condition

$$
\int \phi_0\phi_{0,t} = 0 \tag{13.249}
$$

Subtracting the expectation value from the Heisenberg equation, we get

$$
\begin{aligned}
0 = &\left(\langle\hat{\mu}\rangle - \hat{\mu}\right)\phi_0 + \frac{1}{\sqrt{N}}\left[-i\hbar\lambda_{,t} + (H - \hat{\mu})\,\lambda + u\phi_0^2\left(2\lambda + \lambda^\dagger\right)\right] + \frac{1}{\sqrt{N}}\langle\hat{\mu}\lambda\rangle \\
&+ O\left(N^{-1}\right)
\end{aligned} \tag{13.250}
$$

The orthogonality of ϕ_0 and λ implies

$$
\int \left(\phi_0\lambda_{,t} + \phi_{0,t}\lambda\right) = 0 \tag{13.251}
$$

and from (13.250), (13.248) and (13.247) we get

$$
0 = \langle\hat{\mu}\rangle - \hat{\mu} + \frac{u}{\sqrt{N}}\left(J_3 + J_3^\dagger\right) + O\left(N^{-1}\right) \tag{13.252}
$$

where

$$
J_n = \int \phi_0^n\lambda \tag{13.253}
$$

Observe that this implies

$$
\langle\hat{\mu}\lambda\rangle = O\left(N^{-1/2}\right) \tag{13.254}
$$

The equation for λ simplifies into

$$0=-i\hbar\lambda_{,t}+(H-\hat{\mu})\lambda+u\phi_0^2\lambda+Q\left[u\phi_0^2\left(\lambda+\lambda^{\dagger}\right)\right]+O\left(N^{-1/2}\right) \quad (13.255)$$

where

$$Q[X]=X-\phi_0\int\phi_0X \quad (13.256)$$

The homogeneous case

To get a feeling of the working of the PMC approach, let us apply it to the simplest case of a BEC in a homogeneous box of volume V, with periodic boundary conditions.

In equilibrium, by symmetry, the condensate wavefunction must be homogeneous, and by normalization we must have $\phi_0=V^{-1/2}$. This equation holds to all orders in $1/N$. Therefore

$$\langle\hat{\mu}\rangle=\frac{u}{V}+O\left(N^{-1}\right) \quad (13.257)$$

This gives $\langle\hat{\mu}\rangle=UN/V+\ldots$. By contrast, in the Bogoliubov approximation the chemical potential is $\mu^{Bog}=UN_0/V$ and in the Popov approximation $\mu^{Pop}=(U/V)(2N-N_0)$. We also have

$$\hat{\mu}=\langle\hat{\mu}\rangle+O\left(N^{-1/2}\right) \quad (13.258)$$

and so the lowest order equation for the inhomogeneous mode is

$$0=\ -i\hbar\lambda_{,t}+H\lambda+\frac{UN}{V}\left(\lambda+\lambda^{\dagger}\right) \quad (13.259)$$

These are the Popov equations with N in place of N_0, and so we know the spectrum will be gapless. Moreover, in this case there is no zero mode divergence.

After solving these equations it is simple to compute the higher corrections to $\hat{\mu}$.

13.3.4 Particle number conserving functional approach

One problem with the PNC approach as presented so far is that it is not cast within a functional approach, and therefore lacks the flexibility which has been key to most of the applications of NEqQFT in this book. To be able to give a functional PNC approach, we must revise the measure of integration in the path integral expression for the generating functional we have considered so far. The idea is to define a new generating functional which will agree with the old one in the computation of expectation values for particle number conserving operators, but will lead to different results otherwise. In particular, the expectation value of the field operator in the new approach will be identically zero, as it must be in a system with a finite number of particles.

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The quantum theory of the BEC may be regarded as the quantization of the nonrelativistic classical field theory defined by the action functional (13.39), where the canonical variables are $\Psi(\mathbf{x},t)$ and its conjugate momentum $i\hbar\Psi^*$. This theory conserves particle number (13.213), and we are interested in the case in which particle number takes on a definite value N. We may reinforce this point by adding a constraint on the theory. This is achieved by introducing a Lagrange multiplier $\mu_q(t)$, whereby the action becomes

$$S = \int d^{d+1}x \left[i\hbar\Psi^* \frac{\partial}{\partial t}\Psi + \hbar\mu_q(t)\left(\Psi^*\Psi - \frac{N}{V}\right)\right] - \int dt\, \mathbf{H} \tag{13.260}$$

The original action (13.39) is invariant under a global transformation (13.31) but the new action (13.260) is invariant under the local (in time) transformations (a familiar theory with local U(1) gauge symmetry is electromagnetism)

$$\Psi \to e^{i\theta(t)}\Psi, \qquad \Psi^\dagger \to e^{-i\theta(t)}\Psi^\dagger, \qquad \mu_q \to \mu_q + \frac{d\theta}{dt} \tag{13.261}$$

provided θ vanishes both at the initial and final times (when θ is infinitesimal, these are just the canonical transformations generated by the constraint) [Dir50, Dir58b]. Therefore it must be quantized using the methods developed for gauge theories, such as the Fadeev–Popov method [PesSch95].

The need for a further refinement of the functional measure comes from the fact that now the path integral is redundant, since we may transform the fields as in (13.261). The Fadeev–Popov approach fixes the redundancy by factoring out the gauge group. Choose some function $f_\theta = f\left[\mu_{q\theta}, \Psi_\theta, \Psi_\theta^\dagger\right]$, such that $df_\theta/d\theta \neq 0$. Then

$$1 = \int \frac{df_\theta}{d\theta} d\theta\, \delta\left(f_\theta - c\right) \tag{13.262}$$

Inserting this into the vacuum persistence amplitude and averaging over c with a weight $e^{ic^2/2\sigma}$ we get

$$Z_0 = \Theta \int D\Psi D\mu_q\, e^{iS_{\mu_q,\sigma}/\hbar} \mathrm{Det}\left[\frac{\delta f_\theta}{\delta\theta}\right]_{\theta=0} \tag{13.263}$$

where

$$\Theta = \int D\theta \tag{13.264}$$

is the volume of the gauge group we wish to factor out;

$$S_{\mu,\sigma} = S + \frac{\hbar}{2\sigma}\int dt\, f_0^2 \tag{13.265}$$

where S is defined in (13.260). The determinant is expressed as a path integral over Grassmann fields ζ, η (see Chapter 7)

$$Det\left[\frac{\delta f_\theta}{\delta\theta}\right]_{\theta=0} = \int D\zeta D\eta\, e^{-\frac{1}{\hbar}\int dt\, \zeta \frac{\delta f_\theta}{\delta\theta}\eta} \tag{13.266}$$

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To finalize the set-up, we need to choose the gauge fixing function f_0. Possibly the simplest choice is the "covariant" gauge

$$f_0 = \frac{d\mu_q}{dt} \tag{13.267}$$

which makes the ghost fields decouple. This gauge is employed in [CaHuRe06] to explore the critical regime in the Mott transition. Other choices are also available, and in fact the freedom to choose the gauge fixing condition is one of the main strengths of the approach [DeuDru02, DrDeKh04].

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