# Cold Bosons in Optical Lattices

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#### Abstract

Basic properties of cold Bose atoms in optical lattices are reviewed. The main principles of correct self-consistent description of arbitrary systems with Bose-Einstein condensate are formulated. Theoretical methods for describing regular periodic lattices are presented. A special attention is paid to the discussion of Bose-atom properties in the frame of the boson Hubbard model. Optical lattices with arbitrary strong disorder, induced by random potentials, are treated. Possible applications of cold atoms in optical lattices are discussed, with an emphasis of their usefulness for quantum information processing and quantum computing. An important feature of the present review article, distinguishing it from other review works, is that theoretical fundamentals here are not just mentioned in brief, but are thoroughly explained. This makes it easy for the reader to follow the principal points without the immediate necessity of resorting to numerous publications in the field.

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# **1** Tools for Manipulating Atoms

## 1.1 Cold Atoms

Physics of cold trapped atoms has become nowadays a very fastly developing field of research, both theoretical and experimental. Magnetic, magneto-optical, and all optical traps are employed for trapping atoms. Several atomic species have been cooled down to low temperatures, when their quantum degeneracy could be observed. The Bose-Einstein condensation (BEC) of trapped atoms was experimentally realized [1–3]. At the present time, BEC has been achieved for 12 atomic species: <sup>1</sup>H, <sup>4</sup>He, <sup>7</sup>Li, <sup>23</sup>Na, <sup>39</sup>K, <sup>41</sup>K, <sup>52</sup>Cr, <sup>85</sup>Rb, <sup>87</sup>Rb, <sup>133</sup>Cs, <sup>170</sup>Yb, and <sup>174</sup>Yb. Quantum degeneracy in trapped Fermi gases was achieved for <sup>40</sup>K and <sup>6</sup>Li atoms [4–6]. Now there exist several books [7,8] and review articles treating the Bose-Einstein condensation of Bose atoms [9–14] and the quantum properties of ultracold Fermi gases [15].

An important development has been the realization of optical lattices, formed by interfering laser beams producing a standing wave. Cold atoms can be trapped for a long time in the minima of the created periodic potential [16]. There are several surveys considering the properties of cold atoms in optical lattices, e.g., [17–20].

In the present review paper, the emphasis is made on the theory of cold Bose atoms in periodic potentials. Such potentials are usually formed by optical lattices, though recently magnetic lattices have also been realized [21].

There are two principal features making this review paper distinct from all other review articles. First, the basic theoretical points are thoroughly explained here, but not just mentioned in brief. This should allow the reader to better understand the theoretical fundamentals and to easily follow the logic of the used mathematical methods. The material of this paper can serve as a reference source for researchers in the field. Second, this paper covers the most recent theoretical results that have not yet been described in other review articles.

## **1.2** Control Parameters

Optical lattices with cold atoms provide an extraordinary possibility of creating systems with a wide variety of properties, which can be manipulated in several ways. First of all, the lattice parameters themselves can be varied in a wide range. In experiments, optical lattices can be formed, having different spacing, depth, and filling factors. The latter can be either integer or fractional and can vary between one and  $10^4$  atoms per lattice site [22,23]. The number of lattice sites can also be different. One - two - and three - dimensional lattices can be formed. The lattices can be periodic and quasiperiodic. Different atomic species, or their mixtures, can be loaded in the lattice. The strength of interatomic interactions can be regulated in a very wide range by employing the Feshbach resonance techniques [10,24]. Varying temperature and/or lattice depth, it is possible to induce phase transitions between localized and delocalized states of atoms, as well as between the normal and superfluid phases.

Lattice properties can also be regulated by imposing additional external potentials. In particular, random external fields can be used, producing disordered lattices. By means of alternating external fields, one can manipulate the motion of atomic clouds. Employing special resonant alternating fields makes it possible to create an unusual state of matter, the nonground-state Bose-Einstein condensates.

These rich potentialities of manipulating cold atoms in optical lattices make this object of high importance for various applications. But the latter can become practicable only being based on effective and correct theoretical investigations.

## **1.3** Atomic Fractions

The total number of atoms N, loaded into a lattice, can consist of several parts. An important part of a Bose system is that one forming Bose-Einstein condensate (BEC) of  $N_0$  atoms, which characterizes the coherent portion of atoms. As a rule the arising BEC leads to the appearance of superfluidity involving  $N_{sup}$  atoms. There is no simple relation between  $N_0$ and  $N_{sup}$  and even it is not compulsory that they be present simultaneously. The physical origins of  $N_0$  and  $N_{sup}$  are different. The appearance of BEC manifests the existence of coherence in the system. Superfluidity demonstrates the presence of nontrivial response to a velocity boost, which is caused by strong atomic correlations.

Atoms in a lattice can also be distinguished by the region of their motion. Atoms can be localized in their lattice sites or can be delocalized and moving through the whole sample. The localized atoms are associated with the solid state of matter, possessing small compressibility and a gap in the single-particle spectrum. The number of atoms, forming a solid, will be denoted by  $N_{sol}$ . Delocalized atoms are typical of the liquid or gaseous state of matter, with gapless single-particle spectra.

Since the total number of atoms N, as well as the atomic numbers  $N_0$ ,  $N_{sup}$ , and  $N_{sol}$ , can be very large, it is more appropriate to deal with the related atomic fractions, which are:

the condensate fraction

 $n_0 \equiv \frac{N_0}{N} ,$  $n_{sup} \equiv \frac{N_{sup}}{N} ,$ 

and the solid fraction

superfluid fraction

$$n_{sol} \equiv \frac{N_{sol}}{N}$$
.

Similarly, the number of uncondensed atoms  $N_1$  defines the normal fraction  $n_1 \equiv N_1/N$ . And one can define the fraction of atoms in fluid phase. But the fractions  $n_0$ ,  $n_{sup}$ , and  $n_{sol}$  are the main for the classification of the major system features.

## **1.4** System Classification

The atomic fractions  $n_0$ ,  $n_{sup}$ , and  $n_{sol}$  characterize the basic properties of systems formed by Bose atoms in optical lattices. Thus, the existence of BEC means the presence of coherence, because of which such a system can be termed coherent,

$$n_0 > 0$$
 (coherent)

Vice versa, the absence of BEC permits to call the system incoherent

$$n_0 = 0$$
 (incoherent).

In the same way, the system is superfluid, when there is the superfluid fraction,

$$n_{sup} > 0$$
 (superfluid).

The absence of the superfluid fraction implies that the system is not superfluid, that is, normal,

$$n_{sup} = 0$$
 (normal).

The presence of the solid fraction gives to the system rigidity typical of solids,

$$n_{sol} > 0$$
 (solid).

While, if there is no solid fraction, the system is either liquid or gaseous, generally speaking, fluid,

$$n_{sol} = 0$$
 (fluid).

This terminology allows us to suggest the following classification of admissible systems, depending on the presence or absence of the related atomic fractions.

(1) Incoherent normal fluid:

$$n_0 = 0$$
,  $n_{sup} = 0$ ,  $n_{sol} = 0$ .

Ubiquitous examples are classical liquids and gases.

(2) Coherent normal fluid:

$$n_0 > 0$$
,  $n_{sup} = 0$ ,  $n_{sol} = 0$ .

This case looks a bit exotic, though the situation, when there is BEC but there is no superfluidity can be attributed to what one calls Bose glass, the state that may develop in the presence of disorder.

(3) Incoherent superfluid:

$$n_0 = 0$$
,  $n_{sup} > 0$ ,  $n_{sol} = 0$ .

The known examples are two-dimensional superfluid films without BEC.

(4) Coherent superfluid:

$$n_0 > 0 , \qquad n_{sup} > 0 , \qquad n_{sol} = 0 .$$

This is superfluid  ${}^{4}$ He.

(5) Incoherent normal solid:

$$n_0 = 0$$
,  $n_{sup} = 0$ ,  $n_{sol} > 0$ .

The majority of solids are exactly of this type.

(6) Coherent normal solid:

$$n_0 > 0$$
,  $n_{sup} = 0$ ,  $n_{sol} > 0$ .

This type of solids can also be attributed to the so-called Bose glass.

(7) Incoherent superfluid solid:

$$n_0 = 0$$
,  $n_{sup} > 0$ ,  $n_{sol} > 0$ .

The possibility of such solids is currently under discussion.

(8) Coherent superfluid solid:

$$n_0 > 0$$
,  $n_{sup} > 0$ ,  $n_{sol} > 0$ .

This state looks admissible in optical lattices.

Thus, there can exist 8 classes of systems, depending on the presence or absence of the fractions  $n_0$ ,  $n_{sup}$ , and  $n_{sol}$ . These different states can be achieved by appropriately adjusting the system parameters.

#### 1.5 Cold Molecules

Bose-Einstein condensate can, in principle, be created in different Bose systems. As is mentioned in subsection 1.1, at the present time, BEC has been achieved in 12 atomic species. The latest of them was <sup>170</sup>Yb [25]. In addition, there exist Bose molecules formed of either Bose or Fermi atoms [10,15,24,26,27]. In systems, composed of Bose molecules, BEC can also arise. Thus, BEC was produced in molecular systems, where the molecules were formed by Bose atoms (<sup>23</sup>Na<sub>2</sub>, <sup>85</sup>Rb<sub>2</sub>, <sup>87</sup>Rb<sub>2</sub>, <sup>133</sup>Cs<sub>2</sub>) as well as by Fermi atoms (<sup>6</sup>Li<sub>2</sub>, <sup>40</sup>K<sub>2</sub>). Among other systems, that could exhibit BEC, it is possible to mention boson quark clusters and hadronic molecules [28,29]. Pion condensation in nuclear matter could be one more example [30–34], though in this case the condensate itself possesses a periodic structure.

The theory, presented in the following sections, is applicable to Bose systems of arbitrary nature, whether the constituents are atoms or molecules, or some kind of bosonic clusters. The sole thing is that these constituents are treated as Bose particles, characterized by their masses and interactions. Also, the main attention is paid to particles without internal degrees of freedom. For instance, spins are assumed to be frozen, so that particles can be treated as spinless. The consideration of particles with spin degrees of freedom requires a separate paper.

Theoretical methods are general for describing any type of bosons, whether the latter are atoms or molecules. However, it is important to keep in mind that the possibility of creating molecules provides the way of enriching the system properties. Molecules can also be loaded in optical lattices [35–39].

# 2 Systems with Bose-Einstein Condensate

## 2.1 Bose-Einstein Condensation

Lattices can be periodic, quasiperiodic or even random, representing different external potentials making the system nonuniform. It is worth starting the consideration by formulating the general criteria characterizing the occurrence of BEC in nonuniform systems.

Generally, BEC is the occupation of a single, or several, quantum states by a large number of identical particles. For simplicity, we shall be talking about a single quantum state. The generalization to several macroscopically occupied quantum states is straightforward and will be done in Sec. 2.15.

Historically, BEC was described by Einstein for ideal uniform Bose gas. The history and related historical references can be found in Ref. [40]. The quantum states of a uniform gas are characterized by the momentum **k**. Here and in what follows, we use the system of units, where the Planck constant and the Boltzmann constant are set to one,  $\hbar \equiv 1$ ,  $k_B \equiv 1$ .

In the general case of nonuniform systems, quantum states are labelled by a multi-index k, whose concrete representation depends on the considered problem. There exists the state occupation number  $n_k$  showing the number of particles in a quantum state k. Suppose that among all quantum states there occurs a single state  $k_0$ , for which the occupation number

$$N_0 \equiv n_{k_0} \tag{2.1}$$

is large. Here "large" means not merely that  $N_0$  is much larger than one, but that it is comparable to the total number of particles N, such that  $N_0 \propto N$ . Then we can say that there occurs BEC into the state  $k_0$ .

One says that the condensate state is macroscopically occupied. To make this phrase mathematically accurate, one resorts to the notion of the *thermodynamic limit* 

$$N \to \infty$$
,  $V \to \infty$ ,  $\frac{N}{V} \to const > 0$ , (2.2)

where N is the total number of particles in the system of volume V. The state  $k_0$  is termed macroscopically occupied, when

$$\lim_{N \to \infty} \frac{N_0}{V} > 0 , \qquad (2.3)$$

where the thermodynamic limit (2.2) is implied. Condition (2.3) is, actually, the *Einstein* criterion of BEC.

For trapped atoms, the system volume V may be not well defined. Then the thermodynamic limit can be specified in a different way [41]. If the system contains N trapped atoms, for which extensive observable quantities are defined, then the following limit can be considered. Let  $A_N$  be an extensive observable quantity, then the *effective thermodynamic limit* is

$$N \to \infty$$
,  $\frac{A_N}{N} \to const$ . (2.4)

For instance, taking for the observable quantity the internal energy  $E_N$  of N particles, we have [41] limit (2.4) as

$$N \to \infty$$
,  $\frac{E_N}{N} \to const$ . (2.5)

In what follows, writing  $N \to \infty$ , we shall assume one of the forms of thermodynamic limit.

Confined systems contain finite numbers of atoms N, though the latter is large. All finite systems with  $N \gg 1$  can be treated by the standard methods of statistical mechanics. For finite systems, thermodynamic limits (2.2) or (2.4) and (2.5) are interpreted as *thermodynamic tests*, not merely allowing for the simplification of calculations, but, which is the most important, making it possible to check the correctness of theories.

#### 2.2 Penrose-Onsager Scheme

The Einstein criterion of BEC (2.3) is easily applicable to uniform ideal gases. But for interacting systems, especially for nonuniform cases, to make criterion (2.3) useful requires, first, to specify how the quantum state occupation numbers  $n_k$  could be found. Penrose and Onsager [42] suggested the following scheme.

Assume that the single-particle density matrix  $\rho(\mathbf{r}, \mathbf{r}')$  of the considered system is known. This matrix is a function of the real-space variables  $\mathbf{r}$  and, generally, of time t. The latter does not enter  $\rho(\mathbf{r}, \mathbf{r}')$  for equilibrium systems, but for nonequilibrium systems,  $\rho(\mathbf{r}, \mathbf{r}', t)$  depends on time. In what follows, we shall omit, for the sake of brevity, the time dependence, where this is not important. However, we may keep in mind that the time variable can always be included, when the consideration concerns nonequilibrium cases.

If the density matrix  $\rho(\mathbf{r}, \mathbf{r}')$  is known, then one could solve the eigenvalue problem

$$\int \rho(\mathbf{r}, \mathbf{r}') \varphi_k(\mathbf{r}') \, d\mathbf{r}' = n_k \varphi_k(\mathbf{r}) \,, \qquad (2.6)$$

where the integration is over the whole volume specifying the system. The eigenfunctions  $\varphi_k(\mathbf{r})$  are called the *natural orbitals* [43]. The family  $\{\varphi_k(\mathbf{r})\}$  forms a complete orthonormal basis, for which

$$\int \varphi_k^*(\mathbf{r}) \varphi_p(\mathbf{r}) \ d\mathbf{r} = \delta_{kp}$$

Since the single-particle density matrix is normalized to the total number of particles

$$N = \int \rho(\mathbf{r}, \mathbf{r}) \, d\mathbf{r} \, .$$

the eigenvalues

$$n_k = \int \varphi_k^*(\mathbf{r}) 
ho(\mathbf{r}, \mathbf{r}') \varphi_k(\mathbf{r}') \ d\mathbf{r} d\mathbf{r}'$$

have the meaning of the occupation numbers of quantum states labelled by a multi-index k. In terms of the *natural orbitals*, the density matrix enjoys the *diagonal expansion* 

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_{k} n_k \varphi_k(\mathbf{r}) \varphi_k^*(\mathbf{r}') . \qquad (2.7)$$

Suppose that the maximal of the eigenvalues  $n_k$  corresponds to a quantum state  $k_0$ , for which we may write

$$N_0 \equiv \sup_k n_k = n_{k_0} . \tag{2.8}$$

Separating the state  $k_0$  from sum (2.7) gives

$$\rho(\mathbf{r}, \mathbf{r}') = N_0 \varphi_0(\mathbf{r}) \varphi_0^*(\mathbf{r}') + \sum_{k \neq k_0} n_k \varphi_k(\mathbf{r}) \varphi_k^*(\mathbf{r}') , \qquad (2.9)$$

where  $\varphi_0(\mathbf{r}) \equiv \varphi_{k_0}(\mathbf{r})$ . Then the total number of particles can be written as the sum

$$N = N_0 + N_1$$
,  $N_1 \equiv \sum_{k \neq k_0} n_k$  (2.10)

of the number of particles  $N_0$  in the state  $k_0$  and the number of all other particles  $N_1$ .

One says that there happens BEC into the state  $k_0$ , if the latter is macroscopically occupied, such that the largest eigenvalue (2.8) satisfies condition (2.3) in the sense of one of the thermodynamic limits (2.2) or (2.4). Thus, we return to the Einstein criterion (2.3). The novelty in the Penrose-Onsager scheme is the interpretation of the number of condensed particles (2.1) as the largest eigenvalue (2.8) of the single-particle density matrix.

The Penrose-Onsager interpretation of the Einstein criterion for BEC is very general, being applicable to arbitrary statistical systems, including confined systems of trapped atoms. This is contrary to the concept of the off-diagonal long-range order [44], introducing the number of condensed particles  $N_0$  through the limiting relation

$$\frac{N_0}{V} = \lim_{|\mathbf{r}-\mathbf{r}'|\to\infty} \rho(\mathbf{r},\mathbf{r}') \; .$$

This concept has a meaning solely for uniform infinite systems, while for trapped atoms it is not applicable [9], always strictly giving  $N_0 = 0$ .

## 2.3 Order Indices

The Penrose-Onsager scheme can be generalized by introducing the notion of order indices. The latter can be formulated for arbitrary operators [45]. Let  $\hat{A}$  be an operator possessing a norm  $||\hat{A}||$  and a trace Tr $\hat{A}$ . Then the *operator order index* of  $\hat{A}$  is defined [45] as

$$\omega(\hat{A}) \equiv \frac{\log ||A||}{\log |\mathrm{Tr}\hat{A}|} \,.$$

Here the logarithm can be taken to any convenient base, for instance, it can be the natural logarithm ln.

The reduced density matrices can be treated as matrices with respect to their real-space variables [43]. Thus, the single-particle density matrix defines the first-order density matrix  $\hat{\rho}_1 \equiv [\rho(\mathbf{r}, \mathbf{r}')]$ . Then the order index of  $\hat{\rho}_1$  is

$$\omega(\hat{\rho}_1) = \frac{\log ||\hat{\rho}_1||}{\log \operatorname{Tr} \hat{\rho}_1} \,. \tag{2.11}$$

Similarly, one can introduce the order indices of higher-order density matrices [46–49]. For the order index (2.11), since

$$||\hat{\rho}_1|| = N_0$$
,  $\operatorname{Tr}\hat{\rho}_1 = N$ ,

we obtain

$$\omega(\hat{\rho}_1) = \frac{\log N_0}{\log N} \,. \tag{2.12}$$

This index is not larger than one,  $\omega(\hat{\rho}_1) \leq 1$ , because  $N_0 \leq N$ .

The order indices are convenient for classifying different types of order that can arise in the system. For Bose systems, there can be three possibilities for the order indices (2.11) or (2.12). When

$$\omega(\hat{\rho}_1) \le 0 \qquad (no \ order) , \qquad (2.13)$$

there is no ordering in the system, or at the most, a kind of short-range order may appear. In the interval

$$0 < \omega(\hat{\rho}_1) < 1 \qquad (mid - range), \qquad (2.14)$$

the order index demonstrates the amount of mid-range order. There is no true BEC in this case, but there exists some ordering that can be associated with *quasicondensate*. The true BEC corresponds to the index

$$\omega(\hat{\rho}_1) = 1 \qquad (long - range) , \qquad (2.15)$$

which happens in thermodynamic limit  $N \to \infty$ . In the finite uniform systems, as well as in low-dimensional uniform systems, such as one- and two-dimensional systems, there can be no true BEC, but there can arise quasicondensate. In confined systems, BEC can happen in low-dimensional systems, depending on the type of the trapping potential [41]. The BEC criterion (2.3) is equivalent to condition (2.15) occurring in thermodynamic limit,

$$\omega(\hat{\rho}_1) \to 1 \qquad (N \to \infty) .$$

The notion of order indices is applicable to arbitrary statistical systems, whether finite or infinite, uniform or nonuniform, equilibrium or nonequilibrium. The order indices retain their meaning, when the order parameters cannot be defined [45–49].

#### 2.4 Representative Ensembles

The BEC criteria of the previous sections signals the appearance of BEC. But these criteria assume the knowledge of the density matrix supposed to be found beforehand. Such criteria do not prescribe the way of solving the problem.

The very first step in considering any statistical system is the choice of a statistical ensemble to be used. The *statistical ensemble* is a triplet  $\{\mathcal{F}, \hat{\rho}, \partial t\}$ , in which  $\mathcal{F}$  is the space of microstates,  $\hat{\rho} = \hat{\rho}(0)$  is the initial form of the statistical operator, and  $\partial t$  signifies the evolution law for the considered system. With the given  $\mathcal{F}$  and  $\hat{\rho}$ , one can find the statistical average

$$\langle \hat{A}(t) \rangle \equiv \operatorname{Tr}_{\mathcal{F}} \hat{\rho} \, \hat{A}(t)$$
 (2.16)

for an operator A(t). The prescribed evolution law makes it possible to define the temporal evolution of average (2.16),

$$\frac{\partial}{\partial t} < \hat{A}(t) > = \operatorname{Tr}_{\mathcal{F}} \hat{\rho} \, \frac{\partial \hat{A}(t)}{\partial t} \,. \tag{2.17}$$

The set of all operators  $\hat{A}(t)$ , corresponding to observable quantities, forms the algebra of observables  $\mathcal{O} \equiv \{\hat{A}(t)\}$ . The collection of the statistical averages (2.16) for all operators from the algebra of observables  $\mathcal{O}$  is termed the *statistical state*  $\langle \mathcal{O} \rangle$ .

When defining a statistical ensemble, it is necessary that it would correctly represent the studied statistical system. This means that all conditions and constraints, uniquely defining the system, must be taken into account when constructing the statistical operator  $\hat{\rho}$  and formulating the evolution law. Such an ensemble is called representative.

In the case of equilibrium systems, one usually tells that a statistical ensemble is defined by a Gibbs statistical operator, either canonical or grand canonical. One often calls this the "Gibbs prescription". In many situations, this is sufficient. However in general such a point of view is a strong trivialization of the Gibbs ideas. Gibbs did write [50] that just prescribing a distribution, whether canonical or grand canonical, may be not sufficient, but the description must be complimented by all those constraints and conditions that make the statistical systems uniquely defined. Thus, the idea of representative statistical ensembles is actually due to Gibbs [50]. The term "representative ensembles" was employed by ter Haar [51,52], who discussed the necessity of correctly representing statistical systems. Such ensembles, equipped with additional conditions, are also called conditional [53]. The general theory of equilibrium and quasiequilibrium representative ensembles was described in the review article [54] and book [55]. Representative ensembles for Bose systems with broken gauge symmetry were covered in detail in Refs. [56,57].

To specify the state of microstates, it is necessary to fix the system variables. Suppose we choose as the variables the field operators  $\psi(\mathbf{r})$  and  $\psi^{\dagger}(\mathbf{r})$ , with the Bose commutation relations

$$\left[\psi(\mathbf{r}), \ \psi^{\dagger}(\mathbf{r}')\right] = \delta(\mathbf{r} - \mathbf{r}') ,$$

other relations being zero. The creation operator  $\psi^{\dagger}(\mathbf{r})$  generates the Fock space  $\mathcal{F}(\psi)$ , which is the space of microstates [55]. Then the statistical state is given by the averages (2.16), with the trace over  $\mathcal{F}(\psi)$ .

In order to define the statistical operator  $\hat{\rho}$ , we need to specify the conditions making the statistical ensemble representative. One evident condition is the normalization of the statistical operator,

$$<\hat{1}_{\mathcal{F}}> = 1$$
, (2.18)

where  $\hat{1}_{\mathcal{F}}$  is the unity operator in  $\mathcal{F}(\psi)$ . The Hamiltonian energy operator  $\hat{H}[\psi]$ , which is a functional of  $\psi$  and  $\psi^{\dagger}$ , defines the internal energy

$$\langle \hat{H}[\psi] \rangle = E , \qquad (2.19)$$

which is another statistical condition. The total number of particles N is given by the average

$$\langle \tilde{N}[\psi] \rangle = N , \qquad (2.20)$$

of the number-of-particle operator

$$\hat{N}[\psi] \equiv \int \psi^{\dagger}(\mathbf{r})\psi(\mathbf{r}) \, d\mathbf{r} \,. \tag{2.21}$$

Similarly, there can exist other condition operators  $\hat{C}_i[\psi]$ , with i = 1, 2, ..., whose averages define additional *statistical conditions* 

$$\langle \hat{C}_i[\psi] \rangle = C_i . \tag{2.22}$$

The statistical operator  $\hat{\rho}$  of an equilibrium system is defined as the minimizer of the information functional [55]

$$I[\hat{\rho}] = \operatorname{Tr}\hat{\rho} \,\ln\hat{\rho} + \lambda_0 \left(\operatorname{Tr}\hat{\rho} - 1\right) + \beta \left(\operatorname{Tr}\hat{\rho}\hat{H}[\psi] - E\right) - \beta \mu \left(\operatorname{Tr}\hat{\rho}\hat{N}[\psi] - N\right) + \beta \sum_i \nu_i \left(\operatorname{Tr}\hat{\rho}\hat{C}_i[\psi] - C_i\right) , \qquad (2.23)$$

in which  $\lambda_0$ ,  $\beta$ ,  $\beta\mu$ , and  $\beta\nu_i$  are the appropriate Lagrange multipliers. Minimizing (2.23) gives

$$\hat{\rho} = \frac{\exp(-\beta H[\psi])}{\operatorname{Tr}_{\mathcal{F}(\psi)} \exp(-\beta H[\psi])}, \qquad (2.24)$$

where the trace is over  $\mathcal{F}(\psi)$  and

$$H[\psi] \equiv \hat{H}[\psi] - \mu \hat{N}[\psi] + \sum_{i} \nu_i \hat{C}_i[\psi]$$
(2.25)

is the grand Hamiltonian. The Lagrange multiplier  $\beta = 1/T$  is the inverse temperature and  $\mu$  is called the chemical potential.

After this, one can explicitly define what actually is the single-particle density matrix, which till now has appeared as an abstract notion. This density matrix is

$$\rho(\mathbf{r}, \mathbf{r}') \equiv \langle \psi^{\dagger}(\mathbf{r}')\psi(\mathbf{r}) \rangle . \qquad (2.26)$$

The evolution equations for the field variables  $\psi(\mathbf{r})$  are obtained as follows [57]. By introducing the temporal energy operator

$$\hat{E}[\psi] \equiv \int \psi^{\dagger}(\mathbf{r}, t) i \, \frac{\partial}{\partial t} \, \psi(\mathbf{r}, t) \, d\mathbf{r} \,, \qquad (2.27)$$

we define the action functional

$$\Gamma[\psi] \equiv \int \left( \hat{E}[\psi] - H[\psi] \right) dt . \qquad (2.28)$$

The evolution equations for  $\psi(\mathbf{r}, t)$  and  $\psi^{\dagger}(\mathbf{r}, t)$  are given by the extremization of the action functional,

$$\frac{\delta\Gamma[\psi]}{\delta\psi^{\dagger}(\mathbf{r},t)} = 0 , \qquad (2.29)$$

and by the Hermitian conjugation of the latter variational equation. In view of the action functional (2.28), Eq. (2.29) yields

$$i \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \frac{\delta H[\psi]}{\delta \psi^{\dagger}(\mathbf{r}, t)} .$$
(2.30)

This equation is equivalent [55] to the Heisenberg equation

$$i \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = [\psi(\mathbf{r}, t), H[\psi]]$$

The initial condition for the evolution equation is  $\psi(\mathbf{r}, 0) = \psi(\mathbf{r})$ . The evolution is governed by the same grand Hamiltonian (2.25) as that characterizing the statistical operator (2.24).

In the case of a nonequilibrium statistical system, additional conditions (2.22) should include the information on the initial values  $\langle \hat{A}(0) \rangle$  for the considered operators  $\hat{A}(t)$ .

The procedure, described above, determines the standard way of characterizing a representative statistical ensemble. Here, it is the triplet of the Fock space of microstates  $\mathcal{F}(\psi)$ , the statistical operator (2.24), and of the evolution equations (2.29) or (2.30). For an equilibrium system, the grand Hamiltonian (2.25) may not need the last term with conditional operators.

## 2.5 Field Operators

After a statistical ensemble has been constructed, we may pose the question whether BEC occurs in the system. Then we remember that BEC implies the macroscopic occupation of a single quantum state. Quantum states, labelled by a multi-index k, are associated with an orthonormal basis  $\{\varphi_k(\mathbf{r})\}$ . Expanding the field operator over this basis, we have

$$\psi(\mathbf{r}) = \sum_{k} a_k \varphi_k(\mathbf{r}) , \qquad (2.31)$$

where the operators  $a_k$  obey the commutation relations

$$\begin{bmatrix} a_k, a_p^{\dagger} \end{bmatrix} = \delta_{kp} , \qquad \begin{bmatrix} a_k, a_p \end{bmatrix} = 0 .$$

With expansion (2.31), the density matrix (2.26) takes the form

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_{kp} \langle a_k^{\dagger} a_p \rangle \varphi_p(\mathbf{r}) \varphi_k^*(\mathbf{r}') . \qquad (2.32)$$

For a while, there is arbitrariness in choosing a basis in expansion (2.31). However, BEC is a physical phenomenon and can occur not for an arbitrary chosen quantum state, but for a state naturally related to the considered physical system. This means that the expansion basis  $\{\varphi_k(\mathbf{r})\}$  is not arbitrary, but is to be formed by natural orbitals. In terms of the natural orbitals, the density matrix (2.32) has to enjoy the diagonal expansion [43], which implies the quantum-number conservation condition

$$\langle a_k^{\dagger} a_p \rangle = \delta_{kp} n_k , \qquad (2.33)$$

where

$$n_k \equiv \langle a_k^{\dagger} a_k \rangle \tag{2.34}$$

is the occupation number.

If BEC is associated with a quantum state  $k_0$ , then the field operator (2.31) can be separated into two parts,

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \psi_1(\mathbf{r}) , \qquad (2.35)$$

in which the first term is the operator of condensed particles,

$$\psi_0(\mathbf{r}) \equiv a_0 \varphi_0(\mathbf{r}) , \qquad (2.36)$$

where  $a_0 \equiv a_{k_0}$ , and the second term is the operator of uncondensed particles,

$$\psi_1(\mathbf{r}) \equiv \sum_{k \neq k_0} a_k \varphi_k(\mathbf{r}) . \qquad (2.37)$$

From the quantum-number conservation condition (2.33) it follows that

$$<\psi_0^{\dagger}(\mathbf{r})\psi_1(\mathbf{r}')>=0$$
, (2.38)

since

$$\langle a_0^{\dagger} a_k \rangle = 0 \qquad (k \neq k_0) .$$
 (2.39)

And, because of the orthonormality of the basis  $\{\varphi_k(\mathbf{r})\}\$ , we have the orthogonality condition

$$\int \psi_0^{\dagger}(\mathbf{r})\psi_1(\mathbf{r}) \, d\mathbf{r} = 0 \; . \tag{2.40}$$

The density matrix (2.26) takes the form

$$\rho(\mathbf{r}, \mathbf{r}') = \langle \psi_0^{\dagger}(\mathbf{r}')\psi_0(\mathbf{r}) \rangle + \langle \psi_1^{\dagger}(\mathbf{r}')\psi_1(\mathbf{r}) \rangle .$$
(2.41)

The number-of-particle operators are: for condensed particles,

$$\hat{N}_0[\psi] \equiv \int \psi_0^{\dagger}(\mathbf{r}) \psi_0(\mathbf{r}) \, d\mathbf{r} = a_0^{\dagger} a_0 \,, \qquad (2.42)$$

and for uncondensed particles

$$\hat{N}_1[\psi] \equiv \int \psi_1^{\dagger}(\mathbf{r}) \psi_1(\mathbf{r}) \, d\mathbf{r} = \sum_{k \neq k_0} a_k^{\dagger} a_k \, . \tag{2.43}$$

In view of the orthogonality condition (2.40), the number-of-particle operator for the total number of particles is

$$\hat{N}[\psi] = \hat{N}_0[\psi] + \hat{N}_1[\psi] .$$
(2.44)

The average number of particles in BEC is

$$N_0 = \langle \hat{N}_0[\psi] \rangle = \langle a_0^{\dagger} a_0 \rangle .$$
 (2.45)

And the number of uncondensed particles is

$$N_1 = \langle \hat{N}_1[\psi] \rangle = \sum_{k \neq k_0} n_k .$$
(2.46)

The above equations are valid for any system, whether uniform or not uniform, and for BEC of arbitrary nature, related to a quantum state  $k_0$ .

It is important to stress that operators (2.36) and (2.37) are not separate independent operators, describing different particles, but  $\psi_0(\mathbf{r})$  and  $\psi_1(\mathbf{r})$  are simply two parts of one Bose field operator (2.35). This is evident from the commutation relations for  $\psi_0(\mathbf{r})$ ,

$$\left[\psi_0(\mathbf{r}), \ \psi_0^{\dagger}(\mathbf{r}')\right] = \varphi_0(\mathbf{r})\varphi_0^*(\mathbf{r}') , \qquad (2.47)$$

and for  $\psi_1(\mathbf{r})$ ,

$$\left[\psi_1(\mathbf{r}), \ \psi_1^{\dagger}(\mathbf{r}')\right] = \sum_{k \neq k_0} \varphi_k(\mathbf{r}) \varphi_k^*(\mathbf{r}') , \qquad (2.48)$$

which show that neither  $\psi_0(\mathbf{r})$  nor  $\psi_1(\mathbf{r})$  characterize Bose particles. There exists the sole field operator (2.35) enjoying the Bose commutation relations. This operator is defined on the Fock space  $\mathcal{F}(\psi)$  generated by  $\psi^{\dagger}$ .

Using notation (2.42), the BEC criterion (2.3) can be written as

$$\lim_{N \to \infty} \frac{\langle \hat{N}_0[\psi] \rangle}{N} > 0 , \qquad (2.49)$$

or, equivalently, as

$$\lim_{N \to \infty} \frac{\langle a_0^{\dagger} a_0 \rangle}{N} > 0 .$$
 (2.50)

Calculating the averages, one employs the statistical ensemble with the grand Hamiltonian (2.25) containing the chemical potential  $\mu$ , which is the Lagrange multiplier guaranteeing the normalization condition (2.20). There is here the sole normalization condition, since there exists only one field operator  $\psi(\mathbf{r})$  describing Bose particles.

## 2.6 Gauge Symmetry

Phase transitions from a disordered phase to an ordered phase are usually accompanied by some symmetry breaking [58]. BEC is associated with the global U(1) gauge symmetry breaking. The fundamental question is whether the gauge symmetry breaking is necessary and sufficient for the occurrence of BEC. In literature, one can meet controversial statements, some claiming that BEC does not require any symmetry breaking. This, however, is not correct. The *qauge symmetry breaking is necessary and sufficient for the occurrence of BEC*.

The equivalence of BEC and gauge symmetry breaking has been discussed in recent papers [59–62] and thoroughly explained in the review article [63]. Considering these phenomena, one should always keep in mind that, in finite systems, there are neither rigorously defined phase transitions nor symmetry breaking. Both of them can happen only in thermodynamic limit. So, the existence or absence of these phenomena acquires a correct mathematical meaning only under the thermodynamic limiting test, either in form (2.2) or in forms (2.4) and (2.5). However, one often talks about BEC or symmetry breaking even in the case of a finite, but large, statistical system, with  $N \gg 1$ , keeping in mind that the properties of the system are asymptotically close to those the system would possess in the thermodynamic limit. The U(1) gauge transformation can be represented as the transformation

$$\psi(\mathbf{r}) \longrightarrow \psi(\mathbf{r})e^{i\alpha}$$
(2.51)

for the field operator, with  $\alpha$  being a real number. The Hamiltonian  $H[\psi]$  is assumed to be invariant under the gauge transformation (2.51). The gauge symmetry of the system can be broken by the Bogolubov method of infinitesimal sources [64,65], by defining

$$H_{\varepsilon}[\psi] \equiv H[\varphi] + \varepsilon \sqrt{\rho} \int \left[\psi_0^{\dagger}(\mathbf{r}) + \psi_0(\mathbf{r})\right] d\mathbf{r} , \qquad (2.52)$$

where  $\varepsilon$  is a real parameter and  $\rho$  is the mean particle density. The related statistical operator is

$$\hat{\rho}_{\varepsilon} \equiv \frac{\exp(-\beta H_{\varepsilon}[\psi])}{\operatorname{Tr}\exp(-\beta H_{\varepsilon}[\psi])}, \qquad (2.53)$$

with the trace over  $\mathcal{F}(\psi)$ . The operator averages are defined as

$$\langle \hat{A} \rangle_{\varepsilon} \equiv \operatorname{Tr} \hat{\rho}_{\varepsilon} \hat{A}$$
. (2.54)

According to the Bogolubov method of quasiaverages [64,65], one should, first, take the thermodynamic limit, after which the limit  $\varepsilon \to 0$  is to be taken. There also exist some other methods of symmetry breaking [54,66]. In particular, it would be admissible to make the parameter  $\varepsilon$  a function  $\varepsilon_N$  depending on N, such that it would appropriately tend to zero together with the thermodynamic limit [54,67,68]. But for the sake of clarity, we shall use here the standard Bogolubov method [64,65] of quasiaverages.

One can say that there happens the local spontaneous gauge-symmetry breaking, when

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \langle \psi_0(\mathbf{r}) \rangle_{\varepsilon} \neq 0 , \qquad (2.55)$$

at least for some **r**. And the global spontaneous gauge-symmetry breaking implies that

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{1}{N} \int |\langle \psi_0(\mathbf{r}) \rangle_{\varepsilon}|^2 d\mathbf{r} > 0.$$
(2.56)

Because of definition (2.36), one has

$$\int \left| \langle \psi_0(\mathbf{r}) \rangle_{\varepsilon} \right|^2 d\mathbf{r} = \left| \langle a_0 \rangle_{\varepsilon} \right|^2.$$
(2.57)

Hence, inequality (2.56) of spontaneous gauge-symmetry breaking becomes

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{|\langle a_0 \rangle_{\varepsilon}|^2}{N} > 0.$$
(2.58)

By the Cauchy-Schwarz inequality,

$$|\langle a_0 \rangle_{\varepsilon} | \leq \sqrt{\langle a_0^{\dagger} a_0 \rangle_{\varepsilon}}$$

for any  $\varepsilon$  and N. Therefore

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{|\langle a_0 \rangle_{\varepsilon}|^2}{N} \leq \lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{\langle a_0^{\dagger} a_0 \rangle_{\varepsilon}}{N} .$$
(2.59)

This tells us, that the spontaneous gauge symmetry breaking (2.58) results in BEC, in agreement with condition (2.50).

Moreover, inequality (2.59) can be made the equality. Recall that Hamiltonian (2.52) is a functional

$$H_{\varepsilon}[\psi] \equiv H_{\varepsilon}[\psi_0, \psi_1]$$

of  $\psi_0(\mathbf{r})$  and  $\psi_1(\mathbf{r})$ . And let us introduce the statistical operator

$$\hat{\rho}_{\eta\varepsilon} \equiv \frac{\exp(-\beta H_{\varepsilon}[\eta, \psi_1])}{\operatorname{Tr} \exp(-\beta H_{\varepsilon}[\eta, \psi_1])} , \qquad (2.60)$$

in which the operator  $\psi_0(\mathbf{r})$  is replaced by a function  $\eta(\mathbf{r})$ . The related average of an operator  $\hat{A}$  is

$$\langle \hat{A} \rangle_{\eta\varepsilon} \equiv \operatorname{Tr} \hat{\rho}_{\eta\varepsilon} \hat{A}$$
. (2.61)

Let us also define a class of correlation functions given by the form

$$C_{\varepsilon}(\psi_0,\psi_1) \equiv <\dots \psi_0^{\dagger}\dots \psi_1^{\dagger}\dots \psi_0\dots \psi_1 >_{\varepsilon} .$$
(2.62)

Replacing here all operators  $\psi_0^{\dagger}$  and  $\psi_0(\mathbf{r})$  by functions  $\eta^*(\mathbf{r})$  and  $\eta(\mathbf{r})$ , we get the class of correlation functions

$$C_{\varepsilon}(\eta,\psi_1) \equiv <\dots \eta^* \dots \psi_1^{\dagger} \dots \eta \dots \psi_1 >_{\varepsilon} .$$
(2.63)

It is assumed that the function  $\eta(\mathbf{r})$  is normalized to the same number of condensed particles, as  $\psi_0(\mathbf{r})$ , such that

$$\int \langle \psi_0^{\dagger}(\mathbf{r})\psi_0(\mathbf{r})\rangle_{\varepsilon} d\mathbf{r} = \int |\eta(\mathbf{r})|^2 d\mathbf{r} = N_0 .$$
(2.64)

Then the following statement holds [65].

**Bogolubov theorem**. In thermodynamic limit, the correlation functions (2.62) and (2.63), under normalization condition (2.64), coincide with each other,

$$\lim_{N \to \infty} C_{\varepsilon}(\psi_0, \psi_1) = \lim_{N \to \infty} C_{\varepsilon}(\eta, \psi_1) , \qquad (2.65)$$

for any real  $\varepsilon$ . In particular,

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} C_{\varepsilon}(\psi_0, \psi_1) = \lim_{\varepsilon \to 0} \lim_{N \to \infty} C_{\varepsilon}(\eta, \psi_1) .$$
(2.66)

From the Bogolubov theorem it follows that

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \langle \psi_0(\mathbf{r}) \rangle_{\varepsilon} = \eta(\mathbf{r}) .$$
(2.67)

Also, we have

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \langle \psi_0^{\dagger}(\mathbf{r})\psi_1(\mathbf{r}') \rangle_{\varepsilon} = \eta^*(\mathbf{r}) \lim_{\varepsilon \to 0} \lim_{N \to \infty} \langle \psi_1(\mathbf{r}') \rangle_{\eta\varepsilon} .$$
(2.68)

If  $\eta(\mathbf{r})$  is not identically zero, then the quantum-number conservation condition (2.38) acquires the form

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \langle \psi_1(\mathbf{r}) \rangle_{\eta \varepsilon} = 0.$$
(2.69)

Hence, for the field operator (2.35) one gets

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \langle \psi(\mathbf{r}) \rangle_{\varepsilon} = \eta(\mathbf{r}) .$$
(2.70)

The condition (2.56) of global spontaneous gauge-symmetry breaking becomes

$$\lim_{N \to \infty} \frac{1}{N} \int |\eta(\mathbf{r})|^2 d\mathbf{r} > 0.$$
(2.71)

This, according to normalization (2.64), means the existence of BEC.

To be more precise, we notice that

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{1}{N} \int |\langle \psi_0(\mathbf{r}) \rangle_{\varepsilon}|^2 d\mathbf{r} =$$
$$= \lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{|\langle a_0 \rangle_{\varepsilon}|^2}{N} = \lim_{N \to \infty} \frac{1}{N} \int |\eta(\mathbf{r})|^2 d\mathbf{r} .$$
(2.72)

At the same time, we find

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{\langle \hat{N}_0[\psi] \rangle_{\varepsilon}}{N} = \lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{\langle a_0^{\dagger} a_0 \rangle_{\varepsilon}}{N} = \lim_{N \to \infty} \frac{1}{N} \int |\eta(\mathbf{r})|^2 \, d\mathbf{r} \,. \tag{2.73}$$

Comparing the latter equations, we obtain

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{1}{N} \int |\langle \psi_0(\mathbf{r}) \rangle_{\varepsilon}|^2 d\mathbf{r} = \lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{\langle \hat{N}_0[\psi] \rangle_{\varepsilon}}{N}, \qquad (2.74)$$

or in another form,

$$\lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{|\langle a_0 \rangle_{\varepsilon}|^2}{N} = \lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{\langle a_0^{\dagger} a_0 \rangle_{\varepsilon}}{N}.$$
(2.75)

Equations (2.74) and (2.75) demonstrate that the spontaneous gauge symmetry breaking leads to the existence of BEC. This conclusion holds for any equilibrium system, whether uniform or nonuniform. In the case of uniform systems, Eq. (2.75) was derived in Refs. [59–62].

For uniform systems, there also exist the following theorem [60–62], first, proved by Ginibre [69]. One considers the thermodynamic potentials

$$\Omega_{\varepsilon} \equiv -T \ln \operatorname{Tr} \left( -\beta H_{\varepsilon}[\psi_0, \ \psi_1] \right) \tag{2.76}$$

and

$$\Omega_{\eta\varepsilon} \equiv -T \ln \operatorname{Tr} \left( -\beta H_{\varepsilon}[\eta, \psi_1] \right) , \qquad (2.77)$$

where  $\eta$  is the minimizer of Eq. (2.77), such that

$$\Omega_{\eta\varepsilon} = \inf_x \,\Omega_{x\varepsilon} \,. \tag{2.78}$$

Ginibre theorem. For the thermodynamic potentials (2.76) and (2.77), under condition (2.78), in the thermodynamic limit, one has

$$\lim_{N \to \infty} \frac{\Omega_{\varepsilon}}{N} = \lim_{N \to \infty} \frac{\Omega_{\eta \varepsilon}}{N}$$
(2.79)

for any real  $\varepsilon$ , including  $\varepsilon \to 0$ .

The Bogolubov and Ginibre theorems show that the spontaneous gauge symmetry breaking is a sufficient condition for the occurrence of BEC.

The fact that the symmetry breaking is also a necessary condition for BEC was, first, proved by Roepstorff [70] and recently this proof was generalized by Lieb et al. [60,62]. For this purpose, one compares the average  $\langle a_0^{\dagger}a_0 \rangle$  for a uniform system without symmetry breaking and the average  $\langle a_0 \rangle_{\varepsilon}$  in the presence of the gauge symmetry breaking.

Roepstorff theorem. In the thermodynamic limit,

$$\lim_{N \to \infty} \frac{\langle a_0^{\dagger} a_0 \rangle}{N} \leq \lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{|\langle a_0 \rangle_{\varepsilon}|^2}{N}.$$
(2.80)

This theorem shows that the occurrence of BEC necessarily leads to the gauge symmetry breaking. More details on the relation between BEC and gauge symmetry breaking can be found in the review article [63].

Thus, the conclusion is:

The spontaneous gauge-symmetry breaking is the necessary and sufficient condition for Bose-Einstein condensation.

## 2.7 Bogolubov Shift

Describing a system with BEC, one can follow the procedure of the previous sections, working with the field operator (2.35) defined on the Fock space  $\mathcal{F}(\psi)$ . This operator can formally be partitioned into two terms. However, neither of these terms represents particles, since the commutation relations (2.47) and (2.48) are not of Bose type. Dealing with the field operator (2.35), one should accomplish calculations in finite space, passing after this to the thermodynamic limit. Such an approach has three weak points.

First, in practical calculations, it requires the use of perturbation theory with respect to atomic interactions, as has been done by Belyaev [71]. Hence, it is limited to weakly interacting Bose gases.

Second, the mentioned perturbation theory is singular, being plagued by divergences. So that only the lowest orders of the perturbation theory are meaningful.

Third, the commutation relations (2.47) and (2.48) are cumbersome and not convenient in calculations.

But we know from the theorems of the previous section that in the thermodynamic limit the operator term  $\psi_0(\mathbf{r})$  reduces to a function  $\eta(\mathbf{r})$ . Therefore, it is tempting to replace, from the very beginning, the operator  $\psi(\mathbf{r})$  in Eq. (2.35) by another operator

$$\hat{\psi}(\mathbf{r}) \equiv \eta(\mathbf{r}) + \psi_1(\mathbf{r}) , \qquad (2.81)$$

in which the operator  $\psi_0(\mathbf{r})$  has been replaced by a function  $\eta(\mathbf{r})$ . The procedure of replacing  $\psi(\mathbf{r})$  by  $\hat{\psi}(\mathbf{r})$  is called the *Bogolubov shift* [64,65,72,73].

From the requirement that  $\psi(\mathbf{r})$  is a Bose operator, and because  $\eta(\mathbf{r})$  is a nonoperator function, it follows that  $\psi_1(\mathbf{r})$  is a Bose field operator, with the standard Bose commutation relations

$$\left[\psi_1(\mathbf{r}), \ \psi_1^{\dagger}(\mathbf{r}')\right] = \delta(\mathbf{r} - \mathbf{r}') \ . \tag{2.82}$$

It is evident that to deal with these usual nice commutation relations is much simpler than with the awkward relations (2.47) and (2.48).

In the shifted field operator (2.81), the term  $\eta(\mathbf{r})$  is named the *condensate wave function*, and the term  $\psi_1(\mathbf{r})$  is the operator of uncondensed particles. To be correctly defined, these terms are assumed to preserve the basic properties typical of  $\psi_0(\mathbf{r})$  and  $\psi_1(\mathbf{r})$ . Thus, the orthogonality condition (2.40) now reads as

$$\int \eta^*(\mathbf{r})\psi_1(\mathbf{r}) \, d\mathbf{r} = 0 \; . \tag{2.83}$$

And the quantum-number conservation condition (2.38), similarly to Eq. (2.69), now becomes

$$<\psi_1(\mathbf{r})>=0$$
. (2.84)

The number of condensed atoms (2.42) can be represented as

$$\hat{N}_0 = N_0 \hat{1}_{\mathcal{F}} ,$$
 (2.85)

where,  $\hat{1}_{\mathcal{F}}$  is the unity operator in the appropriate Fock space and  $N_0$ , in agreement with normalization (2.64), is

$$N_0 = \int |\eta(\mathbf{r})|^2 \, d\mathbf{r} \,. \tag{2.86}$$

By analogy with Eq. (2.45), we have

$$N_0 = \langle \dot{N}_0 \rangle . (2.87)$$

The number operator of noncondensed atoms (2.43) is

$$\hat{N}_1 = \int \psi_1^{\dagger}(\mathbf{r}) \psi_1(\mathbf{r}) \, d\mathbf{r} \; .$$

So that the number (2.46) of uncondensed atoms is

$$N_1 = \langle N_1 \rangle . (2.88)$$

Due to the orthogonality condition (2.83), the operator of the total number of particles is the sum

$$\hat{N} \equiv \int \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} = \hat{N}_0 + \hat{N}_1 \,. \tag{2.89}$$

Hence, the total number of particles is

$$N = \langle \hat{N} \rangle = N_0 + N_1$$

The convenience of the Bogolubov shift (2.81) is also in the fact that it explicitly breaks the gauge symmetry since

$$\langle \hat{\psi}(\mathbf{r}) \rangle = \eta(\mathbf{r}),$$
 (2.90)

which is necessary for correctly describing BEC. The latter equation makes it possible to call the condensate wave function  $\eta(\mathbf{r})$  the system order parameter.

The Bogolubov shift (2.81) is the basis for the majority of calculations for weakly nonideal Bose gases at low temperatures, when almost all particles are in BEC [64,65,72,73]. Perturbation theory for asymptotically weak interactions and low temperatures has been developed for uniform [74,75] as well as for nonuniform [76,77] gases.

However, as soon as one tries to describe not asymptotically weak interactions or higher temperatures, one encounters the Hohenberg-Martin dilemma [74]. Hohenberg and Martin [74] showed that the theory, based on the standard grand canonical ensemble, where the gauge symmetry is broken by means of the Bogolubov shift, is internally inconsistent. Depending on the way of calculations, one gets either an unphysical gap in the spectrum of collective excitations, or local conservation laws, together with general thermodynamic relations, become invalid. Recall that the excitation spectrum, according to the Hugenholtz-Pines theorem, must be gapless [65,78]. While conserving approximations [79] usually give a gap in the spectrum [80–82].

The standard attempts to cure the problem are based on what Bogolubov [65] named "the mismatch of approximations". One either arbitrarily adds some phenomenological terms or removes, without justification, other terms. The most popular trick is the omission of anomalous averages, as first, was suggested by Shohno [83] and analysed by Reatto and Straley [84]. In recent years, the Shohno trick [83] is often ascribed to Popov, although, as is easy to infer from the Popov works [85–88], cited in this regard, he has never suggested or used such an unjustified trick.

Of course, all phenomenological attempts, involving the mismatch of approximations, as has already been mentioned by Bogolubov [65], cannot cure the problem. Not self-consistent approaches render the system unstable, spoil thermodynamic relations, and disrupt the Bose-Einstein condensation phase transition from the second-order to the incorrect firstorder transition [89–92]. A detailed analysis of this problem has been done in Ref. [57].

## 2.8 Self-Consistent Approach

The origin of the Hohenberg-Martin dilemma is in the use of a nonrepresentative ensemble for a Bose-condensed system with the gauge symmetry broken by the Bogolubov shift (2.81). Using a representative ensemble [54,55] cures the problem [56,57] and makes it possible to develop a fully self-consistent theory, free of paradoxes [93–95]. This theory is conserving and gapless by construction, independently of the involved approximation [93–98]. To determine a representative ensemble, one should start with the specification of the space of microstates, which depends on the choice of the accepted variables. When one works with the field operator  $\psi(\mathbf{r})$ , as in Secs. 2.4. and 2.5, the corresponding space of microstates is the Fock space  $\mathcal{F}(\psi)$  generated by  $\psi^{\dagger}(\mathbf{r})$ , as is explained in Ref. [55]. But, as soon as the Bogolubov shift (2.81) has been accomplished, the new field operator  $\hat{\psi}(\mathbf{r})$  is defined on another space, which is the Fock space  $\mathcal{F}(\psi_1)$  generated by  $\psi_1^{\dagger}(\mathbf{r})$ , with the spaces  $\mathcal{F}(\psi)$  and  $\mathcal{F}(\psi_1)$  being mutually orthogonal [99]. In the space  $\mathcal{F}(\psi)$ , there was the sole field variable  $\psi(\mathbf{r})$ , while in the space  $\mathcal{F}(\psi_1)$  there are now two variables, the condensate wave function  $\eta(\mathbf{r})$  and the field operator of uncondensed particles  $\psi_1(\mathbf{r})$ . Respectively, instead of one normalization condition (2.20), there are two normalization conditions (2.87) and (2.88).

The conservation-number condition (2.84) can be reduced to the standard form of the statistical conditions (2.22) by defining the Hermitian operator

$$\hat{\Lambda} \equiv \int \left[ \lambda(\mathbf{r}) \psi_1^{\dagger}(\mathbf{r}) + \lambda^*(\mathbf{r}) \psi_1(\mathbf{r}) \right] d\mathbf{r} , \qquad (2.91)$$

which can be called the *linear killer*. This is because the Lagrange multiplier  $\lambda(\mathbf{r})$  has to be chosen so that

$$<\hat{\Lambda}>=0$$
, (2.92)

which requires the absence of the terms linear in  $\psi_1(\mathbf{r})$  in the related grand Hamiltonian [57].

Statistical averages of operators from the algebra of observables  $\mathcal{O} \equiv \{\hat{A}(t)\}\$  are given as

$$\langle \hat{A}(t) \rangle \equiv \operatorname{Tr}_{\mathcal{F}(\psi_1)} \hat{\rho} \hat{A}(t) ,$$
 (2.93)

with a statistical operator  $\hat{\rho} \equiv \hat{\rho}(0)$ . For instance, the energy Hamiltonian

$$\hat{H} = \hat{H}[\hat{\psi}] \equiv \hat{H}[\eta, \psi_1]$$

defines the internal energy

$$E = \langle \hat{H} \rangle . \tag{2.94}$$

In what follows, we shall omit the notation of spaces, over which the trace is taken, in order to avoid cumbersome expressions.

The statistical operator  $\hat{\rho}$  is obtained from the minimization of the information functional  $I[\hat{\rho}]$  under the statistical conditions (2.18), (2.94), (2.87), (2.88), and (2.92). The information functional is

$$I[\hat{\rho}] = \operatorname{Tr}\hat{\rho} \ln \hat{\rho} + \lambda_0 \left(\operatorname{Tr}\hat{\rho} - 1\right) + \beta \left(\operatorname{Tr}\hat{\rho}\hat{H} - E\right) - \beta \mu_0 \left(\operatorname{Tr}\hat{\rho}\hat{N}_0 - N_0\right) - \beta \mu_1 \left(\operatorname{Tr}\hat{\rho}\hat{N}_1 - N_1\right) - \beta \operatorname{Tr}\hat{\rho}\hat{\Lambda}.$$
(2.95)

Its minimization yields the statistical operator

$$\hat{\rho} = \frac{\exp(-\beta H)}{\operatorname{Tr}\exp(-\beta H)}, \qquad (2.96)$$

with the grand Hamiltonian

$$H \equiv \hat{H} - \mu_0 \hat{N}_0 - \mu_1 \hat{N}_1 - \hat{\Lambda} .$$
 (2.97)

This Hamiltonian is, clearly, a functional  $H = H[\eta, \psi_1]$  of  $\eta(\mathbf{r})$  and  $\psi_1(\mathbf{r})$ .

The evolution laws are prescribed by extremizing the action functional, as is described in Sec. 2.4. To this end, we define the temporal energy operator

$$\hat{E} \equiv \int \hat{\psi}^{\dagger}(\mathbf{r}) i \, \frac{\partial}{\partial t} \, \hat{\psi}(\mathbf{r}) \, d\mathbf{r} \, . \tag{2.98}$$

With the Bogolubov shift (2.81), this takes the form

$$\hat{E} = \int \left[ \eta^*(\mathbf{r}) i \, \frac{\partial}{\partial t} \, \eta(\mathbf{r}) + \psi_1^{\dagger}(\mathbf{r}) i \, \frac{\partial}{\partial t} \, \psi_1(\mathbf{r}) \right] \, d\mathbf{r} \,, \qquad (2.99)$$

which shows that  $\hat{E} = \hat{E}[\eta, \psi_1]$  is a functional of  $\eta(\mathbf{r})$  and  $\psi_1(\mathbf{r})$ . The effective action is also a functional of these variables,

$$\Gamma[\eta, \psi_1] \equiv \int \left(\hat{E} - H\right) dt . \qquad (2.100)$$

The evolution laws are given by the extremization of the action functional (2.100) with respect to the condensate wave function,

$$\frac{\delta\Gamma[\eta,\psi_1]}{\delta\eta^*(\mathbf{r},t)} = 0 , \qquad (2.101)$$

and with respect to the field operator of uncondensed particles,

$$\frac{\delta\Gamma[\eta,\psi_1]}{\delta\psi_1^{\dagger}(\mathbf{r},t)} = 0. \qquad (2.102)$$

These evolution equations, owing to the form of the action functional (2.100), are equivalent to the equation

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \frac{\delta H[\eta, \psi_1]}{\delta \eta^*(\mathbf{r}, t)}$$
(2.103)

for the condensate variable, and to the equation

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \frac{\delta H[\eta, \psi_1]}{\delta \psi_1^{\dagger}(\mathbf{r}, t)}$$
(2.104)

for the field variable of uncondensed particles.

Thus, the representative statistical ensemble for a Bose system with the gauge symmetry breaking, induced by the Bogolubov shift (2.81), is the triplet  $\{\mathcal{F}(\psi_1), \hat{\rho}, \partial t\}$  formed by the Fock space  $\mathcal{F}(\psi_1)$ , generated by  $\psi_1^{\dagger}(\mathbf{r})$ , the statistical operator (2.96), with the grand Hamiltonian (2.97), and the evolution laws (2.103) and (2.104).

In the case of an equilibrium system, we can introduce the grand thermodynamic potential

$$\Omega = -T \ln \operatorname{Tr} e^{-\beta H}, \qquad (2.105)$$

defining all thermodynamics of the system. For example, the fraction of condensed atoms is

$$n_0 \equiv \frac{N_0}{N} = -\frac{1}{N} \frac{\partial \Omega}{\partial \mu_0} , \qquad (2.106)$$

and the fraction of uncondensed atoms is

$$n_1 \equiv \frac{N_1}{N} = -\frac{1}{N} \frac{\partial \Omega}{\partial \mu_1} \,. \tag{2.107}$$

The equation for the condensate function is obtained from the statistical averaging of Eq. (2.103), under the condition that, for an equilibrium system,  $\eta(\mathbf{r})$  does not depend on time. Then we get the equation

$$\frac{\delta\Omega}{\delta\eta^*(\mathbf{r})} = \langle \frac{\delta H[\eta, \psi_1]}{\delta\eta^*(\mathbf{r})} \rangle = 0 , \qquad (2.108)$$

which is equivalent to the Bogolubov minimization of the thermodynamic potential with respect to the condensate variable [64,65,72,73].

The free energy can be defined as

$$F = \Omega + \mu_0 N_0 + \mu_1 N_1 . \tag{2.109}$$

At the same time, keeping in mind the standard form of the free energy

$$F = \Omega + \mu N , \qquad (2.110)$$

we find the expression for the system chemical potential

$$\mu = \mu_0 n_0 + \mu_1 n_1 . \tag{2.111}$$

The same form for the chemical potential (2.111) can be derived from the usual definition

$$\mu \equiv \frac{\partial F}{\partial N} . \tag{2.112}$$

The right-hand side here can be written as

$$\frac{\partial F}{\partial N} = \frac{\partial F}{\partial N_0} \frac{\partial N_0}{\partial N} + \frac{\partial F}{\partial N_1} \frac{\partial N_1}{\partial N} ,$$

where

$$\frac{\partial F}{\partial N_0} = \mu_0 , \qquad \frac{\partial F}{\partial N_1} = \mu_1 .$$

Assuming that  $n_0$  and  $n_1$  are fixed in the thermodynamic limit  $N \to \infty$ , from the relations

$$N_0 = n_0 N$$
,  $N_1 = n_1 N$ ,

we have

$$\frac{\partial N_0}{\partial N} = n_0 , \qquad \frac{\partial N_1}{\partial N} = n_1 .$$

Combining these derivatives in definition (2.112), we get the same expression (2.111) for the chemical potential.

It is possible to show [57] that the dispersion of the number-of-particle operator is given by

$$\Delta^2(\hat{N}) = T \,\frac{\partial N}{\partial \mu} \,, \tag{2.113}$$

where the dispersion of a self-adjoint operator  $\hat{A}$  is defined as

$$\Delta^2(\hat{A}) \equiv <\hat{A}^2>-<\hat{A}>^2$$

At the end, the free energy can be represented as a function F = F(T, V, N) of temperature T, volume V, and the particle number N, with the differential

$$dF = -S \, dT - P \, dV + \mu \, dN \,, \tag{2.114}$$

in which S is entropy and P, pressure. And the grand potential (2.105) is a function  $\Omega = \Omega(T, V, \mu)$ , with the differential

$$d\Omega = -S \ dT - P \ dV - N \ d\mu \ . \tag{2.115}$$

All thermodynamics follows from the above expressions. A more detailed discussion is given in Ref. [57].

#### 2.9 Condensate Existence

The existence of BEC, as such, requires the validity of an important necessary condition. Generally, the total number of atoms N is the sum  $\sum_k n_k$  of the occupation numbers for quantum states labelled by a multi-index k. The occurrence of BEC, by definition, means the microscopic occupation of a single quantum state  $k_0$ , when  $N_0 \propto N$ , in agreement with condition (2.3). Only in such a case, it is meaningful to separate out of the sum  $\sum_k n_k$  a single term, related to BEC, obtaining

$$N = N_0 + \sum_{k \neq k_0} n_k . (2.116)$$

Mathematically, the possibility of that separation necessarily implies that, in thermodynamic limit, the distribution  $n_k$  over quantum states diverges when  $k \to k_0$ . Hence, the necessary condition for the BEC existence is

$$\lim_{N \to \infty} \lim_{k \to k_0} \frac{1}{n_k} = 0 , \qquad (2.117)$$

where the thermodynamic limit is invoked in order to make the BEC rigorously defined.

In the representative ensemble of the previous Sec. 2.8, the condensate wave function can be written as

$$\eta(\mathbf{r}) = \sqrt{N_0} \,\varphi_0(\mathbf{r}) \,, \qquad (2.118)$$

while the operator of uncondensed atoms can be expanded over the natural orbitals as

$$\psi_1(\mathbf{r}) = \sum_{k \neq k_0} a_k \varphi_k(\mathbf{r}) . \qquad (2.119)$$

Hence, the occupation numbers are

$$n_k \equiv \langle a_k^{\dagger} a_k \rangle \,, \tag{2.120}$$

with the statistical averaging defined in Eq. (2.93).

If we turn to the terminology of Green functions, then the necessary condition (2.117) can be connected with the properties of the poles of Green functions. Under the spontaneously broken gauge symmetry, the poles of the first-order and second-order Green functions coincide, that is, the single-particle spectrum coincides with the spectrum of collective excitations  $\varepsilon_k$  [65,100]. For the latter, the necessary condition of condensate existence (2.117) translates into

$$\lim_{k \to k_0} \varepsilon_k = 0 , \qquad (2.121)$$

with the condition  $n_k \ge 0$  becoming the stability condition

Re 
$$\varepsilon_k \ge 0$$
, Im  $\varepsilon_k \le 0$ . (2.122)

Conditions (2.117) or (2.121) impose a constraint on the Lagrange multiplier  $\mu_1$ , which has to be such that to make the spectrum  $\varepsilon_k$  gapless in the sense of the limit (2.121).

To illustrate the properties (2.117) and (2.121), let us consider a uniform system, when  $k_0 = 0$ . For a Bose-condensed uniform system, Bogolubov [65] rigorously proved the inequalities for the occupation numbers (2.120) in the case of nonzero temperature,

$$n_k \ge \frac{mn_0T}{2k^2} - \frac{1}{2},$$
 (2.123)

and at zero temperature,

$$n_k \ge \frac{mn_0\varepsilon_k}{4k^2} - \frac{1}{2} \qquad (T=0) , \qquad (2.124)$$

where  $\varepsilon_k$  is the real part of the spectrum of collective excitations. These inequalities can be slightly improved [101], resulting, for finite temperatures, in

$$n_k \ge \frac{mn_0T}{k^2} - \frac{1}{2}$$
 (2.125)

and for zero temperature, in

$$n_k \ge \frac{mn_0\varepsilon_k}{2k^2} - \frac{1}{2} \qquad (T=0).$$
 (2.126)

At zero temperature, one can use the Feynman relation [78,102,103]

$$\varepsilon_k = \frac{k^2}{2mS(\mathbf{k})} \qquad (T=0) , \qquad (2.127)$$

in which  $S(\mathbf{k})$  is the structure factor. Then the Bogolubov inequality (2.126) takes the form

$$n_k \ge \frac{n_0}{4S(\mathbf{k})} - \frac{1}{2} \qquad (T=0) .$$
 (2.128)

At zero temperature, the structure factor possesses the long-wave limit [104] as

$$S(\mathbf{k}) \simeq \frac{k}{2mc}$$
  $(T = 0, \ k \to 0)$ . (2.129)

Hence, from the Feynman relation (2.127), one has

$$\varepsilon_k \simeq ck \qquad (k \to 0) .$$
 (2.130)

The same long-wave limit exists for the spectrum of collective excitations at finite temperatures [65]. That is, limit (2.121) is valid for any T. From the above inequalities, it follows that, for finite temperatures,

$$n_k \geq \frac{mn_0T}{k^2} \qquad (k \to 0) ,$$

and for zero temperature,

$$n_k \geq \frac{mn_0c}{2k} \qquad (T=0, \ k \to 0) \ .$$

Therefore, in any case, the BEC existence condition (2.117) holds true.

Condition (2.117) can also be generalized for nonequilibrium nonuniform systems. But the latter should, at least, be locally equilibrium in order that the meaning of thermodynamic phases be locally preserved. Then for  $\psi_1(\mathbf{r}, t)$  one has the same expansion (2.119), but with  $a_k(t)$  being a function of time. The occupation number (2.120) becomes a function of time,  $n_k = n_k(t)$ . Then condition (2.117) defines the Lagrange multiplier  $\mu_1$  as a function of time  $\mu_1(t)$ . If one employs the local-density approximation, then  $\mu_1$  can also be a function of the spatial variable.

## 2.10 Superfluid Fraction

Expressions, defining the superfluid fraction, can have different forms for uniform and nonuniform systems. It is, therefore, important to recall the most general definition of the superfluid fraction, which could be applied to arbitrary systems, whether uniform or not. This general definition is based on the calculation of the response to a velocity boost imposed on the system.

Let  $\hat{H}$  be the energy Hamiltonian of an immovable system, and let  $\hat{H}_v$  be the energy Hamiltonian of the system moving, as a whole, with velocity  $\mathbf{v}$ . The statistical operator, related to the moving system is denoted as  $\hat{\rho}_v$ . The corresponding statistical average of an operator  $\hat{A}$  is

$$\langle \hat{A} \rangle_v \equiv \operatorname{Tr} \hat{\rho}_v \hat{A}$$
. (2.131)

The return to the immovable system is realized through the limit

$$\langle \hat{A} \rangle = \lim_{v \to 0} \langle \hat{A} \rangle_v$$
 (2.132)

The momentum operator of the total moving system can be represented as

$$\hat{\mathbf{P}}_{v} \equiv \frac{\partial \hat{H}_{v}}{\partial \mathbf{v}} . \tag{2.133}$$

The momentum operator of the immovable system is

$$\hat{\mathbf{P}} = \lim_{v \to 0} \hat{\mathbf{P}}_v . \tag{2.134}$$

The superfluid fraction can be defined as a fraction of particles nontrivially responding to the velocity boost,

$$n_s \equiv \frac{1}{3mN} \lim_{v \to 0} \frac{\partial}{\partial \mathbf{v}} < \hat{\mathbf{P}}_v >_v .$$
(2.135)

This is the most general definition, valid for arbitrary systems [10,57].

For an equilibrium Bose system, with the grand Hamiltonian

$$H_v \equiv \hat{H}_v - \mu_0 \hat{N}_0 - \mu_1 \hat{N}_1 - \hat{\Lambda} , \qquad (2.136)$$

which differs from Eq. (2.97) by the velocity boosted term  $\hat{H}_v$ , the statistical operator is

$$\hat{\rho}_v \equiv \frac{\exp(-\beta H_v)}{\operatorname{Tr} \exp(-\beta H_v)} \,. \tag{2.137}$$

The differentiation in Eq. (2.135) is accomplished according to the rule of differentiation with respect to parameters [105], which gives

$$\frac{\partial}{\partial \mathbf{v}} \cdot \langle \hat{\mathbf{P}}_v \rangle_v = \langle \frac{\partial}{\partial \mathbf{v}} \cdot \hat{\mathbf{P}}_v \rangle_v - \beta \operatorname{cov} \left( \hat{\mathbf{P}}_v, \frac{\partial H_v}{\partial \mathbf{v}} \right) \,.$$

Here the last term is the covariance defined as

$$\operatorname{cov}(\hat{A},\hat{B}) \equiv \frac{1}{2} < \hat{A}\hat{B} + \hat{B}\hat{A} >_v - < \hat{A} >_v < \hat{B} >_v$$
.

Using definition (2.133), we obtain

$$n_s = \frac{1}{3mN} \left[ \lim_{v \to 0} < \frac{\partial}{\partial \mathbf{v}} \cdot \hat{\mathbf{P}}_v > -\beta \Delta^2(\hat{\mathbf{P}}) \right] , \qquad (2.138)$$

where

$$\Delta^2(\hat{\mathbf{P}}) \equiv \langle \hat{\mathbf{P}}^2 \rangle - \langle \hat{\mathbf{P}} \rangle^2$$

The same form (2.138) can be derived from the definition [106,107] of the superfluid fraction

$$n_s \equiv \frac{1}{3mN} \lim_{v \to 0} \frac{\partial^2 \Omega_v}{\partial \mathbf{v}^2} = \frac{1}{3mN} \lim_{v \to 0} \frac{\partial^2 F_v}{\partial \mathbf{v}^2}, \qquad (2.139)$$

applicable to equilibrium systems. Here the grand potential for the moving system is

$$\Omega_v \equiv -T \ln \operatorname{Tr} \exp(-\beta H_v) , \qquad (2.140)$$

and the free energy for that system is

$$F_v \equiv -T \ln \operatorname{Tr} \exp(-\beta \hat{H}_v) . \qquad (2.141)$$

The first derivative gives

$$\frac{\partial F_v}{\partial \mathbf{v}} = \frac{\partial \Omega_v}{\partial \mathbf{v}} = \langle \mathbf{P}_v \rangle_v \quad . \tag{2.142}$$

For an equilibrium system at rest, one has

$$\Delta^2(\hat{\mathbf{P}}) = \langle \hat{\mathbf{P}}^2 \rangle \qquad \left(\langle \hat{\mathbf{P}} \rangle = 0\right) . \tag{2.143}$$

Then, one gets

$$n_s = \frac{1}{3mN} \left( \lim_{v \to 0} < \frac{\partial}{\partial \mathbf{v}} \cdot \hat{\mathbf{P}}_v > -\beta < \hat{\mathbf{P}}^2 > \right) \,. \tag{2.144}$$

Taking into account Eq. (2.143), we see that Eqs. (2.138) and (2.144) coincide.

To specify the expression for the superfluid fraction, we can use the definition for the operator of momentum

$$\hat{\mathbf{P}}_{v} \equiv \int \hat{\psi}_{v}^{\dagger}(\mathbf{r}, t) (-i\nabla) \hat{\psi}_{v}(\mathbf{r}, t) \, d\mathbf{r}$$
(2.145)

of the moving system. The field operator of the moving system can be expressed through the field operator of the system at rest by means of the Galilean transformation

$$\hat{\psi}_{v}(\mathbf{r},t) = \hat{\psi}(\mathbf{r} - \mathbf{v}t,t) \exp\left\{i\left(m\mathbf{v}\cdot\mathbf{r} - \frac{mv^{2}}{2}t\right)\right\}.$$
(2.146)

Consequently,

$$\hat{\mathbf{P}}_{v} = \int \hat{\psi}^{\dagger}(\mathbf{r}) \left(-i\nabla + m\mathbf{v}\right) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} \,. \tag{2.147}$$

The energy Hamiltonian of the system at rest is  $\hat{H} = \hat{H}[\hat{\psi}]$ , while that of the moving system is  $\hat{H}_v = \hat{H}[\hat{\psi}_v]$ . Differentiating Eq. (2.147) gives

$$\frac{\partial}{\partial \mathbf{v}} \cdot \hat{\mathbf{P}}_v = 3m\hat{N}$$

We can define the *dissipated heat* of the considered quantum system as

$$Q \equiv \frac{\Delta^2(\hat{\mathbf{P}})}{2mN} = \frac{\langle \hat{\mathbf{P}}^2 \rangle}{2mN} , \qquad (2.148)$$

which is to be compared with the heat dissipated in a classical system,

$$Q_0 \equiv \frac{3}{2} T . (2.149)$$

Finally, the superfluid fraction (2.144) reduces to the form

$$n_s = 1 - \frac{Q}{Q_0} \,. \tag{2.150}$$

This formula is valid for arbitrary nonuniform equilibrium systems, including periodic lattice potentials.

The superfluid fraction, as is known, is not directly related to the condensate fraction. A straightforward example is the liquid <sup>4</sup>He, which at low temperature  $T \rightarrow 0$  is practically 100% superfluid, while possessing only about 10% of BEC [108]. Superfluidity happens in two-dimensional uniform systems, where BEC cannot exist. For trapped atoms, BEC can occur in low-dimensional systems, depending on the type of the confining potential [41], but again with no direct relation to the superfluid fraction [109–114]. Quasi-low-dimensional atomic systems can be prepared by producing a tight confinement in one or two directions [115]. It is only for ideal Bose gases below  $T_c$  [116–118], when the superfluid and condensate fractions coincide [9]. Generally, superfluidity can exist without BEC, and vice versa.

## 2.11 Equations of Motion

All observable quantities are functionals of the condensate function  $\eta(\mathbf{r})$  and the operator of uncondensed particles  $\psi_1(\mathbf{r})$ . These variables are defined by the evolution equations (2.103) and (2.104). To derive these equations explicitly, we need to specify the Hamiltonian  $\hat{H} = \hat{H}[\eta, \psi_1]$ .

Let us take the energy Hamiltonian in the standard form

$$\hat{H} = \int \hat{\psi}(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U \right) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \int \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}^{\dagger}(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \, d\mathbf{r} d\mathbf{r}' , \qquad (2.151)$$

in which m is atomic mass,  $U = U(\mathbf{r})$  is an external potential, and  $\Phi(\mathbf{r}) = \Phi(-\mathbf{r})$  is the binary atomic interaction potential. After substituting here the Bogolubov shift (2.81), Hamiltonian (2.151) can be rewritten as the sum of five terms, depending on the number of factors of  $\psi_1$ . The same concerns the grand Hamiltonian (2.97), for which we obtain

$$H = \sum_{n=0}^{4} H^{(n)} .$$
 (2.152)

Here the zero-order term is

$$H^{(0)} = \int \eta^*(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \int \Phi(\mathbf{r} - \mathbf{r}') |\eta(\mathbf{r}')|^2 |\eta(\mathbf{r})|^2 \, d\mathbf{r} d\mathbf{r}' \,.$$
(2.153)

To satisfy the quantum-number conservation condition (2.84), the Hamiltonian should not contain the terms linear in  $\psi_1$  [57]. For this purpose, the Lagrange multiplier  $\lambda(\mathbf{r})$  in operator (2.91) is to be taken such that to cancel all linear terms, resulting in

$$H^{(1)} = 0 . (2.154)$$

For the second-order term, we have

$$H^{(2)} = \int \psi_1^{\dagger}(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U - \mu_1 \right) \psi_1(\mathbf{r}) d\mathbf{r} + \int \Phi(\mathbf{r} - \mathbf{r}') \left[ |\eta(\mathbf{r})|^2 \psi_1^{\dagger}(\mathbf{r}') \psi_1(\mathbf{r}') + \eta^*(\mathbf{r}) \eta(\mathbf{r}') \psi_1^{\dagger}(\mathbf{r}') \psi_1(\mathbf{r}) + \frac{1}{2} \eta^*(\mathbf{r}) \eta^*(\mathbf{r}') \psi_1(\mathbf{r}') + \frac{1}{2} \eta(\mathbf{r}) \eta(\mathbf{r}') \psi_1^{\dagger}(\mathbf{r}') \psi_1^{\dagger}(\mathbf{r}) \right] d\mathbf{r} d\mathbf{r}' .$$
(2.155)

The third-order term is

$$H^{(3)} = \int \Phi(\mathbf{r} - \mathbf{r}') \left[ \eta^*(\mathbf{r}) \psi_1^{\dagger}(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) + \psi_1^{\dagger}(\mathbf{r}) \psi_1^{\dagger}(\mathbf{r}') \psi_1(\mathbf{r}') \eta(\mathbf{r}) \right] d\mathbf{r} d\mathbf{r}' . \qquad (2.156)$$

And the fourth-order term is

$$H^{(4)} = \frac{1}{2} \int \psi_1^{\dagger}(\mathbf{r}) \psi_1^{\dagger}(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \, d\mathbf{r} d\mathbf{r}' \,.$$
(2.157)

Inserting Hamiltonian (2.152) into the evolution equation (2.103) yields

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left(-\frac{\nabla^2}{2m} + U - \mu_0\right) \eta(\mathbf{r}, t) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[|\eta(\mathbf{r}')|^2 \eta(\mathbf{r}) + \hat{X}(\mathbf{r}, \mathbf{r}')\right] d\mathbf{r}' , \qquad (2.158)$$

with the correlation operator

$$\hat{X}(\mathbf{r},\mathbf{r}') \equiv \psi_1^{\dagger}(\mathbf{r}')\psi_1(\mathbf{r}')\eta(\mathbf{r}) + \psi_1^{\dagger}(\mathbf{r}')\eta(\mathbf{r}')\psi_1(\mathbf{r}) + \eta^*(\mathbf{r}')\psi_1(\mathbf{r}')\psi_1(\mathbf{r}) + \psi_1^{\dagger}(\mathbf{r}')\psi_1(\mathbf{r}')\psi_1(\mathbf{r}) + \psi_1^{\dagger}(\mathbf{r}')\psi_1(\mathbf$$

And Eq. (2.104), with Hamiltonian (2.152), gives

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \left(-\frac{\nabla^2}{2m} + U - \mu_1\right) \psi_1(\mathbf{r}, t) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[|\eta(\mathbf{r}')|^2 \psi_1(\mathbf{r}) + \eta^*(\mathbf{r}')\eta(\mathbf{r})\psi_1(\mathbf{r}') + \eta(\mathbf{r}')\eta(\mathbf{r})\psi_1^{\dagger}(\mathbf{r}') + \hat{X}(\mathbf{r}, \mathbf{r}')\right] d\mathbf{r}' . \quad (2.159)$$

The equation for the condensate wave function is obtained by averaging Eq. (2.158). For this purpose, let us define the normal density matrix

$$\rho_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1^{\dagger}(\mathbf{r}')\psi_1(\mathbf{r}) \rangle . \qquad (2.160)$$

As soon as the gauge symmetry is broken, there arises the anomalous density matrix

$$\sigma_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1(\mathbf{r}')\psi_1(\mathbf{r}) \rangle . \qquad (2.161)$$

The density of BEC is

$$\rho_0(\mathbf{r}) \equiv |\eta(\mathbf{r})|^2 , \qquad (2.162)$$

and the density of uncondensed atoms is

$$\rho_1(\mathbf{r}) \equiv \rho_1(\mathbf{r}, \mathbf{r}) = \langle \psi_1^{\dagger}(\mathbf{r})\psi_1(\mathbf{r}) \rangle . \qquad (2.163)$$

The diagonal part of Eq. (2.161) is the anomalous average

$$\sigma(\mathbf{r}) \equiv \sigma_1(\mathbf{r}, \mathbf{r}) = \langle \psi_1(\mathbf{r})\psi_1(\mathbf{r}) \rangle . \qquad (2.164)$$

The value  $|\sigma(\mathbf{r})|$  has the meaning of the density of pair-correlated particles [99]. The total density of atoms

$$\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \rho_1(\mathbf{r}) \tag{2.165}$$

is the sum of densities (2.162) and (2.163). Also, we need the notation for the triple correlator

$$\xi(\mathbf{r},\mathbf{r}') \equiv \langle \psi_1^{\dagger}(\mathbf{r}')\psi_1(\mathbf{r}')\psi_1(\mathbf{r}) \rangle \quad .$$
(2.166)

Using the above notation, we get

$$\langle \hat{X}(\mathbf{r},\mathbf{r}') \rangle = \rho_1(\mathbf{r}')\eta(\mathbf{r}) + \rho_1(\mathbf{r},\mathbf{r}')\eta(\mathbf{r}') + \sigma_1(\mathbf{r},\mathbf{r}')\eta^*(\mathbf{r}') + \xi(\mathbf{r},\mathbf{r}')$$

Finally, averaging Eq. (2.158), we obtain

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left(-\frac{\nabla^2}{2m} + U - \mu_0\right) \eta(\mathbf{r}, t) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[\rho(\mathbf{r}')\eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}')\eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}')\eta^*(\mathbf{r}') + \xi(\mathbf{r}, \mathbf{r}')\right] d\mathbf{r}' .$$
(2.167)

This is a general equation for the condensate wave function in the case of an arbitrary Bose system. No approximation has been involved in deriving Eq. (2.167).

For an equilibrium system, we have

$$\frac{\partial}{\partial t} \eta(\mathbf{r}) = 0$$
 (equilibrium).

Then Eq. (2.167) becomes the eigenproblem

$$\left[-\frac{\nabla^2}{2m} + U(\mathbf{r})\right]\eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}')\left[\rho(\mathbf{r}')\eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}')\eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}')\eta^*(\mathbf{r}') + \xi(\mathbf{r}, \mathbf{r}')\right]d\mathbf{r}' = \mu_0\eta(\mathbf{r}) \quad (2.168)$$

defining  $\eta(\mathbf{r})$  and  $\mu_0$ .

The above equations are valid for any interaction potential  $\Phi(\mathbf{r})$ , with the sole restriction that it is integrable [55], so that

$$\left|\int \Phi(\mathbf{r}) \, d\mathbf{r}\right| < \infty \, .$$

For dilute gases, when the interaction radius is much shorter than the mean interatomic distance [7–14], one uses the local interaction potential

$$\Phi(\mathbf{r}) = \Phi_0 \delta(\mathbf{r}) \qquad \left(\Phi_0 \equiv 4\pi \; \frac{a_s}{m}\right) \;, \tag{2.169}$$

in which  $a_s$  is the scattering length. In that case, all equations simplify. For example, the condensate-function equation (2.168) reads as

$$\left[-\frac{\nabla^2}{2m} + U(\mathbf{r})\right]\eta(\mathbf{r}) + \Phi_0\left\{\left[\rho(\mathbf{r}) + \rho_1(\mathbf{r})\right]\eta(\mathbf{r}) + \sigma_1(\mathbf{r})\eta^*(\mathbf{r}) + \xi(\mathbf{r},\mathbf{r})\right\} = \mu_0\eta(\mathbf{r}) .$$
(2.170)

This equation is valid for any nonuniform equilibrium Bose system, which can be treated as dilute.

Note that a dilute gas can, at the same time, be strongly interacting. Really, the gas is dilute, when the interaction radius  $r_0$  is much shorter than the mean interatomic distance

a, that is,  $r_0 \ll a$ . Then the actual form of the interaction potential is not important and this potential can be modelled by the local expression (2.169). The scattering length characterizes the interaction strength, since

$$\Phi_0 = \int \Phi(\mathbf{r}) \ d\mathbf{r} = 4\pi \ \frac{a_s}{m} \ .$$

Nothing precludes the scattering length to be larger that the mean interatomic distance. If  $a_s > a$ , then the average potential energy  $\rho \Phi_0$  is larger than the effective kinetic energy,

$$\rho \Phi_0 > \frac{\rho^{2/3}}{2m} \qquad (a_s > a) ,$$

which means that atoms strongly interact with each other. For a strongly interacting system, atomic correlations can be rather important [10,119–122]. But for dilute gases, the influence of correlations can be taken into account through defining an effective scattering length  $a_s$ .

## 2.12 Uniform System

Though this review article is devoted to nonuniform systems, it is instructive to briefly touch the uniform case. First, this will illustrate the self-consistency of the theory employing the representative statistical ensemble [56,57,93–99]. Second, the theory for uniform systems can be used for generalizing the approach to nonuniform systems by means of the local-density approximation. Also, many formulas in the case of periodic potentials have the structure very similar to that of expressions for the uniform system.

In a uniform system, BEC occurs in the quantum state of zero momentum  $k_0 = 0$ . Atomic densities do not depend on the spatial variable. Thus, the condensate density

$$\rho_0(\mathbf{r}) = \rho_0 \equiv \frac{N_0}{V} , \qquad (2.171)$$

the density of uncondensed atoms

$$\rho_1(\mathbf{r}) = \rho_1 \equiv \frac{N_1}{V} , \qquad (2.172)$$

and the total density

$$\rho(\mathbf{r}) = \rho = \rho_0 + \rho_1 , \qquad (2.173)$$

all are constants.

For the interaction potential  $\Phi(\mathbf{r})$  the Fourier transform

$$\Phi_k = \int \Phi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \, d\mathbf{r} \tag{2.174}$$

is assumed to exist. Plane waves are the natural orbitals  $\varphi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$ . Hence, it is convenient to use everywhere the Fourier transforms.

The problem can be explicitly solved by using the Hartree-Fock-Bogolubov (HFB) approximation for Bose-condensed systems [94–98]. Then the thermodynamic potential (2.105) becomes

$$\Omega = E_B + TV \int \ln\left(1 - e^{-\beta\varepsilon_k}\right) \frac{d\mathbf{k}}{(2\pi)^3} \,. \tag{2.175}$$

Here the first term is the nonoperator expression

$$E_B = E_{HFB} + \frac{1}{2} \sum_{k \neq 0} (\varepsilon_k - \omega_k) , \qquad (2.176)$$

in which

$$E_{HFB} = H^{(0)} - \frac{1}{2} \rho_1^2 \Phi_0 V - \frac{1}{2V} \sum_{k \neq 0} \Phi_{k+p} (n_k n_p + \sigma_k \sigma_p) ,$$
  
$$H^{(0)} = -N_0 \left[ \frac{1}{2} (\rho + \rho_1) \Phi_0 + \frac{1}{V} \sum_{p \neq 0} (n_p + \sigma_p) \Phi_p \right] .$$
(2.177)

The Bogolubov spectrum is

$$\varepsilon_k = \sqrt{\omega_k^2 - \Delta_k^2} \,, \tag{2.178}$$

where

$$\omega_k = \frac{k^2}{2m} + \rho_0 \Phi_k + \frac{1}{V} \sum_{p \neq 0} \left( n_p \Phi_{k+p} - n_p \Phi_p + \sigma_p \Phi_p \right)$$
(2.179)

and

$$\Delta_k = \rho_0 \Phi_k + \frac{1}{V} \sum_{p \neq 0} \sigma_p \Phi_{k+p} .$$
 (2.180)

Equation (2.168) gives

$$\mu_0 = \rho \Phi_0 + \frac{1}{V} \sum_{p \neq 0} (n_p + \sigma_p) \Phi_p . \qquad (2.181)$$

And the condition of the BEC existence (2.117) and (2.121) define

$$\mu_1 = \rho \Phi_0 + \frac{1}{V} \sum_{p \neq 0} (n_p - \sigma_p) \Phi_p . \qquad (2.182)$$

The distributions  $n_p$  and  $\sigma_p$  are the Fourier transforms of the normal density matrix (2.160) and of the anomalous matrix (2.161), respectively. For the former, we have

$$n_k = \frac{\omega_k}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) - \frac{1}{2}, \qquad (2.183)$$

and for the latter, we find

$$\sigma_k = -\frac{\Delta_k}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) . \tag{2.184}$$

The density of uncondensed atoms

$$\rho_1 = \int n_k \, \frac{d\mathbf{k}}{(2\pi)^3} \tag{2.185}$$

defines the condensate density  $\rho_0 = \rho - \rho_1$ . Consequently, the condensate fraction is

$$n_0 = 1 - \frac{\rho_1}{\rho} \,. \tag{2.186}$$
The dissipated heat (2.148) becomes

$$Q = \frac{1}{\rho} \int \frac{k^2}{2m} \left( n_k + n_k^2 - \sigma_k^2 \right) \frac{d\mathbf{k}}{(2\pi)^3} , \qquad (2.187)$$

which, according to Eq. (2.150), gives the superfluid fraction

$$n_s = 1 - \frac{2Q}{3T} \,. \tag{2.188}$$

Again, these expressions are simplified in the case of dilute gases, with the local interaction potential (2.169). Then the Bogolubov spectrum (2.178) takes the standard form

$$\varepsilon_k = \sqrt{(ck)^2 + \left(\frac{k^2}{2m}\right)^2} \,. \tag{2.189}$$

Notation (2.179) gives

$$\omega_k = \frac{k^2}{2m} + mc^2 , \qquad (2.190)$$

while Eq. (2.180) reduces to

$$\Delta_k = (\rho_0 + \sigma_1)\Phi_0 . (2.191)$$

The latter expression defines the sound velocity c through the relation

$$\Delta_k \equiv \Delta \equiv mc^2 . \tag{2.192}$$

And the anomalous average is

$$\sigma_1 \equiv \int \sigma_k \, \frac{d\mathbf{k}}{(2\pi)^3} \,. \tag{2.193}$$

For the Lagrange multipliers (2.181) and (2.182) we obtain

$$\mu_0 = (\rho + \rho_1 + \sigma_1)\Phi_0 \tag{2.194}$$

and, respectively,

$$\mu_1 = (\rho + \rho_1 - \sigma_1)\Phi_0 . \qquad (2.195)$$

Clearly,  $\mu_0 \neq \mu_1$ .

More details on the derivation of the above equations and on the investigation of their properties can be found in the original papers [57,94–98].

#### 2.13 Anomalous Averages

Anomalous averages of the type (2.161), (2.164), and (2.193) appear in all calculations for Bose systems with broken gauge symmetry. They always exist together with BEC, since both of them, the anomalous averages and the phenomenon of BEC, are caused by the same reason, by the spontaneous breaking of symmetry [63]. And when the gauge symmetry is restored, both  $n_0$  as well as  $\sigma_1$  become zero. Therefore,  $n_0$  and  $\sigma_1$  are either simultaneously nonzero, or simultaneously zero. It looks absolutely evident that setting one of them zero, while keeping another nonzero would be principally wrong. It is easy to check that the anomalous averages are often of the same order as the normal averages [123], hence omitting the latter, while keeping the former, is mathematically inappropriate. From these facts, it is clear that neglecting the anomalous averages (as one often does) is principally incorrect. It is also possible to check by direct calculations that the omission of the anomalous averages makes all calculations not self-consistent, dynamics not conserving, thermodynamics incorrect, disturbs the phase transition order, and moreover, renders the system unstable [57,123,124]. Therefore, it is absolutely compulsory to correctly keep account of the anomalous averages.

Dealing with the interaction potentials of finite interaction radii, one can use the results of the previous section, which requires to accomplish numerical calculations. The situation simplifies for the local potential (2.169), when many calculations can be made analytically. The sole thing, however, which does not make the life easier, is that the anomalous average (2.193), for the local potential (2.169), becomes divergent. So, a regularization method is needed.

In the case of the local interaction potential (2.169), the anomalous average (2.193) reads as

$$\sigma_1 = -\int \frac{\Delta}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) \frac{d\mathbf{k}}{(2\pi)^3} \,. \tag{2.196}$$

The integral diverges for all  $T < T_c$ . The divergence is caused by the use of the local potential (2.169), resulting in  $\Delta_k$ , in Eq. (2.192), containing no k-dependence. For interaction potentials, whose Fourier transforms  $\Phi_k$  depend on k, one should use  $\Delta_k$  from Eq. (2.180). Then, for  $\Phi_k$  diminishing at large k not slower than

$$\Phi_k \leq \frac{const}{k^{\alpha}} \qquad (\alpha > 1, \ k \to \infty) ,$$

the integral in Eq. (2.196) converges. However, then, instead of simple Eqs. (2.189) to (2.195), one should return to much more complicated equations, based on expressions (2.178) to (2.184).

Let us denote by

$$\sigma_0 \equiv \lim_{T \to 0} \sigma_1 \tag{2.197}$$

the zero temperature limit of the anomalous average. Equation (2.196) yields

$$\sigma_0 = -\Delta \int \frac{1}{2\varepsilon_k} \frac{d\mathbf{k}}{(2\pi)^3} \,. \tag{2.198}$$

Substituting here the Bogolubov spectrum (2.189), we meet the divergent integral

$$\int \frac{1}{2\varepsilon_k} \frac{d\mathbf{k}}{(2\pi)^3} = \frac{m^2 c}{\pi^2} \int_0^\infty \frac{x \, dx}{\sqrt{1+x^2}} \,. \tag{2.199}$$

The integral in Eq. (2.199) can be regularized by means of the dimensional regularization [11,125], which gives

$$\int_0^\infty \frac{x \, dx}{\sqrt{1+x^2}} \to -1 \, .$$

But, using this procedure, it is necessary to be cautious, keeping in mind that the dimensional regularization has a well defined meaning only in the limit of asymptotically weak interactions, when  $\Phi_0 \rightarrow 0$ . Consequently, using this regularization presupposes that the value of c in Eq. (2.199) has also to be taken in the same weak-coupling limit. In this limit, Eqs. (2.191) and (2.192) give

$$c \simeq c_B \sqrt{n_0} \qquad (\Phi_0 \to 0) , \qquad (2.200)$$

where

$$c_B \equiv \sqrt{\frac{\rho \Phi_0}{m}} \tag{2.201}$$

is the Bogolubov expression for the sound velocity. With this condition  $\Phi_0 \to 0$  in mind, from Eq. (2.199), we get

$$\int \frac{1}{2\varepsilon_k} \frac{d\mathbf{k}}{(2\pi)^3} \simeq -\frac{m^2 c_B}{\pi^2} \sqrt{n_0} \,. \tag{2.202}$$

In this way, in the weak-coupling limit, for the zero-temperature form of the anomalous average (2.198), we obtain

$$\sigma_0 \simeq \frac{\Delta m^2 c_B}{\pi^2} \sqrt{n_0} \qquad (\Phi_0 \to 0) . \tag{2.203}$$

The standard prescription in using the dimensional regularization is to employ the latter in the region of its applicability, after which to analytically continue the result to the whole region of parameters. Using Eq. (2.192), we finally obtain

$$\sigma_0 = \frac{(mc)^2}{\pi^2} \sqrt{m\rho_0 \Phi_0} . \qquad (2.204)$$

One may notice that the procedure of the analytical continuation is not uniquely defined. Fortunately, its different variants do not differ much in the results, provided that the *restoration*symmetry condition

$$\sigma_0 \to 0 \qquad (n_0 \to 0)$$

explicitly holds [97,98]. The meaning of this condition is obvious. As has been discussed above, the anomalous average and the condensate fraction either are together nonzero or together zero. The BEC disappears as soon as the gauge symmetry becomes restored, when  $n_0 \rightarrow 0$ , hence, simultaneously, it should be that  $\sigma_0 \rightarrow 0$ .

To find the low-temperature behavior of  $\sigma_1$ , we may rewrite Eq. (2.196) as

$$\sigma_1 = -\int \frac{\Delta}{2\varepsilon_k} \frac{d\mathbf{k}}{(2\pi)^3} - \int \frac{\Delta}{2\varepsilon_k} \left[ \coth\left(\frac{\varepsilon_k}{2T}\right) - 1 \right] \frac{d\mathbf{k}}{(2\pi)^3} \,. \tag{2.205}$$

The first term here, at low temperatures, can be replaced by form (2.204), which results in

$$\sigma_1 = \simeq \sigma_0 - \frac{\sqrt{2}}{(2\pi)^2} (mc)^3 \int_0^\infty \frac{(\sqrt{1+x^2}-1)^{1/2}}{\sqrt{1+x^2}} \left[ \coth\left(\frac{mc^2}{2T}x\right) - 1 \right] dx .$$
 (2.206)

It is worth stressing that Eqs. (2.205) and (2.206) are not identical. Equation (2.206) is valid only for low temperatures, such that

$$\frac{2T}{mc^2} \ll 1$$
. (2.207)

At these low temperatures, the main contribution to the integral in Eq. (2.206) comes from the region of small x. Then we can use the expansion

$$\frac{\sqrt{2}}{\sqrt{1+x^2}} \left(\sqrt{1+x^2} - 1\right)^{1/2} \simeq x - \frac{5}{8} x^3 + \frac{63}{128} x^5 - \frac{429}{1024} x^7$$

and the integral

$$\int_0^\infty x^{2n-1} \left[ \coth(px) - 1 \right] \, dx = \frac{\pi^{2n} |B_{2n}|}{2np^{2n}}$$

where  $B_n$  are the Bernoulli numbers. Let us introduce the notation

$$\alpha \equiv \left(\frac{\pi T}{2mc^2}\right)^2 \,, \tag{2.208}$$

which is the squared ratio of the typical thermal energy  $\pi T$  to the characteristic kinetic energy

$$\frac{k_0^2}{2m} = 2mc^2 \qquad (k_0 \equiv 2mc) \; .$$

From Eq. (2.206), we find the low-temperature expansion

$$\sigma_1 \simeq \sigma_0 - \frac{(mc)^3}{3\pi^2} \alpha \left( 1 - \alpha + 6\alpha^2 - \frac{429}{5} \alpha^3 \right)$$
 (2.209)

for  $\alpha \to 0$ . In the lowest order in  $\alpha$ , this gives

$$\sigma_1 \simeq \frac{(mc)^3}{\pi^2} \left[ \frac{c_B}{c} \sqrt{n_0} - \frac{\pi^2}{12} \left( \frac{T}{mc^2} \right)^2 \right] \qquad (T \to 0) .$$
 (2.210)

Another asymptotic form of  $\sigma_1$ , which we can find, is its form at  $T \to T_c$ . The critical point  $T_c$  is the temperature, where  $n_0 \to 0$ , hence  $\sigma_1 \to 0$ . Respectively, from Eqs. (2.191) and (2.192), it follows that  $c \to 0$ , as  $T \to T_c$ . Equation (2.196), for any T, can be identically rewritten as

$$\sigma_1 = -\frac{\sqrt{2}}{(2\pi)^2} (mc)^3 \int_0^\infty \frac{\left(\sqrt{1+x^2}-1\right)^{1/2}}{\sqrt{1+x^2}} \coth\left(\frac{mc^2}{2T}x\right) dx .$$
 (2.211)

When  $c \to 0$ , we can use the asymptotic form

$$\operatorname{coth}\left(\frac{mc^2}{2T} x\right) \simeq \frac{2T}{mc^2 x} \qquad (c \to 0)$$

as a result of which, Eq. (2.211) gives

$$\sigma_1 \simeq -\frac{m^2 cT}{2\pi} \qquad (T \to T_c) . \tag{2.212}$$

Thus, the correct anomalous average  $\sigma_1$  should interpolate between the low-temperature behavior (2.210) and the critical asymptotic form (2.212). In order to better illustrate these asymptotic forms, it is convenient to introduce the dimensionless anomalous average

$$\sigma \equiv \frac{\sigma_1}{\rho} \ . \tag{2.213}$$

Also, let us define the dimensionless temperature

$$t \equiv \frac{mT}{\rho^{2/3}} \tag{2.214}$$

and the dimensionless sound velocity

$$s \equiv \frac{mc}{\rho^{1/3}} \,. \tag{2.215}$$

In this notation, the low-temperature expansion (2.209) becomes

$$\sigma \simeq \sigma_0 - \frac{s^3}{3\pi^2} \alpha \left(1 - \alpha + 6\alpha^2\right) , \qquad (2.216)$$

when  $t \to 0$ , with

$$\alpha = \left(\frac{\pi t}{2s^2}\right)^2 \,. \tag{2.217}$$

In the case of the local potential (2.169), it is convenient to introduce the gas parameter

$$\gamma \equiv \rho^{1/3} a_s \ . \tag{2.218}$$

Then the zero-temperature expression for the anomalous average (2.204) reads as

$$\sigma_0 = \frac{2s^2}{\pi^2} \sqrt{\pi \gamma n_0} \,. \tag{2.219}$$

The critical limit (2.212), in dimensionless units takes the form

$$\sigma \simeq -\frac{st}{2\pi} \qquad (t \to t_c) . \tag{2.220}$$

For the critical temperature, we obtain [57,97,98]

$$t_c = 3.312498 . (2.221)$$

This coincides with the BEC temperature for the ideal Bose gas, as it should be in the case of a mean-field picture [57].

It is important to use the correct form for the anomalous average in order to get a selfconsistent description of the system thermodynamics. At low temperatures, outside of the critical region, expression (2.206) can be employed. But in the near vicinity of  $T_c$ , the correct behavior of the anomalous average is prescribed by Eq. (2.212). It is possible to check by direct numerical calculations [98] that the asymptotic form (2.212) guarantees the *second order* of the BEC phase transition for *any value* of the gas parameter (2.218). While, if one takes another expression for the critical behavior of the anomalous average, one can get a first-order transition, which would be incorrect. For instance, omitting the anomalous average, as is done in the Shohno model [83], one always gets the wrong first order of the BEC transition. It is worth stressing that the BEC phase transition must be of second order for arbitrary interaction strength [57].

To emphasize the second order of the BEC transition in the self-consistent theory described above, let us present some asymptotic expansions in powers of the relative temperature

$$\tau \equiv \left| \frac{t - t_c}{t_c} \right| \to 0$$
.

Using the asymptotic expression (2.220), we find the dimensionless sound velocity (2.215),

$$s \simeq \frac{3\pi}{t_c} \tau + \frac{9\pi}{4t_c} \left( 1 - \frac{2\pi}{\gamma t_c^2} \right) \tau^2 ,$$
 (2.222)

the condensate fraction (2.186),

$$n_0 \simeq \frac{3}{2} \tau - \frac{3}{8} \tau^2 , \qquad (2.223)$$

the anomalous average (2.213),

$$\sigma \simeq -\frac{3}{2}\tau + \frac{3}{8}\left(1 + \frac{6\pi}{\gamma t_c^2}\right)\tau^2, \qquad (2.224)$$

and the superfluid fraction (2.188),

$$n_s \simeq \frac{3}{2} \tau - \frac{3}{8} \left( 1 + \frac{132.413}{t_c^3} \right) \tau^2 = \frac{3}{2} \tau - 1.741 \tau^2 .$$
 (2.225)

These expansions explicitly demonstrate the second order of the BEC transition for arbitrary nonzero gas parameters  $\gamma > 0$ .

Let us also recall that liquid <sup>4</sup>He is a strongly interacting system exhibiting superfluid phase transition of *second order* [108,126–130]. At low temperature, superfluid helium can be characterized [130,131] by the gas parameter  $\gamma_{He} \cong 0.6$ . But at high temperatures, more realistic potentials should be used. Such potentials contain, as a rule, hard cores, which requires to take into account short-range correlations [10,119–122]. The latter are often described in the frame of the Jastrow approximation [132–136].

An important point is that the two-body scattering matrix [137] can be shown to be directly related to the total anomalous average (2.180). The latter, for a general nonuniform system, can be represented as

$$\Delta_k = \int \Phi(\mathbf{r} - \mathbf{r}') < \varphi_k^*(\mathbf{r})\varphi_{-k}(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) > d\mathbf{r}d\mathbf{r}' , \qquad (2.226)$$

which describes the scattering of two particles. For a uniform system, the scattering process ends with the plane waves  $\varphi_k(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})/\sqrt{V}$ . Then Eq. (2.226) becomes

$$\Delta_k = \int \Phi(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} < \hat{\psi}(\mathbf{r})\hat{\psi}(0) > d\mathbf{r} . \qquad (2.227)$$

Using here the Bogolubov shift (2.81) gives exactly Eq. (2.180).

On the other hand, the two-body scattering matrix can be defined as a solution of a Lippman-Schwinger equation [138,139], which, in the limit of weak interactions, results in the total anomalous average (2.180) evaluated in the same weak-coupling limit [140–142].

For weak interactions, when  $\rho_0 \approx \rho$ , the anomalous average (2.180), in view of Eq. (2.184), can be rewritten as

$$\Delta_k \simeq \rho \overline{\Phi}_k \qquad (\rho_0 \to \rho) , \qquad (2.228)$$

where the notation for an effective potential

$$\widetilde{\Phi}_{k} = \Phi_{k} - \frac{1}{V} \sum_{p} \widetilde{\Phi}_{p} \frac{\Phi_{k+p}}{2\varepsilon_{p}} \coth\left(\frac{\varepsilon_{p}}{2T}\right)$$
(2.229)

is introduced. As is clear, Eq. (2.229) is nothing but a particular form of the Lippman-Schwinger equation. For a symmetric interaction potential, for which  $\Phi_{-k} = \Phi_k$ , the effective potential  $\widetilde{\Phi}_{-k} = \widetilde{\Phi}_k$  is also symmetric.

Assuming that the potential  $\Phi_k$  fastly diminishes as  $k \to \infty$ , with the maximum of  $\Phi_k$  at the point k = 0, and keeping in mind weak interactions, we can invoke the following approximation:

$$\sum_{p} \widetilde{\Phi}_{p} \, \frac{\Phi_{k+p}}{2\varepsilon_{p}} \coth\left(\frac{\varepsilon_{k}}{2T}\right) \cong \widetilde{\Phi}_{k} \sum_{k} \frac{\Phi_{k+p}}{2\varepsilon_{p}} \left[ \coth\left(\frac{\varepsilon_{k}}{2T}\right) - 1 \right] \,. \tag{2.230}$$

Then Eq. (2.229) is solved for the effective potential

$$\widetilde{\Phi}_{k} = \frac{\Phi_{k}}{1 + \frac{1}{V} \sum_{p} \frac{\Phi_{k+p}}{2\varepsilon_{p}} \left[ \operatorname{coth} \left( \frac{\varepsilon_{k}}{2T} \right) - 1 \right]} \,.$$
(2.231)

For the local potential (2.169), the sum in the denominator of the above expression can be represented as

$$\frac{1}{V} \sum_{p} \frac{1}{2\varepsilon_{p}} \left[ \coth\left(\frac{\varepsilon_{p}}{2T} - 1\right) \right] \equiv m^{2} c J , \qquad (2.232)$$

with the integral

$$J = \frac{\sqrt{2}}{(2\pi)^2} \int_0^\infty \frac{(\sqrt{1+x^2}-1)^{1/2}}{\sqrt{1+x^2}} \left[ \coth\left(\frac{mc^2}{2T}x\right) - 1 \right] dx .$$
 (2.233)

Thus, for the local potential (2.169) since  $\Phi_k = \Phi_0$ , one gets

$$\widetilde{\Phi}_0 = \frac{\Phi_0}{1 + m^2 c J \Phi_0} \,. \tag{2.234}$$

Defining an effective scattering length  $\tilde{a}_s$  through the notation

$$\widetilde{\Phi}_0 \equiv 4\pi \; \frac{\widetilde{a}_s}{m} \;, \tag{2.235}$$

we have

$$\widetilde{a}_s = \frac{a_s}{1 + 4\pi a_s m c J} \ . \tag{2.236}$$

Similarly, one can introduce an *effective gas parameter* 

$$\widetilde{\gamma} \equiv \rho^{1/3} \widetilde{a}_s , \qquad (2.237)$$

for which Eq. (2.236) gives

$$\widetilde{\gamma} = \frac{\gamma}{1 + 4\pi\gamma s J} \,. \tag{2.238}$$

At low temperature, integral (2.233) yields

$$J \simeq \frac{t^2}{12s^4} \qquad (t \to 0) \; .$$

And the effective scattering length (2.236) tends to the scattering length  $a_s$ ,

$$\widetilde{a}_s \simeq \left(1 - \frac{\pi\gamma}{3s^3} t^2\right) a_s \qquad (t \to 0) . \tag{2.239}$$

In the vicinity of the critical temperature, when  $t \to t_c$ , the sound velocity s tends to zero,  $s \to 0$ , according to Eq. (2.222). Then integral (2.233) results in

$$J \simeq \frac{t}{2\pi s^2} \qquad (t \to t_c) \;,$$

hence Eq. (2.236) gives

$$\widetilde{a}_s \simeq \frac{s}{2\gamma t} a_s \qquad (t \to t_c) ,$$
(2.240)

which tends to zero.

The above analysis shows that the use of the two-body scattering matrix is equivalent to the HFB approximation in the weak-coupling limit. However, aiming at considering strong interactions, one is forced to return back to the anomalous average (2.196) expressed through a divergent integral. The latter can be regularized involving some kind of an analytic regularization, such as the dimensional regularization [11,125,143]. The latter gives the zerotemperature anomalous average (2.204). But near the critical temperature the anomalous average behaves as in Eq. (2.212). The correct overall behavior of the anomalous average (2.196) should interpolate between the noncritical form (2.210), valid outside of the critical region, and the critical asymptotic expression (2.212).

### 2.14 Particle Fluctuations

The problem of particle fluctuations in Bose-condensed systems has attracted a great deal of attention provoking controversy in theoretical literature. Many tens of papers have been published claiming the existence of thermodynamically anomalous particle fluctuations in Bose-condensed systems everywhere below the critical temperature. A detailed account of this trend, with many citations, can be found in the recent survey [144]. However, the occurrence of such thermodynamically anomalous particle fluctuations, as has been explained in Refs. [10,93,145,146], contradicts the rigorous theoretical relations as well as contravenes all known experiments. It is therefore important to pay some more attention to this problem.

First of all, it is necessary to specify terminology. Observable quantities are represented by self-adjoint operators. Fluctuations of an observable quantity, associated with an operator  $\hat{A}$ , are characterized by the operator dispersion

$$\Delta^2(\hat{A}) \equiv \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2 .$$
 (2.241)

Generally, in statistical mechanics, one distinguishes intensive and extensive quantities [147]. Fluctuations of intensive quantities are always finite, so that if  $\hat{A}$  represents an intensive quantity, then its dispersion (2.241) is finite. Fluctuations of extensive quantities are described by dispersions (2.241) proportional to the system volume or to the total number of particles N. Fluctuations are termed *thermodynamically normal*, when

$$0 \leq \frac{\Delta^2(\hat{A})}{N} < \infty \tag{2.242}$$

for any N, including the thermodynamic limit  $N \to \infty$ . Condition (2.242) holds for any operators of observables, whether intensive or extensive, which guarantees the system stability [10,93,146].

The number of particles in the system is represented by an operator  $\hat{N}$ . So, particle fluctuations are characterized by the dispersion

$$\Delta^2(\hat{N}) \equiv \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 . \qquad (2.243)$$

Similarly to condition (2.242), particle fluctuations are thermodynamically normal, provided that

$$0 \leq \frac{\Delta^2(\hat{N})}{N} < \infty \tag{2.244}$$

for any N, including  $N \to \infty$ .

The fact why conditions (2.242) or (2.244) are to be valid for any stable statistical system is that the reduced dispersions  $\Delta^2(\hat{A})/N$  describe the system susceptibilities, which also are observable quantities. More precisely, susceptibilities are intensive thermodynamic characteristics, hence, they have to be finite for any stable statistical system, except, may be, the points of phase transitions, where the system is, actually, unstable. But the possible divergence of susceptibilities at phase-transition points should not be confused with their thermodynamic divergence. At a phase-transition point, a susceptibility could become divergent with respect to some thermodynamic parameter, such as temperature, pressure, etc. However it is never divergent with respect to the system volume or number of particles.

Particle fluctuations are directly related to the isothermal compressibility

$$\kappa_T \equiv -\frac{1}{V} \left(\frac{\partial P}{\partial V}\right)_T^{-1} = \frac{\Delta^2(\hat{N})}{\rho T N} , \qquad (2.245)$$

where P is pressure, and to the hydrodynamic sound velocity  $s_T$ , given by the equation

$$s_T \equiv \frac{1}{m} \left( \frac{\partial P}{\partial \rho} \right)_T = \frac{1}{m\rho\kappa_T} = \frac{NT}{m\Delta^2(\hat{N})} \,. \tag{2.246}$$

The structure factor

$$S(\mathbf{k}) = 1 + \rho \int \left[g(\mathbf{r}) - 1\right] e^{-i\mathbf{k}\cdot\mathbf{r}} \, d\mathbf{r} \,, \qquad (2.247)$$

in which  $g(\mathbf{r})$  is a pair correlation function [148], is also expressed through the particle dispersion (2.243), so that

$$S(0) = \rho T \kappa_T = \frac{T}{m s_T^2} = \frac{\Delta^2(N)}{N} .$$
 (2.248)

As is evident, all these observable quantities,  $\kappa_T$ ,  $s_T$ , and  $S(\mathbf{k})$ , are finite then and only then, when the particle fluctuations are normal, satisfying condition (2.244).

Fluctuations of an observable, represented by an operator A, are called *thermodynamically* anomalous, when condition (2.242) does not hold, as a result of which

$$\frac{\Delta^2(\hat{A})}{N} \to \infty \qquad (N \to \infty) \quad (anomalous) \; .$$

Clearly, if particle fluctuations would be thermodynamically anomalous, then the isothermal compressibility (2.245) would be infinite, sound velocity (2.246), zero, and the structure factor (2.248) would also be infinite, all that manifesting the system instability [10,93,146].

The thermodynamically normal properties of susceptibilities do not depend on the used statistical ensemble, provided that the representative ensembles are employed [54,56,57]. The microcanonical ensemble can be considered as a projection of the canonical one, and the canonical ensemble, as a projection of the grand canonical ensemble [149]. For any representative ensemble, susceptibilities should be finite almost everywhere, except the points of phase transitions. For example, in the grand canonical ensemble, the compressibility can be found from the dispersion  $\Delta^2(\hat{N})$ , as in Eq. (2.245). In the canonical ensemble, the total number of particles is fixed. But this does not mean that the compressibility here becomes zero. One simply has to use another formula for calculating the compressibility, which in the canonical ensemble can be calculated by means of the expression

$$\kappa_T = \frac{1}{V} \left( \frac{\partial^2 F}{\partial V^2} \right)_{TN}^{-1} , \qquad (2.249)$$

where F is free energy. The compressibilities (2.245) and (2.249) have to be the same, defining the same observable quantities as the sound velocity (2.246) or the structure factor (2.247). This concerns any statistical system, including Bose-condensed ones [150–152]. In all experiments, whether with cold trapped atoms or with superfluid helium, all intensive quantities below  $T_c$  are, of course, finite, including particle fluctuations measured as  $\Delta^2(\hat{N})/N$  (see Ref. [153]). Divergencies can arise solely at the critical point itself [154].

When one claims the occurrence of thermodynamically anomalous particle fluctuations in Bose-condensed systems [144], one often tells that these anomalous fluctuations may happen not for the total number of particles but only separately for the number of condensed and uncondensed atoms. The operator of the total number of atoms is the sum  $\hat{N} = \hat{N}_0 + \hat{N}_1$ . One assumes that the fluctuations of  $\hat{N}$ , given by the relative dispersion  $\Delta^2(\hat{N})/N$  could be normal, thus, not breaking the system stability, while the fluctuations of  $\hat{N}_0$  and  $\hat{N}_1$  could be anomalous. This assumption is, however, wrong [93,146]. Let us consider two operators  $\hat{A}$  and  $\hat{B}$ , representing some observable quantities. The dispersion of their sum

$$\Delta^{2}(\hat{A} + \hat{B}) = \Delta^{2}(\hat{A}) + \Delta^{2}(\hat{B}) + 2\text{cov}\left(\hat{A}, \hat{B}\right)$$
(2.250)

is expressed through the particle dispersions  $\Delta^2(\hat{A})$  and  $\Delta^2(\hat{B})$  and the covariance

$$cov(\hat{A} + \hat{B}) \equiv \frac{1}{2} < \hat{A}\hat{B} + \hat{B}\hat{A} > - < \hat{A} > < \hat{B} > -$$

The dispersions  $\Delta^2(\hat{A})$  and  $\Delta^2(\hat{B})$  are, by definition, positive or, at least, non-negative, while the covariance can be of any sign. However the covariance cannot compensate the partial dispersions, so that the total dispersion (2.250) is always governed by the largest partial dispersion. This rigorously follows from the theorem below.

**Theorem** (Yukalov [93,146]) The dispersion of the sum of linearly independent selfadjoint operators (2.250) can be represented as

$$\Delta^{2}(\hat{A} + \hat{B}) = \left[\sqrt{\Delta^{2}(\hat{A})} - \sqrt{\Delta^{2}(\hat{B})}\right]^{2} + c_{AB}\sqrt{\Delta^{2}(\hat{A})\Delta^{2}(\hat{B})}, \qquad (2.251)$$

where

$$0 < c_{AB} < 4$$
.

From here it follows that fluctuations of the sum of two operators  $\hat{A} + \hat{B}$  is thermodynamically anomalous then and only then, when at least one of the partial fluctuations of either  $\hat{A}$  or  $\hat{B}$  is anomalous, the anomaly of the total dispersion  $\Delta^2(\hat{A} + \hat{B})$  being governed by the largest partial dispersion. Conversely, fluctuations of the sum  $\hat{A} + \hat{B}$  are thermodynamically normal if and only if all partial fluctuations are thermodynamically normal.

Applying this theorem to the sum  $\hat{N} = \hat{N}_0 + \hat{N}_1$ , we see that, if the total dispersion  $\Delta^2(\hat{N})$  is thermodynamically normal, which is compulsory for any stable system, then both partial dispersions,  $\Delta^2(\hat{N}_0)$  as well as  $\Delta^2(\hat{N}_1)$ , must be normal. Thus, the normality of fluctuations of the total number of particles  $\hat{N}$  necessarily requires the normality of fluctuations of both condensed as well as uncondensed atoms.

A very widespread misconception is that the condensate fluctuations in the grand canonical and canonical ensembles are different; in the grand canonical ensemble the fluctuations are thermodynamically anomalous, such that  $\Delta^2(\hat{N}_0) \sim N^2$ , while in the canonical ensemble they are normal. One even calls this "the grand canonical catastrophe". But there is no any "catastrophe" here. The seeming paradox comes about only because of the use of nonrepresentative ensembles [93]. The problem has been explained long time ago by ter Haar [155]. The anomalous behavior  $\Delta^2(\hat{N}_0) \sim N^2$  appears in the grand canonical ensemble preserving the gauge symmetry, while in the canonical ensemble, the gauge symmetry is effectively broken. However, if the gauge symmetry is also broken in the grand canonical ensemble, then no anomalous behavior of  $\Delta^2(\hat{N}_0)$  arises, this dispersion being the same in both ensembles [93,155]. Recall that the gauge symmetry breaking is necessary and sufficient for describing statistical systems with BEC [63]. Breaking the gauge symmetry by means of the Bogolubov shift (2.81), we pass to the Fock space  $\mathcal{F}(\psi_1)$ , where the number operator of condensed atoms is  $\hat{N}_0 = N_0 \hat{1}_{\mathcal{F}}$ , as in Eq. (2.85). Then  $\Delta^2(\hat{N}_0)$  becomes identically zero. If one prefers to work in the Fock space  $\mathcal{F}(\psi)$ , as is explained in Sec. 2.6, then the field operator  $\psi_0(\mathbf{r})$  becomes a function  $\eta(\mathbf{r})$  in the thermodynamic limit. According to the Bogolubov theorem, it is easy to show [63] that

$$\lim_{N \to \infty} \frac{\Delta^2(N_0)}{N} \equiv 0 \tag{2.252}$$

in the Fock space  $\mathcal{F}(\psi)$ . The latter is orthogonal to the space  $\mathcal{F}(\psi_1)$ . The operator representations on these spaces are unitary nonequivalent [99,156]. But in any case, the limit (2.252) holds true. Therefore, all particle fluctuations are, actually, caused by the uncondensed atoms, since

$$\frac{\Delta^2(\hat{N})}{N} \cong \frac{\Delta^2(\hat{N}_1)}{N} \tag{2.253}$$

for large  $N \to \infty$ .

In the Bogolubov approximation, as well as in the HFB approximation, for a uniform system we have [10,145,146]

$$\frac{\Delta^2(\hat{N}_1)}{N} = \frac{T}{mc^2} , \qquad (2.254)$$

with the sound velocity c in the corresponding approximation. All these fluctuations, described by Eqs. (2.252), (2.253), and (2.254), are clearly thermodynamically normal.

It is worth mentioning that particle fluctuations in uniform systems with BEC are normal for *interacting* systems. For an ideal Bose gas, they are anomalous, which immediately follows from Eq. (2.254), if one sets there  $c \to 0$ , that is, reducing interactions to zero. More precisely, for an ideal uniform Bose-condensed gas, it is easy to find [93] that

$$\frac{\Delta^2(\hat{N}_1)}{N} \sim \left(\frac{mT}{\pi}\right)^2 \frac{N^{1/3}}{\rho^{4/3}} \qquad (ideal \ gas) \ ,$$

which means anomalous fluctuations. This implies that the ideal uniform gas with BEC cannot exist, being an unstable object [10,93,145,146]. Fortunately, the purely ideal gas certainly does not exist, being just a cartoon of weakly interacting systems. Real atoms always interact with each other, at least weakly. No matter how small the interaction, it does stabilize uniform Bose-condensed systems. External fields, forming trapping potentials, can also stabilize an ideal Bose gas, for instance, if the trapping is realized by harmonic potentials [157] or power-law (though not all) potentials [41].

Thus, any stable statistical system of interacting atoms, whether uniform or not, must display thermodynamically normal particle fluctuations. At the same time, as has been emphasized at the beginning of the present section, many papers claim the occurrence of anomalous particle fluctuations everywhere below  $T_c$ , as is summarized in Ref. [144]. These anomalous fluctuations are claimed to be of the type  $\Delta^2(\hat{N}_1) \propto N^{4/3}$  for interacting Bosecondensed systems of any nature, whether uniform or nonuniform trapped clouds. Moreover, since Bose-condensed systems are just one particular example of a very general class of systems with a broken continuous symmetry, the same type of fluctuations has to arise in all such systems [10,146]. This class of systems is really rather wide. In addition to cold trapped atoms, it includes superfluid <sup>4</sup>He, with broken gauge symmetry, isotropic magnets, with broken spin-rotational symmetry, and all solids, with broken transitional and rotational symmetries. If such systems would possess some divergent susceptibilities, this would mean that they could not exist as a stable matter. There would be no superfluids, many magnets, and no solids. It is evident that such an exotic conclusion would be meaningless. - We perfectly know that all that matter does exist and no one experiment has ever revealed any anomalous susceptibility that would persistently be anomalous everywhere below the critical temperature [158,159]. The same concerns theoretical investigations for exactly solvable models [160] as well as correct calculations for other concrete models [58].

It is instructive to consider the magnetic susceptibility of isotropic magnets. If the compressibility of Bose systems would be really divergent as  $N^{1/3}$ , when  $N \to \infty$ , then the magnetic susceptibility would also display the same divergence as  $N^{1/3}$ .

Let us turn, first, to the isotropic ferromagnet described by the Heisenberg model [161,162]. The sample magnetization is given by the vector  $\mathbf{M} = \{M_{\alpha}\}$ , with  $\alpha = x, y, z$ , defined as the statistical average

$$\mathbf{M} = \langle \hat{\mathbf{M}} \rangle, \qquad \hat{\mathbf{M}} = \mu_S N \hat{\mathbf{S}}$$

in which  $\mu_S = g_S \mu_B$ ,  $g_S$  is the gyromagnetic ratio for spin S,  $\mu_B$  is the Bohr magneton, and

$$\mathbf{S} \equiv \frac{1}{N} \sum_{j=1}^{N} \mathbf{S}_j = \{\hat{S}_{\alpha}\}$$

is the reduced spin operator. The susceptibility tensor is defined as the response of the magnetization to the variation of an external field  $\mathbf{H} = \{h_{\alpha}\}$ , so that

$$\chi_{\alpha\beta} \equiv \lim_{h \to 0} \frac{1}{N} \frac{\partial M_{\alpha}}{\partial h_{\beta}} = \frac{\mu_S^2}{T} \operatorname{cov}(\hat{S}_{\alpha}, \hat{S}_{\beta}) .$$
(2.255)

The diagonal magnetic susceptibility

$$\chi_{\alpha\alpha} = \frac{\mu_S^2}{T} \,\Delta^2(\hat{S}_\alpha) \tag{2.256}$$

is expressed through the dispersion of the spin operator  $\hat{S}_{\alpha}$ . Let **M** be directed along the *z*-axis,  $\mathbf{M} = \{M_z, 0, 0\}$ , with

$$M_z = N\mu_S S\sigma$$
,  $\sigma \equiv \frac{\langle S_z \rangle}{S}$ .

Then it is convenient to distinguish the longitudinal susceptibility

$$\chi_{||} \equiv \lim_{h \to 0} \frac{1}{N} \frac{\partial M_z}{\partial h_z} = \frac{\mu_S^2}{T} \Delta^2(\hat{S}_z)$$
(2.257)

and the transverse susceptibility

$$\chi_{\perp} \equiv \lim_{h \to 0} \frac{1}{N} \frac{\partial M_z}{\partial h_x} = \frac{\mu_S^2}{T} \operatorname{cov}(\hat{S}_z, \hat{S}_x) .$$
(2.258)

In the mean-field approximation, the longitudinal susceptibility is

$$\chi_{||} = \frac{S\mu_S^2(1-\sigma)}{2T - JS(1-\sigma)} , \qquad (2.259)$$

where, for spin one-half,

$$\sigma = \tanh \frac{JS\sigma + \mu_S h_0}{2T} ,$$

J is an exchange integral (J > 0), and  $h_0$  is an anisotropy field along the z-axis. Expression (2.259) is finite everywhere below  $T_c$ , even when  $h_0 \rightarrow 0$ . This means, in view of Eq. (2.257), that spin fluctuations are normal.

For the transverse susceptibility (2.258), one gets

$$\chi_{\perp} = \frac{\mu_S S \sigma}{h_0} \,. \tag{2.260}$$

In all real magnets, there always exists an anisotropy field, caused by one of many reasons, such as the natural magnetic lattice anisotropy, spin-orbital interactions, demagnetizing shape factors, and so on, including the Earth magnetic field. Therefore, in real life, the transverse susceptibility (2.260) is finite, no matter how small the anisotropy field.

Even if we consider an ideal situation with no anisotropy, when  $\chi_{\perp}$  diverges with respect to  $h_0 \rightarrow 0$ , this divergence does not make susceptibility (2.260) thermodynamically anomalous. The transverse susceptibility remains *thermodynamically normal*, since it does not diverge with respect to  $N \rightarrow \infty$ .

Recall that the mathematically correct order of the limits, according to the Bogolubov method of quasi-averages [64,65], is in taking first the thermodynamic limit  $N \to \infty$  and only after it, to consider the limit  $h_0 \to 0$ . Since susceptibility (2.260) does not diverge with respect to  $N \to \infty$ , it is thermodynamically normal.

Similarly, the divergence of the longitudinal susceptibility (2.257) with respect to  $T \to T_c$ , when

$$\chi_{||} \propto \left| 1 - \frac{T}{T_c} \right|^{-\gamma} \qquad (T \to T_c) \;,$$

with  $\gamma > 0$ , does not imply thermodynamically anomalous behavior. For any  $T \neq T_c$ , the susceptibility  $\chi_{||}$  is finite under the limit  $N \to \infty$ . So, the above expression  $\chi_{||}$  is also thermodynamically normal. In addition, we should remember that, exactly at the critical temperature  $T_c$ , the system is unstable.

In the same way, one can check that the susceptibilities of isotropic antiferromagnets are also thermodynamically normal [161,163].

The appearance in some theoretical works of thermodynamically anomalous susceptibilities in magnets or thermodynamically anomalous particle fluctuations in Bose-condensed systems is due solely to calculational mistakes. The standard such a mistake, as is explained in Refs. [10,93,145,146], is as follows. One assumes the Bogolubov approximation [72,73], which is a second-order accuracy approximation with respect to the operators of uncondensed particles, or one accepts a hydrodynamic approximation, which, actually, is mathematically equivalent to the Bogolubov approximation, also being a second-order approximation with respect to some field operators. The higher-order terms, higher than two, are not well defined in the second-order theory. Forgetting this, one calculates the fourth-order operator terms in the frame of a second-order theory. This inconsistency results in the arising anomalous expressions, which are just calculational artifacts, and thus have no physical meaning. The detailed explanation can be found in Refs. [10,93,145,146].

The fact that condition (2.242) has to be valid for any observable can be simply understood in the following way. The average of an operator  $\hat{A}$ , associated with an extensive observable quantity, is such that  $\langle \hat{A} \rangle \propto N$ . Hence, condition (2.242) is equivalent to the condition

$$0 \leq \frac{\Delta^2(\hat{A})}{|<\hat{A}>|} < \infty ,$$

meaning that the fluctuations of an observable cannot be infinitely larger than the observable itself.

Thus, in any correct theory, all susceptibilities as well as fluctuations of observables are always thermodynamically normal. Conditions (2.242), or (2.244), are necessary for the stability of statistical systems. There are no experimental observations that would display thermodynamically anomalous susceptibilities in any system with broken continuous symmetry, neither in trapped atoms, nor in liquid helium, nor in magnets, nor in solids.

#### 2.15 Fragmented Condensates

The consideration of the previous sections, treating a Bose system with a sole BEC, can be generalized to the case, when several condensates arise in the system. There exist two principally different situations for the appearance of multiple condensates, depending on how the latter are distinguished. The distinction can be done according to two different kinds of the quantum numbers labelling quantum states. One type of the indices labels collective quantum states. Such has been the index (multi-index) k labelling natural orbitals  $\varphi_k(\mathbf{r})$ in the previous sections. The indices of another type are those characterizing the internal states of each particle, because of which such indices can be termed internal or individual. Examples of the individual indices are spin indices, hyperfine spin or isospin indices, and like that. Briefly speaking, collective indices are associated with collective quantum states of quasiparticles that are members of a statistical system, while individual indices describe the internal states of each separate particle. Respectively, there can be two types of multiple condensates, depending on whether they are distinguished by collective or internal quantum numbers.

In a single-component statistical system, the arising BEC corresponds to the macroscopic occupation of one of the quantum states characterized by natural orbitals, as has been described in Sections 2.1 and 2.2. One can assume that not one but several occupation numbers, related to natural orbitals, become macroscopic. Then the arising multiple condensates are distinguished by the collective quantum index k, labelling the appropriate natural orbitals. This case of multiple condensates is what one calls the condensate fragmentation.

The fragmented condensate is a multiple condensate consisting of several coexisting condensates distinguished by the collective quantum index labelling the natural orbitals.

Probably, the first example of the fragmented condensate was given by Pollock [164], who considered the coexistence of two condensates, one with the zero angular momentum and another with a nonzero angular momentum. The term "fragmented condensates" was

coined by Nozières and Saint James [165], who considered the coexisting condensates with zero and nonzero momenta. These condensates in equilibrium were shown [164,165] to be unstable. This conclusion looks rather clear, since the appearance of a condensate with either a nonzero momentum or nonzero angular momentum rises the system free energy.

In order to remain stable, the fragmented condensate should consist of degenerate parts, such that, though being described by different natural orbitals, they contribute to the system the same energy. An example is the fragmented quasicondensate whose parts possess the same modulus of momentum but various arbitrary momentum directions [166–169]. Here, it is called the quasicondensate, since the order index  $\omega(\hat{\rho}_1)$ , defined in Sec. 2.3., is  $\omega(\hat{\rho}_1) = 1/3$ , which corresponds to mid-range order, as classified in Eq. (2.14) (see details in Ref. [45]).

Fragmented condensates can be created in nonequilibrium systems. For example, in the process of superradiant Rayleigh scattering [170–173] a single BEC separates into several clouds with different momenta. Another example is a Bose system subject to resonant external fields generating nonequilibrium condensates corresponding to different coherent topological modes [174–196].

Fragmented condensates, as they are defined by Pollock [164] and Nozières and Saint James [165], should not be confused with multicomponent condensates. To avoid this confusion, let us give a precise mathematical definition of the fragmented condensates.

Consider a single-component Bose system, whose natural orbitals  $\varphi_k(\mathbf{r})$ , associated with the first-order density matrix, are labelled by a multi-index k. Let the total set  $\{k\}$  of all collective indices k contain a subset  $\{k_{\nu}\}$ , such that  $\{k_{\nu}\} \subset \{k\}$ . The enumeration of the members  $k_{\nu}$  of the subset  $\{k_{\nu}\}$  can be either continuous over a final interval  $0 \leq \nu \leq \nu_{max}$ or can be discrete, when  $\nu = 0, 1, 2, ...$ 

Expanding the field operator over natural orbitals, one has

$$\psi(\mathbf{r}) = \sum_{k} a_k \varphi_k(\mathbf{r}) = \sum_{\nu} \psi_{k_{\nu}}(\mathbf{r}) + \psi_1(\mathbf{r}) . \qquad (2.261)$$

Here the terms

$$\psi_{k_{\nu}}(\mathbf{r}) \equiv a_{k_{\nu}}\varphi_{k_{\nu}}(\mathbf{r}) \tag{2.262}$$

are assumed to be related to the expected fragmented condensates, while the term

$$\psi_1(\mathbf{r}) \equiv \sum_{k \neq k_\nu} a_k \varphi_k(\mathbf{r}) \tag{2.263}$$

corresponds to uncondensed particles. The condition  $k \neq k_{\nu}$  implies that k does not equal any  $k_{\nu}$  from the set  $\{k_{\nu}\}$ .

For  $\varphi_k(\mathbf{r})$  to represent natural orbitals, it is necessary and sufficient that the quantumnumber conservation condition be valid,

$$\langle a_k^{\dagger} a_p \rangle = \delta_{kp} n_k , \qquad n_k \equiv \langle a_k^{\dagger} a_k \rangle .$$
 (2.264)

Then the density matrix

$$\rho(\mathbf{r}, \mathbf{r}') \equiv \langle \psi^{\dagger}(\mathbf{r}')\psi(\mathbf{r}) \rangle = \sum_{k} n_{k}\varphi_{k}(\mathbf{r})\varphi_{k}^{*}(\mathbf{r}') \qquad (2.265)$$

is diagonal in the expansion over natural orbitals.

The terms (2.262) correspond to condensates when

$$\lim_{N \to \infty} \frac{N_{k_{\nu}}}{N} > 0 \qquad (N_{k_{\nu}} \equiv n_{k_{\nu}}) .$$
(2.266)

If so, the density matrix (2.265) can be separated into two parts,

$$\rho(\mathbf{r},\mathbf{r}') = \sum_{\nu} N_{k_{\nu}}\varphi_{k_{\nu}}(\mathbf{r})\varphi_{k_{\nu}}^{*}(\mathbf{r}') + \sum_{k\neq k_{\nu}} n_{k}\varphi_{k}(\mathbf{r})\varphi_{k}^{*}(\mathbf{r}') , \qquad (2.267)$$

where the first sum represents the fragmented condensate.

Realizing the Bogolubov shift, one has to replace the operator  $\psi(\mathbf{r})$  by the field operator

$$\hat{\psi}(\mathbf{r}) = \sum_{\nu} \eta_{\nu} + \psi_1(\mathbf{r}) . \qquad (2.268)$$

The grand Hamiltonian, in the case of the fragmented condensate, is

$$H = \hat{H}[\hat{\psi}] - \sum_{\nu} \mu_{k_{\nu}} \hat{N}_{k_{\nu}} - \mu_1 \hat{N}_1 - \hat{\Lambda} , \qquad (2.269)$$

where  $\hat{H}[\hat{\psi}]$  is the Hamiltonian energy operator (2.151) and the linear killer  $\hat{\Lambda} = \hat{\Lambda}[\psi_1]$  is defined as in Eq. (2.91). The system chemical potential generalizes form (2.111) to

$$\mu = \sum_{\nu} \mu_{k_{\nu}} n_{k_{\nu}} + \mu_1 n_1 , \qquad (2.270)$$

where

$$n_{k_{\nu}} \equiv \frac{N_{k_{\nu}}}{N}$$
,  $n_1 \equiv \frac{N_1}{N}$ .

To stress it again, the fragmented condensate, by definition [164,165], occurs, when several occupation numbers, associated with the *natural orbitals*, become macroscopic. This usually happens for nonequilibrium systems.

#### 2.16 Multicomponent Condensates

Contrary to fragmented condensates, which are rather rare and usually are not equilibrium, the multicomponent condensates are ubiquitous and may happen in any equilibrium system consisting of several kinds of Bose particles, distinguished by different internal numbers. The simplest case, studied long time ago [197–201], is the mixture of several components of Bose particles with different masses and different interactions with each other. Another example is the mixture of atoms with different spins or hyperfine states [202]. And there are plenty of other examples [203]. Among the systems formed by composite bosons, one can remember the systems of bipolarons composed of tightly bound electron pairs and of bound hole pairs [204] and also the mixtures of multiquark bosonic clusters [28,29].

For a multicomponent system, one has several types of field operators  $\psi_{\alpha}(\mathbf{r})$ , labelled by an individual index  $\alpha$ , which can be either discrete or continuous. Respectively, there exist several orthonormal bases  $\{\varphi_{\alpha k}(\mathbf{r})\}\$ , in which  $k = k(\alpha)$  are the indices labelling collective quantum states. Each component may possess BEC in a state labelled by  $k_0 = k_0(\alpha)$ . The related field operator can be expanded over the given basis as

$$\psi_{\alpha}(\mathbf{r}) = \sum_{k} a_{\alpha k} \varphi_{\alpha k}(\mathbf{r}) = \psi_{\alpha 0}(\mathbf{r}) + \psi_{\alpha 1}(\mathbf{r}) , \qquad (2.271)$$

where the first term

$$\psi_{\alpha 0}(\mathbf{r}) \equiv a_{\alpha 0}\varphi_{\alpha 0}(\mathbf{r}) \equiv a_{\alpha k_0}\varphi_{\alpha k_0}(\mathbf{r})$$
(2.272)

is assumed to describe the BEC of the  $\alpha$ -component, and the second term

$$\psi_{\alpha 1}(\mathbf{r}) \equiv \sum_{k \neq k_0} a_{\alpha k} \varphi_{\alpha k}(\mathbf{r})$$
(2.273)

represents uncondensed particle of that component.

If  $\varphi_{\alpha k}(\mathbf{r})$  are chosen as the natural orbitals, then the quantum-number conservation condition must be valid,

$$\langle a_{\alpha k}^{\dagger} a_{\beta p} \rangle = \delta_{\alpha \beta} \delta_{k p} n_{\alpha k} , \qquad n_{\alpha k} \equiv \langle a_{\alpha k}^{\dagger} a_{\alpha k} \rangle , \qquad (2.274)$$

similarly to condition (2.264). This guarantees that the density matrix

$$\rho_{\alpha\beta}(\mathbf{r},\mathbf{r}') \equiv \langle \psi_{\beta}^{\dagger}(\mathbf{r}')\psi_{\alpha}(\mathbf{r}) \rangle$$
(2.275)

be diagonal, such that

$$\rho_{\alpha\beta}(\mathbf{r},\mathbf{r}') = \delta_{\alpha\beta}\rho_{\alpha}(\mathbf{r},\mathbf{r}') , \qquad (2.276)$$

and that it would possess the diagonal expansion

$$\rho_{\alpha}(\mathbf{r}, \mathbf{r}') = \sum_{k} n_{\alpha k} \varphi_{\alpha k}(\mathbf{r}) \varphi_{\alpha k}^{*}(\mathbf{r}') . \qquad (2.277)$$

The  $\alpha$ -component enjoys condensation, when

$$\lim_{N \to \infty} \frac{N_{\alpha 0}}{N} > 0 \qquad (N_{\alpha 0} \equiv n_{\alpha k_0}) .$$
(2.278)

Then matrix (2.277) can be separated into two parts as

$$\rho_{\alpha}(\mathbf{r},\mathbf{r}') = N_{\alpha 0}\varphi_{\alpha 0}(\mathbf{r})\varphi_{\alpha 0}^{*}(\mathbf{r}') + \sum_{k \neq k_{0}} n_{\alpha k}\varphi_{\alpha k}(\mathbf{r})\varphi_{\alpha k}^{*}(\mathbf{r}') . \qquad (2.279)$$

The Bogolubov shift for a multicomponent system implies that each field operator  $\psi_{\alpha}(\mathbf{r})$  is to be replaced by

$$\hat{\psi}_{\alpha}(\mathbf{r}) = \eta_{\alpha}(\mathbf{r}) + \psi_{\alpha 1}(\mathbf{r}) . \qquad (2.280)$$

The corresponding grand Hamiltonian becomes

$$H = \hat{H}\left[\left\{\hat{\psi}_{\alpha}\right\}\right] - \sum_{\alpha} \left(\mu_{\alpha 0}\hat{N}_{\alpha 0} + \mu_{\alpha 1}\hat{N}_{\alpha 1} + \hat{\Lambda}_{\alpha}\right) , \qquad (2.281)$$

where  $\hat{\Lambda}_{\alpha} = \hat{\Lambda}_{\alpha}[\psi_{\alpha 1}].$ 

The total number of particles is

$$N = \sum_{\alpha} N_{\alpha} , \qquad N_{\alpha} = N_{\alpha 0} + N_{\alpha 1} .$$
 (2.282)

If there are no mutual transformations between different components, so that all  $N_{\alpha}$  are fixed, then the system has so many chemical potentials

$$\mu_{\alpha} = \mu_{\alpha 0} n_{\alpha 0} + \mu_{\alpha 1} n_{\alpha 1} \qquad (N_{\alpha} = const) \tag{2.283}$$

how many components it has. But if mutual transformations between components are allowed, so that only the total number of particles N is fixed, then all  $\mu_{\alpha} = \mu$ , and the system possesses the sole chemical potential

$$\mu = \mu_{\alpha 0} n_{\alpha 0} + \mu_{\alpha 1} n_{\alpha 1} \qquad (N = const) .$$
(2.284)

Here, the particle concentrations are

$$n_{\alpha 0} \equiv \frac{N_{\alpha 0}}{N} , \qquad n_{\alpha 1} \equiv \frac{N_{\alpha 1}}{N} . \qquad (2.285)$$

Comparing Sections 2.15 and 2.16, we see that there are important differences between fragmented and multicomponent condensates. Condensate fragmentation occurs in a singlecomponent system, whose several natural orbitals are macroscopically occupied. Multicomponent condensation happens in a multicomponent system, where several of the components acquire their own condensates. Of course, more complicated situations may occur, when multicomponent and fragmented condensates arise simultaneously.

In the case of multicomponent systems, a special care has to be taken with respect to the stability of the considered multicomponent mixture. Depending on the kind of the interactions in a multicomponent system, the latter can be unstable with reference to the component stratification [198–201], when the components spatially separate from each other, rendering the system to a set of single-component parts.

#### 2.17 Model Condensates

Simple models often are useful for quickly catching typical features of more complicated realistic systems. However, one should keep in mind that BEC might exist in a model, though could be absent in a realistic system that has been mimicked by the model. Or the properties of BEC in a cartoon model could be essentially distorted, as compared to the real case. As an example of such a situation, let us consider a very popular two-level model with BEC.

Let us assume that N atoms can occupy only two energy levels, one with energy  $E_1$  and another with energy  $E_2$ , such that  $E_1 < E_2$ . The related field operators,  $a_1$  and  $a_2$ , satisfy the commutation relations

$$\left[a_1, a_1^{\dagger}\right] = \left[a_2, a_2^{\dagger}\right] = 1$$
,  $\left[a_1, a_1\right] = \left[a_1, a_2\right] = \left[a_1, a_2^{\dagger}\right] = \left[a_2, a_2\right] = 0$ .

The condition that all N atoms pertain to one of two levels is

$$a_1^{\dagger}a_1 + a_2^{\dagger}a_2 = N . (2.286)$$

Also suppose that the state, corresponding to energy  $E_1$ , is symmetric with respect to spatial inversion, while the state, associated with energy  $E_2$ , is antisymmetric. The standard situation that is modelled by this picture is an ensemble of trapped atoms with discrete spectrum. When temperature is low and atomic interactions are weak, one assumes that all atoms pile down to the lowest energy levels, say, to the lowest two levels. These assumptions are typical when considering cold atoms in a double-well trap [203].

The symmetric and antisymmetric states can be represented by linear combinations of "left" and "right" field operators,  $c_L$  and  $c_R$ , respectively, so that

$$a_1 = \frac{1}{\sqrt{2}}(c_L + c_R), \qquad a_2 = \frac{1}{\sqrt{2}}(c_L - c_R).$$
 (2.287)

The operator  $a_1$  is symmetric with respect to the interchange of  $c_L$  and  $c_R$ , while the operator  $a_2$  is antisymmetric. The "left" and "right" field operators satisfy the same commutation relations as the operators  $a_1$  and  $a_2$ , in particular,

$$\left[c_L, c_L^{\dagger}\right] = \left[c_R, c_R^{\dagger}\right] = 1 ,$$

and other commutators being zero. Hence equations (2.287) and their converse,

$$c_L = \frac{1}{\sqrt{2}}(a_1 + a_2) , \qquad c_R = \frac{1}{\sqrt{2}}(a_1 - a_2) , \qquad (2.288)$$

represent canonical transformations. The new operators also obey the N-polarity condition

$$c_L^{\dagger}c_L + c_R^{\dagger}c_R = N . \qquad (2.289)$$

By assumption, the states, describing the two considered energy levels, correspond to natural orbitals. Consequently, the quantum-number conservation condition is to be valid,

$$\langle a_1^{\dagger} a_2 \rangle = 0$$
. (2.290)

Then, from Eq. (2.288), we have

$$< c_L^{\dagger} c_L > = < c_R^{\dagger} c_R > = \frac{N}{2} ,$$
 (2.291)

**A** 7

which means that the "left" and "right" sides are equally occupied. Also, we find

$$< c_L^{\dagger} c_R > = \frac{1}{2} \left( < a_1^{\dagger} a_1 > - < a_2^{\dagger} a_2 > \right)$$
 (2.292)

In view of normalization (2.286), we get

$$\langle c_L^{\dagger} c_R \rangle = \langle c_R^{\dagger} c_L \rangle = \langle a_1^{\dagger} a_1 \rangle - \frac{N}{2}$$

The value  $\langle a_1^{\dagger}a_1 \rangle$  depends on the strength of atomic interactions and temperature. These two factors deplete  $\langle a_1^{\dagger}a_1 \rangle$  from N, which can be represented as

$$\langle a_1^{\dagger}a_1 \rangle = N\left(1 - \frac{\delta}{2}\right) \qquad (0 \le \delta \le 1) ,$$

$$(2.293)$$

where  $\delta$  is a depletion factor. The occupation number of the second level becomes

$$\langle a_2^{\dagger} a_2 \rangle = \frac{N}{2} \delta$$
 (2.294)

And Eq. (2.292) yields

$$< c_L^{\dagger} c_R > = \frac{N}{2} (1 - \delta) .$$
 (2.295)

In an ideal gas at zero temperature, there is no depletion,  $\delta = 0$ , so that all atoms condense onto the lowest level,

$$\langle a_1^{\dagger}a_1 \rangle = N$$
,  $\langle a_2^{\dagger}a_2 \rangle = 0$   $(\delta = 0)$ .

For high temperature or strong repulsive interactions, the depletion is maximal,  $\delta = 1$ , which gives

$$\langle a_1^{\dagger} a_1 \rangle = \langle a_2^{\dagger} a_2 \rangle = \frac{N}{2} \qquad (\delta = 1)$$

The latter would mean that there appears the fragmented condensate. Such a conclusion, however, should not be treated seriously, if one remembers that the studied model has meaning only for very low temperatures and weak interactions. High temperatures and strong interactions would destroy any condensate as such, so that the arising fragmented condensate at those conditions is nothing but an artifact of an oversimplified model.

One could notice that the occupation numbers (2.293) and (2.294) are macroscopic for any finite depletion  $\delta > 0$ . Thus one could hope that there exist such low temperatures and weak interactions, when the depletion is already nonzero, however the two-level model is still appropriate, hence, the fragmented condensate could occur. But this hope seems to be invalid. The problem is that in any confining potential, including the double-well potential, the spectrum is countable, so that there are many other levels, except the two considered. The stronger the interactions, the closer the double-well spectrum to that of the harmonic oscillator [205]. No matter how small the temperature and interactions, they will spread atoms over higher levels, making all of them populated, so that the macroscopic population could remain solely on the single lowest level. In any confining potential, the fragmented condensate could exist only during finite time, as a nonequilibrium substance, as it happens for coherent topological modes [174–196]. But an equilibrium fragmented condensate, corresponding to two or more levels, seems to be impossible in a confining potential.

One sometimes calls the fragmented condensate the localized parts of the same condensate in a periodic potential, as in an optical lattice. This terminology, however, is not justified, since the lattice-site indices are not quantum numbers, in the same way as the "left" nd "right" indices in Eq. (2.295) are not good quantum numbers. Till there exists any tunneling between the lattice sites, there is no fragmentation, but there is the sole condensate with a periodic wave function. And if there is no tunneling, then again there is no fragmentation, but there can be merely several spatial separated condensates or no condensate at all, but an insulating Mott phase.

Concluding, equilibrium fragmented condensates could arise in model considerations. However one should be cautious interpreting them as actually existing in real physical systems. One should not forget the limitations of oversimplified models, sometimes yielding artificial results having no counterparts in real physical systems.

# **3** Regular Optical Lattices

#### **3.1** Optical Lattices

Optical lattices are formed by standing waves created by laser beams. Optical potentials are due to the interaction of the laser electric field with atomic transition dipoles corresponding to transitions between two internal atomic energy levels [16]. The laser frequency is taken to be far detuned from the atomic resonance, which allows for the definition of an effective optical potential. For large detuning, the excited level can be eliminated in the adiabatic approximation [16–18,206].

The optical potential, created by laser beams, in three dimensions, has the form

$$V_L(\mathbf{r}) = \sum_{\alpha=1}^3 V_\alpha \sin^2 \left(k_0^\alpha r_\alpha\right) , \qquad (3.1)$$

in which the wave vector  $\mathbf{k}_0 \equiv \{k_0^{\alpha}\}$  has the components

$$k_0^{\alpha} = \frac{2\pi}{\lambda_{\alpha}} = \frac{\pi}{a_{\alpha}} \qquad \left(a_{\alpha} = \frac{\lambda_{\alpha}}{2}\right) ,$$
 (3.2)

related to the laser wavelength  $\lambda_{\alpha}$ . Potential (3.1) can be rewritten as

$$V_L(\mathbf{r}) = \frac{3}{2} V_0 - \frac{1}{2} \sum_{\alpha=1}^{3} V_\alpha \cos(2k_0^{\alpha} r_{\alpha}) , \qquad (3.3)$$

where

$$V_0 \equiv \frac{1}{3} \sum_{\alpha=1}^{3} V_{\alpha} .$$
 (3.4)

The wave vector  $\mathbf{k}_0$  defines the *recoil energy* 

$$E_R \equiv \frac{k_0^2}{2m} \qquad (k_0 \equiv |\mathbf{k}_0|) .$$
 (3.5)

The lattice spacing in the  $\alpha$ -spatial direction is  $a_{\alpha}$ .

It is possible to create optical lattices in one and two dimensions as well. For instance, the one-dimensional optical potential is

$$V_L(z) = V_0 \sin^2(k_0 z) . (3.6)$$

Then the recoil energy (3.5) becomes

$$E_R = \frac{\pi^2}{2ma^2} \qquad \left(k_0 = \frac{\pi}{a}\right) , \qquad (3.7)$$

where a is the lattice spacing.

Keeping in mind, the local interaction potential (2.169), the energy Hamiltonian (2.151) is

$$\hat{H} = \int \hat{\psi}^{\dagger}(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + U + V_L \right) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \Phi_0 \int \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} , \qquad (3.8)$$

in which  $U = U(\mathbf{r})$  is an external, say trapping, potential and  $V_L = V_L(\mathbf{r})$  is an optical potential. The field operator  $\hat{\psi}(\mathbf{r})$  is the Bogolubov-shifted operator (2.81).

For the system to be stable, the particle dispersion

$$\Delta^2(\hat{N}) = T \,\frac{\partial N}{\partial \mu} = N \,\frac{T}{\rho} \,\frac{\partial \rho}{\partial \mu} \tag{3.9}$$

must satisfy the stability condition (2.244), which guarantees that the isothermal compressibility

$$\kappa_T = \frac{\Delta^2(\hat{N})}{\rho T N} = \frac{1}{\rho^2} \frac{\partial \rho}{\partial \mu}$$
(3.10)

is positive and finite.

In an optical lattice, the total number of particles N does not necessarily coincide with the number of the lattice sites  $N_L$ . Hence, the *filling factor* 

$$\nu \equiv \frac{N}{N_L} \qquad (0 < \nu < \infty) \tag{3.11}$$

can be any positive finite number. Defining the mean lattice spacing

$$a \equiv \left(\frac{V}{N_L}\right)^{1/d} \tag{3.12}$$

for a d-dimensional lattice, the filling factor (3.11) can be represented as

$$\rho a^d = \nu . (3.13)$$

Then, compressibility (3.10) takes the form

$$\kappa_T = \frac{a^d}{\nu^2} \frac{\partial \nu}{\partial \mu} \,. \tag{3.14}$$

The general consideration of Bose systems with broken gauge symmetry, given in Sec. 2, is applicable to systems with arbitrary external potentials. Therefore, similarly to Eq. (2.97), the grand Hamiltonian for Bose atoms in an optical lattice is

$$H = \hat{H} - \mu_0 \hat{N}_0 - \mu_1 \hat{N}_1 - \hat{\Lambda} , \qquad (3.15)$$

where  $\hat{H}$  is the energy Hamiltonian (3.8) and  $\hat{\Lambda}$  is the linear killer (2.91).

The lattice parameters can be varied in a rather wide range [16–18]. The typical experimental values for the laser wavelengths, used in creating optical lattices, are of the order  $\lambda \sim 10^{-5} - 10^{-4}$  cm; then the mean lattice spacing is a  $a \sim 10^{-5} - 10^{-4}$  cm and the recoil energy is  $E_R \sim 10^4 - 10^5$  Hz. The ratio of the potential depth  $V_0$  to the recoil energy is  $V_0/E_R \sim 0.1 - 100$ , so that quite deep and very shallow lattices can be formed. The typical linear lattice size is  $L \sim 10^{-3}$  cm.

Generally, it is possible to create not only periodic lattices, but also quasiperiodic lattices, in which at least one of the spatial directions is subject to the action of two or more periodic potentials with incommensurate periods. Such quasiperiodic lattices are similar to quasicrystals [207,208].

#### **3.2** Periodic Structures

The periodic structure of a lattice is characterized by the *lattice vector*  $\mathbf{a} = \{a_{\alpha}\}$ . The lattice is formed by the set  $\{\mathbf{a}_i\}$  of the vectors

$$\mathbf{a}_{i} = \{ n_{i} a_{\alpha} | n_{i} = 0, \pm 1, \pm 2, \ldots \} .$$
(3.16)

The optical potential is periodic with respect to vectors (3.16),

$$V_L(\mathbf{r} + \mathbf{a}_i) = V_L(\mathbf{r}) . \tag{3.17}$$

For the description of periodic structures, one employs the *Bloch functions* 

$$\varphi_{nk}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} f_{nk}(\mathbf{r}) , \qquad (3.18)$$

labelled by the band index n and quasimomentum  $\mathbf{k}$ , with a periodic factor function

$$f_{nk}(\mathbf{r} + \mathbf{a}_i) = f_{nk}(\mathbf{r}) . \tag{3.19}$$

The quasimomentum  $\mathbf{k}$  pertains to the *Brillouin zone* 

$$\mathcal{B} = \left\{ \mathbf{k} : -\frac{\pi}{a_{\alpha}} \le k_{\alpha} \le \frac{\pi}{a_{\alpha}} \right\} .$$
(3.20)

The number of k-points in the Brillouin zone (3.20) equals the number  $N_L$  of the real-space cells in the total lattice,

$$\sum_{k \in \mathcal{B}} 1 = N_L . \tag{3.21}$$

A uniform system can be treated as a degenerate case of the periodic one, when the Bloch function  $\varphi_{nk}(\mathbf{r})$  reduces to the plane wave  $e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$  and the periodic factor function  $f_{nk}(\mathbf{r})$ , to the constant  $1/\sqrt{V}$ .

Without the loss of generality, the factor function (3.19) can be chosen so that the property

$$f_{nk}^*(\mathbf{r}) = f_{n,-k}(\mathbf{r}) \tag{3.22}$$

be valid. As a result, the Bloch function (3.18) satisfies the equation

$$\varphi_{nk}^*(\mathbf{r}) = \varphi_{n,-k}(\mathbf{r}) . \qquad (3.23)$$

The real-space lattice  $\{\mathbf{a}_i\}$  can be related to the reciprocal lattice  $\{\mathbf{g}_i\}$  formed by the vectors  $\mathbf{g}_i$  defined by the condition

$$\mathbf{g}_i \cdot \mathbf{a}_i = \mathbf{g} \cdot \mathbf{a} = 2\pi \;. \tag{3.24}$$

The vectors of the reciprocal lattice and of quasimomentum pertain to different sets, since  $\mathbf{k} \in \mathcal{B}$  and  $\mathbf{g} \in {\mathbf{g}_i}$ , because of which they, generally, do not coincide. Consequently, the property

$$\frac{1}{V} \int e^{i(\mathbf{k}-\mathbf{p}+\mathbf{g})\cdot\mathbf{r}} d\mathbf{r} = \delta_{kp} \delta_{g0}$$
(3.25)

holds. Here and in what follows, the spatial integration is over the whole system volume V.

The periodic function (3.19) can be expanded over the reciprocal lattice as

$$f_{nk}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{g} b_{gnk} e^{i\mathbf{g}\cdot\mathbf{r}} , \qquad (3.26)$$

where the summation is over all reciprocal vectors  $\mathbf{g} \in {\mathbf{g}_i}$ . The coefficient in Eq. (3.26) is

$$b_{gnk} = \frac{1}{\sqrt{V}} \int f_{nk}(\mathbf{r}) e^{-i\mathbf{g}\cdot\mathbf{r}} d\mathbf{r}$$

Using expansion (3.26), the Bloch function (3.18) can be written as

$$\varphi_{nk}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{g} b_{gnk} e^{i(\mathbf{g}+\mathbf{k})\cdot\mathbf{r}} , \qquad (3.27)$$

with

$$b_{gnk} = \frac{1}{\sqrt{V}} \int \varphi_{nk}(\mathbf{r}) e^{-i(\mathbf{g}+\mathbf{k})\cdot\mathbf{r}} d\mathbf{r}$$

The Bloch functions are orthonormal,

$$\int \varphi_{mk}^*(\mathbf{r}) \varphi_{np}(\mathbf{r}) \, d\mathbf{r} = \delta_{mn} \delta_{kp} \,, \qquad (3.28)$$

and generate a complete basis, for which

$$\sum_{n} \sum_{k} \varphi_{nk}(\mathbf{r}) \varphi_{nk}^{*}(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') . \qquad (3.29)$$

Here and in what follows, summation over  $\mathbf{k}$  implies the summation over the Brillouin zone (3.20). From Eq. (3.27), one has

$$\sum_{g} b_{gmk}^* \ b_{gnp} = \delta_{mn} \delta_{kp} \ .$$

Another basis, often employed for describing periodic structures, is formed by Wannier functions, which are related to the Bloch functions through the Fourier transformation

$$w_{nj}(\mathbf{r}) = \frac{1}{\sqrt{N_L}} \sum_k \varphi_{nk}(\mathbf{r}) \ e^{-i\mathbf{k}\cdot\mathbf{a}_j} , \qquad (3.30)$$

with the summation over  $\mathbf{k} \in \mathcal{B}$ , the inverse transform being

$$\varphi_{nk}(\mathbf{r}) = \frac{1}{\sqrt{N_L}} \sum_{j} w_{nj}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{a}_j} , \qquad (3.31)$$

where the summation with respect to j is over the whole lattice  $\{a_j\}$ , with  $j = 1, 2, ..., N_L$ .

The Wannier functions are defined up to a phase factor that can always be chosen such that to make the Wannier functions real and well localized [209,210]. The scalar product between the Bloch and Wannier functions

$$\int \varphi_{mk}^*(\mathbf{r}) w_{nj}(\mathbf{r}) \, d\mathbf{r} = \frac{\delta_{mn}}{\sqrt{N_L}} \, e^{-i\mathbf{k}\cdot\mathbf{a}_j}$$

shows that these functions are asymptotically orthogonal for  $N_L \to \infty$ ,

$$\lim_{N_L \to \infty} \int \varphi_{mk}^*(\mathbf{r}) w_{nj}(\mathbf{r}) \, d\mathbf{r} = 0 \; . \tag{3.32}$$

Using the equations

$$\frac{1}{N_L} \sum_{k} e^{i\mathbf{k} \cdot (\mathbf{a}_i - \mathbf{a}_j)} = \delta_{ij} , \qquad \frac{1}{N_L} \sum_{j} e^{i(\mathbf{k} - \mathbf{p}) \cdot \mathbf{a}_j} = \delta_{kp} ,$$

one can make it sure that Wannier functions are orthonormal,

$$\int w_{mi}^*(\mathbf{r}) w_{nj}(\mathbf{r}) \, d\mathbf{r} = \delta_{mn} \delta_{ij} \,, \qquad (3.33)$$

and form a complete basis, since

$$\sum_{nj} w_{nj}(\mathbf{r}) w_{nj}^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') . \qquad (3.34)$$

As is mentioned above, Wannier functions can be made real, so that

$$w_{nj}^*(\mathbf{r}) = w_{nj}(\mathbf{r}) , \qquad (3.35)$$

which is connected with property (3.23) of Bloch functions.

In view of Eqs. (3.30) and (3.27), one has

$$w_{nj}(\mathbf{r}) = \frac{1}{\sqrt{VN_L}} \sum_{g,k} b_{gnk} e^{i(\mathbf{g}+\mathbf{k})\cdot(\mathbf{r}-\mathbf{a}_j)} .$$
(3.36)

This shows that the Wannier function can be represented as

$$w_{nj}(\mathbf{r}) \equiv w_n(\mathbf{r} - \mathbf{a}_j) . \tag{3.37}$$

From here it follows that the coefficient

$$b_{gnk} = \sqrt{\frac{N_L}{V}} \int w_n(\mathbf{r}) \ e^{-i(\mathbf{g}+\mathbf{k})\cdot\mathbf{r}} \ d\mathbf{r}$$

enjoys the properties

$$b_{gnk} \equiv b_n(\mathbf{g} + \mathbf{k}) , \qquad b_n^*(\mathbf{g} + \mathbf{k}) = b_n(-\mathbf{g} - \mathbf{k}) .$$

The Bloch function (3.31) can be represented as

$$\varphi_{nk}(\mathbf{r}) = \frac{1}{\sqrt{N_L}} \sum_j w_n(\mathbf{r} - \mathbf{a}_j) e^{i\mathbf{k}\cdot\mathbf{a}_j} = \frac{1}{\sqrt{V}} \sum_g b_n(\mathbf{g} + \mathbf{k}) e^{i(\mathbf{g} + \mathbf{k})\cdot\mathbf{r}} .$$
(3.38)

From here, we see that

$$\varphi_{n\,k+g}(\mathbf{r}) = \varphi_{nk}(\mathbf{r}) \,. \tag{3.39}$$

The bases of Bloch functions,  $\{\varphi_{nk}(\mathbf{r})\}$ , and that of Wannier functions,  $\{w_n(\mathbf{r} - \mathbf{a}_j)\}$ , seem to be equivalent for characterizing periodic structures. This, however, is not completely correct. As is discussed in Sec. 2.17, the indices of spatial localization are not good quantum numbers. This concerns as well the lattice indices  $j = 1, 2, \ldots, N_L$ . Because of the latter, Wannier functions cannot serve as natural orbitals. But Bloch functions can. Thus, the Bloch function, corresponding to the lowest band n = 0 and to the zero quasimomentum  $\mathbf{k} = 0$ , is the condensate natural orbital

$$\varphi_0(\mathbf{r}) \equiv \lim_{k \to 0} \varphi_{0k}(\mathbf{r}) . \tag{3.40}$$

According to relation (3.18),

$$\varphi_0(\mathbf{r}) = f_0(\mathbf{r})$$

hence, the condensate natural orbital is purely periodic. It is, by definition, normalized,

$$\int |\varphi_0(\mathbf{r})|^2 \, d\mathbf{r} = 1 \;, \tag{3.41}$$

and, in compliance with Eq. (3.38), is of the form

$$\varphi_0(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_g b_0(\mathbf{g}) e^{i\mathbf{g}\cdot\mathbf{r}} . \qquad (3.42)$$

Its relation to the Wannier functions, given by the equation

$$\varphi_0(\mathbf{r}) = \frac{1}{\sqrt{N_L}} \sum_j w_0(\mathbf{r} - \mathbf{a}_j) , \qquad (3.43)$$

demonstrates that, if  $\varphi_0(\mathbf{r})$  is the condensate natural orbitals, then the associated Wannier function

$$w_0(\mathbf{r} - \mathbf{a}_j) = \frac{1}{\sqrt{N_L}} \sum_k \varphi_{0k}(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{a}_j}$$
(3.44)

is not a condensate natural orbital, since the latter involves the Bloch functions  $\varphi_{0k}(\mathbf{r})$  of uncondensed atoms, with  $\mathbf{k} \neq 0$ .

In thermodynamic limit, when  $N \to \infty$ ,  $V \to \infty$ , and  $N_L \to \infty$ , the summation over quasimomenta is replaced by the integration according to the rule

$$\sum_{k} \longrightarrow V \int_{\mathcal{B}} \frac{d\mathbf{k}}{(2\pi)^{d}}, \qquad (3.45)$$

in which the integration is over the *d*-dimensional Brillouin zone  $\mathcal{B}$ .

#### **3.3** Condensate in Lattices

Bloch functions can serve as natural orbitals. The lowest-band zero-quasimomentum Bloch function corresponds to BEC. The condensate wave function, entering the Bogolubov shift (2.81), is

$$\eta(\mathbf{r}) = \sqrt{N_0} \varphi_0(\mathbf{r}) , \qquad (3.46)$$

with  $\varphi_0(\mathbf{r})$  being the condensate natural orbital (3.40). As usual, the condensate function (3.46) is normalized to the number of condensed particles

$$N_0 = \int |\eta(\mathbf{r})|^2 \, d\mathbf{r} \,. \tag{3.47}$$

In line with expansion (3.43), the condensate function (3.46) reads as

$$\eta(\mathbf{r}) = \sqrt{\frac{N_0}{N_L}} \sum_j w_0(\mathbf{r} - \mathbf{a}_j) . \qquad (3.48)$$

This tells us again that  $w_0(\mathbf{r} - \mathbf{a}_j)$  cannot be treated as the condensate wave function, but only combination (3.48) forms the latter.

The field operators of uncondensed atoms can be expanded over the Bloch functions,

$$\psi_1(\mathbf{r}) = \sum_{nk} a_{nk} \varphi_{nk}(\mathbf{r}) . \qquad (3.49)$$

An expansion over Wannier functions is also admissible,

$$\psi_1(\mathbf{r}) = \sum_{nj} c_{nj} w_n(\mathbf{r} - \mathbf{a}_j) . \qquad (3.50)$$

As is known from Chapter 2, the condensate function, by definition, is orthogonal to the field operator of uncondensed atoms,

$$\int \eta^*(\mathbf{r})\psi_1(\mathbf{r}) \, d\mathbf{r} = 0 \; . \tag{3.51}$$

Substituting here expansion (3.49) requires that

$$\lim_{k \to 0} a_{0k} = 0 , \qquad (3.52)$$

which means that the term with n = 0 and  $\mathbf{k} = 0$  is excluded from sum (3.49).

From relations (3.30) and (3.31) between Bloch and Wannier functions, it follows that

$$\lim_{k \to 0} a_{0k} = \frac{1}{\sqrt{N_L}} \sum_j c_{0j} .$$

$$\sum_j c_{0j} = 0$$
(3.53)

Therefore the property

must hold. Conditions (3.52) and (3.53) assure that the operator of the number of uncondensed atoms

$$\hat{N}_1 \equiv \int \psi_1^{\dagger}(\mathbf{r}) \psi_1(\mathbf{r}) \ d\mathbf{r} = \sum_{nk} a_{nk}^{\dagger} a_{nk} = \sum_{nj} c_{nj}^{\dagger} c_{nj}$$

enters additively into the operator

$$\hat{N} = N_0 + \hat{N}_1 \tag{3.54}$$

of the total number of particles.

Let us write explicitly the grand Hamiltonian (3.15), assuming that there are no external potentials disturbing the lattice, inserting there the Bogolubov shift (2.81), and involving expansion (3.49) over Bloch functions. This gives

$$H = H^{(0)} + H^{(2)} + H^{(3)} + H^{(4)} , \qquad (3.55)$$

where the terms linear in  $\psi_1$  are eliminated by the linear killer (2.91). The first term in sum (3.55) is

$$H^{(0)} = \int \eta^*(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + V_L - \mu_0 \right) \eta(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \, \Phi_0 \, \int |\eta(\mathbf{r})|^4 \, d\mathbf{r} \, .$$
(3.56)

In order to avoid too cumbersome notation, let us combine the two indices  $\{n, \mathbf{k}\}$  into one index k. That is, the Bloch function  $\varphi_{nk}(\mathbf{r})$  will be labelled simply as  $\varphi_k(\mathbf{r})$ , keeping in mind that here k means n, **k**. Then the second term in sum (3.55) writes as

$$H^{(2)} = \sum_{kp} \left[ \int \varphi_k^*(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + V_L - \mu_1 + 2\Phi_0 |\eta|^2 \right) \varphi_p(\mathbf{r}) \, d\mathbf{r} \right] a_k^{\dagger} a_p + \frac{1}{2} \sum_{kp} \left( \Phi_{kp} a_k^{\dagger} a_p^{\dagger} + \Phi_{kp}^* a_p a_k \right) \,, \qquad (3.57)$$

where

$$\Phi_{kp} \equiv \Phi_0 \int \varphi_k^*(\mathbf{r}) \varphi_p^*(\mathbf{r}) \eta^2(\mathbf{r}) \, d\mathbf{r} \; .$$

The third term is

$$H^{(3)} = \sum_{kpq} \left( \Phi_{kpq} a_k^{\dagger} a_p^{\dagger} a_q + \Phi_{kpq}^* a_q^{\dagger} a_p a_k \right) , \qquad (3.58)$$

in which

$$\Phi_{kpq} \equiv \Phi_0 \int \varphi_k^*(\mathbf{r}) \varphi_p^*(\mathbf{r}) \varphi_q(\mathbf{r}) \eta(\mathbf{r}) \, d\mathbf{r} \; .$$

And the last term in Eq. (3.55) reads as

$$H^{(4)} = \frac{1}{2} \sum_{kpql} \Phi_{kpql} a_k^{\dagger} a_p^{\dagger} a_q a_l , \qquad (3.59)$$

with the notation

$$\Phi_{kpql} \equiv \Phi_0 \int \varphi_k^*(\mathbf{r}) \varphi_p^*(\mathbf{r}) \varphi_q(\mathbf{r}) \varphi_l(\mathbf{r}) \, d\mathbf{r} \; .$$

Terms (3.58) and (3.59) can be simplified by invoking the Hartree-Fock-Bogolubov (HFB) approximation. The linear in  $a_k$  terms, appearing in  $H^{(3)}$ , are assumed to be cancelled by the linear killer (2.91). The fourth term (3.59) becomes

$$H^{(4)} = \frac{1}{2} \sum_{kpq} \left( 4\Phi_{kqqp} n_q a_k^{\dagger} a_p + \Phi_{kpqq} \sigma_q a_k^{\dagger} a_p^{\dagger} + \Phi_{kpqq}^* \sigma_q^* a_p a_k \right) - \frac{1}{2} \sum_{kp} \left( 2\Phi_{kppk} n_k n_p + \Phi_{kkpp} \sigma_k^* \sigma_p \right) , \qquad (3.60)$$

in which

$$n_k \equiv \langle a_k^{\dagger} a_k \rangle \,, \qquad \sigma_k \equiv \langle a_k a_{-k} \rangle$$

and the quantum-number conservation conditions, valid for natural orbitals,

$$\langle a_k^{\dagger} a_p \rangle = \delta_{kp} n_k , \qquad \langle a_k a_p \rangle = \delta_{-kp} \sigma_k$$

are taken into account, where -k means n,  $-\mathbf{k}$ .

By introducing the notation

$$\omega_{kp} \equiv \int \varphi_k^*(\mathbf{r}) \left( -\frac{\nabla^2}{2m} + V_L + 2\Phi_0 |\eta|^2 \right) \varphi_p(\mathbf{r}) \, d\mathbf{r} + 2\sum_q \Phi_{kqqp} n_q - \mu_1 \delta_{kp}$$
(3.61)

and

$$\Delta_{kp} \equiv \Phi_{kp} + \sum_{q} \Phi_{kpqq} \sigma_q , \qquad (3.62)$$

the grand Hamiltonian (3.55) acquires the form

$$H = E_{HFB} + \sum_{kp} \omega_{kp} a_k^{\dagger} a_p +$$

$$+ \frac{1}{2} \sum_{kp} \left( \Delta_{kp} a_k^{\dagger} a_p^{\dagger} + \Delta_{kp}^* a_p a_k \right) , \qquad (3.63)$$

in which

$$E_{HFB} \equiv H^{(0)} - \frac{1}{2} \sum_{kp} \left( 2\Phi_{kppk} n_k n_p + \Phi_{kkpp} \sigma_k^* \sigma_p \right) .$$
 (3.64)

Hamiltonian (3.63) can be diagonalized by a canonical transformation. In order to simplify the consideration, we may assume that the diagonal elements in the summation over k and p give the main contribution in Eq. (3.63). This amounts to using the diagonal approximation for  $\omega_{kp}$  and  $\Delta_{kp}$ , so that

$$\omega_{kp} = \delta_{kp}\omega_k , \qquad \Delta_{kp} = \delta_{-kp}\Delta_k , \qquad (3.65)$$

where  $\delta_{-kp}$  implies  $\delta_{mn}\delta_{-kp}$ , since -k means  $n, -\mathbf{k}$ . Then Eq. (3.61) reduces to

$$\omega_{k} = \int \varphi_{k}^{*}(\mathbf{r}) \left( -\frac{\nabla^{2}}{2m} + V_{L} + 2\Phi_{0}|\eta|^{2} \right) \varphi_{k}(\mathbf{r}) d\mathbf{r} + 2\sum_{q} \Phi_{kqqk} n_{q} - \mu_{1}$$
(3.66)

and Eq. (3.62) gives

$$\Delta_k = \Phi_{-kk} + \sum_q \Phi_{-kkqq} \sigma_q . \qquad (3.67)$$

Hamiltonian (3.63) becomes

$$H = E_{HFB} + \sum_{k} \omega_{k} a_{k}^{\dagger} a_{k} + \frac{1}{2} \sum_{k} \left( \Delta_{k} a_{k}^{\dagger} a_{-k}^{\dagger} + \Delta_{k}^{*} a_{-k} a_{k} \right) .$$
(3.68)

This is in direct analogy with the grand Hamiltonian in the HFB approximation for uniform systems [94–98], so that all calculations can be done in the same way. The difference from the uniform case is in different  $\omega_k$  and  $\Delta_k$  defined in Eqs. (3.66) and (3.67) and in the fact that the quasimomentum pertains to the Brillouin zone.

Following the same procedure as for the uniform system [94–98], and restoring the double indexation  $n, \mathbf{k}$  for k, we obtain the Bogolubov-type spectrum

$$\varepsilon_{nk} = \sqrt{\omega_{nk}^2 - \Delta_{nk}^2} , \qquad (3.69)$$

consisting of several branches labelled by the band index  $n = 0, 1, 2, \dots$ 

In agreement with the condensation condition (2.121), we require that

$$\lim_{k \to 0} \varepsilon_{0k} = 0 , \qquad \varepsilon_{0k} \ge 0 . \tag{3.70}$$

This is equivalent to the condition

$$\lim_{k \to 0} (\omega_{0k} - \Delta_{0k}) = 0$$

From here we find the Lagrange multiplier

$$\mu_{1} = \lim_{k \to 0} \left\{ \int \varphi_{k}^{*}(\mathbf{r}) \left( -\frac{\nabla^{2}}{2m} + V_{L} + 2\Phi_{0} |\eta|^{2} \right) \varphi_{k}(\mathbf{r}) d\mathbf{r} - \Phi_{-kk} + \sum_{q} \left( 2\Phi_{kqqk} n_{q} - \Phi_{-kkqq} \sigma_{q} \right) \right\}, \qquad (3.71)$$

where again the short-hand notation is used, with k instead of  $n, \mathbf{k}$ .

The condensate-function equation is derived similarly to Eq. (2.170), which in the HFB approximation for a lattice gives

$$\left\{-\frac{\nabla^2}{2m} + V_L(\mathbf{r}) + \Phi_0[\rho_0(\mathbf{r}) + 2\rho_1(\mathbf{r})]\right\}\eta(\mathbf{r}) + \Phi_0\sigma_1(\mathbf{r})\eta^*(\mathbf{r}) = \mu_0\eta(\mathbf{r}) .$$
(3.72)

Here the densities of condensed and uncondensed atoms and the anomalous average are

$$\rho_0(\mathbf{r}) = |\eta(\mathbf{r})|^2 , \qquad \rho_1(\mathbf{r}) = \sum_{nk} n_{nk} |\varphi_{nk}(\mathbf{r})|^2 ,$$
$$\sigma_1(\mathbf{r}) = \sum_{nk} \sigma_{nk} \varphi_{nk}(\mathbf{r}) \varphi_{n,-k}(\mathbf{r}) . \qquad (3.73)$$

The eigenproblem (3.72) defines the condensate function  $\eta(\mathbf{r})$  and the Lagrange multiplier  $\mu_0$  that guarantees the validity of the normalization condition (3.47). Using the latter yields

$$\mu_{0} = \frac{1}{N_{0}} \int \eta^{*}(\mathbf{r}) \left\{ -\frac{\nabla^{2}}{2m} + V_{L}(\mathbf{r}) + \Phi_{0}[\rho_{0}(\mathbf{r}) + 2\rho_{1}(\mathbf{r})] \right\} \eta(\mathbf{r}) d\mathbf{r} + \frac{\Phi_{0}}{N_{0}} \int \sigma_{1}(\mathbf{r}) \left(\eta^{*}(\mathbf{r})\right)^{2} d\mathbf{r} .$$
(3.74)

This is to be compared with multiplier (3.71). Taking in the latter the limit  $k \to 0$ , we have

$$\begin{split} \lim_{k \to 0} \Phi_{-kk} &= \Phi_0 \int |\eta(\mathbf{r})|^4 \, d\mathbf{r} \;, \\ \lim_{k \to 0} \Phi_{kppk} &= \frac{\Phi_0}{N_0} \; \int \rho_0(\mathbf{r}) |\varphi_p(\mathbf{r})|^2 \; d\mathbf{r} \;, \\ \lim_{k \to 0} \Phi_{-kkpp} &= \frac{\Phi_0}{N_0} \; \int \left[\eta^*(\mathbf{r})\varphi_p(\mathbf{r})\right]^2 \; d\mathbf{r} \;, \end{split}$$

since

$$\lim_{k \to 0} \varphi_k(\mathbf{r}) = \frac{\eta(\mathbf{r})}{\sqrt{N_0}} \,.$$

Taking into consideration Eqs. (3.73), we find

$$\mu_1 = \frac{1}{N_0} \int \eta^*(\mathbf{r}) \left\{ -\frac{\nabla^2}{2m} + V_L(\mathbf{r}) + \Phi_0[\rho_0(\mathbf{r}) + 2\rho_1(\mathbf{r})] \right\} \eta(\mathbf{r}) \, d\mathbf{r} - \frac{1}{N_0} \int \eta^*(\mathbf{r}) \, d\mathbf{r} + \frac{1}{N_0} \int \eta^*(\mathbf{$$

$$- \frac{\Phi_0}{N_0} \int \sigma_1(\mathbf{r}) \left(\eta^*(\mathbf{r})\right)^2 d\mathbf{r} . \qquad (3.75)$$

As is seen,  $\mu_0 \neq \mu_1$ . They coincide only in the limit of asymptotically weak interactions, when the Bogolubov approximation becomes applicable. In this approximation

 $\rho_1(\mathbf{r}) \ \rightarrow \ 0 \ , \qquad \sigma_1(\mathbf{r}) \ \rightarrow \ 0 \qquad (\Phi_0 \rightarrow 0) \ ,$ 

hence

$$\rho_0(\mathbf{r}) \rightarrow \rho(\mathbf{r}) \equiv \rho_0(\mathbf{r}) + \rho_1(\mathbf{r})$$

As a result,

$$\mu_0 \simeq \mu_1 \simeq \frac{1}{N_0} \int \eta^*(\mathbf{r}) \left[ -\frac{\nabla^2}{2m} + V_L(\mathbf{r}) + \Phi_0 \rho(\mathbf{r}) \right] \eta(\mathbf{r}) \, d\mathbf{r} \qquad (\Phi_0 \to 0) \; .$$

The Bogolubov approximation for weakly nonideal gas in tight-binding bands was considered by Ramakumar and Das [211].

## 3.4 Operator of Momentum

The operator of momentum defines the dissipated heat (2.148) and, respectively, the superfluid fraction (2.150). According to Eqs. (2.133) and (2.134), it can be introduced through the relation

$$\hat{\mathbf{P}} \equiv \lim_{v \to 0} \, \frac{\partial H_v}{\partial \mathbf{v}} \,, \tag{3.76}$$

in which  $\hat{H}_v$  is the energy Hamiltonian

$$\hat{H}_{v} = \hat{H} + \int \hat{\psi}(\mathbf{r}) \left( -i\mathbf{v} \cdot \nabla + \frac{mv^{2}}{2} \right) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} \,, \qquad (3.77)$$

obtained by substituting into  $\hat{H}[\hat{\psi}]$  the Galilean-transformed field operator (2.146). This gives the standard form

$$\hat{\mathbf{P}} = \int \hat{\psi}^{\dagger}(\mathbf{r}) \left(-i\nabla\right) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} \,, \qquad (3.78)$$

but with the Bogolubov-shifted field operator (2.81).

We may notice that

$$\int \eta^*(\mathbf{r}) (-i\nabla) \eta(\mathbf{r}) \, d\mathbf{r} = N_0 \sum_g |b_0(\mathbf{g})|^2 \mathbf{g} = 0 \; ,$$

because of the property

$$|b_0(-\mathbf{g})| = |b_0(\mathbf{g})| ,$$

derived in Sec. 3.2. Also,

$$\int \eta^*(\mathbf{r}) (-i\nabla) \psi_1(\mathbf{r}) \, d\mathbf{r} = 0 \; ,$$

due to condition (3.52). Therefore the operator of momentum (3.78) is defined only in terms of the field operators of uncondensed atoms,

$$\hat{\mathbf{P}} = \int \psi_1^{\dagger}(\mathbf{r}) \left(-i\nabla\right) \psi_1(\mathbf{r}) \, d\mathbf{r} \,. \tag{3.79}$$

The field operator  $\psi_1(\mathbf{r})$  can be expanded either over Wannier functions or over Bloch functions, as in Eqs. (3.49) and (3.50), with the relations

$$c_{nj} = \frac{1}{\sqrt{N_L}} \sum_k a_{nk} e^{i\mathbf{k}\cdot\mathbf{a}_j} , \qquad a_{nk} = \frac{1}{\sqrt{N_L}} \sum_j c_{nj} e^{-i\mathbf{k}\cdot\mathbf{a}_j} . \tag{3.80}$$

Defining the matrix elements over Wannier functions,

$$\mathbf{p}_{ij}^{mn} \equiv \int w_m (\mathbf{r} - \mathbf{a}_i) (-i\nabla) w_n (\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r} \,, \qquad (3.81)$$

and over Bloch functions

$$\mathbf{q}_{kp}^{mn} \equiv \int \varphi_{mk}^*(\mathbf{r})(-i\nabla)\varphi_{np}(\mathbf{r}) \, d\mathbf{r} \,, \qquad (3.82)$$

we get the representations of the momentum operator (3.79) in terms of the Wannier,  $c_{nj}$ , or Bloch,  $a_{nk}$ , operators as

$$\hat{\mathbf{P}} = \sum_{mn} \sum_{ij} \mathbf{p}_{ij}^{mn} c_{mi}^{\dagger} c_{nj}$$
(3.83)

and, respectively,

$$\hat{\mathbf{P}} = \sum_{mn} \sum_{kp} \mathbf{q}_{kp}^{mn} a_{mk}^{\dagger} a_{np} .$$
(3.84)

The matrix elements (3.81) and (3.82) are connected through the transformations

$$\mathbf{p}_{ij}^{mn} = \frac{1}{N_L} \sum_{kp} \mathbf{q}_{kp}^{mn} e^{i\mathbf{k}\cdot\mathbf{a}_i - i\mathbf{p}\cdot\mathbf{a}_j} ,$$
$$\mathbf{q}_{kp}^{mn} = \frac{1}{N_L} \sum_{ij} \mathbf{p}_{ij}^{mn} e^{-i\mathbf{k}\cdot\mathbf{a}_i + i\mathbf{p}\cdot\mathbf{a}_j} .$$
(3.85)

In Eq. (3.81), we use the advantage of choosing Wannier functions as being real. This equation can also be written as

$$\mathbf{p}_{ij}^{mn} = \int w_m(\mathbf{r} - \mathbf{a}_{ij})(-i\nabla)w_n(\mathbf{r}) \, d\mathbf{r} \,, \qquad (3.86)$$

where  $\mathbf{a}_{ij} \equiv \mathbf{a}_i - \mathbf{a}_j$ , which allows for the use of the representation

$$\mathbf{p}_{ij}^{mn} \equiv \mathbf{p}_{mn}(\mathbf{a}_{ij}) \ . \tag{3.87}$$

Matrix elements (3.81) have the property

$$\left(\mathbf{p}_{ij}^{mn}\right)^* = \mathbf{p}_{ji}^{nm} = -\mathbf{p}_{ij}^{mn} , \qquad (3.88)$$

from which it follows that

$$\mathbf{p}_{jj}^{nn} = \mathbf{p}_{nn}(0) = 0$$
 (3.89)

Using Eq. (3.87), the second of the matrix elements (3.85) can be rewritten as

$$\mathbf{q}_{kp}^{mn} = \frac{1}{N_L} \sum_{ij} \mathbf{p}_{mn}(\mathbf{a}_{ij}) e^{-i\mathbf{k}\cdot\mathbf{a}_{ij}-i(\mathbf{k}-\mathbf{p})\cdot\mathbf{a}_j} .$$

From here, we get

$$\mathbf{q}_{kp}^{mn} = \delta_{kp} \mathbf{q}_k^{mn} , \qquad (3.90)$$

where the diagonal element is

$$\mathbf{q}_{k}^{mn} = \sum_{j} \mathbf{p}_{mn}(\mathbf{a}_{j}) \ e^{-i\mathbf{k}\cdot\mathbf{a}_{j}} \ . \tag{3.91}$$

The latter enjoys the property

$$\left(\mathbf{q}_{k}^{mn}\right)^{*} = \mathbf{q}_{k}^{nm} = -\mathbf{q}_{-k}^{mn} .$$

$$(3.92)$$

Thence, momentum (3.84) takes the form

$$\hat{\mathbf{P}} = \sum_{mn} \sum_{k} \mathbf{q}_{k}^{mn} a_{mk}^{\dagger} a_{nk} . \qquad (3.93)$$

Using the quantum-number conservation condition

$$\langle a_{mk}^{\dagger}a_{np}\rangle = \delta_{mn}\delta_{kp} \langle a_{nk}^{\dagger}a_{nk}\rangle, \qquad (3.94)$$

we find that the total average momentum

$$\langle \hat{\mathbf{P}} \rangle = \sum_{nk} \mathbf{q}_k^{nm} \langle a_{nk}^{\dagger} a_{nk} \rangle = 0 , \qquad (3.95)$$

owing to property (3.92) and assuming that  $\langle a_{nk}^{\dagger}a_{nk} \rangle$  is symmetric with respect to the inversion **k** to  $-\mathbf{k}$ . This means that in the coordinate frame, coupled with the lattice, the total average momentum is zero, as it should be. If the lattice would be moving, then in the laboratory frame the distribution  $\langle a_{nk}^{\dagger}a_{nk} \rangle$  would not be symmetric with respect to the inversion of **k**.

## 3.5 Tight-Binding Approximation

Since Wannier functions can be made well localized [209,210], one can assume that when atoms are close to the lattice site  $\mathbf{a}_{j}$ , then they feel the potential

$$V_L(\mathbf{r} - \mathbf{a}) \simeq \sum_{\alpha} \frac{m}{2} \omega_{\alpha}^2 \left( r_{\alpha} - a_j^{\alpha} \right)^2 \qquad (\mathbf{r} \approx \mathbf{a}_j) , \qquad (3.96)$$

which is an expansion of the lattice potential (3.1), so that

$$\omega_{\alpha} \equiv 2 \sqrt{E_R V_{\alpha}} . \tag{3.97}$$

It is convenient to define the effective frequency

$$\omega_0 \equiv \left(\prod_{\alpha=1}^d \omega_\alpha\right)^{1/d} \,, \tag{3.98}$$

in which d is space dimensionality, and the effective localization length

$$l_0 \equiv \frac{1}{\sqrt{m\omega_0}} \,. \tag{3.99}$$

Good localization of atomic Wannier functions means that the localization length (3.99) is much smaller than the distance between the nearest neighbors a, which can be expressed in several equivalent inequalities,

$$\frac{l_0}{a} \ll 1$$
,  $k_0 l_0 \ll 1$ , (3.100)

where  $k_0$  is the modulus of the laser wave vector entering the recoil energy (3.5), which also allows us to write down the inequality

$$\frac{E_R}{\omega_0} \ll 1 . \tag{3.101}$$

For the harmonic potential (3.96), the lowest-band localized Wannier function can be approximated by the Gaussian form

$$w(\mathbf{r} - \mathbf{a}_j) = \left(\frac{m\omega_0}{\pi}\right)^{d/4} \prod_{\alpha} \exp\left\{-\frac{m}{2}\omega_{\alpha}\left(r_{\alpha} - a_j^{\alpha}\right)^2\right\}$$
(3.102)

For a cubic lattice, for which  $\omega_{\alpha} = \omega_0$ , this becomes

$$w(\mathbf{r} - \mathbf{a}_j) = \frac{1}{(\sqrt{\pi} \ l_0)^{d/2}} \exp\left\{-\frac{(\mathbf{r} - \mathbf{a}_j)^2}{2l_0^2}\right\} .$$
 (3.103)

The Wannier functions of higher bands could be approximated by the excited wave functions of the harmonic oscillator. If one assumes that in the lattice there are no such strong excitations that would transfer atoms to higher excited bands, then one can limit oneself by considering only the lowest band characterized by the approximate Wannier functions (3.102) or (3.103).

As a first example of using the tight-binding approximation, let us calculate the momentum operator (3.93), with the matrix element (3.91), in the single-band picture. Calculating the matrix element (3.81), we meet the integrals

$$\int_0^\infty e^{-bx^2} \sinh x \, dx = \sqrt{\frac{\pi}{4b}} \, \exp\left(\frac{1}{4b}\right) \Phi\left(\frac{1}{\sqrt{4b}}\right) \,,$$
$$\int_0^\infty x e^{-bx^2} \cosh x \, dx = \frac{1}{2b} + \frac{1}{4b} \sqrt{\frac{\pi}{b}} \, \exp\left(\frac{1}{4b}\right) \Phi\left(\frac{1}{\sqrt{4b}}\right) \,,$$
with the probability integral

$$\Phi(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt .$$

The latter enjoys the property

$$\Phi(x) \simeq 1 \qquad (x \to \infty) \; .$$

Therefore, for small b, we find

$$\int_0^\infty e^{-bx^2} \left(x \cosh x - \sinh x\right) \, dx \simeq \frac{1}{4b} \sqrt{\frac{\pi}{b}} \, \exp\left(\frac{1}{4b}\right) \qquad (b \ll 1) \, .$$

Then, for element (3.81), we obtain

$$\mathbf{p}_{ij} \equiv \mathbf{p}(\mathbf{a}_{ij}) = i \, \frac{\mathbf{a}_{ij}}{a_{ij}^2} \, \exp\left(-\frac{a_{ij}^2}{4l_0^2}\right) \,, \qquad (3.104)$$

where  $a_{ij} \equiv |\mathbf{a}_{ij}|$  and  $\mathbf{a}_{ij} \equiv \mathbf{a}_i - \mathbf{a}_j$ . The diagonal element  $\mathbf{p}_{ii} = 0$ , in agreement with property (3.89).

As is seen, the value of element (3.104) exponentially decays for increasing  $a_{ij}$ , which makes it possible to take into account only the nearest neighbors. Then, for Eq. (3.91), we have

$$\mathbf{q}_k = \sum_{\langle j \rangle} \mathbf{p}(\mathbf{a}_j) \ e^{-i\mathbf{k}\cdot\mathbf{a}_j} \ ,$$

where the summation is over the *nearest neighbors*.

For a *d*-dimensional *cubic lattice*, one has

$$\sum_{\langle j \rangle} \mathbf{a}_j \ e^{-i\mathbf{k}\cdot\mathbf{a}_j} = -2ia \sum_{\alpha=1}^d \sin(k_\alpha a) \mathbf{e}_\alpha \ ,$$

where  $\mathbf{e}_{\alpha}$  is a unit vector, such that

$$\mathbf{e}_{\alpha}^2 = 1$$
,  $\sum_{\alpha=1}^d \mathbf{e}_{\alpha}^2 = d$ .

Keeping in mind a cubic lattice and substituting Eq. (3.104) into Eq. (3.91), we find

$$\mathbf{q}_k = \frac{2}{a} \exp\left(-\frac{a^2}{4l_0^2}\right) \sum_{\alpha} \sin(k_\alpha a) \mathbf{e}_\alpha .$$
(3.105)

This is to be inserted into the operator of momentum (3.93). Or element (3.104) can be used in Eq. (3.83).

# 3.6 Superfluidity in Lattices

The general definition of the superfluid fraction is given by Eq. (2.135), which is valid for arbitrary systems. For an equilibrium system, according to Eq. (2.150), we come to the expression

$$n_s = 1 - \frac{Q}{Q_0} \qquad \left(Q_0 \equiv \frac{3}{2} T\right) ,$$
 (3.106)

in which Q is the dissipated heat

$$Q = \frac{\langle \mathbf{P}^2 \rangle}{2mN}$$

To find the dissipated heat Q, let us treat the single-band case and use the HFB approximation. As usual, the conservation conditions

are taken into account. Then, using the momentum operator (3.93), we obtain

$$\langle \hat{\mathbf{P}}^2 \rangle = \sum_k \left( n_k + n_k^2 - \sigma_k^2 \right) \mathbf{q}_k^2 ,$$
 (3.107)

with the matrix element (3.91). Employing here the explicit expressions for the normal  $n_k$ , and anomalous,  $\sigma_k$ , averages [57,94], we have

$$n_k + n_k^2 - \sigma_k^2 = \frac{1}{4 \sinh^2(\beta \varepsilon_k/2)}$$

where  $\varepsilon_k$  is the Bogolubov spectrum (3.69). Using Eqs. (3.104) and (3.105), we have

$$\mathbf{q}_k^2 = 4|\mathbf{p}(\mathbf{a})|^2 \sum_{\alpha} \sin^2(k_{\alpha}a) , \qquad (3.108)$$

where again a cubic lattice is considered and

$$|\mathbf{p}(\mathbf{a})|^2 = \frac{1}{a^2} \exp\left(-\frac{a^2}{2l_0^2}\right)$$
 (3.109)

Thus, for the dissipated heat, entering the superfluid fraction (3.106), we derive

$$Q = \frac{|\mathbf{p}(\mathbf{a})|^2}{2m\rho} \int_{\mathcal{B}} \frac{\sum_{\alpha} \sin^2(k_{\alpha}a)}{\sinh^2(\beta \varepsilon_k/2)} \frac{d\mathbf{k}}{(2\pi)^d} .$$
(3.110)

The exponential factor in Eq. (3.109) is small, since

$$\frac{a^2}{l_0^2} = 3\pi^2 \sqrt{\frac{V_0}{E_R}} \gg 1$$

by the condition of good localization (3.100). But superfluidity can exist in optical lattices even under well localized atomic Wannier functions.

# 3.7 Transverse Confinement

In experiments, one can create an optical lattice in one direction, while atoms are tightly confined in two other directions. Then one obtains an effective one-dimensional system in a periodic optical potential. To study such a system, let us consider the case of weakly interacting atoms at zero temperature, when practically all atoms are condensed, so that  $N_0 \approx N$ . Then the grand Hamiltonian (3.55) reduces to form (3.56). Let us have a tight transverse trapping potential  $U(\mathbf{r}_{\perp})$ , where  $\mathbf{r}_{\perp}$  is the transverse vector. And let the optical lattice be imposed in the z-direction. Then the Hamiltonian is

$$H = \int \eta^*(\mathbf{r}) \left[ -\frac{\nabla^2}{2m} + U(\mathbf{r}_\perp) + V_L(z) - \mu_0 \right] \eta(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \Phi_0 \int |\eta(\mathbf{r})|^4 \, d\mathbf{r} \,.$$
(3.111)

Let us assume that the transverse confinement is realized by a harmonic potential  $U(\mathbf{r}_{\perp})$ , with the transverse frequency  $\omega_{\perp}$ . Then the transverse localization length is

$$l_{\perp} \equiv \frac{1}{\sqrt{m\omega_{\perp}}} \,. \tag{3.112}$$

Let the lattice have length L in the z-direction. Tight transverse confinement implies that

$$\frac{l_\perp}{L} \ll 1. \tag{3.113}$$

In order to avoid considering atomic scattering on the transverse trapping potential, we assume that the atomic scattering length is much shorter than the transverse localization length (3.112), such that

$$\frac{|a_s|}{l_\perp} \ll 1. \tag{3.114}$$

The equation

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \frac{\delta H}{\delta \eta^*(\mathbf{r}, t)}$$

gives the equation for the condensate function,

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left[ -\frac{\nabla^2}{2m} + U(\mathbf{r}_\perp) + V_L(z) + \Phi_0 |\eta(\mathbf{r}, t)|^2 - \mu_0 \right] \eta(\mathbf{r}, t) .$$
(3.115)

We may look for the solution of this equation in the form

$$\eta(\mathbf{r},t) = \sqrt{N_0} \,\chi(\mathbf{r}_\perp) \,\varphi(z,t) \,e^{-i\omega_\perp t} \,, \qquad (3.116)$$

with the factor functions normalized as

$$\int |\chi(\mathbf{r}_{\perp})|^2 d\mathbf{r}_{\perp} = 1 , \qquad \int_{-L/2}^{L/2} |\varphi(z,t)|^2 dz = 1 .$$
(3.117)

The transverse wave function  $\chi(\mathbf{r}_{\perp})$ , under tight transverse confinement, corresponds to the ground state, given by the equation

$$\left[-\frac{\nabla_{\perp}^2}{2m} + U(\mathbf{r}_{\perp})\right] \chi(\mathbf{r}_{\perp}) = \omega_{\perp} \chi(\mathbf{r}_{\perp}) , \qquad (3.118)$$

in which  $\nabla_{\perp}$  is the transverse part of the Laplacian, entering in  $\nabla^2 = \nabla_{\perp}^2 + \partial^2/\partial z^2$ .

Expression (3.116) is substituted into Eq. (3.115), which is multiplied by  $\chi^*(\mathbf{r}_{\perp})$  and integrated over the transverse variable  $\mathbf{r}_{\perp}$ . To this end, we define the effective one-dimensional interaction parameter

$$\Phi_1 \equiv \frac{N_0}{N_L} \, \Phi_0 \int |\chi(\mathbf{r}_\perp)|^4 \, d\mathbf{r}_\perp \,. \tag{3.119}$$

In the case, when the transverse potential  $U(\mathbf{r}_{\perp})$  is harmonic, then

$$\int |\chi(\mathbf{r}_{\perp})|^4 d\mathbf{r}_{\perp} = \frac{m\omega_{\perp}}{2\pi} . \qquad (3.120)$$

When almost all atoms are condensed,  $N_0 \approx N$ , then the filling factor is

$$\nu \equiv \frac{N}{N_L} \approx \frac{N_0}{N_L} \,. \tag{3.121}$$

For a one-dimensional lattice, the number of lattice sites becomes

$$N_L = \frac{L}{a} . \tag{3.122}$$

And the linear density of atoms is

$$\rho \equiv \frac{N}{L} = \frac{\nu}{a} \,. \tag{3.123}$$

Using the above notation, the effective interaction parameter (3.119) writes as

$$\Phi_1 = \frac{\nu}{2\pi} \, \Phi_0 m \omega_\perp = 2\nu a_s \omega_\perp \,, \qquad (3.124)$$

where Eq. (2.169) for  $\Phi_0$  is taken into account.

Finally, we come to the nonlinear Schrödinger equation

$$i \frac{\partial}{\partial t} \varphi(z, t) = (H_{NLS}[\varphi] - \mu_0) \varphi(z, t) , \qquad (3.125)$$

with the nonlinear Schrödinger Hamiltonian

$$H_{NLS}[\varphi] \equiv -\frac{1}{2m} \frac{\partial^2}{\partial z^2} + V_L(z) + N_L \Phi_1 |\varphi|^2 . \qquad (3.126)$$

One also calls Eq. (3.125) the Gross-Pitaevskii equation.

The one-dimensional nonlinear equation (3.125) has been widely studied. By discretizing the variable  $z \in [-L/2, L/2]$ , Eq. (3.125) allows for a convenient way of its numerical investigation [212]. Stationary solutions to Eq. (3.125) have the form

$$\varphi(z,t) = \varphi(z)e^{-i(E-\mu_0)t} , \qquad (3.127)$$

yielding the stationary nonlinear Schrödinger equation

$$H_{NLS}[\varphi]\varphi(z) = E\varphi(z) . \qquad (3.128)$$

For a system in absolute equilibrium, one has

$$\frac{\partial}{\partial t} \varphi(z,t) = 0$$
 (absolute equilibrium),

hence

$$\mu_0 = \inf_{\varphi} \int \varphi^*(z) H_{NLS}[\varphi] \varphi(z) \, dz \,. \tag{3.129}$$

The nonlinear equation (3.128) may possess different types of solutions. An important class is given by Bloch functions

$$\varphi_{nk}(z) = e^{ikz} f_{nk}(z) . \qquad (3.130)$$

Here n is the band index, k is quasimomentum pertaining to the one-dimensional Brillouin zone  $[-k_B, k_B]$ , with the Brillouin wave number

$$k_B \equiv \frac{\pi}{a} = k_0 . \tag{3.131}$$

The function  $f_{nk}(z)$ , being periodic,

$$f_{nk}(z+a) = f_{nk}(z) ,$$

can be expanded over the reciprocal wave numbers

$$g_j \equiv \frac{2\pi}{a} j$$
  $(j = 0, \pm 1, \pm 2, ...),$ 

which gives

$$f_{nk}(z) = \frac{1}{\sqrt{L}} \sum_{j} b_{jnk} e^{ig_j z} .$$

The coefficients  $b_{jnk}$ , because of normalization (3.117), are normalized as

$$\sum_{j} |b_{jnk}|^2 = 1 \; .$$

The Bloch function (3.130) is a solution to the equation

$$H_{NLS}[\varphi_{nk}] \varphi_{nk}(z) = E_{nk} \varphi_{nk}(z) , \qquad (3.132)$$

while the periodic function  $f_{nk}(z)$  satisfies the equation

$$\left[\frac{(\hat{p}+k)^2}{2m} + V_L(z) + N_L \Phi_1 |f_{nk}(z)|^2\right] f_{nk}(z) = E_{nk} f_{nk}(z) , \qquad (3.133)$$

in which  $\hat{p} \equiv -i\partial/\partial z$ . The eigenvalues  $E_{nk}$  form the *Bloch spectrum*. The lowest value of  $E_{nk}$  defines the chemical potential

$$\mu_0 = \inf_{nk} E_{nk} , \qquad (3.134)$$

in agreement with Eq. (3.129).

To find the compressibility (3.14), we remember that we consider the case, when almost all atoms are condensed, so that  $N_0 \approx N$ , hence,  $N_1 \rightarrow 0$  and  $n_0 \rightarrow 1$ ,  $n_1 \rightarrow 0$ . Therefore, according to relation (2.111),

$$\mu_0 \approx \mu \qquad (N_0 \approx N) \; .$$

Then, we may write

$$\kappa_T = \frac{a}{\nu^2} \frac{\partial \nu}{\partial \mu} = \frac{a}{\nu^2} \left(\frac{\partial \mu}{\partial \nu}\right)^{-1} . \tag{3.135}$$

It is worth noting the following important point. In this section, we have been considering the case of a practically completely condensed system, when  $N_0 \approx N$ . In the grand canonical ensemble with broken gauge symmetry [37,63] the condensate does not fluctuate,  $\Delta^2(\hat{N}_0) = 0$ . Since  $N_0 \approx N$  and N is fixed, then  $\Delta^2(\hat{N}) \approx 0$ . However, as soon as N is fixed, the consideration is reduced to the canonical ensemble. In the latter, the compressibility is not related to  $\Delta^2(\hat{N})$ , as in Eq. (2.245), but has to be calculated differently. In the canonical ensemble,  $\kappa_T$  can be expressed through the derivative of free energy, according to Eq. (2.249). Another ensemble, with a fixed number of particles N, is the Gibbs ensemble in which the role of the thermodynamic potential is played by the chemical potential. Then the compressibility is expressed through the derivative of the chemical potential, as in Eq. (3.155). It would not be correct to say that, when the number of particles is fixed, so that  $\Delta^2(\hat{N}_0) = 0$ , then the compressibility would be zero because of relation (2.245). This relation has meaning only if the number of particles is not fixed. But if N is fixed, one has to invoke other definitions of  $\kappa_T$ , such as Eqs. (2.249) or (3.135).

# 3.8 Bloch Spectrum

The study of the Bloch spectrum is the standard problem of quantum solid-state physics [213,214]. The basic difficulty in the case of cold atoms in optical lattices is the existence of interactions between atoms, which makes the equations nonlinear. To illustrate the properties of the Bloch spectrum, we shall analyze the quasi-one-dimensional optical lattice of the previous Sec. 3.7.

The Bloch spectrum, defined in Eq. (3.132), can be represented as

$$E_{nk} = \int_{-L/2}^{L/2} \varphi_{nk}^*(z) \ H_{NLS}[\varphi_{nk}] \ \varphi_{nk}(z) \ dz \ . \tag{3.136}$$

Its lowest value (3.134) gives the condensate chemical potential

$$\mu_0 = \lim_{k \to 0} \min_n E_{nk} , \qquad (3.137)$$

which, in the considered case of a fully condensed system, equals the system chemical potential,  $\mu_0 = \mu$ .

The Bloch spectrum is a single-particle spectrum, contrary to the Bogolubov spectrum of collective elementary excitations. For atoms in a lattice, these spectra are different [215].

One defines the particle group velocity

$$v_{nk} \equiv \frac{\partial E_{nk}}{\partial k} \tag{3.138}$$

and the effective mass  $m_{nk}^*$ ,

$$\frac{1}{m_{nk}^*} \equiv \frac{\partial^2 E_{nk}}{\partial k^2} \,. \tag{3.139}$$

The long-wave expression of the Bloch spectrum is

$$E_{nk} \simeq \mu_0 + v_{n0}k + \frac{k^2}{2m_{n0}^*} \qquad (k \to 0) , \qquad (3.140)$$

where

$$v_{n0} \equiv \lim_{k \to 0} v_{nk} , \qquad m_{n0}^* \equiv \lim_{k \to 0} m_{nk}^* .$$

Let us consider just one band. Using Eq. (3.136) and expanding the Bloch functions over Wannier functions, as in Eq. (3.31), we have

$$E_k = \frac{1}{N_L} \sum_{ij} \int_{-L/2}^{L/2} w_i(z) H_{NLS}[\varphi_k] w_j(z) e^{-ika_{ij}} dz , \qquad (3.141)$$

where  $a_{ij} \equiv a_i - a_j$ . For an ideal lattice, invoking representation (3.37), that is,  $w_j(z) = w(z - a_j)$ , we get

$$E_k = \sum_j \int_{-L/2}^{L/2} w(z) \ H_{NLS}[\varphi_k] \ w(z - a_j) e^{ika_j} \ dz \ . \tag{3.142}$$

The nonlinear Schrödinger Hamiltonian (3.126) can be written as

$$H_{NLS}[\varphi] = H_L(z) + N_L \Phi_1 |\varphi|^2 ,$$
 (3.143)

where the *linear lattice term* 

$$H_L(z) \equiv -\frac{1}{2m} \frac{\partial^2}{\partial z^2} + V_L(z)$$
(3.144)

is separated out.

Keeping in mind the tight-binding approximation of Sec. 3.5, we shall consider only the nearest-neighbor sites. Then, for the linear term (3.144), there are two types of matrix elements over Wannier functions, the single-site integral

$$h_0 \equiv \int_{-L/2}^{L/2} w(z) H_L(z) w(z) dz \qquad (3.145)$$

and the nearest-neighbor overlap integral

$$h_1 \equiv \int_{-L/2}^{L/2} w(z) H_L(z) w(z-a) \, dz \,. \tag{3.146}$$

The general form of the matrix element of the nonlinear term in Eq. (3.143) is proportional to the integral

$$I_{j_1 j_2 j_3 j_4} \equiv \int_{-L/2}^{L/2} w_{j_1}(z) w_{j_2}(z) w_{j_3}(z) w_{j_4}(z) \, dz \,. \tag{3.147}$$

Treating again only the nearest neighbors, we have three kinds of integrals. The single-site integral is

$$I_0 \equiv \int_{-L/2}^{L/2} w^4(z) \, dz \,. \tag{3.148}$$

The first-order overlap integral is

$$I_1 \equiv \int_{-L/2}^{L/2} w^3(z) w(z-a) \, dz \;. \tag{3.149}$$

And also, we have the second-order overlap integral

$$I_2 \equiv \int_{-L/2}^{L/2} w^2(z) w^2(z-a) \, dz \,. \tag{3.150}$$

Taking only account of the nearest neighbors, Eq. (3.142) reads as

$$E_k = h_0 + 2h_1 \cos ka + \Phi_1 \sum_{j_1 j_2 j_3} I_{0j_1 j_2 j_3} \exp\{-ik(a_{j_1} - a_{j_2} - a_{j_3})\}.$$
(3.151)

The second-order overlap integral (3.150) is smaller than the zero-and first-order integrals (3.148) and (3.149). Therefore, retaining only the overlap integrals up to first order, one has the following terms. The single-site term is

$$\varepsilon_0 \equiv h_0 + \Phi_1 I_0 . \tag{3.152}$$

The first-order overlap integrals define the *tunneling parameter* 

$$J \equiv -h_1 - 4I_1 \Phi_1 \ . \tag{3.153}$$

So that the *Bloch spectrum* (3.151) becomes

$$E_k = \varepsilon_0 - 2J\cos(ka) . \tag{3.154}$$

Taking account of the second-order overlap integral (3.150) would result in an additional term containing  $\cos(2ka)$ .

The chemical potential (3.137) is

$$\mu_0 \equiv \lim_{k \to 0} E_k = \varepsilon_0 - 2J , \qquad (3.155)$$

provided that the lowest band has been considered. This, with Eqs. (3.152) and (3.153), gives

$$\mu_0 = h_0 + 2h_1 + \Phi_1(I_0 + 8I_1) . \tag{3.156}$$

The isothermal compressibility, given in Eq. (3.135), can be approximately defined by taking into account only the dependence of the coupling parameter (3.124) on the filling factor  $\nu$ , but neglecting the possible dependence on  $\nu$  of the Wannier functions. Then

$$\kappa_T = \frac{ma \, l_\perp^2}{2a_s \nu^2 (I_0 + 8I_1)} = \frac{1}{\rho (I_0 + 8I_1) \Phi_1} \,. \tag{3.157}$$

We may notice that, similarly to the case of a uniform system, bosons in a lattice can be stable only in the presence of nonzero repulsive interactions. If atomic interactions would be attractive, such that  $a_s < 0$ , then compressibility (3.157) would be negative. And if the Bose gas would be ideal, such that  $\Phi_1 \rightarrow 0$ , then  $\kappa_T$  would be infinite. In both these cases, the system would be unstable [93,145,146]. In the case of attractive atomic interactions, when  $a_s < 0$ , the system stability can be restored for a *finite* number of atoms by imposing a trapping potential in all directions [9,174,216–218].

With the Bloch spectrum (3.154), the group velocity (3.138) is

$$v_k = 2Ja\sin(ka) \tag{3.158}$$

and the effective mass, given by Eq. (3.139), reads as

$$m_k^* = \frac{1}{2Ja^2\cos(ka)} \,. \tag{3.159}$$

In the limit of  $k \to 0$ , the effective mass is

$$m^* \equiv m_0^* = \frac{1}{2Ja^2} \qquad (k=0) , \qquad (3.160)$$

while the group velocity (3.158) behaves as

$$v_k \simeq 2Ja^2k \qquad (k \to 0) \;.$$

#### **3.9** Spectrum Parameters

To estimate the parameters entering the Bloch spectrum, let us consider the lowest band in the tight-binding approximation. The corresponding Wannier function for a one-dimensional lattice is

$$w(z) = \frac{1}{(\sqrt{\pi} l_0)^{1/2}} \exp\left(-\frac{z^2}{2l_0^2}\right) .$$
 (3.161)

Using this, together with notation (3.99), we find the single-site integral (3.148),

$$I_0 = \frac{1}{\sqrt{2\pi} \, l_0} = \sqrt{\frac{m\omega_0}{2\pi}} \,, \tag{3.162}$$

the first-order overlap integral (3.149),

$$I_1 = I_0 \exp\left(-\frac{3a^2}{8l_0^2}\right) , \qquad (3.163)$$

and the second-order overlap integral (3.150),

$$I_2 = I_0 \exp\left(-\frac{a^2}{2l_0^2}\right) = I_1 \exp\left(-\frac{a^2}{8l_0^2}\right) .$$
 (3.164)

From these expressions, we see that

$$I_2 \ll I_1 \ll I_0 \qquad \left(\frac{l_0}{a} \ll 1\right) , \qquad (3.165)$$

which justifies the neglect of the second-order overlap integral (3.164).

Calculating Eqs. (3.145) and (3.146), we meet the integrals

$$\int_0^\infty \sin^2(bx)e^{-x^2} dx = \frac{\sqrt{\pi}}{4} \left(1 - e^{-b^2}\right) ,$$
$$\int_{-\infty}^{+\infty} \cos[p(x+a)] e^{-x^2} dx = \sqrt{\pi} \cos(pa) \exp\left(-\frac{p^2}{4}\right) .$$

Then, for the single-site integral (3.145), we get

$$h_0 = \frac{\omega_0}{4} + \frac{V_0}{2} \left[ 1 - \exp\left(-k_0^2 l_0^2\right) \right] , \qquad (3.166)$$

and for the overlap integral (3.146), we have

$$h_1 = -\frac{\omega_0 a^2}{8l_0^2} \left\{ 1 - \frac{2l_0^2}{a^2} - \frac{4V_0 l_0^2}{\omega_0 a^2} \left[ 1 + \exp\left(-k_0^2 l_0^2\right) \right] \right\} \exp\left(-\frac{a^2}{4l_0^2}\right) .$$
(3.167)

These can be simplified remembering the conditions (3.100) of good localization, when  $l_0 \ll a$ and  $k_0 l_0 \ll 1$ . Then Eq. (3.166) reduces to

$$h_0 \cong \frac{\omega_0}{4} + \frac{V_0 E_R}{\omega_0} ,$$
 (3.168)

where

$$E_R \equiv \frac{k_0^2}{2m} = \frac{\pi^2}{2ma^2}$$

And Eq. (3.167) simplifies to

$$h_1 \cong -\left(\frac{\pi^2 \omega_0^2}{16E_R} - V_0\right) \exp\left(-\frac{\pi^2 \omega_0}{8E_R}\right) . \tag{3.169}$$

.

The local energy term (3.152) becomes

$$\varepsilon_0 = \frac{\omega_0}{4} + \frac{V_0 E_R}{\omega_0} + \frac{\Phi_1}{2a} \sqrt{\frac{\pi \omega_0}{E_R}} \,. \tag{3.170}$$

The effective frequency  $\omega_0$  can be defined, in first approximation, as in Eq. (3.97),

$$\omega_0 \approx 2 \sqrt{V_0 E_R} \qquad \left(\frac{a_s}{a} \ll 1\right) , \qquad (3.171)$$

which does not take into account atomic interactions. To find the dependence of  $\omega_0$  on the interaction of atoms, we may treat the effective frequency  $\omega_0$  as a trial parameter defined in line with the optimized perturbation theory [219–221]. Accepting the optimization condition as

$$\frac{\partial \varepsilon_0}{\partial \omega_0} = 0 , \qquad (3.172)$$

from Eq. (3.170), we get the equation

$$\omega_0^2 \left( 1 + \frac{\Phi_1}{a} \sqrt{\frac{\pi}{\omega_0 E_R}} \right) = 4V_0 E_R .$$
 (3.173)

Invoking Eq. (3.171), we see that

$$\frac{E_R}{V_0} \approx 4 \left(\frac{E_R}{\omega_0}\right)^2 \ll 1 , \qquad (3.174)$$

according to condition (3.101). Using this in Eq. (3.173), we find

$$\omega_0 \cong 2 \sqrt{V_0 E_R} \left[ 1 - \frac{\Phi_1}{2aE_R} \left( \frac{\pi^2 E_R}{4V_0} \right)^{1/4} \right] . \tag{3.175}$$

Taking account of atomic interactions diminishes the effective frequency  $\omega_0$ .

Recall that we consider weak interactions, since in the other case, the system could not be almost completely condensed. Hence, to a good approximation, one can use the effective frequency estimated in Eq. (3.171). Then expression (3.168) becomes

$$h_0 \cong \sqrt{V_0 E_R} , \qquad (3.176)$$

while Eq. (3.169) reduces to

$$h_1 \cong -\left(\frac{\pi^2}{4} - 1\right) V_0 \exp\left(-\frac{\pi^2}{4} \sqrt{\frac{V_0}{E_R}}\right)$$
 (3.177)

For the tunneling parameter (3.153), we obtain

$$J \cong \left(\frac{\pi^2}{4} - 1\right) V_0 \exp\left(-\frac{\pi^2}{4}\sqrt{\frac{V_0}{E_R}}\right) - 2\sqrt{2\pi} \frac{\Phi_1}{a} \left(\frac{V_0}{E_R}\right)^{1/4} \exp\left(-\frac{3\pi^2}{8}\sqrt{\frac{V_0}{E_R}}\right) .$$
(3.178)

The chemical potential (3.156) reads as

$$\mu_0 \cong \sqrt{V_0 E_R} - \left(\frac{\pi^2}{2} - 2\right) V_0 \exp\left(-\frac{\pi^2}{4} \sqrt{\frac{V_0}{E_R}}\right) +$$

+ 
$$\frac{\Phi_1}{\sqrt{2\pi} l_0} \left[ 1 + 8 \exp\left(-\frac{9\pi^2}{8} \sqrt{\frac{V_0}{E_R}}\right) \right]$$
 (3.179)

And compressibility (3.157) can be simplified to

$$\kappa_T \cong \frac{\sqrt{2\pi} \ l_0}{\rho \Phi_1} , \qquad (3.180)$$

which means that the stability condition  $0 < \kappa_T < \infty$  implies that interactions are repulsive and finite,  $\Phi_1 > 0$ .

### 3.10 Elementary Excitations

Elementary excitations characterize small deviations from the stationary solutions of Eq. (3.128) or Eq. (3.132). Suppose that  $\varphi(z)$ , is an arbitrary stationary solution of Eq. (3.128), with an energy E. Small deviations from the stationary solution are described by the wave function

$$\varphi(z,t) = \left[\varphi(z) + u(z)e^{-i\varepsilon t} + v^*(z)e^{i\varepsilon t}\right]e^{-i(E-\mu_0)t}.$$
(3.181)

Substituting this form into the nonlinear Schrödinger equation (3.125) gives the *Bogolubov* equations

$$(H_{NLS}[\varphi] - E + N_L \Phi_1 |\varphi(z)|^2 - \varepsilon) u(z) + N_L \Phi_1 \varphi^2(z) v(z) = 0 , (H_{NLS}[\varphi] - E + N_L \Phi_1 |\varphi(z)|^2 + \varepsilon) v(z) + N_L \Phi_1 (\varphi^*(z))^2 u(z) = 0 .$$
 (3.182)

As a stationary solution  $\varphi(z)$  with an energy E one can take any Bloch function  $\varphi_{nq}$  with an energy  $E_{nq}$ .

For an equilibrium system, BEC corresponds to the lowest-energy Bloch function  $\varphi_0(z)$  with the energy  $E = \mu_0$ . Considering the elementary excitations above the condensate requires to set as  $\varphi(z)$  in Eq. (3.182) the condensate Bloch function

$$\varphi_0(z) = \frac{1}{\sqrt{N_L}} \sum_j w(z - a_j) .$$
 (3.183)

The Bogolubov functions u(z) and v(z) should be proportional to Bloch functions  $\varphi_k(z)$  with nonzero k. Hence, we take

$$u(z) \equiv u_k \varphi_k(z) , \qquad v(z) \equiv v_k \varphi_k(z) .$$
 (3.184)

Let us introduce the notation

$$\omega_k \equiv \int_{-L/2}^{L/2} \varphi_k^*(z) H_L(z) \varphi_k(z) \, dz \, + \, 2\Delta_k - \mu_0 \,, \qquad (3.185)$$

in which  $H_L(z)$  is the linear lattice Hamiltonian (3.144) and

$$\Delta_k \equiv \Phi_1 N_L \int_{-L/2}^{L/2} |\varphi_k(z)|^2 \varphi_0^2(z) \, dz \,. \tag{3.186}$$

The Bogolubov equations (3.182) reduce to

$$(\omega_k - \varepsilon)u_k + \Delta_k v_k = 0 ,$$
  
$$\Delta_k u_k + (\omega_k + \varepsilon)v_k = 0 , \qquad (3.187)$$

which defines the Bogolubov spectrum of collective excitations

$$\varepsilon_k = \sqrt{\omega_k^2 - \Delta_k^2} \,. \tag{3.188}$$

Calculating quantities (3.185) and (3.186), we employ the tight-binding approximation. The Bloch functions  $\varphi_k(z)$  are expanded over the Wannier functions  $w(z - a_j)$ , as in Eq. (3.31), and w(z) is taken in form (3.161). This yields for Eq. (3.185)

$$\omega_k = \Delta + 4J\sin^2\left(\frac{ka}{2}\right) \,, \tag{3.189}$$

where

$$\Delta \equiv (I_0 + 8I_1)\Phi_1 , \qquad (3.190)$$

while for Eq. (3.186),

$$\Delta_k = \Delta - 8I_1 \Phi_1 \sin^2\left(\frac{ka}{2}\right) . \tag{3.191}$$

Then the Bogolubov spectrum (3.188) is

$$\varepsilon_k = \left[4 \frac{c^2}{a^2} \sin^2\left(\frac{ka}{2}\right) + 16\left(J^2 - 4I_1^2 \Phi_1^2\right) \sin^4\left(\frac{ka}{2}\right)\right]^{1/2} , \qquad (3.192)$$

where c is the sound velocity

$$c \equiv \sqrt{2\Delta(J + 2I_0\Phi_1)a^2} . \tag{3.193}$$

In the long-wave limit, when  $k \to 0$ , one has

$$\omega_k \simeq \Delta + J(ka)^2$$
,  $\Delta_k \simeq \Delta - 2I_1 \Phi_1(ka)^2$ .

And Eq. (3.192) gives the gapless phonon spectrum

$$\varepsilon_k \simeq ck \qquad (k \to 0) .$$
 (3.194)

Comparing the Bloch spectrum (3.154) and the Bogolubov spectrum (3.192), we see that they are quite different [215,222,223]. To stress their difference, we may rewrite the Bloch spectrum (3.154) in the form

$$E_k = \mu_0 + 4J\sin^2\left(\frac{ka}{2}\right) ,$$
 (3.195)

where  $\mu_0$  is the chemical potential (3.155). In the long-wave limit, the Bloch spectrum (3.195) is

$$E_k \simeq \mu_0 + J(ka)^2 \qquad (k \to 0) ,$$

which is, clearly, a single-particle spectrum with the gap  $\mu_0$ , contrary to the gapless phonon spectrum (3.194).

It is important to emphasize that for equilibrium bosons in lattices, in the presence of BEC, when the gauge symmetry is broken, the single-particle spectrum of *uncondensed* atoms (3.69) coincides with the spectrum of elementary excitations (3.188), both of them being the Bogolubov spectra.

Of the Bloch spectrum (3.154), or (3.195), solely one point, where n = 0 and k = 0, and  $E_k = \mu_0$ , corresponds to an equilibrium BEC. But the Bloch spectrum, in general, describes nonequilibrium condensates that are the analog of the coherent modes [174–176]. This is why the Bloch spectrum does not need to coincide with the Bogolubov spectrum

# 3.11 Wave Stability

The condensate wave function  $\varphi_0(z)$  for an equilibrium system is assumed to correspond to a stable system. The related condition of thermodynamic stability is that compressibility (3.135), or (3.157), be positive and finite,  $0 \le \kappa_T < \infty$ .

Other Bloch functions  $\varphi_{nk}(z)$ , which are solutions to Eq. (3.132), as is stressed above, do not correspond to a thermodynamically equilibrium BEC. Though these functions  $\varphi_{nk}(z)$ are stationary solutions, but a statistical system with a condensate, characterized by such a function is not in absolute equilibrium. It is, therefore, useful to study the stability of the Bloch functions  $\varphi_{nk}(z)$ .

There are, in general, several kinds of stability for solutions to differential equations [224– 227]. The most often used is the notion of Lyapunov stability [228]. Let us recall this notion in general terms. Suppose we consider functions of the type  $\varphi(x, t)$ , where x is a variable of arbitrary nature, which can pertain to the continuous manifold  $\mathbb{R}^d$ , or to a discrete manifold, or to their combination, and where  $t \in [0, \infty)$ . Treating x as an enumeration index, one can define the column function  $\varphi(t) \equiv [\varphi(x, t)]$ . Let  $\varphi(t)$  pertain to a Banach space (normed, complete space), where a norm  $||\varphi(t)||$  is defined. When  $\varphi(t)$  pertains to a Hilbert space, the norm is naturally generated by the scalar product. Let us consider the evolution equation

$$\frac{\partial\varphi(t)}{\partial t} = F[\varphi] , \qquad (3.196)$$

in which  $F[\varphi]$  is an operator functional in the same Banach space. It is assumed that, for a given initial condition  $\varphi(0)$ , the Cauchy problem (3.196) enjoys a unique solution.

A solution  $\overline{\varphi}(t)$  is Lyapunov stable, if for any other solution  $\varphi(t)$ , such that

$$||\varphi(0) - \overline{\varphi}(0)|| < \delta_0 , \qquad (3.197)$$

with any  $\delta_0 > 0$ , there exists a positive number  $\delta$ , for which

$$||\varphi(t) - \overline{\varphi}(t)|| < \delta \qquad (t > 0) . \tag{3.198}$$

The solution  $\overline{\varphi}(t)$  is asymptotically stable, when there can be found such  $\delta_0$  in Eq. (3.197) that

$$\lim_{t \to \infty} ||\varphi(t) - \overline{\varphi}(t)|| = 0.$$
(3.199)

The solution  $\overline{\varphi}(t)$  is exponentially stable, if there exists such  $\delta_0$  in Eq. (3.197) that

$$\lim_{t \to \infty} \frac{1}{t} \ln ||\varphi(t) - \overline{\varphi}(t)|| < 0.$$
(3.200)

In particular,  $\overline{\varphi}(t)$  can be a stationary solution, for which  $F[\overline{\varphi}] = 0$ . Exponential stability is a special case of asymptotic stability.

Conversely, if, under condition (3.197): inequality (3.198) is not valid, the solution  $\overline{\varphi}(t)$  is Lyapunov unstable; when limit (3.199) does not follow for any  $\delta_0$ ,  $\overline{\varphi}(t)$  is asymptotically unstable; and if the limit (3.200) becomes positive, then  $\overline{\varphi}(t)$  is exponentially unstable.

From these definitions, it is clear that the Lyapunov stability does not lead to the asymptotic stability and, vice versa, the asymptotic stability does not imply the Lyapunov stability. Also, the Lyapunov instability does not forbid the asymptotic stability for some  $\delta_0$ . And the asymptotic instability does not contradict to the Lyapunov stability.

Lyapunov developed [228] two methods of controlling stability, the direct method and the method of linearization.

Lyapunov direct method is based on the existence of the Lyapunov functional, such that

$$L[\varphi] \ge 0 \tag{3.201}$$

for all  $\varphi(t)$  from the considered Banach space and which does not increase,

$$\frac{\partial}{\partial t} L[\varphi] \le 0 , \qquad (3.202)$$

on the trajectories of Eq. (3.196). If such a Lyapunov functional exists, then the solution  $\varphi(t)$  is Lyapunov stable.

The Lyapunov direct method is global, requiring the validity of condition (3.201) on the whole Banach space. In many cases, one is interested not in the global stability, but in the local stability in the vicinity of a known solution  $\overline{\varphi}(t)$ . Then the direct Lyapunov method is reformulated as follows.

Lyapunov local method assumes the existence of a functional  $L[\varphi]$ , which does not increase on the trajectories, as in Eq. (3.202), and which is minimal in the small vicinity of a given function  $\overline{\varphi}(t)$ , that is, when for  $\varphi = \overline{\varphi} + \delta \varphi$ , one has

$$\delta L[\varphi] = 0 , \qquad \delta^2 L[\varphi] > 0 . \qquad (3.203)$$

If such a functional exists, then the solution  $\overline{\varphi}(t)$  is *locally stable*.

In many cases, the role of the Lyapunov function is played by energy or by an effective energy, if the energy is complimented by additional constraints. When the energy functional  $E[\varphi]$  is an integral of motion, then  $\partial E[\varphi]/\partial t = 0$ , so that condition (3.202) holds. Hence, if  $E[\varphi] \ge 0$ , the motion is Lyapunov stable. This does not mean that the motion is locally stable in the vicinity of a given  $\overline{\varphi}$ . To study the local stability near  $\overline{\varphi}$ , one has to satisfy conditions (3.203) for the Lyapunov functional  $E[\varphi]$ . One says that a solution is *energetically* stable, if

$$\frac{\partial}{\partial t} E[\varphi] \le 0 , \qquad \delta E[\varphi] = 0 , \qquad \delta^2 E[\varphi] > 0 \qquad (3.204)$$

for  $\varphi = \overline{\varphi} + \delta \varphi$ . That is, the *energetic stability* is just an example of the *local stability*, when the Lyapunov functional is represented by an energy functional.

Above, we have considered the variants of the Lyapunov direct method for analysing the stability of solutions to the evolution equation (3.196). The second Lyapunov method is based on the linearization of Eq. (3.196).

Lyapunov linearization method requires the linearization of the evolution equation (3.196) with respect to small deviations from the given solution  $\overline{\varphi}$ . Taking  $\varphi = \overline{\varphi} + \delta \varphi$ , one obtains linear equations for  $\delta \varphi$ , which are subject to the standard stability analysis [228,229]. When all Lyapunov exponents are negative, the solution  $\overline{\varphi}$  is asymptotically stable. If at least one of them is positive, then  $\overline{\varphi}$  is asymptotically unstable. And when some of the Lyapunov exponents are zero, while others being negative, the considered solution is neutrally stable, provided it remains finite for all t > 0. If the linearized equations show that the solution  $\overline{\varphi}$  is either asymptotically stable or neutrally stable, then such a solution is termed dynamically stable.

Suppose that one is interested in the stability of a stationary solution  $\overline{\varphi}$ , for which  $\partial \overline{\varphi} / \partial t = 0$ . Considering small deviations from  $\overline{\varphi}$ , when  $\varphi(t) = \overline{\varphi} + \delta \varphi(t)$ , one can check he local, or energetic stability by means of Eqs. (3.202) and (3.203), or (3.204). Alternatively, one can use the linearization method for the evolution equation (3.196). Then there exists the following relation between different types of stability.

#### **Theorem**. The local stability of a stationary solution yields its dynamic stability.

*Proof.* Let  $\overline{\varphi}$  be a stationary solution of Eq. (3.196), such that  $\partial \overline{\varphi} / \partial t = 0$ . And let this solution be locally stable, which implies that there exists a Lyapunov functional  $L[\varphi]$  satisfying conditions (3.202) and (3.203). Expanding the Lyapunov functional for the perturbed solution  $\varphi(t) = \overline{\varphi} + \delta \varphi(t)$ , we have

$$L[\varphi] = L[\overline{\varphi}] + \delta L[\varphi] + \delta^2 L[\varphi] .$$

From here, in view of Eqs. (3.202) and (3.203), it follows

$$\frac{\partial}{\partial t} \, \delta^2 L[\varphi] = \frac{\partial}{\partial t} \, L[\varphi] \le 0 \; .$$

Taking

$$||\delta\varphi(0)|| \le \delta^2 L[\varphi(0)] ,$$

we find

$$||\delta\varphi(t)|| \le \delta^2 L[\varphi(t)] \le \delta^2 L[\varphi(0)]$$

which shows that the linear deviation  $\delta \varphi(t)$  does not increase with time. Hence,  $\overline{\varphi}$  is dynamically stable.

When the Lyapunov functional is the energy functional, the theorem tells us that the energetic stability of a stationary solution yields its dynamic stability.

The inverse, however, is not true. The dynamic stability does not necessarily yield the local, or energetic, stability. To illustrate this, let us consider a two-component field  $\varphi = \{\varphi_1, \varphi_2\}$ , where  $\varphi_i = \varphi_i(x, t)$ , with the energy functional

$$E[\varphi] = \frac{1}{2} \int \left(\varphi_1|^2 - |\varphi_2|^2 - g|\varphi_1|^2 |\varphi_2|^2\right) dx .$$

The evolution equations are defined in the usual way as

$$i \frac{\partial \varphi_j}{\partial t} = \frac{\delta E[\varphi]}{\delta \varphi_j^*} ,$$

which gives

$$i \frac{\partial \varphi_1}{\partial t} = \frac{1}{2} \varphi_1 \left( 1 - g |\varphi_2|^2 \right) , \qquad i \frac{\partial \varphi_2}{\partial t} = -\frac{1}{2} \varphi_2 \left( 1 + g |\varphi_1|^2 \right) .$$

The stationary solutions of these equations are  $\overline{\varphi}_1 = \overline{\varphi}_2 = 0$ . The linearized equations give

$$\delta \varphi_1 = c_1 e^{-i\omega t} , \qquad \delta \varphi_2 = c_2 e^{i\omega t} ,$$

where  $c_j = c_j(x)$  and  $\omega = 1/2$ . Hence, the deviations  $\delta \varphi_j$  do not increase with time, which means that the stationary solutions  $\overline{\varphi}_1$  and  $\overline{\varphi}_2$  are *dynamically stable*.

For the energy functional, we have

$$\frac{\partial}{\partial t} E[\varphi] = 0 , \qquad \delta E[\varphi] = 0 .$$

However, the second variation

$$\delta^2 E[\varphi] = \frac{1}{2} \int \left( |c_1|^2 - |c_2|^2 \right) \, dx$$

is not positive defined, that is, the stationary solutions  $\overline{\varphi}_j = 0$  do not provide a minimum of  $E[\varphi]$ . Hence these stationary solutions are *energetically unstable*.

For an optical lattice, discussed in the previous sections, we may define the energy functional

$$E[\varphi] \equiv N \int \varphi^*(z) [H_L(z) - E] \varphi(z) dz + \frac{N}{2} N_L \Phi_1 \int |\varphi(z)|^4 dz . \qquad (3.205)$$

The stationarity condition

$$\frac{\delta E[\varphi]}{\delta \varphi^*(z)} = 0 \tag{3.206}$$

results in the stationary nonlinear Schrödinger equation (3.128). The latter, due to its nonlinearity, can possess different types of solutions, including Bloch waves, localized solitons, as well as density waves with a period differing from that of the optical potential [212]. Limiting ourselves by the class of Bloch functions, we come to Eq. (3.132).

The Bloch spectrum  $E_{nk}$ , defined by Eq. (3.132), displays rather nontrivial behavior, caused by the nonlinearity of the eigenproblem. For sufficiently strong nonlinearity, there appears the swallow-tail structure of  $E_{nk}$ , when it is not uniquely defined as a function of k [230–234]. The swallow tails can appear at the edge of the lowest band, with n = 0 and  $k = \pi/a$ , and also in the middle of upper bands, with  $n \ge 1$  and k = 0. This happens when the interaction is sufficiently strong, so that

$$\frac{aV_0}{\Phi_1} < 1 . (3.207)$$

In the presence of nonlinearity, the optical lattice may provoke instability of Bloch waves  $\varphi_{nk}(z)$  for some k. To find the region of stability, one considers small deviations in the vicinity of  $\varphi_{nn}(z)$  by setting

$$\varphi_{nk}(z,t) = \varphi_{nk}(z) + \delta\varphi(z,t) , \qquad (3.208)$$

where

$$\delta\varphi(z,t) = \left[u_{nq}(z)e^{i(qz-\varepsilon t)} + v_{nq}^*(z)e^{-i(qz-\varepsilon t)}\right] .$$
(3.209)

The energetic, or static, stability is defined by substituting Eq. (3.208) into the energy functional (3.205) and taking  $\varepsilon = 0$  in Eq. (3.209). The dynamic stability is analyzed by linearizing the evolution equation

$$i \frac{\partial}{\partial t} \varphi_{nk}(z,t) = (H_{NLS}[\varphi_{nk}] - E_{nk}) \varphi_{nk}(z,t)$$
(3.210)

with respect to the small deviation (3.209). The functions  $\varphi_{nk}(z)$ ,  $u_{nq}(z)$ , and  $v_{nq}(z)$  are Bloch waves.

Linearizing Eq. (3.210) gives for the energy  $\varepsilon$  the spectrum of collective excitations  $\varepsilon_{nkq}$ around the Bloch spectrum  $E_{nk}$ . Dynamic instability occurs when  $\varepsilon_{nkq}$  becomes complex, since then there appears an exponentially increasing term in Eq. (3.209).

From the general theory, expounded at the beginning of this section, it follows that the energetic stability yields the dynamic stability. This means that, if the solution is dynamically unstable, it is also energetically unstable. However, the solution can be dynamically stable, while being energetically unstable. All this is, of course, valid for optical lattices [230–234], as well as for vortex states [235].

It is worth recalling that the Bloch functions  $\varphi_{nk}$ , with n > 0 and k > 0, correspond to excited nonequilibrium condensates. Therefore the stability, in any sense, of such nonequilibrium condensates should be neither required nor expected. What is required is the stability of the equilibrium ground-state BEC, corresponding to the natural Bloch orbital  $\varphi_0$ , with n = 0 and k = 0. The stability of the latter is guaranteed by compressibility (3.135) being positive and finite, which, in view of Eqs. (3.157) and (3.180), requires that atomic interactions be repulsive and finite, that is,  $\Phi_1 > 0$ .

# 3.12 Moving Lattices

Different nonequilibrium states of BEC can be crated by moving the optical lattice. To obtain an effective equation for BEC in a moving lattice, let us assume that the latter moves with velocity v = v(t) along the z-axis. This means that, in the frame of the lattice, the condensate moves with velocity -v(t). The wave function of a moving condensate  $\varphi_v(z,t)$  satisfies the nonlinear Schrödinger equation

$$i \frac{\partial}{\partial t} \varphi_v(z, t) = (H_{NLS}[\varphi_v] - E) \varphi_v(z, t)$$
(3.211)

and is related to the wave function of an immovable condensate through the Galilean transformation

$$\varphi_v(z,t) = \varphi(z+vt,t) \exp\left\{-i\left(mvz + \frac{mv^2}{2}t\right)\right\} .$$
(3.212)

Substituting function (3.212) into Eq. (3.211) and neglecting the term

$$(\hat{p} - mv) \varphi(z + vt, t) \approx 0$$
  $\left(\hat{p} \equiv -i \frac{\partial}{\partial z}\right)$ 

yields

$$i \frac{\partial}{\partial t} \varphi(z + vt, t) = (H_{NLS}[\varphi] - E - m\dot{v}z) \varphi(z + vt, t) , \qquad (3.213)$$

where  $\dot{v} \equiv \partial v / \partial t$ .

There exist two different length scales in the system. One is the intersite distance a, being the lattice period. The typical variation of Bloch functions is on the lattice scale a. And another scale is the effective size L of the studied atomic cloud, being much larger than a,

$$\frac{a}{L} \ll 1. \tag{3.214}$$

The existence of such very different scales allows for the use of averaging techniques [236–239] and of the scale separation approach [240–243]. A similar procedure in electrodynamics is called the slowly varying amplitude approximation [244–249]. In line with such techniques, we may look for the solution of Eq. (3.213) in the form

$$\varphi(z+vt,t) = A(z,t)\varphi_q(z) , \qquad (3.215)$$

where, for simplicity, we consider a single band and assume that the quasimomentum q = q(t) is, generally speaking, a function of time. The factor A(z, t) in Eq. (3.215) is a slowly varying amplitude, such that

$$\left|\frac{\partial A}{\partial z}\right| \ll \left|\frac{\partial \varphi_q}{\partial z}\right| \,. \tag{3.216}$$

While  $\varphi_q(z)$  is a Bloch function given by the equation

$$H_L(z)\varphi_q(z) = E_q\varphi_q(z) , \qquad (3.217)$$

with the linear lattice Hamiltonian (3.144). According to condition (3.216), the function  $\varphi_q(z)$  is fastly varying in space, as compared to the slow amplitude A(z,t). The latter is also called the envelope. It is normalized as

$$\frac{1}{L} \int_{-L/2}^{L/2} |A(z,t)|^2 dz = 1.$$
(3.218)

The Bloch function  $\varphi_q(z)$  satisfies the usual normalization condition

$$\int_{-L/2}^{L/2} |\varphi_q(z)|^2 dz = 1.$$
(3.219)

An important point is the ansatz

$$H_L(z)A(z,t)\varphi_q(z) = [E_{q+\hat{p}}A(z,t)]\varphi_q(z) , \qquad (3.220)$$

whose justification [250] is based on the averaging techniques.

Substituting form (3.215) into Eq. (3.213) yields the equation

$$i\frac{\partial A}{\partial t} = (E_{q+\hat{p}} - E_q)A + \alpha_q |A|^2 A + (\dot{q} - m\dot{v})zA , \qquad (3.221)$$

where A = A(z, t), the overdot means time derivative, and

$$\alpha_q \equiv N_L \Phi_1 \int_{-L/2}^{L/2} |\varphi_q(z)|^4 dz . \qquad (3.222)$$

Deriving (3.221), we have also used the approximate equality

$$\frac{\partial}{\partial q} \varphi_q(z) \approx i z \varphi_q(z)$$

following from the fact that  $\varphi_q \propto e^{iqz}$ .

Expanding

$$E_{q+\hat{p}} \simeq E_q + v_q \hat{p} + \frac{1}{2m_q^*} \hat{p}^2$$
 (3.223)

in powers of  $\hat{p} = -i\partial/\partial z$ , with the group velocity  $v_q$  and effective mass  $m_q^*$  defined by the relations

$$v_q \equiv \frac{\partial E_q}{\partial q} \qquad \frac{1}{m_q^*} \equiv \frac{\partial^2 E_q}{\partial q^2} , \qquad (3.224)$$

we come to the evolution equation for the amplitude

$$i\left(\frac{\partial A}{\partial t} + v_q \;\frac{\partial A}{\partial z}\right) + \frac{1}{2m_q^*} \;\frac{\partial^2 A}{\partial z^2} = \alpha_q |A|^2 A + (\dot{q} - m\dot{v})zA\;. \tag{3.225}$$

# 3.13 Soliton Formation

Suppose that, after moving the lattice and reaching a Bloch state with a quasimomentum q, the motion has been stopped, so that  $\dot{q} = \dot{v} = 0$ . Then Eq. (3.225) reduces to

$$i\left(\frac{\partial A}{\partial t} + v_q \frac{\partial A}{\partial z}\right) + \frac{1}{2m_q^*} \frac{\partial^2 A}{\partial z^2} = \alpha_q |A|^2 A .$$
(3.226)

This is a nonlinear Schrödinger equation supporting soliton solutions [251]. Similar equations are met in laser physics [252], in the theory of turbulent plasma [253,254], in the description of magnetic matter [255], and in the theory of many other nonlinear materials [256,257]. For Bose condensates, Eq. (3.226) was derived by Lenz et al. [258].

Equation (3.226) can be simplified by changing the variable to

$$x \equiv \frac{z - v_q t}{\xi} , \qquad (3.227)$$

where

$$\xi = \frac{1}{\sqrt{2|m_q^*\varepsilon|}} \tag{3.228}$$

is the healing length and  $\varepsilon$  is the soliton energy to be defined by the normalization condition (3.218). Let us introduce a function f(x) through the relation

$$A(z,t) \equiv \sqrt{\frac{\varepsilon}{\alpha_q}} f(x)e^{-i\varepsilon t} . \qquad (3.229)$$

The function f(x) can be chosen real, since Eq. (3.226) is invariant under the global gauge transformation  $A \to Ae^{i\alpha}$ . And let us define

$$\zeta \equiv \operatorname{sgn}(m_q^* \varepsilon) . \tag{3.230}$$

Then Eq. (3.226) can be reduced to

$$\frac{d^2f}{dx^2} + \zeta \left(1 - f^2\right) f = 0.$$
(3.231)

Depending on the sign of  $\zeta$  in Eq. (3.230), there are the following possibilities.

Dark solitons correspond to  $\zeta = 1$  and the boundary conditions

$$\lim_{x \to \pm \infty} f(x) = \pm 1 . \tag{3.232}$$

The name comes from the fact that the density distribution  $|f(x)|^2$  has the lowest value at x = 0. Dark solitons are called cavitons in the theory of plasma [253,254] and in laser physics [252]. There can be two types of dark solitons.

*Normal dark soliton* is formed by atoms with a positive effective mass, repulsive interactions, and with a positive soliton energy,

$$m_q^* > 0 , \qquad \alpha_q > 0 , \qquad \varepsilon > 0 .$$
 (3.233)

*Dark gap soliton* is characterized by a negative effective mass, attractive interactions, and a negative soliton energy,

$$m_q^* < 0 , \qquad \alpha_q < 0 , \qquad \varepsilon < 0 .$$
 (3.234)

It is worth stressing that the signs of the effective interaction  $\alpha_q$  and the soliton energy  $\varepsilon$  are chosen to be the same in order that the expression  $\sqrt{\varepsilon/\alpha_q}$  in Eq. (3.229) be real. This does not limit the generality, but simply takes into account that the amplitude (3.229) is defined up to a phase factor.

The name of the gap soliton is due to the fact that, to achieve a negative effective mass, the atomic cloud has to be shifted to the edge of the Brillouin zone. This shift can be realized by the appropriate motion of the lattice.

The form of the dark soliton, being the solution of Eq. (3.231), with  $\zeta = 1$ , under the boundary conditions (3.232), is

$$f(x) = \tanh \frac{x}{\sqrt{2}} . \tag{3.235}$$

The normalization condition (3.218) for amplitude (3.229), with f(x) from Eq. (3.235), gives

$$\varepsilon = \alpha_q = \frac{1}{2m_q^*\xi^2} \,, \tag{3.236}$$

the healing length (3.228) being

$$\xi = \frac{1}{\sqrt{2m_q^*\alpha_q}} \,. \tag{3.237}$$

Hence, the total dark envelope (3.229) becomes

$$A(z,t) = \tanh\left(\frac{z - v_q t}{\sqrt{2}\,\xi}\right) e^{-i\varepsilon t} \,, \qquad (3.238)$$

with the healing length (3.237) and soliton energy (3.236).

Bright solitons arise for  $\zeta = -1$ , under the boundary conditions

$$\lim_{x \to \pm \infty} f(x) = 0 .$$
 (3.239)

Such solitons correspond to the maximum of the density distribution  $|f(x)|^2$  at x = 0. They are called as well the bell solitons. There are again two possibilities.

*Normal bright soliton* is described by a positive effective mass, though attractive interactions and negative soliton energy,

$$m_q^* > 0 , \qquad \alpha_q < 0 , \qquad \varepsilon < 0 .$$
 (3.240)

Bright gap soliton possesses a negative effective mass, but repulsive interactions and positive soliton energy,

$$m_q^* < 0 , \qquad \alpha_q > 0 , \qquad \varepsilon > 0 .$$
 (3.241)

Again, to make the effective mass negative, it is necessary to move the lattice so that the atomic cloud would acquire a quasimomentum at the edge of the first Brillouin zone.

The bright solution solution, resulting from Eq. (3.231), with  $\zeta = -1$ , under the boundary conditions (3.239), is

$$f(x) = \frac{\sqrt{2}}{\cosh x} \,. \tag{3.242}$$

The normalization condition (3.218) yields the soliton energy

$$\varepsilon = -\frac{m_q^*}{8} (\alpha_q L)^2 = -\frac{1}{2m_q^* \xi^2},$$
 (3.243)

with the healing length

$$\xi = \frac{2}{|m_q^* \alpha_q L|} \,. \tag{3.244}$$

The total bright soliton envelope (3.229) takes the form

$$A(z,t) = \sqrt{\frac{L}{2\xi}} \operatorname{sech}\left(\frac{z - v_q t}{\xi}\right) e^{-i\varepsilon t} , \qquad (3.245)$$

with the healing length (3.244) and soliton energy (3.243). This form is analogous to Langmur solitons in plasma [253,254]. One sometimes distinguishes solitons by their topological charge, defined as

$$\lim_{x \to \infty} [f(x) - f(-x)] \; .$$

When the latter is nonzero, the solitons are termed topological. Thus, dark solitons are topological. If the topological charge is zero, the solitons are called nontopological. Hence, bright solitons are nontopological.

Dark solitons of BEC were generated for repulsive <sup>78</sup>Rb atoms [259,260] and bright solitons in BEC were formed with attractive <sup>7</sup>Li atoms [261,262]. The specific feature of gap solitons is that they can be created only in the presence of a periodic lattice [263]. Gap solitons were observed for <sup>87</sup>Rb atoms [264].

# 3.14 Transverse Resonance

When creating gap solitons, it is necessary to shift an atomic cloud to the boundary of the Brillouin zone, where the effective mass becomes negative. But then the Bloch energy increases, and it may happen that the transverse modes of atomic motion could be excited. In such a case, the quasi-one-dimensional picture for treating a single wave packet is not anymore appropriate, and one has to take into account transverse excitations [265]. This can be done in the following way [250].

When, despite of a strong transverse harmonic confinement, nevertheless, some transverse modes can be excited, then it is necessary, instead of Eq. (3.118), to consider the transverse motion described by the equation

$$\left(-\frac{\nabla_{\perp}^2}{2m} + \frac{m}{2}\,\omega_{\perp}^2 r_{\perp}^2\right)\chi_n(\mathbf{r}_{\perp}) = E_n^{\perp}\chi_n(\mathbf{r}_{\perp}) \;. \tag{3.246}$$

Under the harmonic transverse confinement, the eigenenergy spectrum of Eq. (3.246) is

$$E_n^{\perp} = (2n_r + |m_a| + 1)\omega_{\perp} , \qquad (3.247)$$

where  $n_r = 0, 1, 2, ...$  is a radial quantum number,  $m_a = 0, \pm 1, \pm 2, ...$  is an azimuthal quantum number, and the multi-index  $n = \{n_r, m_a\}$  includes both of these numbers. The lowest energy (3.247) is  $E_0^{\perp} = \omega_{\perp}$ .

When trapped atoms are in the lowest-energy transverse state, then their total spectrum is the sum of the lowest energy of transverse motion,  $\omega_{\perp}$ , and of the Bloch energy  $E_q$ . For an excited transverse state, with an energy  $E_n^{\perp}$ , the total spectrum is the sum  $E_n^{\perp} + E_p$ . Although  $\omega_{\perp} < E_n^{\perp}$ , for  $n \neq 0$ , but if  $q \approx \pi/a$ , there exists such a quasimomentum  $p \in [-\pi/a, \pi/a]$ that  $E_q > E_p$ . And the resonance condition

$$\omega_{\perp} + E_q = E_n^{\perp} + E_p \tag{3.248}$$

can become valid. Then the transverse modes, with the energy  $E_n^{\perp}$ , become excited.

In the presence of the excited transverse modes, the condensate wave function  $\eta(\mathbf{r}, t)$ , satisfying Eq. (3.115), has to be written as

$$\eta(\mathbf{r},t) = \sum_{i} \chi_{n_i}(\mathbf{r}_\perp) B_i(z,t) \varphi_{q_i}(z) \exp\left\{-i \left(E_{n_i}^\perp - \mu_0\right) t\right\} , \qquad (3.249)$$

which generalizes Eqs. (3.116), (3.127), and (3.215). The transverse wave functions  $\chi_n(\mathbf{r}_{\perp})$  are normalized to one, as in Eq. (3.117). The Bloch functions  $\varphi_q(z)$  are normalized as in Eq. (3.219). But the envelopes  $B_i(z,t)$  satisfy the normalization conditions

$$\frac{1}{L} \int_{-L/2}^{L/2} |B_i(z,t)|^2 dz = N_i , \qquad (3.250)$$

where  $N_i = N_i(t)$ , generally, are functions of time. This normalization differs from that in Eq. (3.218).

Now, instead of one interaction parameter (3.222), there are several interaction parameters

$$\alpha_{ijkl} \equiv N_L \Phi_0 \int \chi_{n_i}^* \chi_{n_j}^* \chi_{n_k} \chi_{n_l} \, d\mathbf{r}_\perp \, \int \varphi_{q_i}^* \varphi_{q_j}^* \varphi_{q_k} \varphi_{q_l} \, dz \,. \tag{3.251}$$

Following the same way as in the previous sections, instead of Eq. (3.226), we obtain the set of equations

$$i\left(\frac{\partial B_i}{\partial t} + v_i \frac{\partial B_i}{\partial z}\right) + \frac{1}{2m_i^*} \frac{\partial^2 B_i}{\partial z^2} = \frac{1}{N_L} \sum_{jkl} \alpha_{ijkl} B_j^* B_k B_l$$
(3.252)

for the mode envelopes  $B_i(z,t)$ , with i = 0, 1, 2. The mode envelope  $B_0(z,t)$  corresponds to the central mode of a gap soliton, with  $q = \pi/a$ , while the envelopes  $B_1(z,t)$  and  $B_2(z,t)$ , to the two side modes, for which the resonance condition (3.248) is valid. There are two transverse modes, since the resonance condition (3.248) holds for two Bloch energies  $E_{q_1}$  and  $E_{q_2}$ , for which

$$E_{q_1} = E_{q_2} \qquad \left(q_1 = \frac{\pi}{a} - q \;,\;\; q_2 = \frac{\pi}{a} + q\right) \;.$$
 (3.253)

The form of parameters (3.251) shows that

$$\alpha_{ijkl} = \alpha_{jikl} = \alpha_{ijlk} . \tag{3.254}$$

Also, for the quasimomenta  $q_1$  and  $q_2$ , related as in Eq. (3.253), one has

$$\varphi_{q_1}^*(z) = \varphi_{q_2}(z) . \tag{3.255}$$

For the transverse wave functions, according to condition (3.248), one has

$$\chi_{n_1}(\mathbf{r}_\perp) = \chi_{n_2}(\mathbf{r}_\perp)$$
.

Since the functions  $\chi_0(\mathbf{r}_{\perp})$  and  $\chi_1(\mathbf{r}_{\perp})$  possess different symmetries with respect to the inversion of  $\mathbf{r}_{\perp}$ , not all integrals in Eq. (3.251) are nonzero. These are  $\alpha_{0000}$  and

$$\alpha_{1111} = \alpha_{2222} = \alpha_{1212} , \qquad \alpha_{0101} = \alpha_{0202} = \alpha_{0012} ,$$

as well as all those that are obtained from the above ones using symmetry (3.254) and property (3.255).

An interesting solution of Eqs. (3.252) is represented by a *triple solution* [250], which is a triplet of solitons, one of which corresponds to  $q = \pi/a$ , that is, to a gap soliton, while two

others are the side transverse modes. All three modes are bound with each other, so that they stay localized in space. Bound triplets of solitons are also called tritons [256].

It is worth mentioning that quasi-one-dimensional gap solitons, as those that are considered in Sec. 3.13, are usually unstable with respect to the formation of transverse modes [256]. Hence, gap solitons are, strictly speaking, quasisolitons, that is, the soliton-like solutions that in the long run are unstable, but can live sufficiently long to be observable. However the triple gap soliton can be stable [250].

# 3.15 Lagrange Variation

Instead of solving the system of partial differential equations, it is possible to reduce the problem to the solution of a set of ordinary differential equations by means of the Lagrange variational method. To illustrate the latter, let us consider the system of three partial differential equations (3.252).

Let us define the energy functional

$$E[B] \equiv \sum_{j} \int B_{j}^{*} i \frac{\partial}{\partial t} B_{j} dz , \qquad (3.256)$$

the Hamiltonian functional

$$H[B] \equiv \sum_{j} \int B_{j}^{*} \left( v_{j} \hat{p} + \frac{\hat{p}^{2}}{2m} \right) B_{j} dz + \frac{1}{2L} \sum_{ijkl} \alpha_{ijkl} \int B_{i}^{*} B_{j}^{*} B_{k} B_{l} dz , \qquad (3.257)$$

and the Lagrangian

$$L[B] \equiv E[B] - H[B] . (3.258)$$

Equations (3.252) follow from the Lagrange variational equations

$$\frac{d}{dt} \frac{\delta L[B]}{\delta \dot{B}_j} - \frac{\delta L[B]}{\delta B_j} \,. \tag{3.259}$$

Approximate solutions to Eqs. (3.252) can be constructed by invoking trial forms for the wave packets  $B_i$ , for instance, as the Gaussian envelopes

$$B_j = \frac{C_j}{(\sqrt{\pi} b_j)^{1/2}} \exp\left\{-\frac{(z-z_j)^2}{2b_j}\right\} \exp\left\{-i\left(\alpha_j t - \beta_j z - \gamma_j z^2\right)\right\}, \qquad (3.260)$$

where all variables  $C_j$ ,  $b_j$ ,  $z_j$ ,  $\alpha_j$ ,  $\beta_j$ , and  $\gamma_j$  are treated as functions of time. The evolution equations for all these variables are obtained by applying the Lagrange equations to each of the variables  $C_j$ ,  $b_j$ ,  $z_j$ ,  $\alpha_j$ ,  $\beta_j$ , and  $\gamma_j$ . Then, instead of three equations (3.252) in partial derivatives, one gets a set of 18 equations in ordinary derivatives [250]. The latter are much easier to solve numerically, as well as to analyze the stability of their solutions.

# 4 Boson Hubbard Model

# 4.1 Wannier Representation

In Sec. 3.3 the representation of the grand Hamiltonian (3.15) is given by expanding the field operators over Bloch functions. This results in the Bloch representation of the Hamiltonian (3.55) specified in Eq. (3.56) to (3.59). The field operators could also be expanded over the basis of Wannier functions. Such a Wannier representation, leading to the Hubbard model [266], is widely employed for treating electrons in solid-state lattices and the related metal-insulator phase transition [267–269]. In a particular case of half filling and neglecting double occupancies the Hubbard model can be reduced to the so-called t - J model [270].

For a periodic Bose system with BEC, the field operator can be expanded over Wannier functions,

$$\hat{\psi}(\mathbf{r}) = \sum_{nj} \hat{c}_{ij} w_n(\mathbf{r} - \mathbf{a}_j) .$$
(4.1)

Keeping in mind the Bogolubov-shifted field operator (2.81), that is

$$\hat{\psi}(\mathbf{r}) = \eta(\mathbf{r}) + \psi_1(\mathbf{r}) , \qquad (4.2)$$

we have the expansion

$$\eta(\mathbf{r}) = \sqrt{\frac{N_0}{N_L}} \sum_j w_0(\mathbf{r} - \mathbf{a}_j)$$
(4.3)

for the condensate wave function and the expansion

$$\psi_1(\mathbf{r}) = \sum_{nj} c_{nj} w_n(\mathbf{r} - \mathbf{a}_j) \tag{4.4}$$

for the operator of uncondensed atoms. This means that

$$\hat{c}_{nj} = \sqrt{\frac{N_0}{N_L}} \,\delta_{n0} + c_{nj} \;.$$
(4.5)

Summing this over the lattice yields

$$\sum_{nj} \hat{c}_{nj} = \sqrt{N_0 N_L} + \sum_{nj} c_{nj} .$$
 (4.6)

Remembering the orthogonality property (3.51) and Eq. (3.53), we have

$$\sum_{j} \hat{c}_{0j} = \sqrt{N_0 N_L} , \qquad \sum_{j} c_{0j} = 0 .$$
(4.7)

Substituting expansion (4.1) into the energy Hamiltonian (2.151), we meet the following matrix elements: the single-site term

$$h_i^{mn} \equiv \int w_m^*(\mathbf{r} - \mathbf{a}_i) \ H_L(\mathbf{r}) \ w_n(\mathbf{r} - \mathbf{a}_i) \ d\mathbf{r} , \qquad (4.8)$$

the hopping, or tunneling, term

$$J_{ij}^{mn} \equiv -\int w_m^*(\mathbf{r} - \mathbf{a}_i) \ H_L(\mathbf{r}) \ w_n(\mathbf{r} - \mathbf{a}_j) \ d\mathbf{r} , \qquad (4.9)$$

where  $i \neq j$ , and the interaction term

$$U_{j_1 j_2 j_3 j_4}^{n_1 n_2 n_3 n_4} \equiv \Phi_0 \int w_{n_1}^* (\mathbf{r} - \mathbf{a}_{j_1}) w_{n_2}^* (\mathbf{r} - \mathbf{a}_{j_2}) w_{n_3} (\mathbf{r} - \mathbf{a}_{j_3}) w_{n_4} (\mathbf{r} - \mathbf{a}_{j_4}) \, d\mathbf{r} \,, \tag{4.10}$$

where the local interaction potential (2.169) is assumed and

$$H_L(\mathbf{r}) \equiv -\frac{\nabla^2}{2m} + V_L(\mathbf{r})$$

is the linear lattice Hamiltonian. Then Hamiltonian (2.151) becomes

$$\hat{H} = -\sum_{i \neq j} \sum_{mn} J_{ij}^{mn} \hat{c}_{mi}^{\dagger} \hat{c}_{nj} + \sum_{j} \sum_{mn} h_{j}^{mn} \hat{c}_{mj}^{\dagger} \hat{c}_{nj} + \frac{1}{2} \sum_{\{j\}} \sum_{\{n\}} U_{j_{1}j_{2}j_{3}j_{4}}^{n_{1}n_{2}n_{3}n_{4}} \hat{c}_{n_{1}j_{1}}^{\dagger} \hat{c}_{n_{2}j_{2}}^{\dagger} \hat{c}_{n_{3}j_{3}} \hat{c}_{n_{4}j_{4}} .$$

$$(4.11)$$

To simplify Eq. (4.11), one supposes that the main contribution here comes from the lowest band, so that the single-band approximation can be employed. In so doing, one omits the band indices. Implying that Wannier functions are well localized, one retains in the hopping term only the nearest neighbors, with the tunneling parameter J, and in the interaction term, one keeps only the on-site interaction, with an interaction parameter U. Thus, one arrives at the *Hubbard model* 

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{c}_i^{\dagger} \hat{c}_j + h_0 \sum_j \hat{c}_j^{\dagger} \hat{c}_j + \frac{U}{2} \sum_j \hat{c}_j^{\dagger} \hat{c}_j^{\dagger} \hat{c}_j \hat{c}_j \hat{c}_j , \qquad (4.12)$$

in which  $\langle ij \rangle$  means the summation over nearest neighbors and the parameters J,  $h_0$ , and U do not depend on the lattice-site indices because of the lattice regularity, when other external fields, except the lattice one, are absent.

The Hubbard Hamiltonian (4.12) is widely used for treating electrons in condensed matter [266–270]. The principal difference of the case of bosons, in the presence of BEC, from the case of fermions, is that the Wannier field operators here are Bogolubov-shifted, such that

$$\hat{c}_j \equiv \sqrt{\frac{N_0}{N_L}} + c_j , \qquad (4.13)$$

in agreement with Eq. (4.5).

The Hamiltonian parameters can be calculated in the same way as it was done for the quasi-one-dimensional case of Sec. 3.9. Considering now a three-dimensional lattice in the tight-binding approximation yields

$$h_0 \cong 3E_R \sqrt{\frac{V_0}{E_R}}, \qquad J \cong \frac{3}{4} \left(\pi^2 - 4\right) V_0 \exp\left(-\frac{\pi^2}{4} \sqrt{\frac{V_0}{E_R}}\right),$$

$$U \cong \sqrt{\frac{8}{\pi}} k_0 a_s E_R \left(\frac{V_0}{E_R}\right)^{3/4} . \tag{4.14}$$

The ratio of the on-site interaction to the hopping parameter is

$$\frac{U}{J} \simeq 0.362k_0 a_s \left(\frac{E_R}{V_0}\right)^{1/4} \exp\left(\frac{\pi^2}{4} \sqrt{\frac{V_0}{E_R}}\right) , \qquad (4.15)$$

where  $k_0 = |\mathbf{k}_0|$  is the laser wave vector modulus, being for a cubic lattice  $k_0 = \pi/a$ . As is seen from ratio (4.15), making the lattice deeper by rising the lattice depth  $V_0$  increases the influence of the on-site interaction.

# 4.2 Grand Hamiltonian

For a lattice system with BEC, the Hubbard Hamiltonian (4.12) is a part of the grand Hamiltonian (3.15). It is necessary to deal with a grand Hamiltonian, since the Wannier field operators, as any other field operators, do not conserve the number of particles [271] as well as other normalization conditions. Such conditions and other additional constraints are to be taken into account for constructing a representative statistical ensemble guaranteeing theory self-consistency [56,57,93–99].

Recalling the definition of the condensate fraction,  $n_0$ , the fraction of uncondensed atoms  $n_1$ , and that of the lattice filling factor  $\nu$ ,

$$n_0 \equiv \frac{N_0}{N} , \qquad n_1 \equiv \frac{N_1}{N} , \qquad \nu \equiv \frac{N}{N_L} , \qquad (4.16)$$

we can denote the filling factors of condensed and uncondensed atoms as

$$\frac{N_0}{N} = \nu n_0 , \qquad \frac{N_1}{N_L} = \nu n_1 .$$
 (4.17)

Then the Bogolubov shift (4.13) writes as

$$\hat{c}_j = \sqrt{\nu n_0} + c_j .$$
 (4.18)

The orthogonality condition (4.7) yields

$$\sum_{j} c_j = 0 \qquad (n_0 > 0) . \tag{4.19}$$

The quantum-number conservation condition  $\langle \psi_1 \rangle = 0$  requires that

$$< c_j > = 0$$
. (4.20)

The latter means that there should be no linear in  $c_j$  terms in the grand Hamiltonian [57]. Averaging operator (4.18) gives the condensate order parameter

$$\langle \hat{c}_j \rangle = \sqrt{\nu n_0} . \tag{4.21}$$

The grand Hamiltonian (3.15) includes the Hubbard part (4.12), the number of condensed atoms  $N_0$ , the number operator for uncondensed atoms

$$\hat{N}_1 = \sum_j c_j^{\dagger} c_j , \qquad (4.22)$$

and the linear killer

$$\hat{\Lambda} = \sum_{j} \left( \lambda_j c_j^{\dagger} + \lambda_j^* c_j \right) , \qquad (4.23)$$

which guarantees the absence in H of the terms linear in  $c_i$ , if such occur.

The grand Hamiltonian (3.15), in the Wannier representation, acquires the form

$$H = H^{(0)} + H^{(2)} + H^{(3)} + H^{(4)} , \qquad (4.24)$$

analogously to its Bloch representation (3.55). In the Wannier representation, we have

$$H^{(0)} = -Jz_0 n_0 N + \frac{V}{2} \nu n_0^2 N - (\mu_0 - h_0) n_0 N , \qquad (4.25)$$

where  $z_0$  is the number of nearest neighbors,

$$z_0 \equiv \frac{1}{N} \sum_{\langle ij \rangle} 1$$
 (4.26)

The linear in  $c_j$  term is absent from Eq. (4.24) due to the orthogonality condition (4.19). The second-order term is

$$H^{(2)} = -J \sum_{\langle ij \rangle} c_i^{\dagger} c_j + (2U\nu n_0 - \mu_1 + h_0) \sum_j c_j^{\dagger} c_j + \frac{U}{2} \nu n_0 \sum_j \left( c_j^{\dagger} c_j^{\dagger} + c_j c_j \right) .$$
(4.27)

The third- an fourth-order terms are

$$H^{(3)} = U\sqrt{\nu n_0} \sum_{j} \left( c_j^{\dagger} c_j^{\dagger} c_j + c_j^{\dagger} c_j c_j \right)$$
(4.28)

and, respectively,

$$H^{(4)} = \frac{U}{2} \sum_{j} c_{j}^{\dagger} c_{j}^{\dagger} c_{j} c_{j} c_{j} . \qquad (4.29)$$

The condition of equilibrium,

$$<\frac{\partial H}{\partial N_0}> = 0$$
, (4.30)

defines the Lagrange multiplier  $\mu_0$ . In the Wannier representation, the normal fraction reduces to

$$n_1 = \frac{1}{N} \sum_j < c_j^{\dagger} c_j > ,$$
 (4.31)

while the anomalous average becomes

$$\sigma \equiv \frac{1}{N} \sum_{j} \langle c_j c_j \rangle \quad . \tag{4.32}$$

For an ideal lattice, the averages in the right-hand side of Eqs. (4.31) and (4.32) do not depend on the site index j. Therefore one has

$$< c_j^{\dagger} c_j > = \nu n_1 , \qquad < c_j c_j > = \nu \sigma .$$
 (4.33)

The constant  $h_0$  can be incorporated in the notation of the Lagrange multipliers  $\mu_0$  and  $\mu_1$ . In that way, the condition of equilibrium (4.30) results in

$$\mu_0 = -Jz_0 + \nu n_0 U + \nu U \left[ 2n_1 + \frac{1}{2} \left( \sigma^* + \sigma \right) \right] + \frac{U}{2\sqrt{\nu n_0}} \sum_j \langle c_j^{\dagger} c_j^{\dagger} c_j + c_j^{\dagger} c_j c_j \rangle \quad (4.34)$$

The equations of motion for the operators  $c_j$  are given by the equalities

$$i \frac{\partial c_j}{\partial t} = \frac{\partial H}{\partial c_j^{\dagger}} = [c_j, H],$$

which yield

$$i \frac{\partial c_j}{\partial t} = (-J + 2\nu n_0 U - \mu_1) c_j + \nu n_0 U c_j^{\dagger} + \sqrt{\nu n_0} U \left( 2c_j^{\dagger} c_j + c_j c_j \right) + U c_j^{\dagger} c_j c_j .$$
(4.35)

Let us note that condition (4.30) defines an equilibrium state. When one is interested in a nonequilibrium situation, one should go back to the condensate-function equation (2.167). The condensate wave function  $\eta(\mathbf{r}, t)$  can be expanded over Wannier functions. In a particular case of a purely coherent system, one obtains the Wannier representation for the nonlinear Schrödinger equation [272], which does not take account of either uncondensed atoms or anomalous averages. For more realistic cases, one should deal with the total Eq. (2.167).

#### 4.3 Bose-Condensed System

The description of BEC in an optical lattice, based on the Wannier representation of the grand Hamiltonian (4.24) and on the Hubbard model (4.12), can be done similarly to the way used when dealing with the Bloch representation in Sec. 3.3. The consideration now becomes simpler, since in deriving the Hubbard model (4.12) some simplifications were invoked, which were justified by good localization of Wannier functions.

The field operator of uncondensed atoms, in the single-band approximation, can be expanded either over Wannier or over Bloch functions,

$$\psi_1(\mathbf{r}) = \sum_j c_j w(\mathbf{r} - \mathbf{a}_j) = \sum_k a_k \varphi_k(\mathbf{r}) .$$
(4.36)

Therefore the field operators in the Wannier and Bloch representations are related as

$$c_j = \frac{1}{\sqrt{N_L}} \sum_k a_k e^{i\mathbf{k}\cdot\mathbf{a}_j} , \qquad (4.37)$$

following from the relation

$$\varphi_k(\mathbf{r}) = \frac{1}{\sqrt{N_L}} \sum_j w(\mathbf{r} - \mathbf{a}_j) e^{i\mathbf{k}\cdot\mathbf{a}_j}$$

between the Bloch and Wannier functions. Let us recall that from the orthogonality condition (3.51) one has conditions (3.52) and (3.53), which, for the single-band case, reduce to condition (4.19) and to

$$\lim_{k \to 0} a_k = 0 \qquad (n_0 > 0) . \tag{4.38}$$

Substituting relation (4.37) into Eq. (4.27), assuming a cubic *d*-dimensional lattice, and using the equality d

$$\sum_{\langle ij\rangle} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} = 2N_L \sum_{\alpha=1}^a \cos(k_\alpha a) ,$$

we have

$$H^{(2)} = \sum_{k} \left[ -2J \sum_{\alpha} \cos(k_{\alpha}a) + 2U\nu n_{0} - \mu_{1} \right] a_{k}^{\dagger} a_{k} + \frac{U}{2} \nu n_{0} \sum_{k} \left( a_{k}^{\dagger} a_{-k}^{\dagger} + a_{-k} a_{k} \right) .$$
(4.39)

For the third-order term (4.28), we get

$$H^{(3)} = U \sqrt{\frac{\nu n_0}{N_L}} \sum_{kp} \left( a_k^{\dagger} a_p a_{k+p} + a_{k+p}^{\dagger} a_p a_k \right) .$$
 (4.40)

And the fourth-order term (4.29) becomes

$$H^{(4)} = \frac{U}{2N_L} \sum_{kpq} a_k^{\dagger} a_p^{\dagger} a_{k+q} a_{p-q} . \qquad (4.41)$$

In the Bogolubov approximation, one omits the third-and fourth-order terms (4.40) and (4.41), as has been done in Refs. [273,274]. A more general consideration is based on the Hartree-Fock-Bogolubov (HFB) approximation, in line with the self-consistent approach developed in Refs. [57,93–99].

Applying the HFB approximation to Eqs. (4.40) and (4.41) requires to recall the definition of the normal and anomalous averages

$$n_k \equiv \langle a_k^{\dagger} a_k \rangle, \qquad \sigma_k \equiv \langle a_{-k} a_k \rangle \tag{4.42}$$

and of their integral forms

$$n_1 = \frac{1}{N} \sum_k n_k , \qquad \sigma = \frac{1}{N} \sum_k \sigma_k . \qquad (4.43)$$

The third-order term (4.40) in the HFB approximation is zero because of the orthogonality condition (4.38). And the fourth-order term (4.41) becomes

$$H^{(4)} = \frac{\nu}{2} U \sum_{k} \left( 4n_1 a_k^{\dagger} a_k + \sigma a_k^{\dagger} a_{-k}^{\dagger} + \sigma^* a_{-k} a_k \right) - \frac{\nu}{2} UN \left( 2n_1^2 + |\sigma|^2 \right) .$$
(4.44)

Combining the terms of the grand Hamiltonian (4.24), we employ the notation

$$\omega_k \equiv -2J \sum_{\alpha} \cos(k_{\alpha} a) + 2\nu U - \mu_1 \tag{4.45}$$

and

$$\Delta \equiv \nu U(n_0 + \sigma) . \tag{4.46}$$

Then Eq. (4.24) reduces to the form

$$H = E_{HFB} + \sum_{k} \omega_{k} a_{k}^{\dagger} a_{k} + \frac{1}{2} \sum_{k} \left( \Delta a_{k}^{\dagger} a_{-k}^{\dagger} + \Delta^{*} a_{-k} a_{k} \right) , \qquad (4.47)$$

in which

$$E_{HFB} \equiv H^{(0)} - \nu N \, \frac{U}{2} \left( 2n_1^2 + |\sigma|^2 \right) \,. \tag{4.48}$$

Similarly to the uniform case [57,94], the anomalous average  $\sigma$  can be made real. The Lagrange multiplier (4.34), in the HFB approximation, is

$$\mu_0 = -z_0 J + \nu U (1 + n_1 + \sigma) , \qquad (4.49)$$

where the normalization  $n_0 + n_1 = 1$  is used.

The HFB Hamiltonian (4.47) can be diagonalized by means of the Bogolubov canonical transformation in the same way as it is done for a uniform system [94–98]. This reduces Hamiltonian (4.47) to the Bogolubov form

$$H_B = E_B + \sum_k \varepsilon_k b_k^{\dagger} b_k , \qquad (4.50)$$

in which

$$E_B = E_{HFB} + \frac{1}{2} \sum_{k} (\varepsilon_k - \omega_k)$$
(4.51)

and the Bogolubov spectrum is

$$\varepsilon_k = \sqrt{\omega_k^2 - \Delta^2} . \tag{4.52}$$

As is explained in Sec. 2.9, the condensate existence requires the condensation condition

$$\lim_{k \to 0} \varepsilon_k = 0 , \qquad \text{Re } \varepsilon_k \ge 0 . \tag{4.53}$$

The latter defines the Lagrange multiplier

$$\mu_1 = -z_0 J + \nu U (1 + n_1 - \sigma) , \qquad (4.54)$$

which is different from Eq. (4.49). Recall that  $z_0$  is the coordination number that for a d-dimensional cubic lattice is  $z_0 = 2d$ . Substituting Eq. (4.54) into notation (4.45) yields

$$\omega_k = \Delta + 2J \sum_{\alpha} [1 - \cos(k_{\alpha}a)] = \Delta + 4J \sum_{\alpha} \sin^2\left(\frac{k_{\alpha}a}{2}\right) . \tag{4.55}$$

In the long-wave limit, when  $k \equiv |\mathbf{k}| \to 0$ ,

$$\omega_k \simeq \Delta + J(ka)^2 \qquad (k \to 0) . \tag{4.56}$$

Therefore, spectrum (4.52) is of the phonon type,

$$\varepsilon_k \simeq ck \qquad (k \to 0) , \qquad (4.57)$$

with the sound velocity

$$c = \sqrt{2Ja^2\Delta} . \tag{4.58}$$

When the lattice is not cubic, it is characterized by d lattice spacings  $a_{\alpha}$ , with  $\alpha = 1, 2, \ldots, d$ . Hence, generally, for a d-dimensional lattice, there can be defined d sound velocities

$$c_{\alpha} \equiv \lim_{k \to 0} \frac{\partial \varepsilon_k}{\partial k_{\alpha}} = \sqrt{2J\Delta} a_{\alpha} .$$

Similarly to the uniform case [94-98], for Eqs. (4.42), we get the momentum distribution

$$n_k = \frac{\omega_k}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) - \frac{1}{2}$$
(4.59)

and the anomalous average

$$\sigma_k = -\frac{\Delta_k}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) \,. \tag{4.60}$$

Transforming sums (4.43) to integrals according to Eq. (3.45), we find the fraction of uncondensed atoms

$$n_1 = \frac{1}{\rho} \int_{\mathcal{B}} n_k \, \frac{d\mathbf{k}}{(2\pi)^3} \tag{4.61}$$

and the anomalous average

$$\sigma = \frac{1}{\rho} \int_{\mathcal{B}} \sigma_k \, \frac{d\mathbf{k}}{(2\pi)^3} \,, \tag{4.62}$$

where the integration is over the Brillouin zone.

In the center of the Brillouin zone, functions (4.59) and (4.60) behave as

$$n_k \simeq \frac{T\Delta}{(ck)^2}$$
,  $\sigma_k \simeq -\frac{T\Delta}{(ck)^2}$   $(k \to 0)$ .

At the boundary of the Brillouin zone, one has

$$\omega_k \simeq \Delta + 2z_0 J$$
,  $\varepsilon_k \simeq 2\sqrt{z_0 J(\Delta + z_0 J)}$   $\left(k_\alpha \to \frac{\pi}{a_\alpha}\right)$ .

This shows that both  $n_k$  and  $\sigma_k$  are integrable, so that  $n_1$  as well as  $\sigma$  in Eqs. (4.61) and (4.62) are finite. That is, in the case of a lattice, there are no problems with a divergent anomalous average, as for a uniform system with the local interaction potential, which is discussed in Sec. 2.13. The lattice regularizes  $\sigma$  making it always finite.

The condensate fraction  $n_0 = 1 - n_1$  exists below the BEC phase transition  $T_c$ . This is a second-order phase transition between the normal phase and Bose-condensed phase. At  $T \to T_c$ , one has  $n_0 \to 0$ ,  $\sigma \to 0$ , and  $\Delta \to 0$ . Also,  $\varepsilon_k \to \omega_k$ , when  $T \to T_c$ . At the critical temperature, Eq. (4.55) becomes

$$\omega_k = 4J \sum_{\alpha} \sin^2 \left(\frac{k_{\alpha}a}{2}\right) \qquad (T = T_c) . \tag{4.63}$$

The critical temperature  $T_c$ , where  $n_0 = 0$  and  $n_1 = 1$ , is given by the equation

$$\rho = \frac{1}{2} \int_{\mathcal{B}} \left[ \coth\left(\frac{\omega_k}{2T_c}\right) - 1 \right] \frac{d\mathbf{k}}{(2\pi)^d} , \qquad (4.64)$$

in which  $\omega_k$  is defined in Eq. (4.63) and a *d*-dimensional lattice us considered.

To estimate the critical temperature, let us keep in mind a cubic lattice, for which the filling factor can be written as

$$\nu \equiv \frac{N}{N_L} = \rho a^d . \tag{4.65}$$

By introducing the dimensionless quasimomentum vector

$$\mathbf{x} \equiv \left\{ x_{\alpha} = \frac{k_{\alpha}a}{\pi} : \ \alpha = 1, 2, \dots, d \right\} ,$$

Eq. (4.64) can be represented in the form

$$2^{d+1}\nu = \int_{\overline{\mathcal{B}}} \left\{ \coth\left[\frac{2J}{T_c} \sum_{\alpha=1}^d \sin^2\left(\frac{\pi}{2} x_\alpha\right)\right] - 1 \right\} d\mathbf{x} , \qquad (4.66)$$

in which the integration over each  $x_{\alpha}$  is between -1 and 1, the dimensionless Brillouin zone being

$$\overline{\mathcal{B}} \equiv \{x_{\alpha} \in [-1,1] : \alpha = 1, 2, \dots, d\}.$$

Noticing that the main contribution to integral (4.66) comes from the central region of the Brillouin zone, we can approximate this integral by considering the asymptotic behaviour of the integrand at small  $x_{\alpha}$ . This gives

$$T_c \simeq 2^d \pi^2 \left( \int_{\overline{\mathcal{B}}} \frac{d\mathbf{x}}{\sum_{\alpha} x_{\alpha}^2} \right)^{-1} J\nu .$$
(4.67)

In that approximation, BEC does not happen for one- and two-dimensional lattices,

$$T_c \leq 0 \qquad (d \leq 2) .$$
 (4.68)

For larger dimensionality d > 2, we can evaluate the integral in Eq. (4.67) by invoking the Debye-like approximation. To this end, the integral over the Brillouin zone is replaced by the Debye sphere, whose radius is chosen so that to retain the normalization condition

$$\int_{\mathcal{B}} \frac{d\mathbf{k}}{(2\pi)^d} = \frac{N_L}{V} = \frac{\rho}{\nu} \,. \tag{4.69}$$

The latter, in dimensionless units, reads as

$$\int_{\overline{\mathcal{B}}} d\mathbf{x} = 2^d . \tag{4.70}$$

Then, the Debye approximation implies

$$\int_{\overline{\mathcal{B}}} d\mathbf{x} = \frac{2\pi^{d/2}}{\Gamma(d/2)} \int_0^{x_D} x^{d-1} dx = 2^d .$$
(4.71)

From here, the Debye radius is

$$x_D = \frac{2}{\sqrt{\pi}} \left[ \frac{d}{2} \Gamma \left( \frac{d}{2} \right) \right]^{1/d} . \tag{4.72}$$

In this approximation,

$$\int_{\overline{\mathcal{B}}} \frac{d\mathbf{x}}{\sum_{\alpha} x_{\alpha}^2} = \frac{2\pi^{d/2} x_D^{d-2}}{(d-2)\Gamma(d/2)}$$

Equation (4.67) yields

$$T_c = 2^d \pi^2 \, \frac{(d-2)\Gamma(d/2)}{2\pi^{d/2} x_D^{d-2}} \, J\nu \,. \tag{4.73}$$

For a three-dimensional lattice, one has

$$T_c = \frac{2\pi}{x_D} J\nu$$
,  $x_D = \left(\frac{6}{\pi}\right)^{1/3}$   $(d=3)$ . (4.74)

This results in the BEC temperature

$$T_c \cong 5J\nu \qquad (d=3) . \tag{4.75}$$

A close estimate for the critical temperature of condensation in a lattice follows from the Bogolubov approximation [275].

Thus, in the HFB approximation, the BEC does not occur in one- and two-dimensional lattices. In a three-dimensional lattice, the BEC exists below  $T_c$  given by Eq. (4.75). The transition temperature does not depend on the on-site interaction U. However, one should expect that, for a sufficiently strong repulsion U, the system could go to an insulating state. This means that the HFB approximation for the boson Hubbard model is applicable only for the Bose-condensed phase, but is not suitable for the insulating state. Other approximations will be discussed in the following sections.

# 4.4 Thermodynamic Characteristics

All thermodynamic characteristics can be derived from the system grand potential. For example, when the system is in the Bose-condensed phase, for which the HFB approximation is applicable, the grand potential is

$$\Omega = E_B + TV \int_{\mathcal{B}} \ln\left(1 - e^{-\beta\varepsilon_k}\right) \frac{d\mathbf{k}}{(2\pi)^3} , \qquad (4.76)$$

where  $\varepsilon_k$  is the Bogolubov spectrum (4.52) and

$$E_B = H^{(0)} - \nu N \, \frac{U}{2} \left( 2n_1^2 + \sigma^2 \right) \, + \, \frac{1}{2} \, \sum_k (\varepsilon_k - \omega_k) \tag{4.77}$$

follows from Eq. (4.51).

The system free energy is

$$F = \Omega + \mu N , \qquad (4.78)$$

with the chemical potential

$$\mu = \mu_0 n_0 + \mu_1 n_1 . \tag{4.79}$$

The latter, using the Lagrange multipliers (4.49) and (4.54), becomes

$$\mu = -z_0 J + \nu U (1 + n_1 + \sigma - 2n_1 \sigma) .$$
(4.80)

The internal energy is  $E \equiv \langle H_B \rangle + \mu N$ . Here  $H_B$  is given by Eq. (4.50). Also, from Eqs. (4.25) and (4.49), we have

$$H^{(0)} = \nu n_0 N \, \frac{U}{2} [n_0 - 2(1 + n_1 + \sigma)] \,. \tag{4.81}$$

And Eq. (4.48) gives

$$E_{HFB} = \nu N \frac{U}{2} \left[ n_0^2 - \sigma^2 - 2(1 + n_0 \sigma) \right] .$$
(4.82)

Then for the ground-state energy

$$E_0 \equiv E_B + \mu N = E_{HFB} + \frac{1}{2} \sum_k (\varepsilon_k - \omega_k) + \mu N$$

we find

$$\frac{E_0}{N} = -z_0 J + \nu \, \frac{U}{2} \left( 1 + n_1^2 - \sigma^2 - 2n_1 \sigma \right) \, + \, \frac{1}{2\rho} \, \int_{\mathcal{B}} (\varepsilon_k - \omega_k) \, \frac{d\mathbf{k}}{(2\pi)^3} \, . \tag{4.83}$$

Particle fluctuations are characterized by the dispersion  $\Delta^2(\hat{N})$  of the number-of-particle operator, as defined in Eq. (2.243). For a Bose system, with the broken gauge symmetry by means of the Bogolubov shift, the condensate fluctuations are negligible [57,93], that is,  $\Delta^2(\hat{N}_0) \rightarrow 0$ . Hence, all fluctuations are due to uncondensed particles,

$$\Delta^2(\hat{N}) = \Delta^2(\hat{N}_1) \qquad \left(\hat{N}_1 = \sum_k a_k^{\dagger} a_k\right) . \tag{4.84}$$

Since the HFB approximation results in the Hamiltonian (4.47), quadratic with respect to the filed operators  $a_k$ , then calculating  $\Delta^2(\hat{N}_1)$ , one has to be in the frame of the quadratic approximation, that is, neglecting the terms with  $n_k^2$  and  $\sigma_k^2$ . Similarly to the uniform case [10,93,145,146], for BEC in a lattice, we have

$$\Delta^2(\hat{N}_1) = N[1 + 2\lim_{k \to 0} (n_k + \sigma_k)].$$
(4.85)
From Eqs. (4.59) and (4.60), we find

$$n_k \simeq \frac{T\Delta}{\varepsilon_k^2} + \frac{\Delta}{12T} + \frac{T}{2\Delta} - \frac{1}{2},$$
  
$$\sigma_k \simeq -\frac{T\Delta}{\varepsilon_k^2} - \frac{\Delta}{12T} \qquad (\varepsilon_k \to 0).$$
(4.86)

Therefore,

$$\lim_{k \to 0} (n_k + \sigma_k) = \frac{1}{2} \left( \frac{T}{\Delta} - 1 \right) .$$

$$(4.87)$$

Then Eq. (4.85) gives

$$\Delta^2(\hat{N}_1) = \frac{NT}{\Delta} . \tag{4.88}$$

According to Eq. (4.46), one gets

$$\Delta^{2}(\hat{N}) = \frac{NT}{\nu U(n_{0} + \sigma)} \,. \tag{4.89}$$

The isothermal compressibility reads as

$$\kappa_T = \frac{\Delta^2(\hat{N})}{\rho T N} = \frac{1}{\rho \nu U(n_0 + \sigma)} .$$
 (4.90)

Particle fluctuations are, of course, thermodynamically normal and the compressibility is finite. The latter diverges only at the critical point  $T_c$ , where  $n_0 \to 0$  and  $\sigma \to 0$ . But below  $T_c$ , the compressibility is finite everywhere for  $T < T_c$ , provided that there is a finite interaction U.

## 4.5 Superfluid Fraction

The superfluid fraction can be calculated by employing Eq. (3.106) which has been derived in Sec. 2.10. Equation (3.106) is general and exact. For a lattice, the operator of momentum can be represented in forms (3.83) or (3.84). The latter reduces to Eq. (3.93). In tight-binding approximation, one can invoke Eq. (3.105). The dissipated heat in the HFB approximation is given in Eq. (3.110).

Another possibility is to rederive the superfluid fraction using explicitly the Hubbard Hamiltonian (4.12), in this derivation being based on the general definitions (2.135) or (2.139). For an equilibrium system, both these definitions yield Eq. (2.138). Generalizing the latter for a *d*-dimensional system, we have

$$n_s = \frac{1}{mNd} \left[ \lim_{v \to 0} < \frac{\partial}{\partial \mathbf{v}} \cdot \hat{\mathbf{P}}_v > -\beta \Delta^2(\hat{\mathbf{P}}) \right] .$$
(4.91)

In order to use Eq. (4.91), with the Hubbard Hamiltonian (4.12), it is necessary to find how the Wannier field operators  $\hat{c}_j$  change under the velocity boost. Generally, if the system is boosted with the velocity  $\mathbf{v}$ , the field operator of the moving system can be expanded over the Wannier functions as

$$\hat{\psi}_v(\mathbf{r},t) = \sum_j \hat{c}_j(\mathbf{v},t) w(\mathbf{r}-\mathbf{a}_j) .$$
(4.92)

Being in the frame of the Hubbard model, the single-band case is considered here. Inverting expansion (4.92) gives

$$\hat{c}_j(\mathbf{v},t) = \int w^*(\mathbf{r} - \mathbf{a}_j)\hat{\psi}_v(\mathbf{r},t) \, d\mathbf{r} \,. \tag{4.93}$$

Substituting in Eq. (4.93) the Galilean transformation (2.146), with the expansion

$$\hat{\psi}(\mathbf{r} - \mathbf{v}t, t) = \sum_{j} \hat{c}_{j}(0, t) w(\mathbf{r} - \mathbf{v}t - \mathbf{a}_{j}) , \qquad (4.94)$$

we get the relation

$$\hat{c}_i(\mathbf{v},t) = \sum_j \hat{c}_j(0,t) \exp\left(-i \frac{mv^2}{2} t\right) \int w^*(\mathbf{r} - \mathbf{a}_i) w(\mathbf{r} - \mathbf{v}t - \mathbf{a}_j) e^{im\mathbf{v}\cdot\mathbf{r}} d\mathbf{r} .$$
(4.95)

This is a general relation connecting the Wannier field operators  $\hat{c}_i(\mathbf{v}, t)$  for a moving system with these operators  $\hat{c}_j(0, t)$  for an immovable lattice.

Keeping in mind an equilibrium system, we can set time to zero, introducing the simplified notation

$$\hat{c}_j(\mathbf{v}) \equiv \hat{c}_j(\mathbf{v}, 0) \ . \tag{4.96}$$

Diminishing the velocity to zero, we return to the old notation of the Wannier field operators of an immovable lattice,

$$\hat{c}_j \equiv \lim_{v \to 0} \hat{c}_j(\mathbf{v}) = \lim_{v \to 0} \hat{c}_j(\mathbf{v}, 0) .$$
(4.97)

Then relation (4.95) becomes

$$\hat{c}_i(\mathbf{v}) = \sum_j \hat{c}_j \int w^* (\mathbf{r} - \mathbf{a}_i) w(\mathbf{r} - \mathbf{a}_j) e^{im\mathbf{v}\cdot\mathbf{r}} d\mathbf{r} .$$
(4.98)

Since in the Hubbard model, one assumes well localized Wannier functions, one can use the approximation

$$\int w^*(\mathbf{r} - \mathbf{a}_j) w(\mathbf{r} - \mathbf{a}_j) e^{im\mathbf{v}\cdot\mathbf{r}} \, d\mathbf{r} \cong \delta_{ij} e^{im\mathbf{v}\cdot\mathbf{a}_j} \,. \tag{4.99}$$

Therefore, relation (4.98) simplifies to

$$\hat{c}_j(\mathbf{v}) = \hat{c}_j e^{im\mathbf{v}\cdot\mathbf{a}_j} \ . \tag{4.100}$$

The Hamiltonian (4.12) of the Hubbard model for an immovable system is the functional  $\hat{H} = \hat{H}[\hat{c}_j]$ . For a moving lattice, the latter becomes  $\hat{H}_v = \hat{H}[\hat{c}_j(\mathbf{v})]$ , which gives

$$\hat{H}_{v} = -J \sum_{\langle ij \rangle} \hat{c}_{i}^{\dagger} \hat{c}_{j} e^{-im\mathbf{v} \cdot \mathbf{a}_{ij}} + h_{0} \sum_{j} \hat{c}_{j}^{\dagger} \hat{c}_{j} + \frac{U}{2} \sum_{j} \hat{c}_{j}^{\dagger} \hat{c}_{j}^{\dagger} \hat{c}_{j} \hat{c}_{j}$$
(4.101)

where  $\mathbf{a}_{ij} \equiv \mathbf{a}_i - \mathbf{a}_j$ .

The operator of momentum, according to definition (2.133), is

$$\hat{\mathbf{P}}_{v} \equiv \frac{\partial H_{v}}{\partial \mathbf{v}} = imJ \sum_{\langle ij \rangle} \mathbf{a}_{ij} \hat{c}_{i}^{\dagger} \hat{c}_{j} e^{-im\mathbf{v} \cdot \mathbf{a}_{ij}} .$$
(4.102)

From here it follows that

$$\frac{\partial}{\partial \mathbf{v}} \cdot \hat{\mathbf{P}}_v = m^2 J \sum_{\langle ij \rangle} \mathbf{a}_{ij}^2 \hat{c}_i^\dagger \hat{c}_j e^{-im\mathbf{v} \cdot \mathbf{a}_{ij}}$$

The operator of momentum for an immovable lattice is

$$\hat{\mathbf{P}} \equiv \lim_{v \to 0} \hat{\mathbf{P}}_v = imJ \sum_{\langle ij \rangle} \mathbf{a}_{ij} \hat{c}_i^{\dagger} \hat{c}_j .$$
(4.103)

Substituting here the Bogolubov shift (4.18) and using the orthogonality condition (4.19), we have

$$\hat{\mathbf{P}} = imJ \sum_{\langle ij \rangle} \mathbf{a}_{ij} c_i^{\dagger} c_j \ . \tag{4.104}$$

That is, only the operators of uncondensed atoms contribute to the momentum operator, in agreement with Eq. (3.83). Limiting in the latter the summation by nearest neighbors gives

$$\hat{\mathbf{P}} = \sum_{\langle ij \rangle} \mathbf{p}_{ij} c_i^{\dagger} c_j \qquad (\mathbf{p} = imJ\mathbf{a}_{ij}) \;.$$

Taking into account that in equilibrium  $\langle \hat{\mathbf{P}} \rangle = 0$ , for the superfluid fraction (4.91) we find

$$n_s = \frac{mJ}{Nd} \sum_{\langle ij \rangle} a_{ij}^2 \langle \hat{c}_i^{\dagger} \hat{c}_j \rangle - \frac{\langle \mathbf{P}^2 \rangle}{mTNd} , \qquad (4.105)$$

where  $a_{ij} \equiv |\mathbf{a}_{ij}|$ . From Eq. (4.104), we have

$$\langle \hat{\mathbf{P}}^{2} \rangle = m^{2} J^{2} \sum_{\langle ij \rangle} a_{ij}^{2} \left( \langle c_{i}^{\dagger} c_{j}^{\dagger} c_{j} c_{i} \rangle - \langle c_{i}^{\dagger} c_{i}^{\dagger} c_{j} c_{j} \rangle + \langle c_{i}^{\dagger} c_{i} \rangle \right) .$$
(4.106)

Taking into account the Bogolubov shift (4.18) gives

$$\langle \hat{c}_i^{\dagger}\hat{c}_j \rangle = \nu n_0 + \langle c_i^{\dagger}c_j \rangle$$

Then for the superfluid fraction (4.105) we get

$$n_{s} = \frac{mJ}{Nd} \sum_{\langle ij \rangle} a_{ij}^{2} (\nu n_{0} + \langle c_{i}^{\dagger}c_{j} \rangle) - \frac{mJ^{2}}{TNd} \sum_{\langle ij \rangle} a_{ij}^{2} \left( \langle c_{i}^{\dagger}c_{i} \rangle + \langle c_{i}^{\dagger}c_{j}^{\dagger}c_{j}c_{i} \rangle - \langle c_{i}^{\dagger}c_{i}^{\dagger}c_{j}c_{j}\rangle \right) .$$
(4.107)

On the other hand, the superfluid fraction can be defined by means of Eq. (2.150) that is as general as Eq. (2.138). Generalizing Eq. (2.150) to a *d*-dimensional system yields

$$n_s = 1 - \frac{Q}{Q_0}, \qquad Q \equiv \frac{\langle \mathbf{P}^2 \rangle}{2mN}, \qquad Q_0 \equiv \frac{d}{2} T.$$
 (4.108)

The dissipated heat, according to Eq. (4.106), is

$$Q = \frac{mJ^2}{2N} \sum_{\langle ij \rangle} a_{ij}^2 \left( \langle c_i^{\dagger} c_i \rangle + \langle c_i^{\dagger} c_j^{\dagger} c_j c_i \rangle - \langle c_i^{\dagger} c_i^{\dagger} c_j c_j \rangle \right) .$$
(4.109)

Comparing Eqs. (4.105) and (4.107) with Eqs. (4.108) and (4.109) shows that the expressions for the superfluid fractions differ by the first term. This difference comes from the use of the approximations involved in the derivation of the Hubbard model. However, in the frame of the same approximation scheme, these two terms should be approximately equal. To prove that this is really so, let is notice that

$$\langle c_i^{\dagger} c_j \rangle = \frac{1}{N_L} \sum_k n_k e^{-i\mathbf{k}\cdot\mathbf{a}_{ij}} , \qquad \langle c_i c_j \rangle = \frac{1}{N_L} \sum_k \sigma_k e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} , \qquad (4.110)$$

where  $n_k$  and  $\sigma_k$  are the same as in Eq. (4.42) and enjoy the properties

$$n_k = n_{-k}$$
,  $\sigma_k = \sigma_{-k}$ .

We introduce the mean distance between the nearest neighbors, a, by the formula

$$a^{2} \equiv \frac{1}{z_{0}N_{L}} \sum_{\langle ij \rangle} a_{ij}^{2} . \qquad (4.111)$$

And let us define the effective mass

$$m^* \equiv \frac{1}{2Ja^2} \tag{4.112}$$

by analogy with Eq. (3.160). Also, we may notice that

$$\sum_{\langle ij \rangle} \sum_{k} a_{ij}^2 n_k e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} \cong \sum_{\langle ij \rangle} \sum_{k} a_{ij}^2 n_k$$

Keeping in mind that  $n_0 + n_1 = 1$ , for the first term of Eq. (4.107), we finally obtain

$$\frac{mJ}{Nd} \sum_{\langle ij \rangle} a_{ij}^2 \left( \nu n_0 + \langle c_i^{\dagger} c_j \rangle \right) \cong \frac{mz_0}{m^* 2d} .$$
(4.113)

In order that expressions (4.107) and (4.108) be approximately equal, it is necessary that

$$\frac{mz_0}{m^*2d} \cong 1$$
. (4.114)

The latter holds, for instance, when  $m^* \approx m$  and  $z_0 \approx 2d$ . For a cubic lattice, the coordination number is exactly  $z_0 = 2d$ .

In this way, the superfluid fraction, defined by Eq. (2.139), for the Hubbard model is

$$n_s = \frac{mJ}{Nd} \sum_{\langle ij \rangle} a_{ij}^2 \left( \nu n_0 + \langle c_i^{\dagger} c_j \rangle \right) - \frac{2Q}{Td} , \qquad (4.115)$$

with the dissipated heat (4.109). At the same time, it can also be defined by Eq. (4.108), since the first term in Eq. (4.115), according to Eqs. (4.113) and (4.114), is close to one.

For a d-dimensional cubic lattice, one has

$$\sum_{\langle ij\rangle} a_{ij}^2 e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} = 2a^2 N_L \sum_{\alpha=1}^d \cos(k_\alpha a) \; .$$

From here

$$\sum_{\langle ij \rangle} a_{ij}^2 \langle c_i^{\dagger} c_j \rangle = 2a^2 \sum_k \sum_{\alpha=1}^d n_k \cos(k_{\alpha}a) \,.$$

If one resorts to the HFB approximation, then

$$< c_i^{\dagger} c_j^{\dagger} c_j c_i > = < c_i^{\dagger} c_j >^2 + (\nu n_1)^2 + | < c_i c_j > |^2 ,$$
  
$$< c_i^{\dagger} c_i^{\dagger} c_j c_j > = 2 < c_i^{\dagger} c_j >^2 + |\nu \sigma|^2 .$$

And the dissipated heat (4.109) becomes

$$Q = \frac{mJ^2}{2N} \sum_{\langle ij \rangle} a_{ij}^2 \left( \nu n_1 + \nu^2 n_1^2 - \langle c_i^{\dagger} c_j \rangle^2 - \nu^2 |\sigma|^2 + |\langle c_i c_j \rangle|^2 \right) , \qquad (4.116)$$

where the properties

are used. Taking into account that  $\sigma_k$  in the Fourier transform (4.110) can be made real, for a cubic lattice, one gets

$$\sum_{\langle ij \rangle} a_{ij}^2 \langle c_i c_j \rangle = 2a^2 \sum_k \sum_{\alpha=1}^d \sigma_k \cos(k_\alpha a) ,$$
$$\sum_{\langle ij \rangle} a_{ij}^2 \langle c_i^{\dagger} c_j \rangle^2 = \frac{2a^2}{N_L} \sum_{kp} \sum_{\alpha=1}^d n_k n_p \cos(k_\alpha + p_\alpha) a ,$$
$$\sum_{\langle ij \rangle} a_{ij}^2 |\langle c_i c_j \rangle|^2 = \frac{2a^2}{N_L} \sum_{kp} \sum_{\alpha=1}^d \sigma_k \sigma_p \cos(k_\alpha + p_\alpha) a .$$

Then Eq. (4.116) reads as

$$Q = \frac{mJ\nu}{2m^*N^2} \sum_{kp} \sum_{\alpha=1}^{d} \left[ n_k + 2(n_k n_p - \sigma_k \sigma_p) \sin^2 \left( \frac{k_\alpha + p_\alpha}{2} a \right) \right] .$$
(4.117)

This can be rewritten in a more symmetric form taking into account that

$$2\sum_{p}\sin^{2}(p_{\alpha}a) = N_{L} , \qquad 2\sum_{p}\sin^{2}\left(\frac{k_{\alpha}+p_{\alpha}}{2}a\right) = N_{L} ,$$

Using the latter equalities allow us to rewrite Eq. (4.117) as

$$Q = \frac{1}{N_L} \sum_{kp} \frac{q_{kp}^2}{2mN} \left( n_k + n_k n_p - \sigma_k \sigma_p \right) , \qquad (4.118)$$

where

$$q_{kp}^2 \equiv \frac{2m^2 J}{m^*} \sum_{\alpha=1}^d \sin^2\left(\frac{k_\alpha + p_\alpha}{2} a\right) \,.$$

Assuming that the main contribution to sum (4.118) comes from the diagonal terms results in

$$Q = \sum_{k} \frac{q_k^2}{2mN} \left( n_k + n_k^2 - \sigma_k^2 \right) , \qquad (4.119)$$

with

$$q_k^2 \equiv \frac{2m^2 J}{m^*} \sum_{\alpha=1}^d \sin^2(k_{\alpha}a) \;.$$

Expression (4.119) is in agreement with Eq. (3.107). For the superfluid fraction (4.115), we obtain

$$n_s = \frac{m}{m^*} \left[ n_0 + \frac{1}{N} \sum_k \frac{1}{d} \sum_{\alpha=1}^d n_k \cos(k_\alpha a) \right] - \frac{2Q}{Td} , \qquad (4.120)$$

where the dissipated heat is given by Eq. (4.118) or (4.119). Recall that the first term in Eq. (4.120) is approximately equal to one.

Often, employing definition (2.139) for the superfluid fraction, one transforms the Wannier field operators not as in Eq. (4.100), but by means of a phase factor, that is, replacing  $\hat{c}_j$  by  $\hat{c}_j e^{i\vartheta_j}$ . And, considering the hopping term, one takes  $\vartheta \equiv \vartheta_i - \vartheta_j$ . As a result [276,277], the hopping term in Hamiltonian (4.101) acquires the factor  $e^{-i\vartheta}$ , instead of  $e^{-im\mathbf{v}\cdot\mathbf{a}_{ij}}$ . Hence, one assumes that  $\vartheta = m\mathbf{v}\cdot\mathbf{a}_{ij}$ , which is equivalent to considering a cubic lattice.

#### 4.6 Single-Site Approximation

The tunneling term in the Hubbard Hamiltonian (4.12) can be simplified by means of the single-site approximation [278], assuming the decoupling

$$\hat{c}_{i}^{\dagger}\hat{c}_{j} \cong \langle \hat{c}_{i}^{\dagger} \rangle \ \hat{c}_{j} + \hat{c}_{i}^{\dagger} \langle \hat{c}_{j} \rangle - \langle \hat{c}_{i}^{\dagger} \rangle \langle \hat{c}_{j}^{\dagger} \rangle \qquad (i \neq j) .$$

$$(4.121)$$

This decoupling is equivalent to the Gutzwiller approximation [279], in which the system state is characterized by a product of single-site wave functions [279–282].

According to representation (4.18), the average

$$\langle \hat{c}_j \rangle = \sqrt{\nu n_0} \tag{4.122}$$

is an order parameter for the Bose system in a lattice, and it does not depend on the latticesite index, if the lattice is ideal.

To better understand the meaning of the single-site approximation, let us compare the exact expression

$$\hat{c}_i^{\dagger}\hat{c}_j = \nu n_0 + \sqrt{\nu n_0} \left(c_i^{\dagger} + c_j\right) + c_i^{\dagger}c_j \tag{4.123}$$

with that one following from decoupling (4.121), which gives

$$\hat{c}_i^{\dagger} \hat{c}_j \cong \nu n_0 + \sqrt{\nu n_0} \left( c_i^{\dagger} + c_j \right) \qquad (i \neq j) .$$

$$(4.124)$$

This shows that the single-site approximation neglects the tunneling of the uncondensed atoms,

$$c_i^{\dagger} c_j \cong 0 \qquad (i \neq j, \ n_0 > 0) \ .$$
 (4.125)

Hence, instead of the exact expression

$$\sum_{\langle ij\rangle} \hat{c}_i^{\dagger} \hat{c}_j = z_0 n_0 N + \sum_{\langle ij\rangle} c_i^{\dagger} c_j$$

in the tunneling term, one has

$$\sum_{\langle ij\rangle} \hat{c}_i^{\dagger} \hat{c}_j \cong z_0 n_0 N$$

in the single-site approximation.

Using decoupling (4.121) allows us to present the Hubbard Hamiltonian (4.12) as a sum

$$\hat{H} = \sum_{j} \hat{H}_{j}^{eff} \tag{4.126}$$

of the single-site terms

$$\hat{H}_{j}^{eff} = z_{0}J\left[\nu n_{0} - \sqrt{\nu n_{0}}\left(c_{j}^{\dagger} + \hat{c}_{j}\right)\right] + \frac{U}{2}\,\hat{c}_{j}^{\dagger}\hat{c}_{j}^{\dagger}\hat{c}_{j}\hat{c}_{j}\,\hat{c}_{j}\,\,.$$
(4.127)

This is where the name of the single-site approximation comes from.

In view of the Bogolubov shift (4.18) and the orthogonality condition (4.19), we have

$$\sum_{j} \hat{c}_{j} = \sqrt{\nu n_{0}} N_{L} .$$
(4.128)

Then, instead of sum (4.126), we get

$$\hat{H} = \sum_{j} \hat{H}_{j} \tag{4.129}$$

with

$$\hat{H}_{j} = -z_{0}J\nu n_{0} + \frac{U}{2}\,\hat{c}_{j}^{\dagger}\hat{c}_{j}^{\dagger}\hat{c}_{j}\hat{c}_{j}\,. \qquad (4.130)$$

Substituting here the Bogolubov shift (4.18) yields

$$\hat{H}_j = \sum_{n=0}^4 \hat{H}_j^{(n)} . \tag{4.131}$$

The zero-order term of Eq. (4.131) is

$$\hat{H}_{j}^{(0)} = -z_0 J \nu n_0 + \frac{U}{2} (\nu n_0)^2 . \qquad (4.132)$$

The first-order term, owing to condition (4.19), is zero,  $H^{(1)} = 0$ . The second-order term becomes

$$H_j^{(2)} = \frac{U}{2} \nu n_0 \left( 4c_j^{\dagger}c_j + c_j^{\dagger}c_j^{\dagger} + c_jc_j \right) .$$
(4.133)

The third-order term is

$$\hat{H}_{j}^{(3)} = U\sqrt{\nu n_{0}} \left( c_{j}^{\dagger} c_{j}^{\dagger} c_{j} + c_{j}^{\dagger} c_{j} c_{j} \right) , \qquad (4.134)$$

and the fourth-order one is

$$H_{j}^{(4)} = \frac{U}{2} c_{j}^{\dagger} c_{j}^{\dagger} c_{j} c_{j} = \frac{U}{2} c_{j}^{\dagger} c_{j} \left( c_{j}^{\dagger} c_{j} - 1 \right) .$$
(4.135)

The grand Hamiltonian

$$H = \hat{H} - \mu_0 N_0 - \mu_1 \hat{N}_1 \tag{4.136}$$

is the sum of four terms, as in Eq. (4.24). The zero-order term is the same as in Eq. (4.25), with the constant  $h_0$  being incorporated into the Lagrange multiplier  $\mu_0$ . The second-order term is

$$H^{(2)} = \sum_{j} \hat{H}_{j}^{(2)} - \mu_{1} \hat{N}_{1} = (2U\nu n_{0} - \mu_{1}) \sum_{j} c_{j}^{\dagger} c_{j} + \frac{U}{2} \nu n_{0} \sum_{j} \left( c_{j}^{\dagger} c_{j}^{\dagger} + c_{j} c_{j} \right) , \qquad (4.137)$$

where again  $h_0$  is incorporated into  $\mu_1$ . And the third- and fourth-order terms are

$$H^{(3)} = \sum_{j} \hat{H}_{j}^{(3)} , \qquad H^{(4)} = \sum_{j} \hat{H}^{(4)} , \qquad (4.138)$$

with  $H^{(3)}$  and  $H^{(4)}$  from Eqs. (4.134) and (4.135). Equation (4.137), as compared to Eq. (4.27), does not contain the tunneling of uncondensed atoms.

Because of the no-tunneling condition (4.125), the momentum operator (4.104) vanishes,

$$\hat{\mathbf{P}} = 0$$
  $(c_i^{\dagger} c_j = 0, \ i \neq j)$ . (4.139)

Thence, there is no the dissipated heat, Q = 0. The condensate fraction (4.107), with notations (4.111) and (4.112), becomes

$$n_s = \frac{mz_0}{m^* 2d} \ n_0 \ . \tag{4.140}$$

For a cubic lattice,  $z_0 = 2d$ . Since  $m \approx m^*$ , then  $n_s \approx n_0$ . The fact that the superfluid and condensate fractions practically coincide is the defect of the single-site approximation, which

neglects the tunneling of uncondensed atoms. Comparing Eqs. (4.108) and (4.140) tells us that this approximation is valid, when almost all atoms are condensed, so that  $n_0 \approx 1$ . The latter, in turn, happens when atomic interactions are sufficiently weak. Strong interactions, as is known [94–98], deplete the condensed fraction, while enhance the superfluid fraction, resulting in the inequality  $n_s \gg n_0$ . In the presence of a lattice, strong interactions should lead to the destruction of both BEC and superfluidity and to the appearance of a localized insulating state.

#### 4.7 Localized State

When atomic interactions are much larger than the tunneling rate, so that

$$\frac{U}{J} \gg 1 , \qquad (4.141)$$

than the intersite hopping of atoms is completely suppressed. This can be symbolized by the *localization condition* 

$$c_i^{\dagger}c_j = \delta_{ij}c_i^{\dagger}c_i . \qquad (4.142)$$

When all atoms are localized, global coherence cannot develop. There is no BEC and no gauge symmetry breaking,

$$n_0 = 0$$
,  $n_1 = 1$ . (4.143)

The Hubbard Hamiltonian (4.12) reduces to

$$\hat{H} = \frac{U}{2} \sum_{j} c_{j}^{\dagger} c_{j}^{\dagger} c_{j} c_{j} c_{j} . \qquad (4.144)$$

Using the site-number operator, or *filling operator* 

$$\hat{n}_j \equiv c_j^{\dagger} c_j , \qquad (4.145)$$

Hamiltonian (4.144) can be rewritten as

$$\hat{H} = \frac{U}{2} \sum_{j} \hat{n}_{j} \left( \hat{n}_{j} - 1 \right) .$$
(4.146)

Since there is just one kind of atoms, the sole chemical potential is sufficient. So, the grand Hamiltonian is

$$H \equiv \hat{H} - \mu \hat{N} = \sum_{j} H_j , \qquad (4.147)$$

where the site Hamiltonians are

$$H_j = \frac{U}{2} \, \hat{n}_j^2 - \left(\frac{U}{2} + \mu\right) \hat{n}_j \,, \qquad (4.148)$$

the number-of-particle operator being

$$\hat{N} = \sum_{j} \hat{n}_j \ . \tag{4.149}$$

For an ideal lattice, the average of the site-number operator (4.145) gives the filling factor

$$\nu = \langle \hat{n}_j \rangle$$
 . (4.150)

Explicitly, the latter reads as

$$\nu = \frac{\mathrm{Tr}\hat{n}_j e^{-\beta H}}{\mathrm{Tr}e^{-\beta H}} \,. \tag{4.151}$$

This equation defines the chemical potential  $\mu = \mu(\nu, T)$ . Owing to the additive form of the grand Hamiltonian (4.147), expression (4.151) becomes

$$\nu = \frac{\mathrm{Tr}\hat{n}_j e^{-\beta H_j}}{\mathrm{Tr} e^{-\beta H_j}} \,. \tag{4.152}$$

The eigenproblem for the site-number operators (4.145),

$$\hat{n}_j |n\rangle = n|n\rangle, \qquad (4.153)$$

enjoys, as eigenvalues, the integers n = 0, 1, 2, ..., while  $|n\rangle$  being the occupation-number state [55]. The eigenproblem for the site Hamiltonians (4.148),

$$H_j | n > = e_n | n > , ag{4.154}$$

gives the energy levels

$$e_n = \frac{U}{2} n^2 - \left(\frac{U}{2} + \mu\right) n .$$
 (4.155)

The levels are discrete. One can define the energy gap

$$\Delta e_n \equiv e_{n+1} + e_{n-1} - 2e_n , \qquad (4.156)$$

which gives

$$\Delta e_n = U . \tag{4.157}$$

This is why one tells that the insulator energy spectrum possesses a gap.

With the basis  $\{|n\rangle\}$  of the occupation-number states, the filling factor (4.152) takes the form

$$\nu = \frac{\sum_{n=0}^{\infty} n e^{-\beta e_n}}{\sum_{n=0}^{\infty} e^{-\beta e_n}} \,. \tag{4.158}$$

For high temperature  $(T \gg U)$ , the sums in Eq. (4.158) can be replaced by integrals. But for low temperature  $(T \ll U)$ , the main contribution to the sums comes from the term with the lowest energy  $e_n$ .

Let us consider low temperatures, such that

$$\frac{T}{U} \ll 1. \tag{4.159}$$

The minimum of  $e_n$  is defined by the conditions

$$\frac{\partial e_n}{\partial n} = 0 , \qquad \frac{\partial^2 e_n}{\partial n^2} > 0 . \tag{4.160}$$

This yields the effective number

$$n_{eff} = \frac{2\mu + U}{2U} \qquad (U > 0) . \tag{4.161}$$

For low temperatures, conditioned by inequality (4.159), the filling factor (4.158) is

$$\nu \simeq n_{eff} = \frac{2\mu + U}{2U} . \tag{4.162}$$

This defines the chemical potential

$$\mu \simeq (2\nu - 1) \,\frac{U}{2} \,. \tag{4.163}$$

The grand thermodynamic potential is

$$\Omega \equiv -T \ln \sum_{n=0}^{\infty} e^{-\beta e_n} \simeq e_{\nu} , \qquad (4.164)$$

with

$$e_{\nu} \equiv \frac{U}{2} \nu^2 - \left(\frac{U}{2} + \mu\right) \nu$$
 (4.165)

Substituting here the chemical potential (4.163) yields

$$e_{\nu} = -\frac{U}{2} \nu^2 \,. \tag{4.166}$$

The internal energy reads as

$$E \equiv \langle H \rangle + \mu N \simeq e_{\nu} N_L + \mu N . \qquad (4.167)$$

Hence, the ground-state energy per atom is

$$\frac{E}{N} = (\nu - 1) \frac{U}{2} \qquad (T = 0) . \tag{4.168}$$

The fluctuations of particles are characterized by the dispersion  $\Delta^2(\hat{N})$ , as is described in Sec. 2.14. With the number-of-particle operator (4.149), we have [93,94]

$$\Delta^2(\hat{N}) = \sum_j \Delta^2(\hat{n}_j) + \sum_{i \neq j} \operatorname{cov}(\hat{n}_i, \hat{n}_j) .$$

For the considered localized state,

$$<\hat{n}_i\hat{n}_j> = <\hat{n}_i> <\hat{n}_j> \qquad (i \neq j) ,$$

because of which  $cov(\hat{n}_i, \hat{n}_j) = 0$ . The dispersion of the filling operator (4.145) is

$$\Delta^2(\hat{n}_j) \equiv \langle \hat{n}_j^2 \rangle - \langle \hat{n}_j \rangle^2 = T \frac{\partial \nu}{\partial \mu} .$$
(4.169)

This, according to Eq. (3.14), defines the compressibility

$$\kappa_T = \frac{a^d}{\nu^2} \frac{\partial \nu}{\partial \mu} = \frac{a^d \Delta^2(\hat{n}_j)}{\nu^2 T} \,. \tag{4.170}$$

At low temperatures, satisfying inequality (4.159), we have

$$\langle \hat{n}_j \rangle \simeq \nu$$
,  $\langle \hat{n}_j^2 \rangle \simeq \nu^2$ .

Therefore  $\Delta^2(\hat{n}_j) \simeq 0$  and  $\kappa_T \simeq 0$ . In that sense, one tells that the localized state is incompressible.

## 5 Phase States and Transitions

#### 5.1 Existence of Pure Phases

To locate the phase transition between the purely delocalized and localized states, one can compare the corresponding thermodynamic potentials. For instance, one can consider the grand potential of the Bose-condensed superfluid phase,  $\Omega_{sup} = \Omega_{sup}(\nu, J, U, T)$ , given, e.g., by Eq. (4.76). From another side, one has the grand potential of the localized phase,  $\Omega_{loc} = \Omega_{loc}(\nu, U, T)$ , given, e.g., by Eq. (4.164). The phase boundary could be described by the equality  $\Omega_{sup} = \Omega_{loc}$ . However, for finite temperature, the system cannot be completely localized, but contains a portion of wandering atoms [283–285]. The same concerns the noninteger filling factors  $\nu$ , for which the system is not absolutely localized [286]. Complete localization can occur for integer filling factors  $\nu = 1, 2, \ldots$  at zero temperature. Such a completely localized state is called the Mott insulator [267,268]. The phase transition between the superfluid state and Mott insulator, occurring for an integer filling at zero temperature, has been studied in various approximations. One usually starts with the Hubbard Hamiltonian

$$\hat{H} = -J \sum_{\langle ij \rangle} c_i^{\dagger} c_j + \frac{U}{2} \sum_j c_j^{\dagger} c_j^{\dagger} c_j c_j + \sum_j h_j c_j^{\dagger} c_j , \qquad (5.1)$$

where, for generality, the site-dependent term with  $h_j$  is included to. The quantity  $h_j$  represents some external fields, like a confining field. It may also represent additionally imposed fields, regular or random. Pure superfluid or insulating phases can exist only under special values of the system parameters.

### 5.2 Hard-Core Lattice Gas

In the limit of an infinite on-site interaction,  $U \to \infty$ , one comes to the hard-core lattice-gas model. In that limit, there can be at most one particle at each site, which is symbolized by the hard-core condition

$$\left(c_{j}^{\dagger}\right)^{2} = 0 , \qquad c_{j}^{2} = 0 .$$
 (5.2)

The Hamiltonian (5.1) reduces to

$$\hat{H} = -J \sum_{\langle ij \rangle} c_i^{\dagger} c_j + \sum_j h_j c_j^{\dagger} c_j .$$
(5.3)

The hard-core boson operators, with condition (5.2), can be transformed as

$$c_{j} = S_{j}^{x} - iS_{j}^{y} \equiv S_{j}^{-}, \qquad c_{j}^{\dagger} = S_{j}^{x} + iS_{j}^{y} \equiv S_{j}^{+},$$
$$c_{j}^{\dagger}c_{j} = \frac{1}{2} + S_{j}^{z}, \qquad (5.4)$$

being expressed through the quasispin operators

$$S_{j}^{x} = \frac{1}{2} \left( c_{j} + c_{j}^{\dagger} \right) , \qquad S_{j}^{y} = \frac{i}{2} \left( c_{j} - c_{j}^{\dagger} \right) , \qquad S_{j}^{z} = c_{j}^{\dagger} c_{j} - \frac{1}{2}$$

This transforms Hamiltonian (5.3) to the quasispin representation

$$\hat{H} = -J \sum_{\langle ij \rangle} S_i^+ S_j^- + \sum_j h_j S_j^z + \frac{h}{2} N_L , \qquad (5.5)$$

in which

$$h \equiv \frac{1}{N_L} \sum_j h_j \,. \tag{5.6}$$

The hopping term in Eq. (5.5) can be rewritten using the equality

$$\sum_{\langle ij \rangle} S_i^+ S_j^- = \sum_{\langle ij \rangle} \left( S_i^x S_j^x + S_i^y S_j^y \right)$$

For three-dimensional lattices, at sufficiently large tunneling parameter J, there can arise the BEC state, while for low J, the Mott insulator state can develop [287–289]. For a onedimensional lattice, there can arise only quasi-long-range order, that is, not the true BEC but a quasicondensate [290].

The ground state of hard-core lattice bosons has also been analyzed by involving the Girardeau Bose-Fermi mapping [13,291,292] by Lin and Wu [293]. They found that in a one-dimensional lattice there can exist the Mott insulator and a normal nonlocalized Bose system if the filling factor is noninteger, but no real BEC, though quasicondensate can exist.

## 5.3 Effective Interaction Parameter

In the more realistic case, when the on-site interaction is finite, there should exist a critical value of this interaction at which the superfluid-insulator phase transition occurs. It is convenient to define the dimensionless parameter

$$u \equiv \frac{U}{z_0 J} \,. \tag{5.7}$$

The critical value of this parameter can be simply estimated as follows. The tunneling energy of each particle approximately is  $z_0 J$ . The energy of a pair interaction of two particles in each lattice site is U/2, hence, the potential energy per particle at one site is U/4. The total potential energy for the lattice is  $N_L U/4$ . So, the potential energy per particle is  $N_L U/4N = U/4\nu$ . The phase transition happens when the tunneling energy  $z_0 J$  equals the potential energy  $U/4\nu$ . This defines the critical parameter (5.7) as

$$u_c = 4\nu . (5.8)$$

Here it has been assumed that there are no external fields.

### 5.4 Gutzwiller Single-Site Approximation

This approximation involves the use of variational wave functions of the Gutzwiller type, which are represented as products over the lattice sites [278–282,294]. At zero temperature, the critical parameter (5.8) is found to be

$$u_c = \left(\sqrt{\nu} + \sqrt{1+\nu}\right)^2 \,. \tag{5.9}$$

For the unity filling  $\nu = 1$ , this gives

$$u_c = 5.8 \qquad (\nu = 1) .$$
 (5.10)

The critical value (5.10) does not depend on the lattice dimensionality, which is usual for mean-field-type approximations. Generally, the microscopic dynamics of the localization-delocalization transition is influenced by the space dimensionality [295].

## 5.5 Dynamical Mean-Field Approximation

Another type of a mean-field approximation was employed by Amico and Penna [296]. They found that, at zero temperature, the superfluid-insulator transition is located at

$$u_c = 4\nu , \qquad (5.11)$$

in exact agreement with the simple estimate (5.8). Again, the result does not depend on the lattice dimensionality. One may notice that the Gutzwiller-approximation value (5.9) reduces to either Eq. (5.8) or Eq. (5.11) for large coordinate numbers  $\nu$ .

#### 5.6 Small-System Numerical Diagonalization

Direct numerical diagonalization can be done for small one-dimensional lattices, of about 10 sites, at zero temperature [276]. This gives, for the unity filling factor, the critical value

$$u_c = 2.3 \qquad (\nu = 1, \ d = 1) .$$
 (5.12)

For one-dimensional lattices, value (5.12) is lower than the values predicted by mean-filed estimates because of the stronger influence of fluctuations that are underestimated in mean-field approximations.

## 5.7 Density-Matrix Renormalization Group

This is another numerical method that can be applied to small one-dimensional lattices [297] giving

$$u_c = 1.7$$
  $(\nu = 1, d = 1)$ . (5.13)

This is close to value (5.12) found by the numerical diagonalization.

#### 5.8 Strong-Coupling Perturbation Theory

Perturbation theory in powers of J/U can be used, with the following summation of series, e.g., by means of Padé approximants [298-300]. One-, two-, and three-dimensional cubic (square) lattices have been considered. The results are

$$u_{c} = 1.9 \qquad (\nu = 1, \ d = 1 \ [299]) ,$$
  

$$u_{c} = 4.2 \qquad (\nu = 1, \ d = 2 \ [299]) ,$$
  

$$u_{c} = 4.9 \qquad (\nu = 1, \ d = 3 \ [298]) . \qquad (5.14)$$

The value for the one-dimensional lattice is close to the numbers obtained by the small-system numerical diagonalization (5.12) and by the density-matrix renormalization group (5.13).

### 5.9 Monte Carlo Simulations

The simulations are accomplished for a finite number of bosons, which can reach  $N \simeq 10^3$  atoms. One-, two-, and three-dimensional rectangular lattices have been investigated [301–305]. The most recent results are presented below:

$$u_{c} = 1.8 \qquad (\nu = 1, \ d = 1 \ [302]) ,$$
  

$$u_{c} = 4.2 \qquad (\nu = 1, \ d = 2 \ [305]) ,$$
  

$$u_{c} = 4.9 \qquad (\nu = 1, \ d = 3 \ [304]) . \qquad (5.15)$$

All these quantities agree well with the strong-coupling perturbation theory. The finitetemperature phase diagram at filling factor  $\nu = 1$  is also found [304,305]. The critical temperature  $T_c = T_c(U)$  as a function of the on-site interaction displays a nonmonotonic behavior, as has been suggested by Kleinert et al. [275]. When U increases from zero,  $T_c$ , first rises, reaches the maximum at around  $U/J \approx 5$ , and then diminishes to zero at the critical value  $U_c/J$ .

#### 5.10 Order of Phase Transition

The transition between the superfluid and Mott insulator phases, occurring at zero temperature and integer filling factors, is an example of the quantum phase transitions. This is a continuous transition, that is, a second-order phase transition. The role of an order parameter is played by the condensate fraction  $n_0$ . Considering the latter as a function  $n_0 = n_0(u)$  of the dimensionless parameter (5.7), one has the following behavior. In the absence of interaction,  $n_0(0) = 1$ . Then, the condensate fraction diminishes with increasing u, and drops continuously to zero at the critical value  $u_c$ . The continuous nature of the superfluid-Mott insulator quantum phase transition in any dimension follows from the fact that the *d*-dimensional Hubbard model with BEC pertains to the universality class of a d + 1-dimensional XY-model [306].

## 5.11 Experiments on Superfluid-Insulator Transition

Several experiments observing the superfluid-insulator phase transition of cold bosons in optical lattices have been accomplished. Actually, because of the finiteness of the lattices, it is not a sharp phase transition that has been observed, but a gradual crossover between the superfluid and Mott insulator states, occurring around the critical values  $u_c$  predicted by theory.

The first experiment was by Greiner et al. [307] with <sup>87</sup>Rb BEC at zero temperature. A three-dimensional lattice was formed by three optical standing waves aligned orthogonal to each other. The laser beams operated at a wavelength  $\lambda = 852$  nm, forming the cubic three-dimensional lattice with the lattice spacing  $a = 4.26 \times 10^{-5}$  cm. The existence of coherence in the superfluid Bose-condensed phase and its absence in the insulating localized phase was analysed by studying the level of interference after suddenly turning off the trapping potential and allowing atoms to expand freely. For the unity filling factor, the superfluid-insulator crossover was localized around  $u_c \approx 6$ .

In the experiment by Stöferle et al. [308], a one-dimensional optical lattice was realized with <sup>87</sup>Rb atoms. The optical lattice was formed by laser beams at a wavelength  $\lambda = 826$ nm, which translated into the lattice spacing  $a = 4.13 \times 10^{-5}$  cm. Bragg spectroscopy was employed for investigating the excitation spectrum. The superfluid insulator crossover, at the unity filling factor, was observed close to  $u_c \approx 5.8$ , though for one-dimensional lattices it should happen at  $u_c \approx 1.8$ . This disagreement could be due to the finite size of the trap. A very important finding was that for strongly interacting Bose systems in optical lattices the superfluid fraction could be significantly different from the coherent BEC fraction.

Different types of lattices, one-, two-, and three-dimensional optical lattices were created by Köhl et al. [309] for <sup>87</sup>Rb atoms. The optical lattices were formed by retro-reflected laser beams at a wavelength  $\lambda = 826$  nm, which corresponded to the lattice spacing  $a = 4.13 \times 10^{-5}$  cm. The superfluid-insulator crossover was investigated by using Bragg spectroscopy for studying the excitation spectra. The appearance of the discrete spectrum structure, associated with the Mott insulating phase, was observed between u = 4 and u = 8.

A three-dimensional lattice, filled by sodium <sup>23</sup>Na atoms, was formed by Xu et al. [310]. A dye laser operated at  $\lambda = 594.7$  nm. Hence, the lattice spacing was  $a = 2.97 \times 10^{-5}$  cm. The system properties were studied by the time-off-flight images. The filling factors could be varied between  $\nu = 1$  to  $\nu = 5$ . The superfluid-insulator crossovers were observed around the critical values  $u_c$  given by the single-site approximation (5.9).

In the experiment by Spielman et al. [311] the BEC of <sup>87</sup>Rb atoms was loaded into a two-dimensional optical lattice formed by laser light of  $\lambda = 820$  nm. This gave the lattice spacing  $a = 4.1 \times 10^{-5}$  cm. The system properties were analysed by studying the timeof-flight images. For the unity filling factor, the superfluid-insulator crossover was located around the critical value  $u_c \approx 4$ , which was in agreement with the Monte Carlo simulations as could be seen from Eq. (5.15).

## 5.12 Layered Superfluid-Insulator Structure

When, in addition to the optical lattice potential, there is an external trapping potential, the system becomes nonuniform, so that the lattice is no longer ideal. Then in some spatial parts

the conditions could be created for the occurrence of the insulating phase, while in other spatial locations the superfluid phase would be preferable. This results in the formation of a shell structure, where the layers of Mott insulating phases alternate with the layers of superfluid phases. This layered structure was studied by Monte Carlo methods [312], by employing a pseudospin approximation [313], and was observed in experiment [314].

### 5.13 Models with Neighbor Interactions

The Hubabrd model (5.1) contains only the on-site atomic interaction U. This is, of course, a simplification. When deriving the Hubabrd Hamiltonian in Sec. 4.1, we could see that the Wannier representation (4.11) of the general system Hamiltonian (2.151) includes interactions between all lattice sites. Strictly speaking, all these interactions are nonzero even for the local interaction potential, as follows from the matrix element (4.10). Considering solely the on-site interaction assumes that the interaction potential is of short-range type and Wannier functions are well localized at their lattice sites. But when the lattice optical potential is shallow, the corresponding Wannier functions may be not so well localized. Or, if the pair atomic interaction potential is not short-range, then the interactions of atoms at neighboring sites can be sufficiently important and not negligible. For example, the dipolar quantum gas of <sup>52</sup>Cr possesses long-range dipolar interactions [315,316]. Therefore, there are realistic situations, when the different-site interactions could be important. This requires to consider the *extended Hubbard model* 

$$\hat{H} = -J \sum_{\langle ij \rangle} c_i^{\dagger} c_j + \frac{U}{2} \sum_j c_j^{\dagger} c_j^{\dagger} c_j c_j c_j + \frac{1}{2} \sum_{i \neq j} U_{ij} c_i^{\dagger} c_j^{\dagger} c_i c_j + \sum_j h_j c_j^{\dagger} c_j , \qquad (5.16)$$

in which, in addition to the on-site term, intersite atomic interactions are taken into account. One usually considers the nearest-neighbor  $(U_1)$  and next-nearest-neighbor  $(U_2)$  interactions. Because of the complexity of Hamiltonian (5.16), such extended models are mainly studied by means of numerical techniques, e.g., by using the density-matrix renormalization group method [317,318] or quantum Monte Carlo simulations [319–322]. With additional parameters, the phase diagram of the extended model becomes essentially more rich. There can exist pure superfluid and insulator phases, there can arise a spatially separated mixture of these phases, striped solid phases can develop, and staggered patterns of alternating empty and multiply occupied sites can occur. For noninteger fillings, the states can appear with simultaneous diagonal order, corresponding to a solid, and off-diagonal long-range order, typical of the BEC state, accompanied by superfluidity. The latter state, combining solid, superfluid, and BEC properties, is an example of the coherent superfluid solid, according to the classification of Sec. 1.4.

## 5.14 Quasiperiodic Optical Lattices

In experiment, it is possible to create not only periodic optical potentials, as in Eq. (3.1), but also quasiperiodic potentials [323,324]. The general form of a quasiperiodic potential is a superposition of several periodic functions with incommensurate periods, as in the expression

$$V_L(\mathbf{r}) = \sum_{\alpha=1}^d \sum_{\mu} V_{\alpha\mu} \sin^2 \left( k_{\mu}^{\alpha} r_{\alpha} \right) \; .$$

One usually considers one-dimensional quasiperiodic lattices with the potential

$$V_L(z) = V_0 \sin^2(k_0 z) + V_1 \sin^2(q_0 z) , \qquad (5.17)$$

in which neither  $k_0/q_0$  nor  $q_0/k_0$  are integers. The physics of the one-dimensional systems with the quasiperiodic lattice potential (5.17) has been studied in different approximations [325–328] as well as numerically [329–331]. Quasiperiodic systems were found to have an intermediate behavior between periodic ones and random systems. Depending on the system parameters, there can exist the superfluid phase, Mott-insulator phase, as well as the coexisting superfluid and normal phases. In addition, an incommensurate density wave can arise, representing the incommensurate insulator, whose period is incommensurate with the lattice periods. Also, the Bose glass phase can develop, in which there is BEC,  $n_0 > 0$ , but there is no superfluidity,  $n_s = 0$ .

In order to demonstrate how the Hubbard model for a quasiperiodic lattice could be constructed, let us consider the one-dimensional case with the bichromatic optical potential (5.17). The derivation of the Hubbard model can be done in the same way as in Sec. 4.1, if one treats one of the sublattices as primary and accomplishes the expansions over Wannier functions associated with this primary sublattice. For instance, the first term in potential (5.17) can be treated as primary, hence, the primary sublattice having the period a, related to the laser wavevector  $k_0 = \pi/a$ .

The lattice local Hamiltonian can be separated into two parts,

$$H_L(z) = -\frac{\nabla^2}{2m} + V_L(z) = H_L^0(z) + \Delta H_L(z) , \qquad (5.18)$$

the first part including the primary potential,

$$H_L^0(z) \equiv -\frac{\nabla^2}{2m} + V_0 \sin^2(k_0 z) , \qquad (5.19)$$

and the addition being

$$\Delta H_L(z) \equiv V_1 \sin^2(q_0 z) . \qquad (5.20)$$

The primary term (5.19) is periodic over the sublattice  $\{a_j\}$ , so that

$$H_L^0(z+a_j) = H_L^0(z)$$
.

The Hubbard parameters are defined in Eqs. (4.8), (4.9), and (4.10). As in Eq. (4.12), we shall consider the single-band Hubbard model.

For the tunneling term, we have

$$J_{ij} = J_{ij}^{0} + \Delta J_{ij} , \qquad J_{ij}^{0} \equiv -\int w(z - a_i) H_L^0(z) w(z - a_j) \, dz ,$$
$$\Delta J_{ij} \equiv -\int w(z - a_i) \Delta H_L(z) w(z - a_j) \, dz . \qquad (5.21)$$

Respectively, the single-site term  $h_j$  becomes

$$h_j = h_0 + \Delta h_j$$
,  $h_0 \equiv \int w(z) H_L^0(z) w(z) dz$ ,

$$\Delta h_j \equiv \int w(z - a_j) \Delta H_L(z) w(z - a_j) \, dz \,. \tag{5.22}$$

Using for Wannier functions the Gaussian approximation (3.161), we follow calculations similar to those in Sec. 3.9. Then we have the primary parameters

$$J = \left(\frac{\pi^2}{4} - 1\right) V_0 \exp\left(-\frac{a^2}{4l_0^2}\right) , \qquad h_0 = \sqrt{V_0 E_R} , \qquad (5.23)$$

where J is  $J_{ij}^0$  for nearest neighbors. The additional term for the tunneling parameter is

$$\Delta J_{ij} = -\frac{V_1}{2} \exp\left(-\frac{a^2}{4l_0^2}\right) \left\{1 - \exp\left(-q_0^2 l_0^2\right) \cos[q_0(a_i + a_j)]\right\} , \qquad (5.24)$$

and the addition to the single-site term is

$$\Delta h_j = \frac{V_1}{2} \left[ 1 - \exp(-q_0^2 l_0^2) \cos(2q_0 a_j) \right] .$$
(5.25)

The latter equations can be simplified, when there is good localization, not only with respect to the primary sublattice, such that  $k_0 l_0 \ll 1$ , but also with respect to the secondary sublattice, so that

$$q_0 l_0 \ll 1$$
 . (5.26)

Then Eq. (5.24) becomes

$$\Delta J_{ij} \simeq -V_1 \exp\left(-\frac{a^2}{4l_0^2}\right) \sin^2\left(q_0 \,\frac{a_i + a_j}{2}\right) \,, \tag{5.27}$$

while Eq. (5.25) reduces to

$$\Delta h_j \cong V_1 \sin^2(q_0 a_j) . \tag{5.28}$$

The on-site interaction parameter U remains the same as in Eq. (4.14).

Thus, the Hubbard parameters J and  $h_0$  acquire the site-dependent terms (5.27) and (5.28). Comparing these additional terms with the primary values J and  $h_0$ , we have

$$\left|\frac{\Delta J_{ij}}{J}\right| \le 0.7 \, \frac{V_1}{V_0} \,, \qquad \frac{\Delta h_j}{h_0} \le \frac{V_1}{2V_0} \,\sqrt{\frac{V_0}{E_R}} \,.$$
 (5.29)

And the Hubbard Hamiltonian for the quasiperiodic bichromatic potential takes the form

$$\hat{H} = -\sum_{\langle ij \rangle} J_{ij} c_i^{\dagger} c_j + \sum_j h_j c_j^{\dagger} c_j + \frac{U}{2} \sum_j c_j^{\dagger} c_j^{\dagger} c_j c_j c_j \,.$$
(5.30)

If the amplitude of the second term in potential (5.17) is comparable with that of the first term, then, as follows from ratio (5.29), Hamiltonian (5.30) describes a very nonideal lattice with strong dependence of  $J_{ij}$  and  $h_j$  on site numbers. Therefore, one usually considers the case, when the second term in potential (5.17) plays the role of perturbation, so that  $V_1 \ll V_0$ . In such a case,  $|\Delta J_{ij}| \ll J$ , and one can neglect the variation of the tunneling parameter J. However, even when  $V_1 \ll V_0$ , but the primary sublattice is sufficiently deep, so that  $E_R \ll V_0$ , then  $\Delta h_j$  can be of order of  $h_0$ , as it is seen from Eq. (5.22). Therefore, the variation of the single-site parameter  $h_j$  cannot be neglected. In that situation, one can replace in the Hubbard Hamiltonian (5.30) the tunneling  $J_{ij}$  by the site-independent value J, while keeping  $h_j$  as the sum  $h_0 + \Delta h_j$ , with the site-varying part (5.28). The properties of quasiperiodic optical lattices have much in common with those of quasicrystals [207,208].

## 5.15 Rotating Optical Lattices

When a Bose system with BEC is rotated, vortices appear after the rotation frequency  $\Omega$  reaches the critical value. An optical lattice, in principle, also can be rotated sufficiently fast in order that vortices could grow in it. Two interesting situations can occur, when rotating one-dimensional lattices, with the lattice direction either along the vortex, that is, along the rotation frequency  $\Omega$ , or perpendicular to the latter, hence, perpendicular to the vortex. Both these cases were studied theoretically in Refs. [332,333] and [334,335], respectively. Experimentally these cases have not yet been realized.

When an axisymmetric BEC with a single vortex on the axis of symmetry is subject to a lattice optical potential along the same axis, then this one-dimensional lattice would slice the rotating BEC into many circular disks [332,333,336]. The resulting periodic array forms a set of quasi-two-dimensional condensate layers. Each effectively two-dimensional condensate becomes a single pancake vortex.

A rotating Bose system is conveniently described in the rotating reference frame. Then the system Hamiltonian acquires an additional centrifugal term

$$\hat{U}_{rot} = -\int \psi^{\dagger}(\mathbf{r}) \ \mathbf{\Omega} \cdot \hat{\mathbf{L}} \ \psi(\mathbf{r}) \ d\mathbf{r} \ ,$$

where  $\Omega$  is the angular rotation frequency and  $\mathbf{\hat{L}} = \mathbf{r} \times \mathbf{p}$  is angular momentum. Passing to the Wannier representation transforms the centrifugal term into

$$\hat{U}_{rot} = -\sum_{i \neq j} J_{ij}^{rot} c_i^{\dagger} c_j + \sum_j h_j^{rot} c_j^{\dagger} c_j ,$$

with

$$J_{ij}^{rot} \equiv \int w^* (\mathbf{r} - \mathbf{a}_i) (\mathbf{\Omega} \cdot \hat{\mathbf{L}}) w(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r} \,,$$
$$h_j^{rot} \equiv -\int w^* (\mathbf{r} - \mathbf{a}_j) (\mathbf{\Omega} \cdot \hat{\mathbf{L}}) w(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r} \,.$$

This means that rotating a lattice induces additional atomic tunneling and a single-site energy term.

Thus, optical lattices provide the possibility of creating Bose systems with a wide variety of properties, which can be employed in different applications.

# 6 Optical Lattices with Disorder

## 6.1 Random Potentials

The presence of an externally incorporated disorder can essentially change the system properties. And the possibility of varying the level of disorder presents a powerful tool for achieving different states of matter. This problem has been considered in solid state physics for many years, with applications to conducting properties of materials [337–340], magnetic properties of spin glasses [341,342], to real-space glasses [343,344], amorphous alloys [345,346], and to physics of caking [347]. Disorder can also be introduced by the boundaries of finite systems [101,348] and by domain walls [349,350].

Recently, several experiments [351–354] have studied <sup>87</sup>Rb in random optical potentials created by optical speckles. It has been observed that the speckle randomness induces damping of collective excitations [351] and inhibition of expansion [352–354]. The effects of a disordered optical potential on the transport and phase coherence of a BEC of <sup>7</sup>Li atoms has also been studied, and inhibition of transport and damping of dipole excitations have been observed [355]. An ultracold bosonic gas of <sup>87</sup>Rb in a 3-dimensional optical lattice was investigated, with disorder induced by a small contribution of fermionic <sup>40</sup>K impurity atoms [356]. The random admixture was found to favor the localization of bosonic atoms. It was suggested [357] that a one-dimensional BEC in a weak random potential can exhibit Anderson localization [358].

The Hamiltonian of atoms in an optical lattice potential  $V_L(\mathbf{r})$ , and also subject to the action of an additional random potential  $\xi(\mathbf{r})$ , has the form

$$\hat{H} = \int \psi^{\dagger}(\mathbf{r}) \left[ -\frac{\nabla^2}{2m} + V_L(\mathbf{r}) + \xi(\mathbf{r}) \right] \psi(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \Phi_0 \int \psi^{\dagger}(\mathbf{r}) \psi^{\dagger}(\mathbf{r}) \psi(\mathbf{r}) \psi(\mathbf{r}) \, d\mathbf{r} \,, \quad (6.1)$$

where  $\Phi_0 \equiv 4\pi a_s/m$ . The random potential is real

$$\xi^*(\mathbf{r}) = \xi(\mathbf{r}) \ . \tag{6.2}$$

Without the loss of generality, it can be taken as zero-centered, so that its stochastic averaging be

$$\ll \xi(\mathbf{r}) \gg = 0. \tag{6.3}$$

The stochastic averaging of the pair product

$$\ll \xi(\mathbf{r})\xi(\mathbf{r}') \gg = R(\mathbf{r} - \mathbf{r}')$$
(6.4)

is characterized by a random-potential correlation function that is real and symmetric, such that

$$R^*(\mathbf{r}) = R(\mathbf{r}) = R(-\mathbf{r}) . \tag{6.5}$$

Details of defining the stochastic averaging can be found in the book [359].

When using the Bloch representation for the field operator

$$\psi(\mathbf{r}) = \sum_{nk} a_{nk} \varphi_{nk}(\mathbf{r})$$

it is convenient to introduce the matrix element of the random potential

$$\beta_{kp}^{mn} \equiv \int \varphi_{mk}^*(\mathbf{r})\xi(\mathbf{r})\varphi_{np}(\mathbf{r}) \, d\mathbf{r} \,. \tag{6.6}$$

Then the term of Hamiltonian (6.1), containing the random potential, is

$$\int \psi^{\dagger}(\mathbf{r})\xi(\mathbf{r})\psi(\mathbf{r}) d\mathbf{r} = \sum_{mn} \sum_{kp} \beta_{kp}^{mn} a_{mk}^{\dagger} a_{np}$$

If, when considering a lattice, one prefers the Wannier representation

$$\psi(\mathbf{r}) = \sum_{nj} c_{nj} w_n(\mathbf{r} - \mathbf{a}_j) \; ,$$

then one meets the matrix element

$$\gamma_{ij}^{mn} \equiv \int w_m^*(\mathbf{r} - \mathbf{a}_i)\xi(\mathbf{r})w_n(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r} \,. \tag{6.7}$$

And the random term in Eq. (6.1) becomes

$$\int \psi^{\dagger}(\mathbf{r})\xi(\mathbf{r})\psi(\mathbf{r}) d\mathbf{r} = \sum_{mn} \sum_{ij} \gamma_{ij}^{mn} c_{mi}^{\dagger} c_{nj}$$

The matrix elements (6.6) and (6.7) are connected through the Fourier transformations

$$\beta_{kp}^{mn} = \frac{1}{N_L} \sum_{ij} \gamma_{ij}^{mn} e^{-i\mathbf{k}\cdot\mathbf{a}_i + i\mathbf{p}\cdot\mathbf{a}_j} , \qquad \gamma_{ij}^{mn} = \frac{1}{N_L} \sum_{kp} \beta_{kp}^{mn} e^{i\mathbf{k}\cdot\mathbf{a}_i - i\mathbf{p}\cdot\mathbf{a}_j} . \tag{6.8}$$

In the uniform limit, when the Bloch functions  $\varphi_{nk}(\mathbf{r})$  tend to the plane waves  $e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$ , it is convenient to define the Fourier transform of the random potential

$$\xi_k \equiv \frac{1}{\sqrt{V}} \int \xi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \, d\mathbf{r} \,, \qquad \xi(\mathbf{r}) \equiv \frac{1}{\sqrt{V}} \sum_k \xi_k e^{i\mathbf{k}\cdot\mathbf{r}} \,. \tag{6.9}$$

Then one has

$$\beta_{kp}^{mn} = \frac{1}{\sqrt{V}} \,\xi_{k-p} \,. \tag{6.10}$$

In the presence of BEC, one has to break the global gauge symmetry [63], which can be done by the Bogolubov shift of the field operator

$$\psi(\mathbf{r}) \rightarrow \hat{\psi}(\mathbf{r}) \equiv \eta(\mathbf{r}) + \psi_1(\mathbf{r}) ,$$
 (6.11)

as is described in Sec. 2.7. This implies, in agreement with Sec. 3.3, the corresponding shift of the Bloch field operator

$$a_{nk} \rightarrow \hat{a}_{nk} \equiv \delta_{n0} \,\delta_{k0} \sqrt{N_0} \,+\, a_{nk} \tag{6.12}$$

and of the Wannier field operator

$$c_{nj} \rightarrow \hat{c}_{nj} \equiv \delta_{n0} \sqrt{\nu n_0} + c_{nj} . \qquad (6.13)$$

The Bogolubov shift realizes unitary nonequivalent operator representations [99,360–362].

The grand Hamiltonian of a system with BEC is

$$H = \hat{H} - \mu_0 N_0 - \mu_1 \hat{N}_1 .$$
(6.14)

The type of disorder induced by an external random potential is termed the *frozen* disorder or *quenched* disorder. The corresponding grand thermodynamic potential is defined as

$$\Omega = -T \ll \ln \operatorname{Tr} e^{-\beta H} \gg .$$
(6.15)

And the free energy is

$$F = \Omega + \mu N$$
,  $\mu = \mu_0 n_0 + \mu_1 n_1$ 

It is important to emphasize that there are two kinds of averaging for quantum random systems. One type of averaging is the stochastic averaging, denoted by the double angle brackets  $\ll \ldots \gg$ , characterizing the averaging over the distribution of random potentials. And there is the quantum statistical averaging, which for an operator  $\hat{A}$  is defined as

$$\langle \hat{A} \rangle_H \equiv \text{Tr} \hat{\rho} \hat{A}$$
, (6.16)

with the statistical operator

$$\hat{\rho} = \frac{\exp(-\beta H)}{\operatorname{Tr} \exp(-\beta H)} \,. \tag{6.17}$$

The total averaging

$$\langle \hat{A} \rangle \equiv \ll \operatorname{Tr} \hat{\rho} \hat{A} \gg$$
 (6.18)

includes both, the quantum as well as stochastic averaging procedures.

The condensate fraction  $n_0 = 1 - n_1$  is expressed through the fraction of uncondenced atoms

$$n_1 \equiv \frac{1}{N} \int \langle \psi_1^{\dagger}(\mathbf{r})\psi_1(\mathbf{r}) \rangle d\mathbf{r} = \frac{1}{N} \sum_{nk} \langle a_{nk}^{\dagger} a_{nk} \rangle = \frac{1}{N} \sum_{nj} \langle c_{nj}^{\dagger} c_{nj} \rangle .$$
(6.19)

The anomalous average is

$$\sigma \equiv \frac{1}{N} \int \langle \psi_1(\mathbf{r}) \psi_1(\mathbf{r}) \rangle d\mathbf{r} = \frac{1}{N} \sum_{nk} \langle a_{nk} a_{n,-k} \rangle = \frac{1}{N} \sum_{nj} \langle c_{nj} c_{nj} \rangle .$$
(6.20)

For random systems, it is possible to define an additional order parameter, the glassy fraction

$$n_G \equiv \frac{1}{N} \int \ll |\langle \psi_1(\mathbf{r}) \rangle_H|^2 \gg d\mathbf{r} , \qquad (6.21)$$

which is analogous to the Edwards-Anderson order parameter for spin glasses [341,342]. Though the total average  $\langle \psi_1(\mathbf{r}) \rangle = 0$ , the partial, quantum, average  $\langle \psi_1(\mathbf{r}) \rangle_H$  is not necessarily zero. Respectively, the quantum averages

$$\alpha_{nk} \equiv \langle a_{nk} \rangle_H , \qquad \overline{\alpha}_{nj} \equiv \langle c_{nj} \rangle_H \tag{6.22}$$

are not zero, contrary to the total averages

$$\langle \psi_1(\mathbf{r}) \rangle = \langle a_{nk} \rangle = \langle c_{nj} \rangle = 0.$$
 (6.23)

From here it follows that

$$\ll \alpha_{nk} \gg = \ll \overline{\alpha}_{nj} \gg = 0.$$
 (6.24)

The glassy fraction (6.21) can be rewritten as

$$n_G = \frac{1}{N} \sum_{nk} \ll |\alpha_{nk}|^2 \gg = \frac{1}{N} \sum_{nj} \ll |\overline{\alpha}_{nj}|^2 \gg .$$
 (6.25)

The presence of random fields induces in the system additional fluctuations, which is typical of random and chaotic systems [363]. Without disordering fields, the condensate is depleted by atomic interactions and temperature. The inclusion of random fields depletes the condensate even more and creates the glassy fraction (6.21).

### 6.2 Uniform Limit

A uniform system is a limiting case of a very shallow lattice. Then, in the Bloch representation, the Bloch functions are plane waves. Uniform Bose-condensed systems in random potentials have been studied for asymptotically weak atomic interactions and asymptotically weak strength of disorder [364-366]. A theory for arbitrary strong random potentials and interactions was developed in Refs. [367,368]. When a disordered potential is created inside a trap, then the BEC properties can be investigated by means of time-of -flight experiments [369].

For a system, uniform on average, the condensate fraction is

$$n_0 = \frac{1}{\rho} |\eta(\mathbf{r})|^2 \qquad (\eta(\mathbf{r}) = \sqrt{\rho_0}) .$$
 (6.26)

The fraction of uncondensed atoms (6.19) can be written as

$$n_1 = \frac{1}{N} \sum_k n_k \qquad \left( n_k \equiv \langle a_k^{\dagger} a_k \rangle \right) . \tag{6.27}$$

The anomalous average (6.20) takes the form

$$\sigma = \frac{1}{N} \sum_{k} \sigma_k \qquad (\sigma_k \equiv \langle a_k a_{-k} \rangle) . \tag{6.28}$$

And the glassy fraction (6.21) becomes

$$n_G = \frac{1}{N} \sum_k \ll |\alpha_k|^2 \gg , \qquad (6.29)$$

where the notation

$$\alpha_k \equiv \langle a_k \rangle_H \tag{6.30}$$

is introduced.

Accomplishing in Eq. (6.1) the Bogolubov shift (6.11) and passing to the Fourier-transformed field operators  $a_k$ , for the grand Hamiltonian (6.14), we obtain

$$H = \sum_{n=0}^{4} H^{(n)} + H_{ext} , \qquad (6.31)$$

in which the terms in the sum are

$$H^{(0)} = \left(\frac{1}{2}\rho_{0}\Phi_{0} - \mu_{0}\right)N_{0}, \qquad H^{(1)} = 0,$$

$$H^{(2)} = \sum_{k\neq 0} \left(\frac{k^{2}}{2m} + 2\rho_{0}\Phi_{0} - \mu_{1}\right)a_{k}^{\dagger}a_{k} + \frac{1}{2}\sum_{k\neq 0}\rho_{0}\Phi_{0}\left(a_{k}^{\dagger}a_{-k}^{\dagger} + a_{-k}a_{k}\right),$$

$$H^{(3)} = \sqrt{\frac{\rho_{0}}{V}}\sum_{kp(\neq 0)}\Phi_{0}\left(a_{k}^{\dagger}a_{k+p}a_{-p} + a_{-p}^{\dagger}a_{k+p}^{\dagger}a_{k}\right),$$

$$H^{(4)} = \frac{1}{2V}\sum_{q}\sum_{kp(\neq 0)}\Phi_{0}a_{k}^{\dagger}a_{p}^{\dagger}a_{k-q}a_{p+q} \qquad (6.32)$$

and the last term, caused by the random potential, is

$$H_{ext} = \rho_0 \xi_0 \sqrt{V} + \sqrt{\rho_0} \sum_{k \neq 0} \left( a_k^{\dagger} \xi_k + \xi_k^* a_k \right) + \frac{1}{\sqrt{V}} \sum_{kp(\neq 0)} a_k^{\dagger} a_p \xi_{k-p} .$$
(6.33)

The correlation function of a disordered potential, defined in Eq. (6.4), is assumed to possess a Fourier transform

$$R_k = \int R(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \, d\mathbf{r} \,, \qquad R(\mathbf{r}) = \frac{1}{V} \, \sum_k R_k e^{i\mathbf{k}\cdot\mathbf{r}} \,. \tag{6.34}$$

From properties (6.2) and (6.5), it follows that

$$\xi_k^* = \xi_{-k} , \qquad R_k^* = R_{-k} = R_k .$$
 (6.35)

And the stochastic averaging (6.4) gives

$$\ll \xi_k^* \xi_p \gg = \delta_{kp} R_k . \tag{6.36}$$

In the case of white noise, one has

$$R(\mathbf{r}) = R_0 \delta(\mathbf{r}) , \qquad R_k = R_0 .$$
(6.37)

Thence, Eq. (6.36) reduces to

$$\ll \xi_k^* \xi_p \gg = \delta_{kp} R_0 . \tag{6.38}$$

The Hamiltonian terms in Eq. (6.32) can be simplified by using the Hartree-Fock-Bogolubov approximation, as in Refs. [57,94–99]. But the random Hamiltonian term (6.33) should be treated with care. If one would use the standard mean-field decoupling for the last term in Eq. (6.33), one would kill in this term all quantum effects because of Eqs. (6.3) and (6.23). Therefore it is necessary to invoke a more delicate decoupling procedure. For this purpose, it is convenient to employ the *stochastic mean-field approximation* suggested and used earlier for other physical systems [241,242,370–373]. This approximation in the present case yields

$$a_k^{\dagger} a_p \xi_{k-p} = \left( a_k^{\dagger} \alpha_p + \alpha_k^* a_p - \alpha_k^* \alpha_p \right) \xi_{k-p} .$$
(6.39)

Then Hamiltonian (6.31) can be diagonalized by the use of the *nonuniform nonlinear* canonical transformation

$$a_k = u_k b_k + v_{-k}^* b_{-k}^\dagger + w_k \varphi_k , \qquad (6.40)$$

which generalizes the standard uniform Bogolubov transformation. The diagonalization implies that the resulting Hamiltonian should be diagonal in terms of the operators  $b_k^{\dagger}$  and  $b_k$ , so that

$$\langle b_k \rangle_H = \langle b_k b_p \rangle_H = 0 \; .$$

Hence, relation (6.40) gives

$$\langle a_k \rangle_H = w_k \varphi_k . \tag{6.41}$$

This diagonalization results in

$$u_k^2 = \frac{\omega_k + \varepsilon_k}{2\varepsilon_k} , \qquad v_k^2 = \frac{\omega_k - \varepsilon_k}{2\varepsilon_k} , \qquad w_k = -\frac{1}{\omega_k + mc^2} ,$$
$$\omega_k = \frac{k^2}{2m} + mc^2 , \qquad \omega_k^2 = \varepsilon_k^2 + (mc^2)^2 , \qquad (6.42)$$

where

$$\varepsilon_k = \sqrt{(ck)^2 + \left(\frac{k^2}{2m}\right)^2} \tag{6.43}$$

is the Bogolubov spectrum, with the sound velocity c defined by the equation

$$mc^2 = (n_0 + \sigma)\rho\Phi_0$$
 . (6.44)

The random variable  $\varphi_k$  in transformation (6.40) satisfies the Fredholm equation

$$\varphi_k = \sqrt{\rho_0} \,\xi_k \ - \ \frac{1}{\sqrt{V}} \sum_p \ \frac{\xi_{k-p}\varphi_p}{\omega_p + mc^2} \,. \tag{6.45}$$

The nonuniform nonlinear transformation (6.40) reduces the grand Hamiltonian (6.31) to the form

$$H = E_B + \sum_k \varepsilon_k b_k^{\dagger} b_k + \varphi_0 \sqrt{N_0} , \qquad (6.46)$$

with

$$E_B = \frac{1}{2} \sum_k (\varepsilon_k - \omega_k) - \left[ 1 - n_0^2 + \frac{1}{2} (n_0 + \sigma)^2 \right] \rho^2 \Phi_0 N .$$
 (6.47)

The diagonal Hamiltonian (6.46) allows us to find the momentum distribution

$$n_k = \frac{\omega_k}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) - \frac{1}{2} + \ll |\alpha_k|^2 \gg$$
(6.48)

and the anomalous average

$$\sigma_k = -\frac{mc^2}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) + \ll |\alpha_k|^2 \gg .$$
(6.49)

The random variable (6.30), in view of Eqs. (6.41) and (6.42), is

$$\alpha_k = w_k \varphi_k = -\frac{\varphi_k}{\omega_k + mc^2} \,. \tag{6.50}$$

Therefore

$$\ll |\alpha_k|^2 \gg = \frac{\ll |\varphi_k|^2 \gg}{(\omega_k + mc^2)^2} \,. \tag{6.51}$$

The fraction of uncondensed atoms (6.27) becomes a sum of two terms,

$$n_1 = n_N + n_G , (6.52)$$

in which the first term

$$n_N = \frac{1}{2\rho} \int \left[ \frac{\omega_k}{\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) - 1 \right] \frac{d\mathbf{k}}{(2\pi)^3}$$
(6.53)

is the fraction of uncondensed atoms, due to finite temperature and interactions, while the second term

$$n_G = \frac{1}{\rho} \int \frac{\ll |\varphi_k|^2 \gg}{(\omega_k + mc^2)^2} \frac{d\mathbf{k}}{(2\pi)^3}$$
(6.54)

is the glassy fraction (6.29), caused by the random potential. The anomalous average (6.28) is also a sum of two terms,

$$\sigma = \sigma_N + n_G , \qquad (6.55)$$

with the first term

$$\sigma_N = -\frac{1}{2\rho} \int \frac{mc^2}{\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) \frac{d\mathbf{k}}{(2\pi)^3}$$
(6.56)

and the second term (6.54).

To find the superfluid fraction, we resort to the general definition of Sec. 2.10,

$$n_s = 1 - \frac{2Q}{3T} \qquad \left(Q \equiv \frac{\langle \mathbf{P}^2 \rangle}{2mN}\right) \,. \tag{6.57}$$

The dissipated heat consists of two parts,

$$Q = Q_N + Q_G . ag{6.58}$$

The first part

$$Q_N = \frac{1}{8m\rho} \int \frac{k^2}{\sinh^2(\varepsilon_k/2T)} \frac{d\mathbf{k}}{(2\pi)^3}$$
(6.59)

is the heat dissipated by uncondensed atoms related to finite temperature and interactions. And the second part

$$Q_G = \frac{1}{2m\rho} \int \frac{k^2 \ll |\varphi_k|^2 \gg}{\varepsilon_k(\omega_k + mc^2)} \coth\left(\frac{\varepsilon_k}{2T}\right) \frac{d\mathbf{k}}{(2\pi)^3}$$
(6.60)

is the heat dissipated by the glassy fraction of atoms.

The analysis [367,368] of the derived equations shows that for weak interactions and sufficiently strong disorder, the superfluid fraction can become smaller than the condensate fraction, in agreement with Monte Carlo simulations [374]. But at relatively strong interactions, the superfluid fraction is larger than the condensate fraction for any strength of disorder. The condensate and superfluid fractions, and the glassy fraction always coexist, being together either nonzero or zero. In the presence of disorder, the condensate fraction becomes a nonmonotonic function of the interaction strength, displaying an antidepletion effect caused by the competition between the stabilizing role of the atomic interaction and the destabilizing role of the disorder. An ideal Bose gas with BEC is stochastically unstable, the BEC being destroyed by infinitesimally weak disorder. Finite atomic interactions stabilize the system. When the strength of disorder is increased, reaching a critical value  $\zeta_c$ of the disorder parameter

$$\zeta \equiv \frac{7m^2 R_0}{4\pi \rho^{1/3}} = \frac{a}{l_L} \; ,$$

in which

$$l_L \equiv \frac{4\pi}{7m^2R_0} \qquad a \equiv \frac{1}{\rho^{1/3}} ,$$

the condensate and superfluid fractions drop to zero by a first-order phase transition. The characteristic length  $l_L$  practically coincides with the Larkin length [375]. The critical value of the disorder parameter  $\zeta_c$ , where the first-order phase transition occurs, depends on the interaction strength and temperature. More details on the properties of the disordered superfluid can be found in Refs. [367,368].

After the strength of disorder reaches its critical value, characterized by the critical value of the disorder parameter  $\zeta_c$ , the global coherence becomes destroyed and there is no global BEC occupying the whole system. Also, there is no superfluidity. But for  $\zeta > \zeta_c$ , the condensate can decay into fragments each of the size of the Larkin length  $l_L$ , so that the phase transition at  $\zeta_c$  could be interpreted as a spatial condensate fragmentation [376]. For  $\zeta > \zeta_c$ , the local remnants of the condensate could remain, while superfluidity being absent. Such a state, according to the classification of Sec. 1.4, corresponds to the Bose glass. The destruction of superfluidity, with increasing disorder, through a first-order transition, was also found in Ref. [377].

#### 6.3 Disordered Lattice

Passing from the initial Hamiltonian (6.1) to the Wannier representation, we may, as usual, consider the single-band case. Then the matrix element (6.7) of the random potential  $\xi(\mathbf{r})$  reads as

$$\gamma_{ij} = \int w^*(\mathbf{r} - \mathbf{a}_i)\xi(\mathbf{r})w(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r} \,. \tag{6.61}$$

For the single-site effective potential, we have

$$h_j = h_0 + \gamma_j , \qquad (6.62)$$

in which the constant term

$$h_0 \equiv \int w^*(\mathbf{r}) H_L(\mathbf{r}) w(\mathbf{r}) \, d\mathbf{r}$$

in what follows can be neglected without the loss of generality. The random term in Eq. (6.62) is

$$\gamma_j \equiv \gamma_{jj} = \int |w(\mathbf{r} - \mathbf{a}_j)|^2 \xi(\mathbf{r}) \, d\mathbf{r} \,. \tag{6.63}$$

This diagonal term is real because of Eq. (6.2),

$$\gamma_j^* = \gamma_j \ . \tag{6.64}$$

From Hamiltonian (6.1), the Hubbard Hamiltonian follows

$$\hat{H} = -\sum_{\langle ij \rangle} \tilde{J}_{ij} c_i^{\dagger} c_j + \sum_j \gamma_j c_j^{\dagger} c_j + \frac{U}{2} \sum_j c_j^{\dagger} c_j^{\dagger} c_j c_j , \qquad (6.65)$$

with the tunneling integral

$$\tilde{J}_{ij} = J - \gamma_{ij} \tag{6.66}$$

renormalized by the random variable (6.61).

To understand how substantial this change of the tunneling parameter could be, let us consider the stochastic average

$$\ll \gamma_i \gamma_j \gg = \int |w(\mathbf{r} - \mathbf{a}_i)|^2 R(\mathbf{r} - \mathbf{r}') |w(\mathbf{r} - \mathbf{a}_j)|^2 d\mathbf{r} d\mathbf{r}' .$$
 (6.67)

As is common, we may assume that the correlation length of the correlation function  $R(\mathbf{r})$  is short, such that

$$\left| \frac{\int r^2 R(\mathbf{r}) \, d\mathbf{r}}{\int R(\mathbf{r}) \, d\mathbf{r}} \right| \ll a^2$$

Then the white-noise approximation for the random potential is applicable. In that case, Eq. (6.67) reduces to

$$\ll \gamma_i \gamma_j \gg = R_0 \int |w(\mathbf{r} - \mathbf{a}_{ij})w(\mathbf{r})|^2 d\mathbf{r}$$
 (6.68)

Using the tight-binding approximation of Sec. 3.5, we have

$$\ll \gamma_i \gamma_j \gg = R_0 \left(\frac{m\omega_0}{2\pi}\right)^{3/2} \exp\left(-\frac{3a_{ij}^2}{2l_0^2}\right) ,$$
 (6.69)

where

$$\omega_0 = 2\sqrt{E_R V_0}$$
,  $l_0 \equiv \frac{1}{\sqrt{m\omega_0}}$ .

For the white-noise case,

$$\ll \gamma_{ij}\gamma_{ij} \gg = \ll \gamma_i\gamma_j \gg , \qquad (6.70)$$

therefore it is sufficient to consider the stochastic averages (6.68) and (6.69).

Taking the nearest neighbors for  $i \neq j$  in Eq. (6.69) and considering a cubic lattice gives

$$\ll \gamma_i \gamma_j \gg = \frac{R_0 k_0^3}{(2\pi)^{3/2}} \left(\frac{V_0}{E_R}\right)^{3/4} \exp\left(-\frac{3\pi^2}{2}\sqrt{\frac{V_0}{E_R}}\right).$$
 (6.71)

This is to be compared with the tunneling parameter J defined in Eq. (4.14). Using the latter yields

$$\frac{\ll \gamma_i \gamma_j \gg}{J^2} = \frac{\zeta}{136} \left(\frac{E_R}{V_0}\right)^{5/4} \exp\left(-\pi^2 \sqrt{\frac{V_0}{E_R}}\right) , \qquad (6.72)$$

where the relation

$$\frac{R_0}{a^3 E_R^2} = \frac{16}{7\pi^3} \,\zeta$$

is employed and

$$\zeta \equiv \frac{a}{l_L} \qquad \left( l_L \equiv \frac{4\pi}{7m^2R_0} \right) \tag{6.73}$$

being the disorder parameter.

From Eq. (6.72) it is seen that if the disorder is not extremely strong, then

$$\frac{\ll \gamma_i \gamma_j \gg}{J^2} \ll 1 , \qquad (\zeta \ll \zeta_{max}) , \qquad (6.74)$$

where

$$\zeta_{max} \equiv 136 \left(\frac{V_0}{E_R}\right)^{5/4} \exp\left(\pi^2 \sqrt{\frac{V_0}{E_R}}\right)$$

For deep lattices, when  $E_R \ll V_0$ ,  $\zeta_{max}$  is very large. Even for quite shallow lattices, one has

$$\zeta_{max} \gg 1 \qquad \left(\frac{E_R}{V_0} \ll 100\right)$$

If the disorder is so strong that  $\zeta > \zeta_{max}$ , then the lattice, as such, can be destroyed, and one would return to the uniform limit. Hence considering a lattice model is meaningful only for  $\zeta < \zeta_{max}$ . Under condition (6.74), the random part  $\gamma_{ij}$  in the renormalized tunneling integral (6.66) can be neglected, so that

$$\tilde{J}_{ij} \cong J \qquad (\zeta \ll \zeta_{max})$$

for  $i \neq j$  pertaining to the nearest neighbors.

In this way, for the realistic cases of optical lattices, Hamiltonian (6.65) simplifies to

$$\hat{H} = -J \sum_{\langle ij \rangle} c_i^{\dagger} c_j + \sum_j \gamma_j c_j^{\dagger} c_j + \frac{U}{2} \sum_j c_j^{\dagger} c_j^{\dagger} c_j c_j \,. \tag{6.75}$$

For treating the lattice with BEC, one has to break the gauge symmetry by means of the Bogolubov shift (6.13), replacing the operators  $c_j$  by  $\hat{c}_j$ .

## 6.4 Disordered Superfluid

To study the property of the superfluid state in a disordered lattice, we have to follow the standard prescriptions. In the Hubbard Hamiltonian (6.75), we make the Bogolubov shift (6.13) and then define the grand Hamiltonian (6.14). This yields

$$H = -J \sum_{\langle ij \rangle} \hat{c}_i^{\dagger} \hat{c}_j + \frac{U}{2} \sum_j \hat{c}_j^{\dagger} \hat{c}_j^{\dagger} \hat{c}_j \hat{c}_j + H_{ext} - \mu_0 N_0 - \mu_1 \hat{N}_1 , \qquad (6.76)$$

where  $\hat{N}_1$  is given in Eq. (4.22) and the term

$$H_{ext} \equiv \sum_{j} \gamma_j \hat{c}_j^{\dagger} \hat{c}_j \tag{6.77}$$

is due to the external random potential. The last term (6.77), with the Bogolubov shift (6.13), reads as

$$H_{ext} = \sum_{j} \gamma_j \left[ \nu n_0 + \sqrt{\nu n_0} \left( c_j^{\dagger} + c_j \right) + c_j^{\dagger} c_j \right] \,. \tag{6.78}$$

Expanding the random variable over the lattice, we have

$$\gamma_j = \frac{1}{\sqrt{N_L}} \sum_k \beta_k e^{i\mathbf{k}\cdot\mathbf{a}_j} , \qquad \beta_k = \frac{1}{\sqrt{N_L}} \sum_j \gamma_j e^{-i\mathbf{k}\cdot\mathbf{a}_j} . \tag{6.79}$$

Because of property (6.64),

$$\beta_k^* = \beta_{-k} \qquad (\gamma_j^* = \gamma_j) . \tag{6.80}$$

The relation of the variable  $\beta_k$  with  $\beta_{kp}$ , defined in Eq. (6.8), follows from the fact that  $\gamma_j \equiv \gamma_{jj}$ , hence

$$\gamma_j = \frac{1}{N_L} \sum_{kp} \beta_{kp} e^{i(\mathbf{k} - \mathbf{p}) \cdot \mathbf{a}_j}$$

Then Eqs. (6.79) give

$$\beta_k = \frac{1}{\sqrt{N_L}} \sum_p \beta_{k+p,p} \, .$$

The random variables  $\gamma_j$  enjoy the properties

$$\ll \gamma_j \gg = 0$$
,  $\ll \gamma_i \gamma_j \gg = R_{ij}$ , (6.81)

where the correlation function  $R_{ij}$  is given by Eq. (6.67). In the particular case of white noise, according to Eq. (6.68), one has

$$R_{ij} = R_0 \int |w(\mathbf{r} - \mathbf{a}_{ij})w(\mathbf{r})|^2 \, d\mathbf{r} \,. \tag{6.82}$$

For the tight-binding approximation, this reduces to Eq. (6.69).

The variables  $\beta_k$  have the properties

$$\ll \beta_k \gg = 0$$
,  $\ll \beta_k^* \beta_p \gg = \tilde{R}_{kp}$ , (6.83)

with

$$\tilde{R}_{kp} \equiv \frac{1}{N_L} \sum_{ij} R_{ij} e^{i\mathbf{k}\cdot\mathbf{a}_i - i\mathbf{p}\cdot\mathbf{a}_j} .$$
(6.84)

Considering the random Hamiltonian (6.78), we take into account that

$$\frac{1}{\sqrt{N_L}} \sum_j \gamma_j = \beta_0 , \qquad \sum_j \gamma_j c_j = \sum_k \beta_k^* a_k , \qquad \sum_j \gamma_j c_j^\dagger c_j = \frac{1}{\sqrt{N_L}} \sum_{kp} \beta_{k-p} a_k^\dagger a_p .$$

Thence Eq. (6.78) takes the form

$$H_{ext} = \nu n_0 \beta_0 \sqrt{N_L} + \sqrt{\nu n_0} \sum_k \left( a_k^{\dagger} \beta_k + \beta_k^* a_k \right) + \frac{1}{\sqrt{N_L}} \sum_{kp} \beta_{k-p} a_k^{\dagger} a_p .$$
(6.85)

Following the same procedure as in Sec. 6.2, we can employ the stochastic mean-field approximation, simplifying the last term in Eq. (6.85) as

$$a_k^{\dagger} a_p \beta_{k-p} = \left( a_k^{\dagger} \alpha_p + \alpha_k^* a_p - \alpha_k^* \alpha_p \right) \beta_{k-p} , \qquad (6.86)$$

which is analogous to Eq. (6.39), and where

$$\alpha_k \equiv \langle a_k \rangle_H , \qquad \ll \alpha_k \gg = \langle a_k \rangle = 0 .$$
(6.87)

For the third- and fourth-order terms, with respect to the operators  $a_k$ , the HFB approximation can be used.

Minimizing the grand potential (6.15) over  $N_0$  defines

$$\mu_0 = -z_0 J + \nu U (1 + n_1 + \sigma) + \mu_G , \qquad (6.88)$$

where the additional term

$$\mu_G \equiv \frac{1}{2\sqrt{\nu n_0} N_L} \sum_k \ll \alpha_k^* \beta_k + \beta_k^* \alpha_k \gg$$
(6.89)

is due to the presence of the random potential.

Similarly to Eq. (6.45), we introduce a random variable  $\varphi_k$  satisfying the Fredholm equation

$$\varphi_k = \sqrt{\nu n_0} \,\beta_k + \frac{1}{\sqrt{N_L}} \,\sum_p \alpha_p \beta_{k-p} \,. \tag{6.90}$$

With this variable, Hamiltonian (6.85) transforms into

$$H_{ext} = \sqrt{N_0} \varphi_0 + \sum_k \left( a_k^{\dagger} \varphi_k + \varphi_k^* a_k - \alpha_k^* \varphi_k \right) .$$
 (6.91)

Owing to properties (6.80), the random variable  $\varphi_k$  satisfies the conditions

$$\varphi_k^* = \varphi_{-k} , \qquad \varphi_0^* = \varphi_0 . \tag{6.92}$$

The variable  $\varphi_0$ , according to Eq. (6.90), obeys the equation

$$\varphi_0 = \sqrt{\nu n_0} \beta_0 + \frac{1}{\sqrt{N_L}} \sum_p \alpha_p^* \beta_p . \qquad (6.93)$$

Using the latter reduces Eq. (6.89) to the form

$$\mu_G = \frac{\ll \varphi_0 \gg}{\sqrt{N_0}} . \tag{6.94}$$

Since

$$\ll \varphi_k \gg = 0 \qquad (\ll \alpha_k \gg = 0) ,$$
 (6.95)

one gets

$$\mu_G = 0 . (6.96)$$

Keeping in mind a cubic lattice, for which

$$\sum_{\langle ij\rangle} c_i^{\dagger} c_j = 2 \sum_k \sum_{\alpha} \cos(k_{\alpha} a) a_k^{\dagger} a_k \,,$$

let us define the quantities

$$\omega_k \equiv -2J \sum_{\alpha} \cos(k_{\alpha} a) + 2\nu U - \mu_1 \tag{6.97}$$

and

$$\Delta \equiv \nu (n_0 + \sigma) U . \tag{6.98}$$

Then the grand Hamiltonian (6.76) transforms into

$$H = E_{HFB} + \sum_{k} \omega_{k} a_{k}^{\dagger} a_{k} + \frac{1}{2} \sum_{k} \Delta \left( a_{k}^{\dagger} a_{-k}^{\dagger} + a_{-k} a_{k} \right) + H_{ext} , \qquad (6.99)$$

where the random part is given by Eq. (6.91) and the first term is

$$E_{HFB} = -z_0 J n_0 N + \frac{U}{2} \nu n_0^2 N - \mu_0 n_0 N - \frac{U}{2} \left( 2n_1^2 + \sigma^2 \right) N ,$$

in which

$$n_1 = \frac{1}{N} \sum_k n_k , \qquad \sigma = \frac{1}{N} \sum_k \sigma_k .$$

To diagonalize Hamiltonian (6.99), we employ the nonuniform nonlinear transformation (6.40), for which we find

$$u_k^2 = \frac{\omega_k + \varepsilon_k}{2\varepsilon_k}$$
,  $v_k^2 = \frac{\omega_k - \varepsilon_k}{2\varepsilon_k}$ ,  $w_k = -\frac{1}{\omega_k + \Delta}$ 

Here  $\omega_k$  and  $\Delta$  are defined in Eqs. (6.97) and (6.98) and the Bogolubov spectrum is

$$\varepsilon_k = \sqrt{\omega_k^2 - \Delta^2} . \tag{6.100}$$

As in Sec. 4.3, the Lagrange multiplier  $\mu_1$  is defined by the condensation condition (4.53), which yields

$$\mu_1 = -z_0 J + \nu U(1 + n_1 - \sigma) . \qquad (6.101)$$

Substituting the latter into Eq. (6.97) gives

$$\omega_k = \Delta + 4J \sum_{\alpha} \sin^2\left(\frac{k_{\alpha}a}{2}\right) , \qquad (6.102)$$

where a cubic lattice is assumed.

The diagonalized form of Hamiltonian (6.99) is

$$H = E_B + \sum_k \varepsilon_k b_k^{\dagger} b_k + H_{\varphi} , \qquad (6.103)$$

in which  $E_B$  is the same as in Eq. (4.51), but Hamiltonian (6.103) differs from Eq. (4.50) by the random term

$$H_{\varphi} = \varphi_0 \sqrt{N_0} - \sum_k \left( \alpha_k^* + \frac{\varphi_k^*}{\omega_k + \Delta} \right) \varphi_k .$$
 (6.104)

Since the quantum averaging with Hamiltonian (6.103) gives

$$\langle b_k \rangle_H = \langle b_k b_p \rangle_H = 0 ,$$

from transformation (6.40), we have

$$\alpha_k = -\frac{\varphi_k}{\omega_k + \Delta} \,. \tag{6.105}$$

Using this reduces the random part (6.104) to the simple form

$$H_{\varphi} = \varphi_0 \sqrt{N_0} . \tag{6.106}$$

We may notice that because of condition (6.95),

$$\langle H_{\varphi} \rangle = \ll H_{\varphi} \gg = 0.$$
 (6.107)

For the normal and anomalous averages

$$n_k \equiv \langle a_k^{\dagger} a_k \rangle \,, \qquad \sigma_k \equiv \langle a_k a_{-k} \rangle \,,$$

we find

$$n_k = n_k^N + \ll |\alpha_k|^2 \gg , \qquad \sigma_k = \sigma_k^N + \ll |\alpha_k|^2 \gg , \qquad (6.108)$$

where

$$n_k^N = \frac{\omega_k}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) - \frac{1}{2} , \qquad \sigma_k^N = -\frac{\Delta}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) . \tag{6.109}$$

According to Eq. (6.105),

$$\ll |\alpha_k|^2 \gg = \frac{\ll |\varphi_k|^2 \gg}{(\omega_k + \Delta)^2} \,. \tag{6.110}$$

The fraction of uncondensed atoms is the sum

$$n_1 = n_N + n_G , (6.111)$$

in which the first term

$$n_N = \frac{1}{\rho} \int_{\mathcal{B}} n_k^N \frac{d\mathbf{k}}{(2\pi)^d} \tag{6.112}$$

is due to finite interactions and temperature, while the second term

$$n_G = \frac{1}{\rho} \int_{\mathcal{B}} \frac{\ll |\varphi_k|^2 \gg d\mathbf{k}}{(\omega_k + \Delta)^2} \frac{d\mathbf{k}}{(2\pi)^d}$$
(6.113)

is caused by the random potential.

The anomalous average (6.28) becomes

$$\sigma = \sigma_N + n_G , \qquad (6.114)$$

where

$$\sigma_N = \frac{1}{\rho} \int_{\mathcal{B}} \sigma_k^N \frac{d\mathbf{k}}{(2\pi)^d} , \qquad (6.115)$$

and  $n_G$  is given by Eq. (6.113).

To find the superfluid fraction, we follow the discussion of Sec. 4.5. For the dissipated heat (4.109), we get

$$Q = Q_N + Q_G , \qquad (6.116)$$

similarly to Eq. (6.58). Keeping in mind a *d*-dimensional cubic lattice and envoking the same approximations as is Sec. 4.5, we obtain

$$Q_N = \frac{1}{8m\rho} \int_{\mathcal{B}} \frac{q_k^2}{\sinh^2(\varepsilon_k/2T)} \frac{d\mathbf{k}}{(2\pi)^d}$$
(6.117)

and

$$Q_G = \frac{1}{2m\rho} \int_{\mathcal{B}} \frac{q_k^2 \ll |\varphi_k|^2 \gg}{\varepsilon_k(\omega_k + \Delta)} \coth\left(\frac{\varepsilon_k}{2T}\right) \frac{d\mathbf{k}}{(2\pi)^d} \,. \tag{6.118}$$

Here

$$q_k^2 \equiv \left(\frac{m}{m^*}\right)^2 \frac{1}{a^2} \sum_{\alpha=1}^d \sin^2(k_\alpha a) ,$$

with  $m^* \equiv 1/2Ja^2$ . In the long-wave limit,  $q_k^2$  behaves as

$$q_k^2 \simeq \left(\frac{m}{m^*}\right)^2 k^2 \qquad (k \to 0)$$

To realize actual calculations, one has to solve Eq. (6.90), which, taking account of relation (6.105), acquires the form

$$\varphi_k = \sqrt{\nu n_0} \beta_k - \frac{1}{\sqrt{N_L}} \sum_p \frac{\beta_{k-p} \varphi_p}{\omega_p + \Delta}.$$
(6.119)

The solution of Eq. (6.119) can be accomplished following the way of Ref. [367].

The superfluid fraction can be calculated using either definition (4.108) or Eq. (4.120). The condensate fraction is defined by the normalization condition  $n_0 + n_1 = 1$ , which in view of Eq. (6.111), reads as

$$n_0 + n_N + n_G = 1 . (6.120)$$

The approximations, involved in the present section, describe well the superfluid state of disordered optical lattices. However, with increasing interactions and the strength of disorder, the system can undergo phase transitions into an insulating or Bose-glass phases. The description of the latter phases requires the use of other approximations or numerical calculations.

### 6.5 Phase Diagram

The influence of disorder on the boson Hubbard model has been studied for lattices of different dimensionalities and in several approaches. Scaling arguments [378–381] and renormalization group techniques [382–387] were used [306,388,389]. There have been employed numerical calculations for small ( $4 \le N \le 25$ ) systems [390], strong-coupling expansions [298], density matrix renormalization group [391], mean-field single-site approximation [392–394], and Monte Carlo simulations [395–404].

The general physical properties of disordered boson lattices have been described by Fisher et al. [306]. Depending on the system parameters, several states can be realized. There exists the usual superfluid coherent phase, where  $n_s > 0$  and  $n_0 > 0$ . This phase possesses a finite compressibility and has no gap in the spectrum of collective excitations. The Mott insulating phase can occur at zero temperature and integer filling. This phase has zero compressibility and a gap for particle-hole excitations. The superfluid-Mott insulator phase transition is a second-order transition being in the universality class of the (d+1)-dimensional XY model. When an additional trapping potential is imposed on the lattice, the phase transition point could be slightly shifted [405].

Except these two phases that also exist in regular optical lattices, for disordered lattices, there can arise a novel phase called the Bose glass [306]. This third phase, due to the presence of disorder, is insulating because of the localization effects of the randomness, it is characterized by a finite compressibility and no gap in the spectrum. The Bose glass exhibits no superfluidity ( $n_s = 0$ ), but possesses local remnants of BEC ( $n_0 > 0$ ). Such a Bose-glass phase can also develop in a quasiperiodic bichromatic lattice [406].

At nonzero temperature and noninteger filling, there can be no Mott insulator, but localized and delocalized atoms coexist. The itinerant component can be either superfluid or normal. To realize pure phases, one usually considers the zero-temperature and integerfilling case. The lattice disorder is commonly introduced as a random term in the Hubbard model (6.75), with a site dependent, uniformly distributed, on-site potential,  $-D < \gamma_j < D$ , so that the related stochastic distribution is

$$p(\gamma_j) = \begin{cases} \frac{1}{2D}, & |\gamma_j| < D\\ 0, & |\gamma_j| > D \end{cases}$$

The most often discussed phase diagram concerns the case of zero temperature and integer filling, when the pure Mott insulating phase can exist. The disorder is introduced through a uniformly distributed on-site potential, as is explained above. It is generally accepted that when increasing disorder, the Mott insulating phase transforms, through a first-order phase transition, into the Bose glass phase. While increasing the tunneling parameter yields the superfluid phase with BEC. Under sufficiently strong disorder, the Bose glass transforms into superfluid through a second-order transition, provided the uniformly distributed disorder is bounded by a finite D.

There exist, however, a controversy with regard to the transformation of the Mott insulator into superfluid. Fisher et al. [306] argued that, in the presence of any finite disorder, the transition from the Mott insulator to superfluid occurs only through the intermediate Bose-glass phase. This picture has been supported by several numerical calculations
[298,391,399,401]. The corresponding quantitative phase diagram is shown in Fig. 1. Precise numerical values depend on the lattice dimensionality and can be found in the cited references.



Figure 1: Possible qualitative phase portrait for a disordered lattice with an integer filling factor at zero temperature.

Other researches claim that there are two different regimes in a disordered boson Hubbard model. For weak disorder, the Mott insulating phase is sustained up to the *direct* transition into a superfluid. Strong disorder changes the nature of the transition to that of the Bose glass to superfluid transition. Thus, contrary to the above cited works, it is stated that at weak disorder the direct Mott insulator to superfluid phase transition does occur, without an intervening Bose glass phase. This picture is also based on several numerical investigations [389,393,396,398,400,402,403]. The related qualitative phase diagram is presented in Fig. 2.



Figure 2: Possible qualitative phase diagram for a disordered lattice with an integer filling factor at zero temperature.

# 7 Nonstandard Lattice Models

#### 7.1 Coexisting States

For noncommensurate filling, a mixture of localized and delocalized atoms exists in the lattice [407] at all temperatures, including zero. Such a mixture of coexisting localized and delocalized states occurs at finite temperatures for any filling, including integer. Finally, there are indications [408] that, even at zero temperature and integer filling, close to the boundary between the superfluid and Mott insulating phases, there can arise an itinerant-localized dual structure, where the localized and itinerant states coexist.

The coexistence of two different states could be described phenomenologically, involving the Ginzburg-Landau functional [409] generalized to the mixture of several states [54]. But, of course, it is more important to have a microscopic model characterizing such a coexistence of delocalized and localized atoms.

Let us assume that a superfluid state coexists with a portion of localized atoms. Then, in addition to the Bogolubov shifted field operator  $\eta(\mathbf{r}) + \psi_1(\mathbf{r})$ , there exists the field operator  $\psi_2(\mathbf{r})$ , so that  $\eta(\mathbf{r})$  is the condensate wave function,  $\psi_1(\mathbf{r})$  is the field operator of uncondensed delocalized atoms, and  $\psi_2(\mathbf{r})$  is the field operator of uncondensed localized atoms. Each of these operators can be expanded over Wannier functions,

$$\eta(\mathbf{r}) = \sqrt{\nu n_0} \sum_j w_0(\mathbf{r} - \mathbf{a}_j) , \qquad \psi_1(\mathbf{r}) = \sum_j c_j w(\mathbf{r} - \mathbf{a}_j) ,$$
$$\psi_2(\mathbf{r}) = \sum_j b_j w(\mathbf{r} - \mathbf{a}_j) .$$
(7.1)

The field operators of delocalized and localized atoms commute with each other,

$$[\psi_1(\mathbf{r}), \psi_2(\mathbf{r}')] = [\psi_1(\mathbf{r}), \psi_2^{\dagger}(\mathbf{r}')] = 0 , \qquad [c_i, b_j] = [c_i, b_j^{\dagger}] = 0 .$$
(7.2)

The Bose commutation relations are valid for each type of the field operators.

Thus, the starting point is the assumption of the existence of two types of atoms differing from each other by their localization property. The delocalized atoms are characterized by an operator  $c_j$ , while the localized atoms, by  $b_j$ . This is somewhat close to the consideration of a two-component system [288]. Another analogy is the picture of a crystal where a portion of atoms are localized, while a part of atoms can jump between lattice sites [220,410]. Probably, the most direct interpretation of the existence of two types of atoms is the consideration of the multiband Hamiltonian (4.11), in which two bands are taken into account. One band is the conducting band, whose atoms are itinerant, being characterized by the field operator  $\hat{c}_j$ . Another band is that of bound states, with localized atoms described by an operator  $b_j$ .

The localized atoms of bound states are considered as normal, such that

$$\langle b_j \rangle = 0$$
. (7.3)

This requires [57] that the related Hamiltonian be invariant under the global gauge transformation  $b_j \to b_j e^{i\alpha}$ , with a real  $\alpha$ . So, the two-band Hubabrd Hamiltonian can be written down as

$$\hat{H} = -\sum_{\langle ij \rangle} \left( J \hat{c}_i^{\dagger} \hat{c}_j + J_2 b_i^{\dagger} b_j \right) + \sum_j \left( \frac{U}{2} \, \hat{c}_j^{\dagger} \hat{c}_j^{\dagger} \hat{c}_j \hat{c}_j \hat{c}_j + U_1 \hat{c}_j^{\dagger} \hat{c}_j b_j^{\dagger} b_j + \frac{U_2}{2} \, b_j^{\dagger} b_j^{\dagger} b_j b_j \right) \,.$$
(7.4)

A correct introduction of different degrees of freedom has to be such that to exclude the double counting [411]. This requires that the field operators of different types be orthogonal to each other,

$$\int \eta^*(\mathbf{r})\psi_1(\mathbf{r}) \, d\mathbf{r} = 0 , \qquad \int \eta^*(\mathbf{r})\psi_2(\mathbf{r}) \, d\mathbf{r} = 0 , \qquad \int \psi_1^{\dagger}(\mathbf{r})\psi_2(\mathbf{r}) \, d\mathbf{r} = 0 .$$
(7.5)

With expansions (7.1), this yields

$$\sum_{j} c_{j} = 0 , \qquad \sum_{j} b_{j} = 0 , \qquad \sum_{j} c_{j}^{\dagger} b_{j} = 0 ,$$
$$\sum_{j} \hat{c}_{j}^{\dagger} b_{j} = 0 , \qquad (\hat{c}_{j} \equiv \sqrt{\nu n_{0}} + c_{j}) .$$
(7.6)

To distinguish the bound states of localized atoms from the conducting-band states of nonlocalized atoms, it is necessary to impose the *localization condition* 

$$b_i^{\dagger} b_j = \delta_{ij} b_j^{\dagger} b_j . \tag{7.7}$$

This removes the second tunneling term in Eq. (7.4). In other respects, the atoms can be treated as similar, possessing the same interaction parameter  $U = U_1 = U_2$ .

Then the two-band Hamiltonian (7.4), describing the conducting and bound-state bands, takes the form

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{c}_{i}^{\dagger} \hat{c}_{j} + \frac{U}{2} \sum_{j} \left( \hat{c}_{j}^{\dagger} \hat{c}_{j}^{\dagger} \hat{c}_{j} \hat{c}_{j} + 2 \hat{c}_{j}^{\dagger} \hat{c}_{j} b_{j}^{\dagger} b_{j} + b_{j}^{\dagger} b_{j}^{\dagger} b_{j} b_{j} \right) .$$
(7.8)

For the conducting-band operators, the Bogolubov shift (6.13) is assumed in order to take into account the possible appearance of BEC.

The delocalized atoms can include a Bose-condensed fraction and a part of uncondensed atoms, while all localized atoms, by their definition, are not condensed. The operators of uncondensed atoms are

$$\hat{N}_1 = \sum_j c_j^{\dagger} c_j , \qquad \hat{N}_2 = \sum_j b_j^{\dagger} b_j .$$
 (7.9)

For the corresponding numbers of particles, we have

$$N_{0} = \nu n_{0} N_{L} , \qquad N_{1} = \sum_{j} \langle c_{j}^{\dagger} c_{j} \rangle ,$$
$$N_{2} = \sum_{j} \langle b_{j}^{\dagger} b_{j} \rangle , \qquad N_{0} + N_{1} = \sum_{j} \langle \hat{c}_{j}^{\dagger} \hat{c}_{j} \rangle .$$
(7.10)

The related atomic fractions are defined as

$$n_0 \equiv \frac{N_0}{N}$$
,  $n_1 \equiv \frac{N_1}{N}$ ,  $n_2 \equiv \frac{N_2}{N}$ , (7.11)

with the normalization condition

$$n_0 + n_1 + n_2 = 1 . (7.12)$$

For an ideal lattice, Eqs. (7.10) give

$$\langle c_j^{\dagger} c_j \rangle = \nu n_1 , \qquad \langle b_j^{\dagger} b_j \rangle = \nu n_2 , \qquad \langle \hat{c}_j^{\dagger} \hat{c}_j \rangle = \nu (n_0 + n_1) .$$
 (7.13)

Anomalous averages can exist for delocalized atoms, while the former are absent for localized bound-state atoms,

$$\langle c_j c_j \rangle \equiv \nu \sigma$$
,  $\langle b_j b_j \rangle \equiv 0$ . (7.14)

The grand Hamiltonian for the system is

 $2\pi$ 

$$H = \hat{H} - \mu_0 N_0 - \mu_1 \hat{N}_1 - \mu_2 \hat{N}_2 . \qquad (7.15)$$

The grand potential and free energy are

$$\Omega = -T \ln \operatorname{Tr} e^{-\beta H}, \qquad F = \Omega + \mu N, \qquad (7.16)$$

where  $\mu$  is the system chemical potential. The latter is defined as

$$\mu = \frac{\partial F}{\partial N} = \frac{\partial F}{\partial N_0} \frac{\partial N_0}{\partial N} + \frac{\partial F}{\partial N_1} \frac{\partial N_1}{\partial N} + \frac{\partial F}{\partial N_2} \frac{\partial N_2}{\partial N}$$

Under relations

$$\begin{aligned} \frac{\partial F}{\partial N_0} &= \mu_0 , \qquad \frac{\partial F}{\partial N_1} = \mu_1 , \qquad \frac{\partial F}{\partial N_2} = \mu_2 , \\ \frac{\partial N_0}{\partial N} &= n_0 , \qquad \frac{\partial N_1}{\partial N} = n_1 , \qquad \frac{\partial N_2}{\partial N} = n_2 , \end{aligned}$$

we get

$$\mu = \mu_0 n_0 + \mu_1 n_1 + \mu_2 n_2 . \tag{7.17}$$

The Lagrange multiplier  $\mu_0$  is defined by the minimization of the grand thermodynamical potential  $\Omega$  with respect to the number of condensed atoms  $N_0$ , under the fixed numbers of atoms  $N_1$  and  $N_2$ . The multiplier  $\mu_1$  is defined from the condition of the BEC existence, as is explained in Sec. 2.9, and which is equivalent to the condition of the gapless spectrum. But what defines  $\mu_2$ ? The latter could be found if the number  $N_2$  of localized atoms would be fixed. This, however, is not the case, since only the total number N can be fixed.

The Lagrange multiplier  $\mu_2$  can be found from the condition that the system is in stable equilibrium, when  $\delta F = 0$ , with the variation over the numbers of atoms, so that

$$\frac{\partial F}{\partial N_0} \,\delta N_0 + \frac{\partial F}{\partial N_1} \,\delta N_1 + \frac{\partial F}{\partial N_2} \,\delta N_2 = 0 \,. \tag{7.18}$$

Using the relation  $N_2 = N - N_0 - N_1$ , one has

$$\delta N_2 = -\delta N_0 - \delta N_1 \; .$$

And Eq. (7.18) gives

$$(\mu_0 - \mu_2)\delta N_0 + (\mu_1 - \mu_2)\delta N_1 = 0$$

or, equivalently,

$$[(\mu_0 - \mu_2)n_0 + (\mu_1 - \mu_2)n_1]\delta N = 0$$

This is valid for an arbitrary variation of N, hence

$$(\mu_0 - \mu_2)n_0 + (\mu_1 - \mu_2)n_1 = 0$$

From here

$$\mu_2 = \frac{\mu_0 n_0 + \mu_1 n_1}{n_0 + n_1} \,. \tag{7.19}$$

Substituting the latter into Eq. (7.17) yields

$$\mu = \mu_2 = \frac{\mu_0 n_0 + \mu_1 n_1}{n_0 + n_1} . \tag{7.20}$$

When there exist only delocalized atoms, hence  $N_2 = 0$  and  $n_0 + n_1 = 1$ , Eq. (7.20) acquires the standard form (2.111).

Hamiltonian (7.8) consists of the parts corresponding to the atoms of the conducting band, the atoms of the bound-state band, and contains the term

$$\hat{H}_{int} \equiv U \sum_{j} \hat{c}_{j}^{\dagger} \hat{c}_{j} b_{j}^{\dagger} b_{j}$$
(7.21)

associated with the interband atomic interaction. With the operator  $\hat{c}_j$ , given in Eq. (7.6), we have

$$\hat{c}_j^{\dagger}\hat{c}_jb_j^{\dagger}b_j = \nu n_0 b_j^{\dagger}b_j + \sqrt{\nu n_0} \left(c_j^{\dagger} + c_j\right)b_j^{\dagger}b_j + c_j^{\dagger}c_jb_j^{\dagger}b_j \ .$$

The operators of the different types can be decoupled as follows:

$$c_{j}^{\dagger}b_{j}^{\dagger}b_{j} = \langle c_{j}^{\dagger} \rangle b_{j}^{\dagger}b_{j} + c_{j}^{\dagger} \langle b_{j}^{\dagger}b_{j} \rangle - \langle c_{j}^{\dagger} \rangle \langle b_{j}^{\dagger}b_{j} \rangle ,$$
  

$$c_{j}^{\dagger}c_{j}b_{j}^{\dagger}b_{j} = c_{j}^{\dagger}c_{j} \langle b_{j}^{\dagger}b_{j} \rangle + \langle c_{j}^{\dagger}c_{j} \rangle b_{j}^{\dagger}b_{j} - \langle c_{j}^{\dagger}c_{j} \rangle \langle b_{j}^{\dagger}b_{j} \rangle .$$
(7.22)

Since  $\langle c_j \rangle = 0$  and because of conditions (7.6) one gets

$$\sum_j c_j^{\dagger} b_j^{\dagger} b_j = \nu n_2 \sum_j c_j^{\dagger} = 0 \; .$$

The interaction term (7.21) transforms into

$$\hat{H}_{int} = \nu U \sum_{j} \left[ n_2 c_j^{\dagger} c_j + (n_0 + n_1) b_j^{\dagger} b_j \right] - \nu n_1 n_2 U N .$$
(7.23)

The grand Hamiltonian (7.15) reduces to the sum

$$H = H_{del} + H_{loc} - \nu U n_1 n_2 N , \qquad (7.24)$$

in which the first term describes delocalized atoms, while the second, localized atoms. The Hamiltonian of delocalized atoms reads as

$$H_{del} = \sum_{n=0}^{4} H^{(n)} . (7.25)$$

The zero- and the second-order terms are

$$H^{(0)} = \left(-z_0 J + \frac{U}{2} \nu n_0 - \mu_0\right) n_0 N ,$$
  
$$H^{(2)} = -J \sum_{\langle ij \rangle} c_i^{\dagger} c_j + (2\nu U n_0 + \nu U n_2 - \mu_1) \sum_j c_j^{\dagger} c_j + \frac{U}{2} \nu n_0 \sum_j \left(c_j^{\dagger} c_j^{\dagger} + c_j c_j\right) .$$
(7.26)

The first-order term is zero, because of conditions (7.6), that is,  $H^{(1)} = 0$ . The third- and fourth-order terms are

$$H^{(3)} = \sqrt{\nu n_0} U \sum_j \left( c_j^{\dagger} c_j^{\dagger} c_j + c_j^{\dagger} c_j c_j \right)$$
(7.27)

and, respectively,

$$H^{(4)} = \frac{U}{2} \sum_{j} c_{j}^{\dagger} c_{j}^{\dagger} c_{j} c_{j} c_{j} . \qquad (7.28)$$

The term in Eq. (7.24), describing the localized atoms, can be written as

$$H_{loc} = \sum_{j} H_j , \qquad (7.29)$$

where

$$H_j = \frac{U}{2} b_j^{\dagger} b_j \left( b_j^{\dagger} b_j - 1 \right) + \left[ \nu U(n_0 + n_1) - \mu b_j^{\dagger} b_j \right].$$
(7.30)

The Hamiltonian (7.25) of delocalized atoms can be treated in the HFB approximation, as is done in Secs. 4.2 and 4.3. Following the same procedure, and minimizing the grand potential over  $N_0$ , we get

$$\mu_0 = -z_0 J + \nu U(n_0 + 2n_1 + \sigma) . \tag{7.31}$$

Introducing the notation

$$\omega_k \equiv -2J \sum_{\alpha} \cos(k_{\alpha} a) + \nu U(1 + n_0 + n_1) - \mu_1 , \qquad \Delta \equiv \nu U(n_0 + \sigma) , \qquad (7.32)$$

we keep in mind a cubic lattice and use the relation

$$2(n_0 + n_1) + n_2 = 1 + n_0 + n_1 .$$

The condition (4.53) of condensate existence can be represented as

$$\lim_{k \to 0} (\omega_k - \Delta) = 0.$$
(7.33)

The latter yields

$$\mu_1 = -z_0 J + \nu U (1 + n_1 - \sigma) . \tag{7.34}$$

In this way, we obtain the same forms of the expressions as in Eq. (4.55), of the spectrum (4.52), and of Eq. (4.59) and (4.60) defining the momentum distribution  $n_k$  and the anomalous average  $\sigma_k$ , respectively.

The subsystem of localized atoms, with Hamiltonian (7.29) can be considered as in Sec. 4.7. The eigenvalues of the single-site Hamiltonian (7.30) are

$$e_n = \frac{U}{2} n^2 \left[ \nu U(n_0 + n_1) - \frac{U}{2} - \mu \right] n , \qquad (7.35)$$

where n = 0, 1, 2, ... Minimizing  $e_n$  with respect to n gives the effective number

$$n_{eff} = \frac{2\mu + U[1 - 2\nu(n_0 + n_1)]}{2U} .$$
(7.36)

Since  $\langle b_j^{\dagger} b_j \rangle = \nu n_2$ , for an ideal lattice, we have

$$\nu n_2 = \frac{\operatorname{Tr} \hat{n}_j e^{-\beta H_j}}{\operatorname{Tr} e^{-\beta H_j}} \,. \tag{7.37}$$

At low temperature, this gives

$$\nu n_2 \simeq n_{eff} \qquad (T \ll U) . \tag{7.38}$$

Hence,

$$n_2 \simeq \frac{2\mu + U[1 - 2\nu(n_0 + n_1)]}{2\nu U} \,. \tag{7.39}$$

In view of the normalization condition (7.12), the chemical potential, following from Eq. (7.39), becomes

$$\mu \simeq (2\nu - 1) \frac{U}{2} \qquad (T \ll U) .$$
 (7.40)

At the same time, from Eqs. (7.20), (7.31), and (7.34), we have

$$\mu = -z_0 J + \nu U \left[ n_0 + n_1 + \sigma + \frac{(1 - 2\sigma)n_1}{n_0 + n_1} \right] .$$
(7.41)

Expressions (7.40) and (7.41) give the equality

$$\left[\left(\nu - \frac{1}{2}\right)U + z_0 J\right](1 - n_2) = \nu U\left[(1 - n_2 + \sigma)(1 - n_2) + n_1(1 - 2\sigma)\right]$$
(7.42)

connecting  $n_2$  with  $n_1$  and  $\sigma$ . The latter are defined in Eqs. (4.61) and (4.62), respectively.

The single-particle spectrum (7.35), with the chemical potential (7.40), reads as

$$e_n = nU\left(\frac{n}{2} - \nu n_2\right) . \tag{7.43}$$

The effective energy level is

$$e_{eff} \equiv \lim_{n \to n_{eff}} e_n = -\frac{U}{2} (\nu n_2)^2 .$$
 (7.44)

When delocalized atoms coexist with localized ones, there are two types of spectra. The spectrum of collective excitations, caused by the delocalized atoms, is given by the Bogolubov

form (4.52). The spectrum is gapless, displaying in the long-wave limit the asymptotic behavior  $\varepsilon_k \simeq ck$ , as in Eq. (4.57), with the sound velocity

$$c = \sqrt{2Ja^2\Delta} = \sqrt{\frac{\Delta}{m^*}} , \qquad (7.45)$$

according to Eq. (4.58) and the notation  $m^* = 1/2Ja^2$  for the effective mass. At the same time, there exists the single-particle spectrum (7.43) possessing the gap  $\Delta e_n = U$ , which is defined as in Eq. (4.156). Both these spectra can be experimentally observed. The spectrum of collective excitations describes density fluctuations due to delocalized atoms in the conducting band. And the single-particle spectrum describes discrete energy levels of localized atoms in the bound-state band. The energy gap in the single-particle spectrum characterizes the quantity of energy that is necessary for transferring an atom from the bound-state band to the conducting band.

# 7.2 Vibrational Excitations

In the extended Hubbard model (5.16), one considers atomic interactions between different lattice sites. Such intersite interactions can become important when atoms interact through long-range forces, for instance, through dipolar interactions [315,316,412]. Then one should consider the extended Hubbard model, which has been treated in a number of papers [317–322].

It is worth noting that for short-range interactions, the intersite forces can also be rather strong, when the effective scattering length becomes very large due to Feshnach resonance [10,24] or to geometric resonances in waveguides [413,414]. But, anyway, the intersite interactions are much smaller than the on-site interactions. Thus, for a three-dimensional cubic lattice in the tight-binding approximation, as follows from Secs. 3.5. and 3.9, we have the on-site interaction

$$U = \frac{\Phi_0}{(2\pi)^{3/2} l_0^3}$$

with the localization length

$$l_0 = \frac{1}{\sqrt{m\omega_0}} = \frac{a}{\pi} \left(\frac{E_R}{V_0}\right)^{1/4} \,.$$

While for the nearest-neighbor interactions, we get

$$U_{ij} = U \exp\left(-\frac{3a^2}{2l_0^2}\right) \,.$$

For well-localized atoms, for which  $l_0 \ll a$ , one has  $|U_{ij}/U| \ll 1$ . So that the intersite interactions are negligible as compared to the on-site interactions. These short-range interactions could be comparable only for very shallow lattices, for which, however, the Hubbard model as such would be not a good approximation to reality. But for long-range interactions, the extended Hubbard model is well justified.

As soon as there are atomic interactions between different sites, there appear collective vibrational excitations, that is, phonons. Their introduction into the extended Hubbard model can be done similarly to the quantization of collective coordinates for extended quantum systems [415,416].

In the Hubbard model (5.16), there is the single-site term containing the quantity  $h_j$ , defined in Eq. (4.8), which for a single-band model becomes

$$h_j \equiv \int w^*(\mathbf{r} - \mathbf{a}_j) \left[ -\frac{\nabla^2}{2m} + V_L(\mathbf{r}) \right] w(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r} \,. \tag{7.46}$$

Let us introduce the notation

$$\mathbf{p}_j^2 \equiv \int w^* (\mathbf{r} - \mathbf{a}_j) (-\nabla^2) w(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r} \,. \tag{7.47}$$

Then Eq. (7.46) writes as

$$h_j = \frac{\mathbf{p}_j^2}{2m} + \int w^*(\mathbf{r}) V_L(\mathbf{r}) w(\mathbf{r}) \, d\mathbf{r} \,. \tag{7.48}$$

The second term in Eq. (7.48) is a constant and can be omitted. The extended Hubbard model takes the form

$$\hat{H} = -J \sum_{\langle ij \rangle} c_i^{\dagger} c_j + \sum_j \frac{\mathbf{p}_j^2}{2m} c_j^{\dagger} c_j + \frac{U}{2} \sum_j c_j^{\dagger} c_j^{\dagger} c_j c_j c_j + \frac{1}{2} \sum_{i \neq j} U_{ij} c_i^{\dagger} c_j^{\dagger} c_j c_i .$$
(7.49)

Accomplishing the quantization of collective variables assumes that the quantities  $\mathbf{p}_j$  and  $U_{ij}$  become operators, so that

$$\mathbf{p}_j \to \hat{\mathbf{p}}_j, \qquad U_{ij} \to \hat{U}_{ij}, \qquad (7.50)$$

where

$$\hat{U}_{ij} \equiv U(\hat{\mathbf{r}}_{ij}) \qquad (\hat{\mathbf{r}}_{ij} \equiv \hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j) . \tag{7.51}$$

The coordinate operator

$$\hat{\mathbf{r}}_j = \mathbf{a}_j + \hat{\mathbf{u}}_j \tag{7.52}$$

is such that

$$\langle \hat{\mathbf{r}}_j \rangle = \mathbf{a}_j , \qquad (7.53)$$

hence

$$\langle \hat{\mathbf{u}}_j \rangle = 0$$
 . (7.54)

The operator  $\hat{\mathbf{u}}_j$  describes the deviation from the average equilibrium position  $\mathbf{a}_j$ . It is assumed that  $\hat{\mathbf{u}}_j = \{\hat{u}_i^{\alpha}\}$  characterizes small fluctuations around the lattice site  $\mathbf{a}_j$ .

The operator function (7.51) can be expanded in powers of  $u_j^{\alpha}$ . Such a second-order expansion reads as

$$U(\hat{\mathbf{r}}_{ij}) \simeq U_{ij} + \sum_{\alpha} \Phi^{\alpha}_{ij} \left( \hat{u}^{\alpha}_{i} - \hat{u}^{\alpha}_{j} \right) + \sum_{\alpha\beta} \Phi^{\alpha\beta}_{ij} \left( \hat{u}^{\alpha}_{i} \hat{u}^{\beta}_{j} - \frac{1}{2} \hat{u}^{\alpha}_{i} \hat{u}^{\beta}_{i} - \frac{1}{2} \hat{u}^{\alpha}_{j} \hat{u}^{\beta}_{j} \right) , \qquad (7.55)$$

where

$$U_{ij} \equiv U(\mathbf{a}_{ij}) \qquad (\mathbf{a}_{ij} \equiv \mathbf{a}_i - \mathbf{a}_j) ,$$

$$\Phi_{ij}^{\alpha} \equiv \frac{\partial U_{ij}}{\partial a_i^{\alpha}} , \qquad \Phi_{ij}^{\alpha\beta} \equiv \frac{\partial^2 U_{ij}}{\partial a_i^{\alpha} \partial a_j^{\beta}} . \tag{7.56}$$

Atomic interactions, as usual, are symmetric with respect to spatial inversion,

$$U(\mathbf{a}_{ji}) = U(\mathbf{a}_{ij}) , \qquad U_{ji} = U_{ij} .$$
 (7.57)

From here, it follows that

$$\Phi_{ij}^{\alpha} = -\Phi_{ji}^{\alpha} , \qquad \Phi_{ij}^{\alpha\beta} = \Phi_{ij}^{\beta\alpha} = \Phi_{ji}^{\beta\alpha} = \Phi_{ji}^{\alpha\beta} .$$
(7.58)

For an ideal lattice, the sum

$$\sum_{j(\neq i)} U_{ij} = \sum_{j(\neq i)} U(\mathbf{a}_{ij})$$

does not depend on  $\mathbf{a}_i$ . Therefore

$$\sum_{j(\neq i)} \Phi_{ij}^{\alpha} = \frac{\partial}{\partial a_i^{\alpha}} \sum_{j(\neq i)} U_{ij} = 0 , \qquad \sum_{j(\neq i)} \Phi_{ij}^{\alpha\beta} = -\frac{\partial^2}{\partial a_i^{\alpha} \partial a_i^{\beta}} \sum_{j(\neq i)} U_{ij} = 0 , \qquad (7.59)$$

where the property

$$\frac{\partial U(\mathbf{a}_{ij})}{\partial a_i^{\alpha}} = - \frac{\partial U(\mathbf{a}_{ij})}{\partial a_j^{\alpha}}$$

is employed. Consequently, Eq. (7.55) satisfies the relation

$$\sum_{i \neq j} U(\hat{\mathbf{r}}_{ij}) = \sum_{i \neq j} U_{ij} + \sum_{i \neq j} \sum_{\alpha \beta} \Phi_{ij}^{\alpha \beta} \hat{u}_i^{\alpha} \hat{u}_j^{\beta} .$$
(7.60)

Also, because of condition (7.54), one has

$$\langle \hat{U}_{ij} \rangle = U_{ij} + \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} \left( \langle \hat{u}_i^{\alpha} \hat{u}_j^{\beta} \rangle - \langle \hat{u}_j^{\alpha} \hat{u}_j^{\beta} \rangle \right) .$$

$$(7.61)$$

To simplify the problem, let us resort to the mean-field decoupling

$$\langle c_i^{\dagger} c_i c_j^{\dagger} c_j \rangle = \langle c_i^{\dagger} c_i \rangle \langle c_j^{\dagger} c_j \rangle \qquad (i \neq j)$$

$$(7.62)$$

for the atomic operators. And let us decouple the atomic and phonon variables as follows:

$$\hat{\mathbf{p}}_{j}^{2}c_{j}^{\dagger}c_{j} = \hat{\mathbf{p}}_{j}^{2} < c_{j}^{\dagger}c_{j} > + < \hat{\mathbf{p}}_{j}^{2} > c_{j}^{\dagger}c_{j} - < \hat{\mathbf{p}}_{j}^{2} > < c_{j}^{\dagger}c_{j} > ,$$
$$\hat{U}_{ij}c_{i}^{\dagger}c_{j}^{\dagger}c_{j}c_{i} = \hat{U}_{ij} < c_{i}^{\dagger}c_{j}^{\dagger}c_{j}c_{i} > + < \hat{U}_{ij} > c_{i}^{\dagger}c_{j}^{\dagger}c_{j}c_{i} - < \hat{U}_{ij} > < c_{i}^{\dagger}c_{j}^{\dagger}c_{j}c_{i} > .$$
(7.63)

Also, let us recall the notation for the filling factor

$$\nu \equiv \frac{N}{N_L} = \frac{1}{N_L} \sum_{j} \langle c_j^{\dagger} c_j \rangle = \langle c_j^{\dagger} c_j \rangle, \qquad (7.64)$$

where again an ideal lattice is assumed.

Accomplishing quantization (7.50) in Hamiltonian (7.49) and decoupling the atomic and phonon variables according to Eq. (7.63), we come to the Hamiltonian

$$\hat{H} = E_{sh} + \hat{H}_{at} + \hat{H}_{ph} \tag{7.65}$$

with the separated variables. Here the first term shifts Hamiltonian (7.65) by the nonoperator quantity

$$E_{sh} = -\nu \sum_{j} \frac{\langle \hat{\mathbf{p}}_{j}^{2} \rangle}{2m} - \frac{\nu^{2}}{2} \sum_{i \neq j} \langle \hat{U}_{ij} \rangle .$$
 (7.66)

The second term in Eq. (7.65) is an effective atomic Hamiltonian

$$\hat{H}_{at} = -J \sum_{\langle ij \rangle} c_i^{\dagger} c_j + \sum_j \frac{\langle \hat{\mathbf{p}}_j^2 \rangle}{2m} c_j^{\dagger} c_j + \frac{U}{2} \sum_j c_j^{\dagger} c_j^{\dagger} c_j c_j + \frac{1}{2} \sum_{i \neq j} \langle \hat{U}_{ij} \rangle c_i^{\dagger} c_j^{\dagger} c_j c_i .$$
(7.67)

And the last term in Eq. (7.65) is an effective phonon Hamiltonian

$$\hat{H}_{ph} = \nu \sum_{j} \frac{\hat{\mathbf{p}}_{j}^{2}}{2m} + \frac{\nu^{2}}{2} \sum_{i \neq j} \sum_{\alpha \beta} \Phi_{ij}^{\alpha \beta} u_{i}^{\alpha} u_{j}^{\beta} .$$

$$(7.68)$$

The quantity  $\Phi_{ij}^{\alpha\beta}$  is called the dynamical matrix. The eigenproblem

$$\frac{\nu^3}{m} \sum_{j(\neq i)} \sum_{\beta} \Phi_{ij}^{\alpha\beta} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} e_{ks}^{\beta} = \omega_{ks}^2 e_{ks}^{\alpha}$$
(7.69)

defines the phonon spectrum  $\omega_{ks}$  and the polarization vectors  $\mathbf{e}_{ks} = \{e_{ks}^{\alpha}\}$ , in which  $s = 1, 2, \ldots, d$  is a polarization index. The phonon spectrum and polarization vectors can be chosen to be symmetric with respect to the inversion of the wave vector  $\mathbf{k}$ , so that

$$\omega_{-ks} = \omega_{ks} , \qquad \mathbf{e}_{-ks} = \mathbf{e}_{ks} .$$

The polarization vectors enjoy the properties

$$\mathbf{e}_{ks} \cdot \mathbf{e}_{ks'} = \delta_{ss'} , \qquad \sum_{s} e^{\alpha}_{ks} e^{\beta}_{ks} = \delta_{\alpha\beta} ,$$

meaning that they form a complete orthonormal basis.

The variables  $\hat{\mathbf{u}}_j$  and  $\hat{\mathbf{p}}_j$  can be expanded over the polarization-vector basis,

$$\hat{\mathbf{u}}_{j} = \sum_{ks} \frac{\nu \mathbf{e}_{ks}}{\sqrt{2mN\omega_{ks}}} \left( b_{ks} + b_{-ks}^{\dagger} \right) e^{i\mathbf{k}\cdot\mathbf{a}_{j}} ,$$
$$\hat{\mathbf{p}}_{j} = -i\sum_{ks} \sqrt{\frac{m\omega_{ks}}{2N}} \mathbf{e}_{ks} \left( b_{ks} - b_{-ks}^{\dagger} \right) e^{i\mathbf{k}\cdot\mathbf{a}_{j}} , \qquad (7.70)$$

with the quasimomentum **k** in the Brillouin zone. Here  $b_{ks}$  and  $b_{ks}^{\dagger}$  are the phonon field operators satisfying the Bose commutation relations

$$[b_{ks}, b_{ps'}] = 0$$
,  $[b_{ks}, b_{ps'}^{\dagger}] = \delta_{kp} \delta_{ss'}$ .

This guarantees that  $\hat{\mathbf{u}}_j$  and  $\hat{\mathbf{p}}_j$  are mutually conjugate variables and obey the commutation relations

$$[\hat{u}_{i}^{\alpha}, \hat{u}_{j}^{\beta}] = 0$$
,  $[\hat{p}_{i}^{\alpha}, \hat{p}_{j}^{\beta}] = 0$ ,  $[\hat{u}_{i}^{\alpha}, \hat{p}_{j}^{\beta}] = i\delta_{\alpha\beta}\delta_{ij}$ .

With expansion (7.70), the phonon Hamiltonian (7.68) becomes

$$\hat{H}_{ph} = \sum_{ks} \omega_{ks} \left( b_{ks}^{\dagger} b_{ks} + \frac{1}{2} \right) .$$
(7.71)

The phonon-spectrum equation follows from eigenproblem (7.69), which yields

$$\omega_{ks}^2 = \frac{\nu^3}{m} \sum_{j(\neq i)} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} e_{ks}^{\alpha} e_{ks}^{\beta} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} .$$
(7.72)

In the long-wave limit, this gives

$$\omega_{ks}^2 \simeq -\frac{\nu^3}{m} \sum_{j(\neq i)} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} e_{ks}^{\alpha} e_{ks}^{\beta} (\mathbf{k} \cdot \mathbf{a}_{ij})^2 , \qquad (7.73)$$

where  $k \to 0$ . We may note that

$$\Phi_{ij}^{\alpha\beta} \equiv \frac{\partial^2 U(\mathbf{a}_{ij})}{\partial a_i^{\alpha} \partial a_j^{\beta}} = -\frac{\partial^2 U(\mathbf{a}_{ij})}{\partial a_i^{\alpha} \partial a_i^{\beta}}$$

Therefore  $\omega_{ks}^2 \ge 0$ , tending to zero in the limit  $k \to 0$ . For a *d*-dimensional lattice, the polarization index  $s = 1, 2, \ldots, d$ . Hence Eq. (7.73) defines *d* phonon branches.

For Hamiltonian (7.71), we have

$$\langle b_{ks}^{\dagger}b_{ks}\rangle = \left[\exp\left(\frac{\omega_{ks}}{T}\right) - 1\right]^{-1}$$
 (7.74)

This yields

$$\langle \hat{\mathbf{p}}_{j}^{2} \rangle = \frac{m}{2N} \sum_{ks} \omega_{ks} \operatorname{coth}\left(\frac{\omega_{ks}}{2T}\right)$$

Then the mean phonon kinetic energy per particle is

$$K \equiv \frac{\langle \mathbf{p}_j^2 \rangle}{2m} = \frac{1}{4N} \sum_{ks} \omega_{ks} \operatorname{coth} \left(\frac{\omega_{ks}}{2T}\right) \,. \tag{7.75}$$

For the correlation function of atomic displacements, we have

$$\langle \hat{u}_{i}^{\alpha}\hat{u}_{j}^{\beta}\rangle = \frac{\delta_{ij}\nu^{2}}{2N} \sum_{ks} \frac{e_{ks}^{\alpha}e_{ks}^{\beta}}{m\omega_{ks}} \coth\left(\frac{\omega_{ks}}{2T}\right) .$$

$$(7.76)$$

The average total phonon energy is

$$\langle \hat{H}_{ph} \rangle = 2NK = \frac{1}{2} \sum_{ks} \omega_{ks} \operatorname{coth}\left(\frac{\omega_{ks}}{2T}\right)$$
 (7.77)

Denoting the interaction average (7.61) as

$$\tilde{U}_{ij} \equiv \langle \hat{U}_{ij} \rangle = U_{ij} + \Delta U_{ij} , \qquad (7.78)$$

we have

$$\Delta U_{ij} = -\frac{\nu^2}{2N} \sum_{ks} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} \frac{e_{ks}^{\alpha} e_{ks}^{\beta}}{m\omega_{ks}} \coth\left(\frac{\omega_{ks}}{2T}\right) \,. \tag{7.79}$$

The latter quantity shows how atomic interactions change in the presence of phonon excitations.

The energy shift (7.66), in view of properties (7.59), becomes

$$E_{sh} = -\left(K + \frac{\nu}{2} \Phi\right) N , \qquad (7.80)$$

where the notation

$$\Phi \equiv \frac{1}{N_L} \sum_{i \neq j} U_{ij}$$

is employed.

## 7.3 Phonon-Induced Interactions

The atomic Hamiltonian (7.67), with Eqs. (7.75), (7.78), and (7.79), takes the form

$$\hat{H}_{at} = -J \sum_{\langle ij \rangle} c_i^{\dagger} c_j + K \sum_j c_j^{\dagger} c_j + \frac{U}{2} \sum_j c_j^{\dagger} c_j^{\dagger} c_j c_j + \frac{1}{2} \sum_{i \neq j} \tilde{U}_{ij} c_i^{\dagger} c_j^{\dagger} c_j c_i .$$
(7.81)

Comparing Eqs. (7.49) and (7.81), we see that phonon excitations increase the total energy of atoms by the second term in Eq. (7.81), containing the kinetic phonon energy (7.75). The second term here is the energy of the vibrational atomic motion. In the grand canonical ensemble, the energy K can be incorporated into the chemical potential.

Atomic vibrations renormalize the interaction potential of atoms. Now the effective atomic interaction is shifted according to Eq. (7.78). In order to evaluate how substantial this renormalization is, let us resort to the isotropic approximation, keeping in mind a cubic lattice, when the phonon spectrum is the same for all polarizations, so that  $\omega_{ks}$  can be replaced by the average  $\omega_k$ , defined as

$$\omega_k^2 \equiv \frac{1}{d} \sum_{s=1}^d \omega_{ks}^2 .$$
 (7.82)

And let us introduce the *effective dynamical matrix* 

$$D_{ij} \equiv \frac{1}{d} \sum_{\alpha=1}^{d} \frac{\partial^2 U(\mathbf{a}_{ij})}{\partial a_i^{\alpha} \partial a_i^{\alpha}} = -\frac{1}{d} \sum_{\alpha=1}^{d} \Phi_{ij}^{\alpha\alpha} .$$
(7.83)

Since  $D_{ij}$  enters everywhere in the sums with  $i \neq j$ , for the simplicity of notation, we can set

$$D_{jj} \equiv 0 . \tag{7.84}$$

Recall that, due to the properties described in Eq. (7.59), one has

$$\sum_{j} D_{ij} = 0$$

From Eq. (7.72), the phonon spectrum in the isotropic approximation is given by

$$\omega_k^2 = -\frac{\nu^3}{m} \sum_j D_{ij} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} .$$
(7.85)

In the long-wave limit, this yields

$$\omega_k^2 \simeq \frac{\nu^3}{2m} \sum_j D_{ij} (\mathbf{k} \cdot \mathbf{a}_{ij})^2 \qquad (k \to 0) .$$
(7.86)

Taking into account only the nearest neighbors reduces Eq. (7.85) to

$$\omega_k^2 = \frac{4\nu^3}{m} D_0 \sum_{\alpha} \sin^2\left(\frac{k_{\alpha}a_{\alpha}}{2}\right) , \qquad (7.87)$$

where  $D_0$  is  $D_{ij}$  for the nearest neighbors,

$$D_0 \equiv \frac{1}{d} \sum_{\alpha=1}^d \frac{\partial^2 U(\mathbf{a})}{\partial a_{\alpha}^2} , \qquad (7.88)$$

with  $\mathbf{a} = \{a_{\alpha}\}$  being the elementary lattice vector. Then the long-wave limit (7.86) becomes

$$\omega_k \simeq c_0 k \qquad (k \to 0) , \qquad (7.89)$$

with the sound velocity

$$c_0 \equiv \sqrt{\frac{\nu^3}{m} D_0 a^2} \,. \tag{7.90}$$

Passing from summation to integration, according to the rule

$$\sum_{k} \rightarrow V \int_{\mathcal{B}} \frac{d\mathbf{k}}{(2\pi)^{d}} ,$$

for the interaction shift (7.79), we obtain

$$\Delta U_{ij} = \frac{\nu^2 d}{2m\rho} D_{ij} \int_{\mathcal{B}} \frac{1}{\omega_k} \coth\left(\frac{\omega_k}{2T}\right) \frac{d\mathbf{k}}{(2\pi)^d} .$$
(7.91)

The main contribution to this integral comes from the region of long waves, when  $k \to 0$ . It is, therefore, possible to invoke the Debye approximation, in which the phonon spectrum is taken in the long-wave form (7.89), while the integration over the Brillouin zone is replaced by the integration over the Debye sphere by means of the substitution

$$\int_{\mathcal{B}} d\mathbf{k} \to \frac{2\pi^{d/2}}{\Gamma(d/2)} \int_0^{k_D} k^{d-1} dk .$$
(7.92)

The Debye radius  $k_D$  is defined so that to preserve the correct normalization

$$V \int_{\mathcal{B}} \frac{d\mathbf{k}}{(2\pi)^d} = N_L , \qquad \rho a^d = \nu ,$$

that is, from the equation

$$\frac{2\pi^{d/2}V}{\Gamma(d/2)(2\pi)^d} \int_0^{k_D} k^{d-1} dk = N_L \,.$$

The latter results in

$$k_D^d = \frac{2^d \pi^{d/2} d}{2\nu} \,\Gamma\left(\frac{d}{2}\right) \rho \,. \tag{7.93}$$

In particular, in three dimensions,

$$k_D^3 = \frac{6\pi^2}{\nu} \rho = \frac{6\pi^2}{a^3} \qquad (d=3) .$$
(7.94)

A characteristic lattice temperature, related to the Debye radius  $k_D$ , is the Debye temperature

$$T_D \equiv c_0 k_D = \sqrt{4\pi} \left[ \frac{d}{2} \Gamma\left(\frac{d}{2}\right) \right]^{1/d} \frac{c_0}{a} .$$
(7.95)

This temperature separates the region of low temperatures  $(T \ll T_D)$  from that of high temperatures  $(T \gg T_D)$  with respect to phonon characteristics.

Another important quantity is the mean-square atomic displacement

$$r_0^2 \equiv \frac{1}{d} \sum_{\alpha=1}^d \langle \hat{u}_j^{\alpha} \hat{u}_j^{\alpha} \rangle .$$
 (7.96)

Using Eq. (7.76) for a cubic lattice gives

$$r_0^2 = \frac{\nu^2}{2m\rho} \int_{\mathcal{B}} \frac{1}{\omega_k} \coth\left(\frac{\omega_k}{2T}\right) \frac{d\mathbf{k}}{(2\pi)^d} \,. \tag{7.97}$$

Then the phonon-induced interaction (7.91) can be represented as

$$\Delta U_{ij} = D_{ij} r_0^2 d . aga{7.98}$$

Hence, the phonon-induced interaction strongly depends on the amplitude of atomic vibrations described by the mean-square deviation (7.96) or (7.97).

First of all, we may notice that integral (7.97) diverges for any finite temperature T > 0, if the space dimensionality is  $d \leq 2$ . This means that, for these low dimensions, atoms cannot be localized in a lattice. Their mean-square deviations (7.97) become infinite. And the phonon-induced interaction (7.98) is also infinite. It is important to stress that interaction (7.98) becomes infinite for any finite  $D_{ij}$ . And the dynamical matrix  $D_{ij}$  is always finite for any nonvanishing atomic interactions. As is discussed in Sec. 7.2, the matrix  $D_{ij}$  is finite, though may be small, even for the local interactions, proportional to  $\delta(\mathbf{r})$ . Thus, for such local interactions and well localized atoms, for which  $l_0 \ll a$ , one has

$$U(\mathbf{a}_{ij}) \approx U \exp\left(-\frac{\mathbf{a}_{ij}^2 d}{2l_0^2}\right) ,$$

from where

$$D_{ij} \approx \frac{a^2 d^2}{l_0^4} U(\mathbf{a}_{ij}) \; .$$

Therefore the localized states of the low-dimensional lattices, with  $d \leq 2$ , at finite temperature T > 0, are unstable with respect to vibrational excitations. That is, in such lattices, a purely insulating stable phase cannot exist.

At zero temperature, the localized state in a one-dimensional lattice also cannot exist, since integral (7.97) diverges for d = 1 even when T = 0. Thence, the Mott insulating phase cannot be a stable phase in a one-dimensional lattice. However, it can exist in quasione-dimensional lattices, which, actually, are just three-dimensional lattices elongated in one direction and tightly confined in two other directions. What one realizes in experiments are always quasi-low-dimensional lattices, but never purely one-dimensional or purely two-dimensional ones. So, what is measured in experiments with low-dimensional lattices does not need to exactly coincide with numerical calculations accomplished for purely lowdimensional lattices.

For *d*-dimensional lattices at zero temperature, the Debye approximation gives

$$\int_{\mathcal{B}} \frac{1}{\omega_k} \frac{d\mathbf{k}}{(2\pi)^d} = \frac{\rho d}{(d-1)\nu T_D} ,$$

where  $T_D$  is the Debye temperature (7.95). Then Eq. (7.97) yields

$$r_0^2 = \frac{\nu d}{2(d-1)mT_D} \qquad (T=0) . \tag{7.99}$$

Hence the phonon-induced interaction (7.98) is

$$\Delta U_{ij} = \frac{\nu d^2}{2(d-1)mT_D} D_{ij} \qquad (T=0) .$$
(7.100)

These formulas again confirm that the localized states in one-dimensional lattices cannot exist. But the localized states in two-dimensional lattices can occur at zero temperature. Three-dimensional lattices with localized atoms are also stable at zero temperature.

At finite temperatures, such that  $T \gg T_D$ , the Debye approximation gives

$$\int_{\mathcal{B}} \frac{1}{\omega_k} \coth\left(\frac{\omega_k}{2T}\right) \frac{d\mathbf{k}}{(2\pi)^d} \simeq \frac{2\rho T d}{(d-2)\nu T_D^2}$$

And the mean-square deviation (7.97) becomes

$$r_0^2 \simeq \frac{\nu T d}{(d-2)mT_D^2}$$
 (7.101)

Then the phonon-induced interaction (7.98) is

$$\Delta U_{ij} \simeq \frac{\nu T d^2}{(d-2)mT_D^2} D_{ij} .$$
 (7.102)

From Eqs. (7.101) and (7.102), we again see that the two-dimensional lattices with localized atoms are unstable at nonzero temperature. But such localized states can arise for three-dimensional lattices.

To evaluate how strong the phonon-induced interaction  $\Delta U_{ij}$  is, being compared to the bare interaction  $U_{ij}$ , let us consider a cubic lattice with nearest-neighbor interactions, when

$$D_{ij} = D_0 = \frac{\partial^2 U(\mathbf{a})}{\partial a^2} \,. \tag{7.103}$$

Suppose that atoms interact through dipole forces, for which  $U(\mathbf{a}) \sim a^{-3}$ . As a result,

$$D_0 = \frac{12}{a^2} U(\mathbf{a}) . \tag{7.104}$$

Then the phonon sound velocity (7.90) is

$$c_0 = \sqrt{\frac{12}{m} \nu^3 U(\mathbf{a})}$$
 (7.105)

At zero temperature, the phonon-induced interaction (7.100) writes as

$$\Delta U_{ij} = \frac{d^2}{(d-1)k_D a^2} \sqrt{\frac{3}{\nu m} U(\mathbf{a})} .$$
 (7.106)

Using the relation

$$E_R = \frac{k_0^2}{2m} = \frac{\pi^2}{2ma^2} \; ,$$

we find

$$\frac{\Delta U_{ij}}{U_{ij}} = \frac{\sqrt{6} d^2}{\pi (d-1)k_D a} \sqrt{\frac{E_R}{\nu U_{ij}}}, \qquad (7.107)$$

where

$$k_D a = \sqrt{4\pi} \left[ \frac{d}{2} \Gamma\left(\frac{d}{2}\right) \right]^{1/d}$$

For two-and three-dimensional lattices we have

$$k_D a = \sqrt{4\pi} = 3.545$$
  $(d = 2)$ ,  
 $k_D a = 3.898$   $(d = 3)$ .

Therefore Eq. (7.107) yields

$$\frac{\Delta U_{ij}}{U_{ij}} = 0.9 \sqrt{\frac{E_R}{\nu U_{ij}}} \qquad (T = 0; \ d = 2, 3) \ . \tag{7.108}$$

At finite temperatures, such that  $T \gg T_D$ , the phonon-induced interaction is given by Eq. (7.102), from where

$$\frac{\Delta U_{ij}}{U_{ij}} \simeq \frac{d^2}{(d-2)(k_D a)^2} \left(\frac{T}{\nu U_{ij}}\right) \,. \tag{7.109}$$

For a three-dimensional lattice, this gives

$$\frac{\Delta U_{ij}}{U_{ij}} \simeq 0.6 \ \frac{T}{\nu U_{ij}} \qquad (T > T_D, \ d = 3) \ . \tag{7.110}$$

Equations (7.108) and (7.110) show that phonons can substantially renormalize atomic interactions.

The extended Hubbard model (5.16) has been studied theoretically for one-dimensional [317–322] and two-dimensional [417] lattices. However, it is necessary to be cautious interpreting the results of numerical calculations. As follows from the above analysis, the localized states in one-dimensional lattices are unstable with respect to phonon excitations at any temperature. The Mott insulating phase, strictly speaking, cannot be realized in such lattices even at zero temperature. In two- and three-dimensional lattices, the Mott insulating phase can happen at zero temperature. But, investigating the phase diagram, one should take into account the phonon-induced renormalization of atomic interactions.

The boundary between the insulating and Bose-condensed phases can be defined by studying the behavior of the condensate fraction [418]. One should keep in mind that this boundary can be shifted because of the influence of the phonon-induced interactions.

For optical lattices with disorder, the phase diagram essentially depends on the presence of the order-parameter fluctuations [419]. The existence of the vibrational atomic fluctuations can also strongly influence the phase portrait of disordered optical lattices. For the latter, the phonon excitations can occur to be even more dramatic than for ideal lattices.

# 8 Double-Well Optical Lattices

# 8.1 Effective Hamiltonians

Recently, a double-well optical lattice was realized experimentally [420], being a lattice each site of which is represented by a double-well potential. Dynamics of cold atoms in a separate double-well has been considered in several publications [421–423]. But to study the properties of the whole double-well lattice, it is necessary to have an appropriate lattice Hamiltonian.

We should start with the general Hamiltonian in the Wannier representation, given by Eq. (4.11). Contrary to the case of the standard Hubbard model (4.12), for the double-well lattice, it is impossible to resort to the single-band approximation. This is because the tunneling of atoms between the wells of a double well results in the splitting of the ground-state level onto two energy levels that can be very close to each other [205]. Without taking

account of this splitting there would be no atomic tunneling between the wells. Since, in addition, atoms interact with each other, this tunneling is essentially nonlinear [424,425].

Thus, for the double-well lattices, we have to retain not less than two lowest energy levels, that is, we have to deal with at least a two-band case. It is important to stress that in the expansion of the field operator

$$\psi(\mathbf{r}) = \sum_{nj} c_{nj} w_n (\mathbf{r} - \mathbf{a}_j)$$
(8.1)

the index n enumerates the quantum bands, that is, the quantum energy levels, but not "left" or "right" positions. The latter, as is explained in Sec. 2.17, are not good quantum numbers. The necessity of taking into account several energy levels is typical of atoms in complex multi-well configurations [426–428] as well as can occur for some metastable systems [429].

Introducing the notation

$$E_{ij}^{mn} \equiv \int w_m^*(\mathbf{r} - \mathbf{a}_i) H_L(\mathbf{r}) w_n(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r} \,, \qquad (8.2)$$

in which

$$H_L(\mathbf{r}) \equiv -\frac{\nabla^2}{2m} + V_L(\mathbf{r}) \; ,$$

Hamiltonian (4.11) can be rewritten as

$$\hat{H} = \sum_{ij} \sum_{mn} E_{ij}^{mn} c_{mi}^{\dagger} c_{nj} + \frac{1}{2} \sum_{\{j\}} \sum_{\{n\}} U_{j_1 j_2 j_3 j_4}^{n_1 n_2 n_3 n_4} c_{n_1 j_1}^{\dagger} c_{n_2 j_2}^{\dagger} c_{n_3 j_3} c_{n_4 j_4} .$$
(8.3)

The indices m and n here have to take at least two values, m, n = 1, 2. When there is BEC in the lattice, so that the gauge symmetry becomes broken, the field operators  $c_{nj}$  should be replaced by the Bogolubov-shifted operators (4.5).

In order to find the relation between the matrix element (8.2) and the Bloch energy  $E_{nk}$ , which is the eigenvalue of the equation

$$H_L(\mathbf{r})\varphi_{nk}(\mathbf{r}) = E_{nk}\varphi_{nk}(\mathbf{r}) ,$$

we can employ the expansion of the Bloch functions  $\varphi_{nk}(\mathbf{r})$  over the Wannier functions. Then the above eigenproblem transforms into the equation

$$H_L(\mathbf{r})w_n(\mathbf{r}-\mathbf{a}_i) = \frac{1}{N_L} \sum_{jk} E_{nk} e^{-i\mathbf{k}\cdot\mathbf{a}_{ij}} w_n(\mathbf{r}-\mathbf{a}_j) \ .$$

This shows that the Wannier functions, strictly speaking, are not the eigenfunctions of the lattice Hamiltonian  $H_L(\mathbf{r})$ . Using this equation, for the matrix element (8.2), we find

$$E_{ij}^{mn} = \delta_{mn} E_{ij}^n$$

where

$$E_{ij}^n = \frac{1}{N_L} \sum_k E_{nk} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} \; .$$

The latter expression can be represented in the form

$$E_{ij}^{n} = \delta_{ij} E_{n} + (1 - \delta_{ij}) J_{ij}^{n} , \qquad (8.4)$$

in which

$$E_n = \int w_n^*(\mathbf{r} - \mathbf{a}_j) H_L(\mathbf{r}) w_n(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r} = \frac{1}{N_L} \sum_k E_{nk} \, ,$$
$$J_{ij}^n = \int w_n^*(\mathbf{r} - \mathbf{a}_i) H_L(\mathbf{r}) w_n(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r} = \frac{1}{N_L} \sum_k E_{nk} e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} \, , \qquad (i \neq j) \, .$$

There is a temptation to reduce the number of these parameters by assuming that the above quantities do not depend on the band indices. This, however, is not a good idea. The tunneling between the wells of a single double-well depends on the nonzero value of the difference  $E_{jj}^{22} - E_{jj}^{11}$ . But this difference would be zero, if the values  $E_{ij}^{mn}$  would not depend on the band indices. In oder not to kill the tunneling between the wells of a double well, one has to retain the dependence on the band indices. The consideration of model (8.3), with many independent parameters, is rather complicated and can be done by setting some of these parameters to zero [430].

There is, however, a case, when Hamiltonian (8.3) can be essentially simplified. This is when the filling factor is strictly fixed to one, so that the double occupancy of a lattice site is prohibited, which is manifested by the *unipolarity conditions* 

$$\sum_{n} c_{nj}^{\dagger} c_{nj} = 1 , \qquad c_{nj} c_{nj} = 0 .$$
(8.5)

Let us also assume that the lattice is in the insulating state, such that the atomic hopping between different lattice sites is negligible,

$$\left|\frac{J_{ij}}{E_n}\right| \ll 1 \qquad (i \neq j) \ . \tag{8.6}$$

Under this condition, Wannier functions become approximate eigenfunctions of  $H_L(\mathbf{r})$ , in the sense that

$$H_L(\mathbf{r})w_n(\mathbf{r}-\mathbf{a}_j)\simeq E_nw_n(\mathbf{r}-\mathbf{a}_j)$$

Under conditions (8.5) and (8.6), Hamiltonian (8.3) reduces to the form

$$\hat{H} = \sum_{nj} E_n c_{nj}^{\dagger} c_{nj} + \frac{1}{2} \sum_{i \neq j} \sum_{mnm'n'} V_{ij}^{mnm'n'} c_{mi}^{\dagger} c_{nj}^{\dagger} c_{m'j} c_{n'i} , \qquad (8.7)$$

in which

$$V_{ij}^{mnm'n'} \equiv V_{ijji}^{mnm'n'} + V_{ijij}^{mnm'm'}$$

Retaining only the two lowest bands implies that n = 1, 2. Then the unipolarity conditions (8.5) are

$$c_{1j}^{\dagger}c_{1j} + c_{2j}^{\dagger}c_{2j} = 1$$
,  $c_{1j}c_{1j} = c_{2j}c_{2j} = 0$ .

For this two-band case, it is possible to resort to the pseudospin representation, similar to that used for some ferroelectrics [431,432]. The pseudospin operators are defined as

$$S_{j}^{x} = \frac{1}{2} \left( c_{1j}^{\dagger} c_{1j} - c_{2j}^{\dagger} c_{2j} \right) , \qquad S_{j}^{y} = \frac{i}{2} \left( c_{1j}^{\dagger} c_{2j} - c_{2j}^{\dagger} c_{1j} \right) ,$$

$$S_j^z = \frac{1}{2} \left( c_{1j}^{\dagger} c_{2j} + c_{2j}^{\dagger} c_{1j} \right) .$$
(8.8)

This gives

$$c_{1j}^{\dagger}c_{1j} = \frac{1}{2} + S_j^x , \qquad c_{2j}^{\dagger}c_{2j} = \frac{1}{2} - S_j^x ,$$
  

$$c_{1j}^{\dagger}c_{2j} = S_j^z - iS_j^y , \qquad c_{2j}^{\dagger}c_{1j} = S_j^z + iS_j^y . \qquad (8.9)$$

To clarify the physical meaning of the pseudospin operators (8.8), one can introduce the left,  $c_{jL}$ , and the right,  $c_{jR}$ , operators by the relations

$$c_{1j} = \frac{1}{\sqrt{2}} (c_{jL} + c_{jR}) , \qquad c_{2j} = \frac{1}{\sqrt{2}} (c_{jL} - c_{jR}) ,$$
  
$$c_{jL} = \frac{1}{\sqrt{2}} (c_{1j} + c_{2j}) , \qquad c_{jR} = \frac{1}{\sqrt{2}} (c_{1j} - c_{2j}) . \qquad (8.10)$$

Then operators (8.8) become

$$S_{j}^{x} = \frac{1}{2} \left( c_{jL}^{\dagger} c_{jR} + c_{jR}^{\dagger} c_{jL} \right) , \qquad S_{j}^{y} = -\frac{i}{2} \left( c_{jL}^{\dagger} c_{jR} - c_{jR}^{\dagger} c_{jL} \right) ,$$
$$S_{j}^{z} = \frac{1}{2} \left( c_{jL}^{\dagger} c_{jL} - c_{jR}^{\dagger} c_{jR} \right) .$$
(8.11)

These equations demonstrate that  $S_j^x$  describes the tunneling intensity between the left and right wells of a double-well potential centered at the *j*-site;  $S_j^y$  characterizes the Josephson current between the left and right wells; and  $S_j^z$  is the displacement operator for the imbalance between the wells.

The ground-state wave function and that of the first excited state in a double-well possess different symmetry properties and differing topology [205]. For instance, the ground-state wave function  $w_1(\mathbf{r})$  is symmetric with respect to spatial inversion, while the excited-state wave function  $w_2(\mathbf{r})$  is antisymmetric,

$$w_1(-\mathbf{r}) = w_1(\mathbf{r}) , \qquad w_2(-\mathbf{r}) = -w_2(\mathbf{r}) .$$
 (8.12)

Due to the symmetry properties (8.12), some of the matrix elements  $V_{ij}^{mnm'n'}$  can become zero. Concretely, these are the matrix elements that are nondiagonal with respect to the band indices.

Let us consider the integral

$$\Phi_{ij}^{1112} \equiv \int \Phi(\mathbf{r} - \mathbf{r}') w_1^*(\mathbf{r} - \mathbf{a}_i) |w_1(\mathbf{r}' - \mathbf{a}_j)|^2 w_2(\mathbf{r} - \mathbf{a}_i) d\mathbf{r} d\mathbf{r}' ,$$

in which  $\Phi(-\mathbf{r}) = \Phi(\mathbf{r})$  is any symmetric pair-interaction potential and  $i \neq j$ . Shifting here  $\mathbf{r}$  by  $\mathbf{a}_i$  and  $\mathbf{r}'$  by  $\mathbf{a}_j$  gives an equivalent form

$$\Phi_{ij}^{1112} \equiv \int \Phi(\mathbf{r} - \mathbf{r}' + \mathbf{a}_{ij}) w_1^*(\mathbf{r}) |w_1(\mathbf{r}')|^2 w_2(\mathbf{r}) d\mathbf{r} d\mathbf{r}' .$$

Accomplishing here the spatial inversion of  $\mathbf{r}$  and  $\mathbf{r}'$ , using the symmetry of the interaction potential, and invoking the symmetry properties (8.12), we have

$$\Phi_{ij}^{1112} = -\int \Phi(\mathbf{r} - \mathbf{r}' - \mathbf{a}_{ij}) w_1^*(\mathbf{r}) |w_1(\mathbf{r}')|^2 w_2(\mathbf{r}) d\mathbf{r} d\mathbf{r}' .$$

From the last two equations, keeping in mind that the Wannier functions form an orthonormal basis and can be made well localized, we find

$$\Phi_{ij}^{1112} \cong -\Phi_{ij}^{1112} \cong 0$$
.

In the same way, it is easy to show that other nondiagonal matrix elements of the interaction potential are practically zero. As a result, we obtain

$$V_{ij}^{1112} = V_{ij}^{1121} = V_{ij}^{1211} = V_{ij}^{2111} = V_{ij}^{2221} = V_{ij}^{2212} = V_{ij}^{2122} = V_{ij}^{1222} = 0.$$
(8.13)

Choosing real Wannier functions yields

$$V_{ij}^{1212} = V_{ij}^{2121} = V_{ij}^{2211} = V_{ij}^{1122} , \qquad V_{ij}^{2112} = V_{ij}^{1221} .$$
(8.14)

These matrix elements are nonzero.

Let us introduce the notation

$$E_0 \equiv \frac{1}{2} \left( E_1 + E_2 \right) \tag{8.15}$$

and the following combinations of the interaction matrix elements:

$$A_{ij} \equiv \frac{1}{4} \left( V_{ij}^{1111} + V_{ij}^{2222} + 2V_{ij}^{1221} \right) , \qquad B_{ij} \equiv \frac{1}{2} \left( V_{ij}^{1111} + V_{ij}^{2222} - 2V_{ij}^{1221} \right) ,$$
$$C_{ij} \equiv \frac{1}{2} \left( V_{ij}^{2222} - V_{ij}^{1111} \right) , \qquad I_{ij} \equiv -2V_{ij}^{1122} . \tag{8.16}$$

Also, let us define the quantity

$$\Omega \equiv E_2 - E_1 + \sum_{j(\neq i)} C_{ij} , \qquad (8.17)$$

playing the role of a tunneling parameter characterizing the tunneling between the wells of a double-well potential.

As a result, Hamiltonian (8.7) reduces to the pseudospin form

$$\hat{H} = E_0 N + \frac{1}{2} \sum_{i \neq j} A_{ij} - \Omega \sum_j S_j^x + \sum_{i \neq j} B_{ij} S_i^x S_j^x - \sum_{i \neq j} I_{ij} S_i^z S_j^z .$$
(8.18)

By their definitions, the diagonal matrix elements  $V_{ij}^{1111}$ ,  $V_{ij}^{2222}$ , and  $V_{ij}^{1221}$ , by their absolute values, can be close to each other, but much larger than the exchange matrix element  $I_{ij}$ , so that

$$|V_{ij}^{1122}| \ll |V_{ij}^{1111}| . \tag{8.19}$$

Then, from Eqs. (8.16), it follows that

$$|C_{ij}| \ll |A_{ij}|, \qquad |I_{ij}| \ll |A_{ij}|.$$
 (8.20)

However the term, containing  $A_{ij}$ , is not an operator, hence can be omitted from the Hamiltonian, as well as the term  $E_0N$ . The remaining terms, with  $B_{ij}$ ,  $I_{ij}$ , and  $\Omega$ , can be of the same order. By varying the shape of a double well, it is possible to make the energy difference  $E_2 - E_1$  quite large or exponentially small [205]. Thence the tunneling parameter  $\Omega$  in Eq. (8.17) can be varied in a wide range. That is, in general, the term with  $B_{ij}$  cannot be omitted. It can be neglected only when the tunneling parameter  $\Omega$  is sufficiently large, such that it is much larger than  $B_{ij}$ . Note that the tunneling between different lattice sites can be modulated by shaking the lattice [433]. In a similar way, one could also modulate the effective tunneling between the adjacent wells of a double-well potential.

#### 8.2 Phase Transitions

To study what kind of phase transitions occurs for Hamiltonian (8.18), let us resort to the mean-field approximation

$$S_{i}^{\alpha}S_{j}^{\beta} = \langle S_{i}^{\alpha} \rangle S_{j}^{\beta} + S_{i}^{\alpha} \langle S_{j}^{\beta} \rangle - \langle S_{i}^{\alpha} \rangle \langle S_{j}^{\beta} \rangle \qquad (i \neq j) .$$
(8.21)

And let us introduce the notation

$$A \equiv \frac{1}{N_L} \sum_{i \neq j} A_{ij} , \qquad B \equiv \frac{1}{N_L} \sum_{i \neq j} B_{ij} , \qquad I \equiv \frac{1}{N_L} \sum_{i \neq j} I_{ij} . \tag{8.22}$$

Under the unipolarity conditions (8.5), the filling factor is strictly one, and  $N_L = N$ . Also, we define the effective tunneling

$$\overline{\Omega} \equiv \Omega - 2B < S_j^x > . \tag{8.23}$$

Then Hamiltonian (8.18) acquires the form

$$\hat{H} = H_{non} - \overline{\Omega} \sum_{j} S_j^x - 2I \sum_{j} \langle S_i^z \rangle S_j^z , \qquad (8.24)$$

in which the first term is the nonoperator quantity

$$H_{non} = NE_0 + \frac{N}{2} \left( A - 2B < S_i^x >^2 + 2I < S_i^z >^2 \right) .$$
(8.25)

By introducing an effective "magnetic" field

$$\mathbf{H}_{eff} \equiv \{H_{eff}^{\alpha}\} \equiv \{\overline{\Omega}, \ 0, \ 2I < S_j^z >\}, \qquad (8.26)$$

Hamiltonian (8.24) can be rewritten as

$$\hat{H} = H_{non} - \sum_{j} \mathbf{H}_{eff} \cdot \mathbf{S}_{j} .$$
(8.27)

The corresponding free energy is

$$F = H_{non} - NT \ln \left( 2 \cosh \frac{H_{eff}}{2T} \right) , \qquad (8.28)$$

where  $H_{eff} \equiv |\mathbf{H}_{eff}|$ , which gives

$$H_{eff} = \sqrt{\overline{\Omega}^2 + 4I^2 < S_j^z >^2} .$$
 (8.29)

The average values  $< S_j^\alpha >$  can be found from the equation

$$< S_j^{lpha} > = -\frac{1}{N} \frac{\partial F}{\partial H_{eff}^{lpha}} \,.$$

This yields the equations for the x-component (tunneling intensity)

$$\langle S_j^x \rangle = \frac{\overline{\Omega}}{2H_{eff}} \tanh\left(\frac{H_{eff}}{2T}\right) ,$$
 (8.30)

the y-component (Josephson current)

$$\langle S_j^y \rangle = 0$$
, (8.31)

and the z-component (well imbalance)

$$\langle S_j^z \rangle = \langle S_j^z \rangle \frac{I}{H_{eff}} \tanh\left(\frac{H_{eff}}{2T}\right)$$
 (8.32)

Let us define the averages

$$x \equiv 2 < S_j^x > , \qquad y \equiv 2 < S_j^y > , \qquad z \equiv 2 < S_j^z > .$$
 (8.33)

It is convenient to introduce the dimensionless quantities

$$\omega \equiv \frac{\Omega}{I+B} , \qquad b \equiv \frac{B}{I+B} . \tag{8.34}$$

Using these, we have

$$\frac{\Omega}{I+B} = \omega - bx , \qquad \frac{I}{I+B} = 1 - b .$$
(8.35)

Also, let us define the dimensionless quantity

$$h \equiv \frac{H_{eff}}{I+B} , \qquad (8.36)$$

which is

$$h = \sqrt{(\omega - bx)^2 + (1 - b)^2 z^2} .$$
(8.37)

The nonoperator part (8.25) of Hamiltonian (8.24) reads as

$$\frac{H_{non}}{N} = E_0 + \frac{A}{2} + \frac{I+B}{4} \left[ (1-b)z^2 - bx^2 \right] .$$
(8.38)

Employing the dimensionless quantities, defined above, the temperature T will be measured in units of I + B.

In the dimensionless notation, the averages (8.30), (8.31), and (8.32) yield the tunneling intensity

$$x = \frac{\omega - bx}{h} \tanh\left(\frac{h}{2T}\right) , \qquad (8.39)$$

the Josephson current

$$y = 0$$
, (8.40)

and the well imbalance

$$z = z \, \frac{1-b}{h} \tanh\left(\frac{h}{2T}\right) \,. \tag{8.41}$$

These variables satisfy the condition

$$x^{2} + y^{2} + z^{2} = \tanh^{2}\left(\frac{h}{2T}\right)$$
 (8.42)

Equations (8.39) and (8.41) are invariant under the replacement

$$x \to -x$$
,  $\omega \to -\omega$ ,  $z \to -z$ .

Therefore, without the loss of generality, we can consider only the case, when  $x \ge 0$ ,  $\omega \ge 0$ , and  $z \ge 0$ . The inequality  $\omega \ge 0$  is in agreement with the accepted enumeration of the energy levels in a double-well potential, when  $E_1 < E_2$ .

Equation (8.41) shows that there can be two types of solutions, when  $z \neq 0$  and when z = 0. The well-imbalance z plays the role of an order parameter. If  $z \neq 0$ , this means that atoms are mainly shifted to one of the double wells. While if z = 0, then atoms on the average equally populate both wells. The thermodynamic phase with  $z \neq 0$  is called ordered, while that with z = 0 is termed disordered.

For the ordered phase, when  $z \neq 0$ , Eq. (8.41) gives

$$\frac{1-b}{h}\tanh\left(\frac{h}{2T}\right) = 1 , \qquad (8.43)$$

which defines z. Using Eq. (8.43) in Eq. (8.39) yields

$$x = \frac{\omega - bx}{1 - b} \; ,$$

from where it follows

$$x = \omega . \tag{8.44}$$

Since, by definition, the variable x is positive and less than one, we see that the ordered phase can exist if

$$0 \le \omega \le 1$$
  $(0 \le x \le 1)$ . (8.45)

Equation (8.43), with

$$h = (1-b) \sqrt{\omega^2 + z^2} , \qquad (8.46)$$

defines z > 0 for  $T < T_c$ . The critical temperature is

$$T_c = \frac{(1-b)\omega}{2\operatorname{artanh}\omega} , \qquad (8.47)$$

where

artanh 
$$\omega = \frac{1}{2} \ln \frac{1+\omega}{1-\omega}$$

When  $\omega \to 0$ , then

$$T_c \simeq \frac{1-b}{2} \qquad (\omega \ll 1)$$

which in dimensional units becomes  $T_c \simeq I/2$ . And if  $\omega \to 1$ , then  $T_c \to 0$ . Thus, the ordered phase, with z > 0, can exist when both  $T < T_c$  and  $\omega \leq 1$ .

In the disordered phase,

$$z = 0$$
 . (8.48)

Equation (8.37) gives

$$h = \omega - bx . \tag{8.49}$$

Then Eq. (8.39) yields

$$x = \tanh\left(\frac{\omega - bx}{2T}\right) \,. \tag{8.50}$$

For x to be non-negative, it should be that

$$\omega \ge bx \qquad (x \ge 0) . \tag{8.51}$$

The disordered phase arises, when the ordered phase cannot exist, that is, when either  $T > T_c$  or  $\omega > 1$ .

The transition between the ordered and disordered phases happens when either the temperature or the tunneling parameter are varied. For example, at zero temperature T = 0, the ordered phase has

$$x = \omega$$
,  $z = \sqrt{1 - \omega^2}$  ( $\omega < 1$ ). (8.52)

While the disordered phase is described by

$$x = 1$$
,  $z = 0$ ,  $(\omega > 1)$ . (8.53)

At the value  $\omega = 1$ , the quantum phase transition occurs.

The reduced internal energy

$$E \equiv \frac{1}{N} < \hat{H} >$$

is

$$E = \frac{H_{non}}{N} - \frac{I+B}{2} \left[ (\omega - bx)x + (1-b)z^2 \right] .$$
 (8.54)

In view of Eq. (8.38), this gives

$$E = E_0 + \frac{A}{2} + \frac{I+B}{4} \left[ bx^2 - 2\omega - (1-b)z^2 \right] .$$
(8.55)

The energy of the ordered phase,

$$E = E_0 + \frac{A}{2} - \frac{I+B}{4} \left(1 - b + \omega^2\right) \qquad (\omega < 1)$$

is always lower than the energy of the disordered phase,

$$E = E_0 + \frac{A}{2} + \frac{I+B}{4} (b-2\omega) \qquad (\omega > 1).$$

These energies coincide at the critical value  $\omega = 1$ .

# 8.3 Collective Excitations

The dynamics of the pseudospin operators follows from the Heisenberg equations

$$i \ \frac{dS_j^{\alpha}}{dt} = \left[S_j^{\alpha}, \hat{H}\right] \ ,$$

with the commutation relations

$$[S_i^x, S_j^y] = i\delta_{ij}S_j^z , \qquad [S_i^y, S_j^z] = i\delta_{ij}S_j^x , \qquad [S_i^z, S_j^x] = i\delta_{ij}S_j^y .$$

Using the pseudospin Hamiltonian (8.18) results in the equations of motion

$$\frac{dS_i^x}{dt} = 2S_i^y \sum_{j(\neq i)} I_{ij}S_j^z , \qquad \frac{dS_i^y}{dt} = \Omega S_i^z - 2S_i^x \sum_{j(\neq i)} I_{ij}S_j^z - 2S_i^z \sum_{j(\neq i)} B_{ij}S_j^x ,$$
$$\frac{dS_i^z}{dt} = -\Omega S_i^y + 2S_i^y \sum_{j(\neq i)} B_{ij}S_j^x . \tag{8.56}$$

Collective excitations in the random-phase approximation can be found by representing the pseudospin operators as

$$S_j^{\alpha} = \langle S_j^{\alpha} \rangle + \delta S_j^{\alpha} \tag{8.57}$$

and considering  $\delta S_j^{\alpha}$  as a small deviation from an equilibrium average. Equation (8.57) is to be substituted into Eqs. (8.56), which are linearized with respect to  $\delta S_j^{\alpha}$ . In the zero order, one gets

$$\frac{dx}{dt} = 0 , \qquad \frac{dy}{dt} = (\overline{\Omega} - Ix)z , \qquad \frac{dz}{dt} = 0 .$$
(8.58)

For the ordered phase, when  $z \neq 0$ , one has  $x = \omega$ ; and for the disordered phase, z = 0. Therefore the second equation in Eqs. (8.58) becomes dy/dt = 0. So, all averages, x, y, and z, do not depend on time, as it should be for equilibrium quantities. In the first order, one has

$$\frac{d}{dt} \,\delta S_i^x = Iz\delta S_i^y \;,$$
$$\frac{d}{dt} \,\delta S_i^y = -Iz\delta S_i^x - z\sum_{j(\neq i)} B_{ij}\delta S_j^x \;+\; \overline{\Omega}\delta S_i^z \;-\; x\sum_{j(\neq i)} I_{ij}\delta S_j^z \;,$$

$$\frac{d}{dt}\,\delta S_i^z = -\overline{\Omega}\delta S_i^y \,. \tag{8.59}$$

One defines the Fourier transforms

$$\delta S_j^{\alpha} = \frac{1}{N_L} \sum_k \sigma_k^{\alpha} e^{i(\mathbf{k} \cdot \mathbf{a}_j - \varepsilon t)} , \qquad \sigma_k^{\alpha} = \sum_j \delta S_j^{\alpha} e^{-i(\mathbf{k} \cdot \mathbf{a}_j - \varepsilon t)} .$$
(8.60)

Similarly, Fourier transforms are introduced for the interaction functions,

$$B_{ij} = \frac{1}{N_L} \sum_k B_k e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} , \qquad B_k = \sum_i B_{ij} e^{-i\mathbf{k}\cdot\mathbf{a}_{ij}} ,$$
$$I_{ij} = \frac{1}{N_L} \sum_k I_k e^{i\mathbf{k}\cdot\mathbf{a}_{ij}} , \qquad I_k = \sum_i I_{ij} e^{-i\mathbf{k}\cdot\mathbf{a}_{ij}} . \tag{8.61}$$

Then Eqs. (8.59) yield

$$i\varepsilon\sigma_k^x + zI\sigma_k^y = 0$$
,  $(I+B_k)z\sigma_k^x - i\varepsilon\sigma_k^y + (xI_k - \overline{\Omega})\sigma_k^z = 0$ ,  
 $\overline{\Omega}\sigma_k^y - i\varepsilon\sigma_k^z = 0$ . (8.62)

The condition for the existence of nontrivial solutions to Eqs. (8.62) gives the equation

$$\varepsilon \left[ \varepsilon^2 - (\overline{\Omega} - xI_k) - I(I + B_k)z^2 \right] = 0 , \qquad (8.63)$$

in which

$$\overline{\Omega} = \Omega - Bx \; .$$

Equation (8.63) defines three branches for the spectrum of collective excitations. One branch is trivial,

$$\varepsilon_1(\mathbf{k}) = 0 \ . \tag{8.64}$$

And two other branches are given by the equation

$$\varepsilon_{2,3}^2(\mathbf{k}) = \overline{\Omega}(\overline{\Omega} - xI_k) + I(I + B_k)z^2 . \qquad (8.65)$$

The branches of spectrum (8.65) describe the pseudospin oscillations. These branches possess gaps for both ordered as well as disordered phases, and, in the long-wave limit, they vary as  $k^2$ .

#### 8.4 Nonequilibrium States

Nonequilibrium states in lattices appear, when atoms are subject to temporal external fields. This is possible to accomplish by varying the shape of the lattice, for instance, by changing the configuration of the double-well potential in each lattice site. Atomic interactions can be modulated by means of the Feshbach resonance techniques. A nonequilibrium situation arises in the process of loading atoms into the lattice.

The nonequilibrium behavior of atoms in a double well lattice can be characterized by considering the temporal evolution of the average quantities (8.33). The evolution equations for these quantities are to be obtained from averaging the operator equations (8.56). When

accomplishing such an averaging, it is customary to invoke the mean-field approximation (8.21). This standard way has a principal defect of not taking into account atomic collisions resulting in the appearance of damping. Not taking account of the latter can lead to incorrect dynamics and wrong physical conclusions.

The existence of atomic collisions yielding the arising attenuation, can be included in the dynamics by employing the local-field approximation. This approximation is based on the fact that a kind of local equilibrium exists even in strongly nonequilibrium systems [434-436]. Then one can consider atomic collisions as occurring in an effective local field of other particles [437]. The resulting attenuation effects are included into the evolution equations through the damping parameters, characterizing the longitudinal,  $\gamma_1$ , and transverse,  $\gamma_2$ , relaxation. The values of these parameters can be calculated in the same way as is done for magnetic systems [438].

The local fields for variables (8.33) are defined through expressions (8.39), (8.40), and (8.41) as

$$x_t \equiv \frac{\omega - bx}{h} \tanh\left(\frac{h}{2T}\right) , \qquad y_t = 0 , \qquad z_t \equiv \frac{1 - b}{h} z \tanh\left(\frac{h}{2T}\right) , \qquad (8.66)$$

where h is given by Eq. (8.37). Averaging Eqs. (8.56) in the local-field approximation results in the evolution equations for the tunneling intensity

$$\frac{dx}{dt} = (1-b)yz - \gamma_2(x-x_t) , \qquad (8.67)$$

Josephson current

$$\frac{dy}{dt} = (\omega - x)z - \gamma_2(y - y_t) , \qquad (8.68)$$

and the well imbalance

$$\frac{dz}{dt} = (bx - \omega)y - \gamma_1(z - z_t) , \qquad (8.69)$$

with the local fields (8.66). These equations describe the time evolution of x = x(t), y = y(t), and z = z(t) under the given initial conditions

$$x_0 = x(0)$$
,  $y_0 = y(0)$ ,  $z_0 = z(0)$ . (8.70)

Here the dimensionless parameters (8.34) are employed and time is measured in units of 1/(I+B).

The evolution equations (8.67), (8.68), and (8.69), depending on the parameters b and  $\omega$ , can show two types of behavior, attenuating to two different fixed points, one corresponding to the ordered stationary solution and another, to the disordered stationary solution.

#### 8.5 Heterophase Lattices

It may happen that a double-well lattice is neither completely ordered nor completely disordered, but consists of the ordered regions intermixed with disordered parts. The spatial distribution of these differently ordered regions is random, as well as their sizes and shapes. Such an object composed of a random mixture of different phases is called the *heterophase* 

system. In condensed matter, there are plenty of examples of such systems, as has been reviewed in the articles [54,66]. A schematic picture of a heterophase double-well lattice is shown in Fig. 3, where the ordered regions are marked by arrows, while the disordered regions are left empty. Because of their random distribution in space and because they often arise randomly, that is, in a fluctuational way, in time, the heterophase regions inside a statistical system are called heterophase fluctuations. Such fluctuations can be provoked by the environmental randomness [439], even when the latter corresponds to a very weak noise. But they can also be due to intrinsic causes, such as local fluctuations of entropy or temperature [440], fluctuations of density or composition fluctuations [441], and other internal perturbations generated by the system itself [442]. The nuclei of one phase inside another are also termed droplets or clusters [443]. The system with heterophase fluctuations can be more stable than a pure-phase sample. What kind of internal structure is more profitable for a system is chosen by the system itself, which self-organizes for reaching an optimal state [444,445]. A thorough description of possible origins of heterophase fluctuations is given in the review articles [54,66]. A general microscopic theory of statistical systems with heterophase fluctuations has been developed [67,446–453] and reviewed in Refs. [54,66]. Below, this theory is applied to describing the heterophase double-well lattices.



Figure 3: Schematic picture of a heterophase double-well lattice. Arrows show the regions of the ordered phase. Empty space corresponds to the regions of the disordered phase

Each thermodynamic phase is characterized by its typical states forming a Hilbert space. The coexistence of several phases corresponds to the direct sum of the Hilbert spaces, related to particular phases. The Fock space over the direct sum of Hilbert spaces is identified with the tensor product of Fock spaces over each of the Hilbert space [454].

Suppose that the considered system is a mixture of several thermodynamic phases enumerated by the index f = 1, 2, ... Each phase is characterized by a Fock space  $\mathcal{F}_f$  of microscopic states typical of the given phase [54]. The total Fock space of the whole system is the fiber space

$$\tilde{\mathcal{F}} = \bigotimes_{f} \mathcal{F}_{f} . \tag{8.71}$$

After averaging over heterophase configurations [54], the system is described by a renormal-

ized Hamiltonian

$$\tilde{H} = \bigoplus_{f} \hat{H}_{f} , \qquad (8.72)$$

which is a direct sum of the partial Hamiltonians associated with the related phases. In a double-well lattice, there can be two different thermodynamic phases, the ordered phase and the disordered one, as is described in Sec. 8.2. Therefore the fiber space is

$$\tilde{\mathcal{F}} = \mathcal{F}_1 \bigotimes \mathcal{F}_2 , \qquad (8.73)$$

while the renormalized Hamiltonian is

$$\tilde{H} = \hat{H}_1 \bigoplus \hat{H}_2 . \tag{8.74}$$

The ordered and disordered phases are characterized by different values of the averages of the imbalance operator  $S_j^z$ . The average of an operator  $\hat{A}$ , related to an *f*-phase, is defined as

$$\langle \hat{A} \rangle_f \equiv \operatorname{Tr}_{\mathcal{F}_f} \hat{\rho}_f \hat{A}_f ,$$
 (8.75)

where the statistical operator is

$$\hat{\rho}_f = \frac{\exp(-\beta \hat{H}_f)}{\operatorname{Tr}_{\mathcal{F}_f} \exp(-\beta \hat{H}_f)}$$
(8.76)

and  $\hat{A}_f$  is a representation of the operator  $\hat{A}$  on the Fock space  $\mathcal{F}_f$ . Let us ascribe the index f = 1 to the ordered phase, while the index f = 2, to the disordered phase. Then these phases are defined as those for which

$$\langle S_j^z \rangle_1 \neq 0, \qquad \langle S_j^z \rangle_2 \equiv 0.$$
 (8.77)

As a result of averaging over heterophase configurations, the renormalized Hamiltonian (8.74) depends on the geometric probabilities of the phases,  $w_f$ , which satisfy the conditions

$$w_1 + w_2 = 1$$
,  $0 \le w_f \le 1$ . (8.78)

Following the general procedure [54], for the considered case of the double-well lattice, we have

$$\hat{H}_{f} = w_{f}E_{0}N + \frac{w_{f}^{2}}{2}\sum_{i\neq j}A_{ij} - w_{f}\Omega\sum_{j}S_{j}^{x} + w_{f}^{2}\sum_{i\neq j}B_{ij}S_{i}^{x}S_{j}^{x} - w_{f}^{2}\sum_{i\neq j}I_{ij}S_{i}^{z}S_{j}^{z}.$$
 (8.79)

Resorting again to the mean-field approximation (8.21) and introducing the notation

$$\Omega_f \equiv \Omega - 2w_f B < S_j^x >_f \tag{8.80}$$

yields

$$\hat{H}_f = H_f^{non} - w_f \Omega_f \sum_j S_j^x - 2w_f^2 I \sum_j \langle S_i^z \rangle_f S_j^z , \qquad (8.81)$$

with the first, nonoperator, term being

$$H_f^{non} = w_f E_0 N + \frac{w_f^2}{2} \left( A - 2B < S_i^x >_f^2 + 2I < S_i^z >_f^2 \right) N .$$
(8.82)

By defining the effective field

$$\mathbf{H}_f^{eff} \equiv \{ w_f \Omega_f, \ 0, \ 2w_f^2 I < S_j^z >_f \}$$

reduces Hamiltonian (8.81) to the form

$$\hat{H}_f = H_f^{non} - \sum_j \mathbf{H}_f^{eff} \cdot \mathbf{S}_j .$$
(8.83)

The free energy of the whole system is

$$F = F_1 + F_2 , (8.84)$$

with

$$F_f = H_f^{non} - NT \ln\left(2\cosh\frac{H_f^{eff}}{2T}\right) , \qquad (8.85)$$

where

$$H_f^{eff} = w_f \sqrt{\Omega_f^2 + 4w_f^2 I^2 < S_j^z >_f^2} .$$
(8.86)

For the averages of the pseudospin operators, we get

$$\langle S_j^x \rangle_f = w_f \frac{\Omega_f}{2H_f^{eff}} \tanh\left(\frac{H_f^{eff}}{2T}\right) ,$$
  
$$\langle S_j^y \rangle_f = 0 , \qquad \langle S_j^z \rangle_f = w_f^2 \langle S_j^z \rangle_f \frac{I}{H_f^{eff}} \tanh\left(\frac{H_f^{eff}}{2T}\right) . \tag{8.87}$$

It is convenient to employ the reduced variables

$$x_f \equiv 2 < S_j^x >_f, \qquad y_f \equiv 2 < S_j^y >_f, \qquad z_f \equiv 2 < S_j^z >_f$$
(8.88)

and use the dimensionless quantities (8.34). We define the effective tunneling frequency

$$\omega_f \equiv \omega - b w_f x_f \tag{8.89}$$

and introduce the notation

$$h_f \equiv w_f \,\sqrt{\omega_f^2 + (1-b)^2 w_f^2 z_f^2} \,. \tag{8.90}$$

Then averages (8.87) transform into

$$x_f = w_f \frac{\omega_f}{h_f} \tanh\left(\frac{h_f}{2T}\right), \qquad y_f = 0, \qquad z_f = w_f^2 z_f \frac{1-b}{h_f} \tanh\left(\frac{h_f}{2T}\right), \qquad (8.91)$$

where the temperature T is measured in units of I + B.

Condition (8.77), distinguishing the ordered and disordered phases, becomes

$$z_1 \neq 0$$
,  $z_2 \equiv 0$ . (8.92)

For the ordered phase,  $z_1$  is defined by the equation

$$w_1^2 \frac{1-b}{h_1} \tanh\left(\frac{h_1}{2T}\right) = 1$$
, (8.93)

while  $x_1$ , by the equation

$$x_1 = \frac{\omega_1}{(1-b)w_1}$$

The latter, in view of Eq. (8.89), gives

$$x_1 = \frac{\omega}{w_1} \ . \tag{8.94}$$

From here, it follows that the ordered component can exist if

$$0 \le \omega \le w_1 \qquad (0 \le x_1 \le 1) .$$
 (8.95)

Expressions (8.89) and (8.90) reduce to

$$\omega_1 = (1-b)\omega$$
,  $h_1 = (1-b)w_1 \sqrt{\omega^2 + w_1^2 z_1^2}$ . (8.96)

When  $z_1$  tends to zero, this can happen at the temperature

$$T_c = \frac{w_1(1-b)\omega}{2\operatorname{artanh}(\omega/w_1)}, \qquad (8.97)$$

where  $w_1 = w_1(T_c)$ .

For the disordered component, for which  $z_2 = 0$ , we have

$$\omega_2 = \omega - bw_2 x_2 , \qquad h_2 = w_2 \omega_2 .$$
 (8.98)

And  $x_2$  is defined by the equation

$$x_2 = \tanh\left(\frac{w_2\omega_2}{2T}\right) \ . \tag{8.99}$$

The proportions of the phases are prescribed by the system stability. The equations for the phase probabilities  $w_f$  can be found by minimizing the free energy (8.84) under the normalization condition (8.78). For that purpose, we define

$$w_1 \equiv w , \qquad w_2 \equiv 1 - w .$$
 (8.100)

Then, the free energy F = F(w) is minimized with respect to w. From the equation

$$\frac{\partial F(w)}{\partial w} = 0 , \qquad (8.101)$$

we find

$$w_{1} = \frac{2u + \omega_{1}x_{1} - \omega_{2}x_{2}}{4u - (1 - b)z_{1}^{2}},$$

$$w_{2} = \frac{2u - \omega_{1}x_{1} + \omega_{2}x_{2} - (1 - b)z_{1}^{2}}{4u - (1 - b)z_{1}^{2}},$$
(8.102)

where the notation

$$u \equiv \frac{A}{I+B} \tag{8.103}$$

is used.

Let us analyze the obtained equations for the case of zero temperature. Then we have

$$x_1 = \frac{\omega}{w_1} , \qquad x_2 = 1 ,$$
  
$$z_1 = \sqrt{1 - \frac{\omega^2}{w_1^2}} , \qquad z_2 = 0 \qquad (T = 0) . \qquad (8.104)$$

Also,

$$\omega_1 = (1-b)\omega$$
,  $\omega_2 = \omega - bx_2$ ,  $h_1 = (1-b)w_1^2$ ,  $h_2 = w_2(\omega - bw_2)$ . (8.105)

Probabilities (8.102) reduce to

$$w_1 = \frac{2u+b-\omega}{4u+2b-1}$$
,  $w_2 = \frac{2u+b+\omega-1}{4u+2b-1}$ . (8.106)

By definition,  $0 \le w_f \le 1$ . This imposes the constraints under which the heterophase mixture can exist,

$$1 - b - 2u < \omega < 2u + b. (8.107)$$

In particular, one can notice that

$$w_1 = w_2 = \frac{1}{2}$$
,  $z_1 = 0$   $\left(\omega = \frac{1}{2}\right)$ . (8.108)

To check whether the energy of the heterophase mixture is lower than that of a pure phase, let us consider the internal energy

$$E_{mix} \equiv \frac{1}{N} < \tilde{H} > = E_1 + E_2 ,$$
 (8.109)

in which

$$E_f \equiv \frac{1}{N} < \hat{H}_f >_f$$
 (8.110)

For the Hamiltonian (8.81), we find

$$E_f = \frac{H_f^{non}}{N} - \frac{I+B}{2} w_f \left[ \omega_f x_f + (1-b) w_f z_f^2 \right] ,$$

with

$$\frac{H_f^{non}}{N} = w_f E_0 + \frac{I+B}{4} w_f^2 \left[ 2u - bx_f^2 + (1-b)z_f^2 \right] .$$

Combining the latter two expressions, we get

$$E_f = w_f E_0 - \frac{I+B}{2} \omega w_f x_f + \frac{I+B}{4} w_f^2 \left[ 2u + bx_f^2 - (1-b)z_f^2 \right] .$$
(8.111)

For the ordered and disordered components, Eq. (8.111) gives, respectively

$$E_{1} = w_{1}E_{0} + \frac{I+B}{4} \left[ w_{1}^{2}(2u+b-1) - \omega^{2} \right] ,$$
  

$$E_{2} = w_{2}E_{0} + \frac{I+B}{4} \left[ w_{2}^{2}(2u+b) - 2\omega w_{2} \right] .$$
(8.112)

The total sum (8.109) becomes

$$E_{mix} = E_0 + \frac{I+B}{4} \left[ 2u+b-2\omega-\omega^2 - 2w(2u+b-\omega) + w^2(4u+2b-1) \right] , \quad (8.113)$$

where notation (8.100) is employed.

Minimizing Eq. (8.113) with respect to w implies that

$$\frac{\partial E_{mix}}{\partial w} = 0 , \qquad \frac{\partial^2 E_{mix}}{\partial w^2} > 0 . \tag{8.114}$$

From Eq. (8.113), we have

$$\frac{\partial E_{mix}}{\partial w} = \frac{I+B}{2} \left[ w(4u+2b-1) - 2u - b + \omega \right], \qquad \frac{\partial^2 E_{mix}}{\partial w^2} = \frac{I+B}{2} \left( 4u + 2b - 1 \right).$$

The first of Eqs. (8.114) yields the expressions for the phase probabilities (8.106). And the second condition in Eqs. (8.114) requires that

$$4u + 2b - 1 > 0. (8.115)$$

If one compares the energy (8.113) of the heterophase mixture with the energy of the pure ordered phase

$$E_{ord} \equiv E_{mix}$$
  $(w_1 = 1, w_2 = 0),$  (8.116)

then one gets the difference

$$E_{mix} - E_{ord} = -\frac{(2u+b+\omega-1)^2}{4(4u+2b-1)} (I+B) , \qquad (8.117)$$

which shows that the energy of the mixture is lower than that of the pure ordered phase under the same condition (8.115).

The difference of the ordered-phase energy (8.116) with the disordered-phase energy

$$E_{dis} \equiv E_{mix}$$
  $(w_1 = 0, w_2 = 1)$  (8.118)

reads as

$$E_{ord} - E_{dis} = -\frac{(\omega - 1)^2}{4} \left( I + B \right) \,. \tag{8.119}$$

Hence,  $E_{ord} \leq E_{dis}$  for all  $\omega$ . Therefore the energy of the heterophase mixture (8.113) satisfies the inequality

$$E_{mix} < E_{ord} \leq E_{dis} , \qquad (8.120)$$

provided that conditions (8.107) and (8.115) are valid. That is, under these conditions, the mixed state is more profitable than the pure phases.

# 9 Tools for Quantum Computing

#### 9.1 Entanglement Production

Cold atoms in optical lattices are considered as a very promising tool for realizing quantum information processing and quantum computation [17,455]. General problems of quantum computation and information are described in the books [456,457] and reviews [458,459]. Here we concentrate our attention on the possibility of employing cold atoms in optical lattices as a tool for this purpose.

Probably, the main advantage of quantum devices for information processing and computation is the feasibility of creating entanglement. This purely quantum property, which is absent in classical devices, should make quantum processors much more powerful and miniature.

The notion of entanglement has two sides. The entanglement of a quantum state describes the structure of this state. However, quantum states, as such, are not measurable quantities, so that their entanglement could be used only indirectly. Also, there is no uniquely defined measure of entanglement for quantum states, especially when the latter are mixed [456–459].

The other notion is the *entanglement production*, which shows how much entanglement is generated by a quantum operation. There exists a general measure of entanglement production, valid for arbitrary systems [460,461]. This measure of entanglement production is introduced below, with keeping in mind its application to lattices.

Let us have a lattice whose lattice sites are enumerated with the index  $j = 1, 2, ..., N_L$ . For the purpose of information processing, it is necessary to have a deep lattice potential, so that atoms be well localized in the lattice sites. The appearance of BEC diminishes the level of entanglement [461]. Therefore the insulating state is preferable. Finite temperature reduces the feasibility of manipulating atoms. Hence the system is to be deeply cooled down, so that atoms be almost at zero temperature.

Suppose that atoms in a *j*-site can have different quantum numbers labelled by the index  $n_j$ , such that these states  $|n_j\rangle$  form a basis  $\{|n_j\rangle\}$ . The closed linear envelope over this basis is the Hilbert space

$$\mathcal{H}_j \equiv \overline{\mathcal{L}}\{|n_j\rangle\} \,. \tag{9.1}$$

Denoting a given set  $\{n_j\}$  of the indices  $n_j$  by **n**, one can define the states

$$|\mathbf{n}\rangle \equiv \bigotimes_{j} |n_{j}\rangle \qquad (\mathbf{n} \equiv \{n_{j}\}).$$
 (9.2)
Using states (9.2) as a basis  $\{|\mathbf{n}_{\mathbf{j}} >\}$  makes it possible to construct the closed linear envelope over this basis, which yields the Hilbert space

$$\mathcal{H} \equiv \overline{\mathcal{L}}\{ |\mathbf{n}\rangle \} = \bigotimes_{j} \mathcal{H}_{j} .$$
(9.3)

The states of space (9.3) can be represented as

$$\varphi = \sum_{\mathbf{n}} c_{\mathbf{n}} | \mathbf{n} > \qquad (\varphi \in \mathcal{H}) .$$
(9.4)

Generally, these states do not have the form of a tensor product  $\otimes_j \varphi_j$ , with  $\varphi_j \in \mathcal{H}_j$ . Let us separate out of the space  $\mathcal{H}$  the *disentangled set* 

$$\mathcal{D} \equiv \{ f = \bigotimes_{j} \varphi_{j} | \varphi_{j} \in \mathcal{H}_{j} \} , \qquad (9.5)$$

whose members have the form of the tensor products. Then the compliment  $\mathcal{H} \setminus \mathcal{D}$  is the set of entangled states.

For any quantum operation, represented by an operator  $\hat{A}$  on  $\mathcal{H}$ , we can introduce the norm over  $\mathcal{D}$ ,

$$||\hat{A}||_{\mathcal{D}} \equiv \sup_{f,f'} |(f, \hat{A}f')|,$$
 (9.6)

where

 $f \in \mathcal{D}$ ,  $f' \in \mathcal{D}$ , ||f|| = ||f'|| = 1,

with the norm  $||f|| \equiv \sqrt{f, f}$  generated by the scalar product.

It is worth noting that the restricted norm (9.6) over the set  $\mathcal{D}$  can also be defined as a norm over a weighted Hilbert space [54,66]. With this aim in view, we can introduce the weighted Hilbert space  $\mathcal{H}_{\mathcal{D}}$  as a projected space, in which the scalar product is defined as

$$(f, f')_{\mathcal{H}_{\mathcal{D}}} \equiv (P_f \varphi, P_{f'} \varphi')_{\mathcal{H}},$$

where  $P_f$  is a projector, such that

$$P_f \varphi \equiv f \in \mathcal{D}$$
.

The norm of  $\hat{A}$  over the weighted Hilbert space  $\mathcal{H}_{\mathcal{D}}$  is defined as

$$||\hat{A}||_{\mathcal{H}_{\mathcal{D}}} \equiv ||P_{\mathcal{D}}\hat{A}P_{\mathcal{D}}||_{\mathcal{H}},$$

where

$$P_{\mathcal{D}} = \{ P_f | P_f \varphi = f \in \mathcal{D} \} .$$

By this definition

$$||\hat{A}||_{\mathcal{D}} = ||\hat{A}||_{\mathcal{H}_{\mathcal{D}}} .$$

Let us introduce the compliment space

$$\mathcal{H} \setminus \mathcal{H}_j = \bigotimes_{i(\neq j)} \mathcal{H}_i \tag{9.7}$$

and define the partially traced operator

$$\hat{A}_j \equiv \operatorname{Tr}_{\mathcal{H} \setminus \mathcal{H}_j} \hat{A} . \tag{9.8}$$

Then we construct the *factor operator* 

$$\hat{A}^{\otimes} \equiv \frac{\operatorname{Tr}_{\mathcal{H}}\hat{A}}{\operatorname{Tr}_{\mathcal{D}}\bigotimes_{j}\hat{A}_{j}}\bigotimes_{j}\hat{A}_{j} , \qquad (9.9)$$

for which

$$\operatorname{Tr}_{\mathcal{D}}\hat{A}^{\otimes} = \operatorname{Tr}_{\mathcal{H}}\hat{A}$$

The measure of entanglement generated by the operator  $\hat{A}$  is defined [460,461] as

$$\varepsilon(\hat{A}) \equiv \log \; \frac{||\hat{A}||_{\mathcal{D}}}{||\hat{A}^{\otimes}||_{\mathcal{D}}} , \qquad (9.10)$$

where *log* is to the base two. This measure can be employed for any operator possessing a trace. For example, one can consider how much entanglement is produced by a Hamiltonian in a finite Hilbert space. More often, one is interested in the level of entanglement produced by a statistical operator.

### 9.2 Topological Modes

To realize any scheme of information processing it is necessary to possess objects that could be transferred into different quantum states. In the case of cold atoms, these could be internal atomic states [17]. Another possibility is to generate topological coherent modes in BEC, as suggested in Ref. [174]. Various properties of these modes, representing nonground-state Bose condensates, have been studied in several papers [174–196,462-466]. The generation of such modes can be accomplished in two ways. One method is the modulation of the trapping potential with the frequency in resonance with the transition frequency between two coherent modes [174–176]. The other way, as has been mentioned in Refs. [189,190,192] and analysed in Ref. [464], is by the resonant modulation of the atomic scattering length. Both these techniques are illustrated below.

Let us consider a deep lattice, in each site of which there are many Bose atoms. Optical lattices with large filling factors, reaching  $\nu \sim 10^4$ , are readily available in experiment [22,23]. All atoms inside a lattice site can be made well localized, with the intersite tunneling almost completely suppressed. Temperature can be kept low, so that practically all atoms piling down to BEC.

Since lattice sites are very deep, we can start the consideration from a single site, representing a kind of a trap. At low temperature and weak interactions, the system inside the trap is described by the condensate wave function satisfying the Gross-Pitaevskii equation

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left[ -\frac{\nabla^2}{2m} + U(\mathbf{r}, t) - \mu_0 + \Phi_0(t) |\eta(\mathbf{r}, t)|^2 \right] \eta(\mathbf{r}, t) .$$
(9.11)

The condensate wave function is normalized to the number of atoms inside the trap, that is, to the filling factor

$$\int |\eta(\mathbf{r},t)|^2 \, d\mathbf{r} = \nu \;. \tag{9.12}$$

The external potential

$$U(\mathbf{r},t) = U(\mathbf{r}) + V(\mathbf{r},t)$$
(9.13)

consists of a trapping potential  $U(\mathbf{r})$ , characterizing the optical potential at the considered lattice site, and of an additional modulating potential  $V(\mathbf{r}, t)$ . The interaction strength can also be made time-dependent by means of the Feshbach resonance techniques.

For convenience, one can use the relation

$$\eta(\mathbf{r},t) \equiv \sqrt{\nu} \,\varphi(\mathbf{r},t) \;, \tag{9.14}$$

defining the function  $\varphi(\mathbf{r}, t)$  normalized to one,

$$\int |\varphi(\mathbf{r},t)|^2 \, d\mathbf{r} = 1 \,. \tag{9.15}$$

Then Eq. (9.11) reads as

$$i \frac{\partial}{\partial t} \varphi(\mathbf{r}, t) = \left[ -\frac{\nabla^2}{2m} + U(\mathbf{r}, t) - \mu_0 + \nu \Phi_0(t) |\varphi(\mathbf{r}, t)|^2 \right] \varphi(\mathbf{r}, t) .$$
(9.16)

For a stationary case, when there is no modulating field,  $V(\mathbf{r}, t) = 0$ , and atomic interactions are constant,  $\Phi_0(t) = \Phi_0$ , Eq. (9.16) becomes

$$i \frac{\partial}{\partial t} \varphi_n(\mathbf{r}, t) = \left[ -\frac{\nabla^2}{2m} + U(\mathbf{r}) - \mu_0 + \nu \Phi_0 |\varphi_n(\mathbf{r}, t)|^2 \right] \varphi_n(\mathbf{r}, t) , \qquad (9.17)$$

where a multi-index n enumerates quantum states. In stationary solutions, the spatial and temporal variables can be separated as follows:

$$\varphi_n(\mathbf{r},t) = \varphi_n(\mathbf{r})e^{-i\omega_n t} . \qquad (9.18)$$

As a result, Eq. (9.17) reduces to the eigenproblem

$$\left[-\frac{\nabla^2}{2m} + U(\mathbf{r}) + \nu \Phi_0 |\varphi_n(\mathbf{r})|^2\right] \varphi_n(\mathbf{r}) = E_n \varphi_n(\mathbf{r}) , \qquad (9.19)$$

in which the eigenvalues

$$E_n \equiv \omega_n + \mu_0 \tag{9.20}$$

have the property

$$\min_n E_n = \mu_0 , \qquad \min_n \omega_n = 0 .$$

The eigenfunctions  $\varphi_n(\mathbf{r})$  of Eq. (9.19) are the *topological coherent modes* [174–176]. Equally, the condensate functions

$$\eta_n(\mathbf{r}) = \sqrt{\nu} \,\varphi_n(\mathbf{r}) \tag{9.21}$$

can also be called the topological coherent modes. The condensate function (9.21), corresponding to the lowest energy  $E_n = \mu_0$ , characterizes the standard BEC. The higher modes of  $\eta_n(\mathbf{r})$  describe the *nonground-state condensates* [174–176]. The functions  $\varphi_n(\mathbf{r})$  and  $\eta_n(\mathbf{r})$ differ solely by their normalizations

$$\int |\varphi_n(\mathbf{r})|^2 d\mathbf{r} = 1 , \qquad \int |\eta_n(\mathbf{r})|^2 d\mathbf{r} = \nu .$$

In equilibrium, only the standard BEC is realized. To produce the macroscopic occupation of the higher levels, it is necessary to apply additional fields making the system nonequilibrium.

The modulating trapping potential can be taken in the form

$$V(\mathbf{r},t) = V_1(\mathbf{r})\cos\omega t + V_2(\mathbf{r})\sin\omega t . \qquad (9.22)$$

Similarly, the interaction strength can be made time-dependent as

$$\Phi_0(t) = \Phi_0 + \varepsilon_1 \cos \omega t + \varepsilon_2 \sin \omega t . \qquad (9.23)$$

It is of principal importance to choose the frequency of the alternating potentials to be tuned to a resonance with a transition frequency related to the energy levels we wish to connect. Let us consider two energy levels,  $E_1$  and  $E_2$ , with the transition frequency being

$$\omega_{21} \equiv E_2 - E_1 . \tag{9.24}$$

Then the resonance condition is

$$\left|\frac{\Delta\omega}{\omega_{21}}\right| \ll 1 \qquad (\Delta\omega \equiv \omega - \omega_{21}) . \tag{9.25}$$

For instance,  $E_1$  can correspond to the lowest energy level, equal to  $\mu_0$ .

We can look for the solution to the temporal Eq. (9.16) in the form of the expansion over the coherent modes,

$$\varphi(\mathbf{r},t) = \sum_{n} c_n(t)\varphi_n(\mathbf{r},t) . \qquad (9.26)$$

The coefficient functions can be treated as slow in time, compared to the exponential oscillations in Eq. (9.18), such that

$$\frac{1}{\omega_n} \left| \frac{dc_n}{dt} \right| \ll 1.$$
(9.27)

The latter condition requires that atomic interactions and the pumping alternating fields would not be too strong, which is easily realized in experiment [174–176,182]. The normalization condition

$$\sum_{n} |c_n(t)|^2 = 1 \tag{9.28}$$

is assumed.

When there are two time scales, one can resort to the averaging techniques [236,237] and to the scale separation approach [240–242]. To this end, we substitute expansion (9.26) into Eq. (9.16), multiply the latter by  $\varphi_n^*(\mathbf{r}, t)$ , integrate over  $\mathbf{r}$ , and accomplish the time averaging according to the rule

$$\{f(t)\}_t \equiv \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau f(t) dt$$
, (9.29)

where the slow variables are kept as quasi-integrals of motion [240–242]. For example, averaging (9.29) gives

$$\left\{e^{i(\omega_m-\omega_n)t}\right\}_t = \delta_{mn} ,$$

from where

$$\{\varphi_m^*(\mathbf{r},t)\varphi_n(\mathbf{r},t)\}_t = \delta_{mn}|\varphi_n(\mathbf{r})|^2$$

Therefore, the functions  $\varphi_n(\mathbf{r}, t)$  are orthogonal on average, though the functions  $\varphi_n(\mathbf{r})$  can be not orthogonal. Also, we have

$$\left\{e^{i(\omega_m+\omega_n-\omega_k-\omega_p)t}\right\}_t = \delta_{mk}\delta_{np} + \delta_{mp}\delta_{nk} - \delta_{mk}\delta_{np}\delta_{mn} \; .$$

Let us introduce the notation for the matrix elements of the interaction

$$\alpha_{mn} \equiv \nu \Phi_0 \int |\varphi_m(\mathbf{r})|^2 \left[ 2|\varphi_n(\mathbf{r})|^2 - |\varphi_m(\mathbf{r})|^2 \right] d\mathbf{r} , \qquad (9.30)$$

of the pumping potential

$$\beta_{mn} \equiv \int \varphi_m^*(\mathbf{r}) [V_1(\mathbf{r}) - iV_2(\mathbf{r})] \varphi_n(\mathbf{r}) \, d\mathbf{r} \,, \qquad (9.31)$$

and of the interaction modulation

$$\gamma_n \equiv \nu(\varepsilon_1 - i\varepsilon_2) \int \varphi_1^*(\mathbf{r}) |\varphi_n(\mathbf{r})|^2 \varphi_2(\mathbf{r}) \, d\mathbf{r} \,. \tag{9.32}$$

Then Eq. (9.16) yields

$$i \frac{dc_n}{dt} = \sum_{m(\neq n)} \alpha_{nm} |c_m|^2 c_n + \frac{1}{2} \delta_{n1} e^{i\Delta\omega t} \left[ 2 \sum_{m(\neq 2)} \gamma_m |c_m|^2 c_2 + \gamma_2 |c_2|^2 c_2 + \beta_{12} c_2 \right] + \frac{1}{2} \delta_{n1} e^{-i\Delta\omega t} \gamma_1^* c_2^* c_1^2 + \frac{1}{2} \delta_{n2} e^{-i\Delta\omega t} \left[ 2 \sum_{m(\neq 1)} \gamma_m^* |c_m|^2 c_1 + \gamma_1^* |c_1|^2 c_1 + \beta_{12}^* c_1 \right] + \frac{1}{2} \delta_{n2} e^{i\Delta\omega t} \gamma_2 c_1^* c_2^2 .$$
(9.33)

It is not difficult to notice [182] that, if at the initial time t = 0,  $c_n(0) = 0$  for  $n \neq 1, 2$ , then  $c_n(t) = 0$  for all  $t \ge 0$  and  $n \ne 1, 2$ . Hence Eq. (9.33) can be separated into two equations

$$i \frac{dc_1}{dt} = \alpha_{12} |c_2|^2 c_1 + \frac{1}{2} e^{i\Delta\omega t} \left( 2\gamma_1 |c_1|^2 c_2 + \gamma_2 |c_2|^2 c_2 + \beta_{12} c_2 \right) + \frac{1}{2} e^{-i\Delta\omega t} \gamma_1^* c_2^* c_1^2 ,$$
  
$$i \frac{dc_2}{dt} = \alpha_{21} |c_1|^2 c_2 + \frac{1}{2} e^{-i\Delta\omega t} \left( 2\gamma_2^* |c_2|^2 c_1 + \gamma_1^* |c_1|^2 c_1 + \beta_{12}^* c_1 \right) + \frac{1}{2} e^{i\Delta\omega t} \gamma_2 c_1^* c_2^2 .$$
(9.34)

The solutions to these equations define the temporal behavior of the *fractional mode populations* 

$$p_n(t) \equiv |c_n(t)|^2$$
 (9.35)

The properties of Eqs. (9.34) have been studied in detail for the case of the mode generation by means of the trapping-potential modulation, when  $\beta_{12} \neq 0$  while  $\gamma_n = 0$ , in Refs. [174–176,179,180,182,184–186,192–196]. The generalization for the case of the multiple mode generation has been given [189,190]. It has also been shown that the generation of the nonground-state condensate is achievable at nonzero temperature [193,465]. The creation of the topological coherent modes by the modulation of the interaction strength, when  $\beta_{12} = 0$ but  $\gamma_n \neq 0$ , is considered in Ref. [464].

#### 9.3 Coherent States

Now let us turn to the situation, when there is a lattice with  $N_L$  sites. In each site a deep well is formed by an optical potential. The number of atoms in a *j*-lattice site is  $\nu_j \gg 1$ . For an ideal lattice, the filling factor  $\nu_j$  does not depend on the site index. But, in general, the lattice can be nonideal. Then  $\nu_j$  can be different for different sites.

By employing the resonant generation, described in the previous section, one can excite in the *j*-site the topological coherent modes labelled by a multi-index  $n_j$ . Suppose that  $\eta_{n_j}$  are the coherent fields associated with the *j*-site and normalized to the corresponding occupation number

$$\int |\eta_{n_j}(\mathbf{r})|^2 \, d\mathbf{r} = \nu_j \,. \tag{9.36}$$

Similarly to Eq. (9.21), we can also define the functions  $\varphi_{n_j}(\mathbf{r})$  normalized to one, such that

$$\eta_{n_j}(\mathbf{r}) = \sqrt{\nu_j} \,\varphi_{n_j}(\mathbf{r}) \,. \tag{9.37}$$

Being the solutions to the nonlinear Schrödinger equation of type (9.19), the coherent fields  $\eta_{n_i}(\mathbf{r})$  and  $\eta_{n_i}(\mathbf{r})$ , with  $i \neq j$ , are not, generally, orthogonal, that is, the scalar product

$$\int \eta_{n_i}^*(\mathbf{r})\eta_{n_j}(\mathbf{r}) \, d\mathbf{r} \equiv \nu_{ij} \tag{9.38}$$

is not necessarily zero for  $i \neq j$ . The diagonal quantity

$$\nu_{jj} = \nu_j \tag{9.39}$$

is the occupation number of the j-site.

In the Fock space, the coherent state, associated with the  $n_j$ -mode, is given by the column

$$|n_j \rangle = \left[ \frac{\exp(-\nu_j/2)}{\sqrt{n!}} \prod_{k=0}^n \eta_{n_j}(\mathbf{r}_k) \right] ,$$
 (9.40)

where n = 0, 1, 2, ... Expression (9.40) is the short-hand notation for the column state of the type

$$|m\rangle = e^{-\nu/2} \begin{bmatrix} 1 \\ \eta_{m}(\mathbf{r}_{1}) \\ \frac{1}{\sqrt{2!}} \eta_{m}(\mathbf{r}_{1})\eta_{m}(\mathbf{r}_{2}) \\ \cdot \\ \cdot \\ \frac{1}{\sqrt{n!}} \eta_{m}(\mathbf{r}_{1})\eta_{m}(\mathbf{r}_{2}) \dots \eta_{m}(\mathbf{r}_{n}) \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} .$$
(9.41)

The coherent states (9.40) are not necessarily orthogonal to each other, so that the scalar product

$$\langle n_i | n_j \rangle = \exp\left(-\frac{\nu_i + \nu_j}{2} + \nu_{ij}\right)$$

$$(9.42)$$

is not, in general, zero for  $i \neq j$ . But the coherent states (9.40) are normalized to one, since

$$< n_j | n_j > = 1$$
. (9.43)

However, as follows from Eqs. (9.38) and (9.42), the coherent states are asymptotically orthogonal [467,468] in the sense that

$$\langle n_i | n_j \rangle \simeq \delta_{ij} \qquad (\nu_i + \nu_j \gg 1) .$$
 (9.44)

They also are asymptotically complete in the weak sense,

$$\sum_{n_j} |n_j \rangle < n_j| \simeq 1 \qquad (\nu_i + \nu_j \gg 1) .$$
(9.45)

Therefore the states  $|\mathbf{n}\rangle$ , defined in Eq. (9.2), form the asymptotically orthogonal and complete basis  $\{|\mathbf{n}\rangle\}$  in the Hilbert space (9.3).

#### 9.4 Coherent-Mode Register

The topological coherent modes can be used as a tool for a quantum register of information processing. These modes possess a rich variety of interesting properties [174–196,462–466]. The most important, for the purpose of quantum information processing, is the feasibility of producing entangled states [192,467–469]. Entanglement production with topological coherent modes and its temporal evolution can be regulated by external fields [465,467–469].

The statistical state of a lattice with coherent modes generated in its lattice sites, is characterized by the statistical operator  $\hat{\rho}$  which can be expanded over the basis { $|\mathbf{n}\rangle$ } of the coherent states,

$$\hat{\rho} = \sum_{\mathbf{n}} p_{\mathbf{n}} |\mathbf{n}\rangle \langle \mathbf{n}| .$$
(9.46)

The normalization condition

$$\mathrm{Tr}_{\mathcal{H}}\hat{\rho} = \sum_{\mathbf{n}} p_{\mathbf{n}} = 1$$

is assumed. Following the procedure of Sec. 9.1, we construct the factor operator

$$\hat{\rho}^{\otimes} \equiv \bigotimes_{j} \hat{\rho}_{j} , \qquad \hat{\rho}_{j} \equiv \operatorname{Tr}_{\mathcal{H} \setminus \mathcal{H}_{j}} \hat{\rho} .$$
(9.47)

The normalization conditions are valid:

$$\operatorname{Tr}_{\mathcal{H}_j}\hat{\rho}_j = 1$$
  $\operatorname{Tr}_{\mathcal{H}}\hat{\rho}^{\otimes} = \prod_j \operatorname{Tr}_{\mathcal{H}_j}\hat{\rho}_j = 1$ ,

where

$$\hat{\rho}_j = \sum_{\mathbf{n}} p_{\mathbf{n}} |n_j > < n_j|$$

Using the measure of entanglement production (9.10), we define the level of entanglement produced by the statistical operator (9.46),

$$\varepsilon(\hat{\rho}) = \log \frac{||\hat{\rho}||_{\mathcal{D}}}{||\hat{\rho}^{\otimes}||_{\mathcal{D}}}.$$
(9.48)

Here

$$||\hat{\rho}||_{\mathcal{D}} = \sup_{\mathbf{n}} p_{\mathbf{n}} , \qquad ||\hat{\rho}_j||_{\mathcal{H}_j} = \sup_{n_j} \sum_{\mathbf{n}(\neq n_j)} p_{\mathbf{n}} , \qquad ||\hat{\rho}^{\otimes}||_{\mathcal{D}} = \prod_j ||\hat{\rho}_j||_{\mathcal{H}_j}$$

As a result, Eq. (9.48) yields

$$\varepsilon(\hat{\rho}) = \log \frac{\sup_{\mathbf{n}} p_{\mathbf{n}}}{\prod_{j} \sup_{n_{j}} \sum_{\mathbf{n}(\neq n_{j})} p_{\mathbf{n}}} \,.$$
(9.49)

Entanglement in the lattice is generated when

$$\sup_{\mathbf{n}} p_{\mathbf{n}} \neq \prod_{j} \sup_{n_{j}} \sum_{\mathbf{n}(\neq n_{j})} p_{\mathbf{n}} ,$$

that is, when the lattice sites are somehow correlated. There are several sources of their correlation. First, this is the common history of the condensate preparation. Second, the lattice sites are never completely independent, but there always exists at least a weak tunneling. Third, atoms from different sites do interact, even though this interaction can be rather weak. Finally, the modulating resonant fields, producing the coherent modes, can be common for all sites of the lattice. The maximal correlation between the modes from different sites happens when all sites are identical and modulated synchronously, so that

$$p_{\mathbf{n}} = p_n \prod_j \delta_{nn_j} \; .$$

Then the statistical operator (9.46) is

$$\hat{\rho} = \sum_{n} p_n |nn \dots n| < nn \dots n|$$

And we have

$$\sup_{\mathbf{n}} p_{\mathbf{n}} = p_n , \qquad \sum_{\mathbf{n}(\neq n_j)} p_{\mathbf{n}} = p_n \delta_{nn_j} , \qquad \sup_{n_j} p_n \delta_{nn_j} = p_n .$$

The entanglement-production measure (9.49) reduces to

$$\varepsilon(\hat{\rho}) = -(N_L - 1) \log \sup_{n} p_n .$$
(9.50)

The quantity  $p_n = p_n(t)$  is the same as in Eq. (9.35), hence, is defined by the evolution equations (9.34). If the number of sites  $N_L$  is large, measure (9.50) can be made very large. Since the value  $p_n(t)$  can be regulated, the evolution of measure (9.50) can also be regulated [465,467,469], thus, allowing for the realization of the coherent-mode lattice register.

The specific features of the coherent-mode register are:

(i) The working objects, multimode condensates, are mesoscopic. Entanglement is accomplished for these mesoscopic objects, but not for separate particles.

(ii) A very strong level of entanglement can be produced, when  $\varepsilon(\hat{\rho}) \sim N_L \gg 1$ .

(iii) The computation dimension is very large. For  $N_L$  lattice sites, with M modes in each, the computation dimension is  $M^{N_L}$ . Thus, for two modes (M = 2) in a lattice of  $N_L = 100$  sites, the computation dimension is  $10^{30}$ .

(iv) The properties of the lattice, the strength of atomic interactions, and the resonant modulating fields can be varied in a very wide range, thus, making the mode register highly controllable.

(v) It is feasible to organize parallel computation by producing operations in different parts of the lattice.

(vi) Erasing memory is a simple process that can be done by appropriately varying the modulating fields.

(vii) The decoherence time is sufficiently long. Estimates [182,465] give it of the order of 10 - 100 seconds.

#### 9.5 Double-Well Register

Double-well lattices are considered as a very promising tool for quantum information processing and quantum computing. Recently, such double-well lattices have been realized experimentally in two-dimensional [420] and three-dimensional [470–474] configurations. The lattices were loaded by <sup>87</sup>Rb atoms. The total number of lattice sites was around  $3 \times 10^3$ . The filling factor could be varied between one and about 200 atoms. The properties of the double wells, such as the barrier height, the distance between the wells, and the relative energy offset, could be dynamically controlled. The atoms could be transferred between the left and right wells in a controllable way.

The possibility of dynamically varying the properties of the double-well lattices allows for the regulation of their states and dynamics [475]. This controllable regulation is of high importance for realizing quantum information processing and quantum computing with double-well lattices. For the latter purpose, the lattices with the filling factor one seem to be the most appropriate. The properties of such double-well lattices are described in Chapter 8. Note that the double-well potentials can be made asymmetric, which provides additional possibilities for regulating the system properties [476].

Quantum information protocols hold the promise of technological applications unattainable by purely classical means. In order to realize both, the storage of quantum information and the faithful long-distance communication, combined systems of atoms interacting with photons seem to be good candidates [477]. It would be interesting to consider the interaction of coherent electromagnetic fields with atoms located at the cites of a double-well lattice.

## **10** Brief Concluding Remarks

The material, covered in the present review article, is so extensive that it would take too much space for a more or less detailed concluding discussion. And listing in short the considered topics would duplicate the Contents. Therefore, instead of having a concluding summary, the reader is advised to survey again the Contents. At the present time, optical lattices is a fastly developing field of research. There permanently appear new interesting results. For instance, density modulations in an elongated BEC with a disorder potential were observed [478]. The direct observation of the Anderson localization [358] of boson matter waves in a one-dimensional non-interacting BEC with disorder was announced [479,480]. The Anderson localization is a phenomenon typical of the ideal gases, while rather weak interactions destroy this effect [481].

The phenomenon of the Anderson localization occurs in real space. There exists an analogous effect, called the dynamical localization [482], happening in momentum space. Such a dynamical localization can be realized by means of the quasiperiodic kicked-rotator model [483].

Despite the variety of novel experimental observations, the basic theoretical points remain the same. In this review, the emphasis was exactly on the main theoretical ideas and methods. Therefore the material of this review should remain useful in future for any researcher in the field of optical lattices.

Many techniques, related to periodic potentials, like those treated in the review, are actually common for Bose as well as for Fermi systems. Although the physics of the latter, in many respects, is different. The most detailed description of the state of the art of ultracold Fermi gases has recently been given by Ketterle and Zwierlein [484] (see also [15,485]).

In conclusion, it is worth mentioning that many properties of trapped atoms are similar to those of particles in quantum dots, finite nuclei, and clusters. The discussion of the latter systems can be found in the review articles [486–490].

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