Topical Review

Dipolar and spinor bosonic systems

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Received 28 September 2017
Accepted for publication 3 October 2017
Published 11 April 2018

Abstract
The main properties and methods of describing dipolar and spinor atomic systems, composed of bosonic atoms or molecules, are reviewed. The general approach for the correct treatment of Bose-condensed atomic systems with nonlocal interaction potentials is explained. The approach is applied to Bose-condensed systems with dipolar interaction potentials. The properties of systems with spinor interaction potentials are described. Trapped atoms and atoms in optical lattices are considered. Effective spin Hamiltonians for atoms in optical lattices are derived. The possibility of spintronics with cold atom is emphasized. The present review differs from the previous review articles by concentrating on a thorough presentation of basic theoretical points, helping the reader to better follow mathematical details and to make clearer physical conclusions.

Keywords: cold atoms, dipolar interactions, spinor interactions, Bose–Einstein condensate, optical lattices, effective spin Hamiltonians, spintronics with cold atoms

(Some figures may appear in colour only in the online journal)

1. Introduction

Cold atomic and molecular bosonic systems have recently been the objects of intensive research, both experimental and theoretical. First, the attention has been concentrated on dilute systems, composed of particles characterized by local interaction potentials, independent of spins, whose properties are well described by the $s$-wave scattering length. There are several books [1–4] and review articles [5–19] covering different aspects of such bosonic systems with spin-independent local interaction potentials.

In the present review, bosonic atoms or molecules are treated interacting through nonlocal interaction potentials, such as dipolar potential, and interacting through spinor forces that are local but depending on the effective spins related to hyperfine states. Although there exist reviews devoted to dipolar [20–25] and spinor [26, 27] systems (see also [3, 28]) the present paper differs from them in the following aspects. First, our aim here is not a brief enumeration of particular cases, numerical calculations, and different experiments, but the attention here is concentrated on the principal theoretical points allowing for the correct treatment of dipolar and spinor systems. Second, more attention is paid to the derivation of effective spin Hamiltonians for atoms and molecules in optical lattices. Third, the possibility of spintronics with cold atoms and molecules, interacting through dipolar and spinor forces, is discussed.

The exposition of the material is organized so that the main mathematical points be clear to the reader. More technical details can be found in the tutorials [29, 30]. Throughout the paper, the system of units is employed where the Boltzmann and Planck constants are set to one, $k_B = 1$ and $\hbar = 1$.

2. Nonlocal interaction potentials

2.1. General approach

The system of particles interacting through a nonlocal potential $\Phi(\mathbf{r})$ is described by the energy Hamiltonian
\[ \hat{H} = \int \hat{\psi}^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U(\mathbf{r})\right) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \int \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \, d\mathbf{r} d\mathbf{r}', \quad (2.1) \]

in which \( U = U(\mathbf{r}, t) \) is an external potential, generally, depending on spatial, \( \mathbf{r} \), and temporal, \( t \), variables. The field operators \( \hat{\psi}(\mathbf{r}) = \psi(\mathbf{r}, t) \) contain time that, for short, is not written explicitly. Bose–Einstein condensation is assumed.

When Bose–Einstein condensate appears in the system, the global gauge symmetry becomes broken, being the necessary and sufficient condition for Bose–Einstein condensation [1, 12, 18]. The gauge symmetry breaking is the most conveniently realized by the Bogolubov [31, 32] shift
\[ \hat{\psi}(\mathbf{r}) = \eta(\mathbf{r}) + \psi_1(\mathbf{r}), \quad (2.2) \]
where \( \eta(\mathbf{r}) \) is the condensate function and \( \psi_1(\mathbf{r}) \) is the operator of uncondensed particles. These variables are orthogonal to each other,
\[ \int \eta^\ast(\mathbf{r}) \psi_1(\mathbf{r}) \, d\mathbf{r} = 0. \quad (2.3) \]

Note that shift (2.2) is an exact canonical transformation, but not an approximation, as one sometimes incorrectly writes.

The condensate function plays the role of the system order parameter defined as the statistical average
\[ \eta(\mathbf{r}) = \langle \hat{\psi}(\mathbf{r}) \rangle, \quad (2.4) \]
which implies that
\[ \langle \psi_1(\mathbf{r}) \rangle = 0. \quad (2.5) \]

The condensate function is normalized to the number of condensed particles,
\[ N_0 = \int |\eta(\mathbf{r})|^2 \, d\mathbf{r}, \quad (2.6) \]
while the number of uncondensed particles is the average
\[ N_1 = \langle \hat{N}_1 \rangle \quad (2.7) \]
of the operator
\[ \hat{N}_1 = \int \psi_1^\dagger(\mathbf{r}) \psi_1(\mathbf{r}) \, d\mathbf{r} \quad (2.8) \]

More generally, condition (2.5) is represented as the average
\[ \langle \hat{\Lambda} \rangle = 0 \quad (2.9) \]
of the operator
\[ \hat{\Lambda} = \int \left[ \lambda(\mathbf{r}) \psi_1^\dagger(\mathbf{r}) + \lambda^\ast(\mathbf{r}) \psi_1(\mathbf{r}) \right] \, d\mathbf{r}. \quad (2.10) \]

The effective action functional, taking into account conditions (2.6), (2.7), and (2.9), is
\[ A[\eta, \psi_1] = \int \left[ \hat{L}[\hat{\psi}] + \mu_0 N_0 + \mu_1 \hat{N}_1 + \hat{\Lambda} \right] \, d\mathbf{r}, \quad (2.11) \]

with the Lagrangian
\[ \hat{L}[\hat{\psi}] = \int \hat{\psi}^\dagger(\mathbf{r}) \left(i \frac{\partial}{\partial t}\right) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} - \hat{H}. \quad (2.12) \]
The action functional can also be written as
\[ A[\eta, \psi_1] = \int L[\eta, \psi_1] \, d\mathbf{r}, \quad (2.13) \]
through the generalized Lagrangian
\[ L[\eta, \psi_1] = \int \hat{\psi}^\dagger(\mathbf{r}) \left(i \frac{\partial}{\partial t}\right) \hat{\psi}(\mathbf{r}) \, d\mathbf{r} - \hat{H}. \quad (2.14) \]

with the grand Hamiltonian
\[ \hat{H} = \hat{H} - \mu_0 N_0 - \mu_1 \hat{N}_1 - \hat{\Lambda}. \quad (2.15) \]
The quantities \( \mu_0, \mu_1, \) and \( \lambda(\mathbf{r}) \) play the role of Lagrange multipliers.

The evolution equations for the variables \( \eta(\mathbf{r}, t) \) and \( \psi_1(\mathbf{r}, t) \) are given by the extremization of the action functional:
\[ \left\langle \frac{\delta A[\eta, \psi_1]}{\delta \eta^\ast(\mathbf{r}, t)} \right\rangle = 0 \quad (2.16) \]
and
\[ \left\langle \frac{\delta A[\eta, \psi_1]}{\delta \psi_1^\dagger(\mathbf{r}, t)} \right\rangle = 0. \quad (2.17) \]
The extremization equations can be rewritten in the form
\[ i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left\langle \frac{\delta H}{\delta \eta^\ast(\mathbf{r}, t)} \right\rangle \quad (2.18) \]
and
\[ i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \frac{\delta H}{\delta \psi_1^\dagger(\mathbf{r}, t)}. \quad (2.19) \]

Note that the variational derivatives are related to commutators by the equation [18, 33]
\[ \frac{\delta H}{\delta \psi_1^\dagger(\mathbf{r}, t)} = [\psi_1(\mathbf{r}, t), \hat{H}]. \]

Hence equation (2.19) is equivalent to the Heisenberg equation of motion.

The above equations make it straightforward to derive the evolution equations for various operators. For instance, the evolution equation for the operator density of uncondensed particles is
\[ i \frac{\partial}{\partial t} \left[ \psi_1^\dagger(\mathbf{r}, t) \psi_1(\mathbf{r}, t) \right] = \left[ \psi_1^\dagger(\mathbf{r}, t) \psi_1(\mathbf{r}, t), \hat{H} \right] \]
\[ = \psi_1^\dagger(\mathbf{r}, t) \frac{\delta H}{\delta \psi_1^\dagger(\mathbf{r}, t)} - \frac{\delta H}{\delta \psi_1(\mathbf{r}, t)} \psi_1(\mathbf{r}, t). \quad (2.20) \]

2.2. Grand Hamiltonian

With the Bogolubov shift (2.2), the grand Hamiltonian (2.15) becomes the sum of five terms distinguished by the power of the operators \( \psi_1 \).
\[ H = \sum_{n=0}^{\infty} H^{(n)}. \]

The zero-order term contains no operators \( \psi_1 \),
\[ H^{(0)} = \int \eta^*(r) \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(r) \, dr + \frac{1}{2} \int \Phi(r - r')|\eta(r')|^2|\eta(r')|^2 \, dr \, dr'. \]

To satisfy condition (2.5), there should be no first-order terms with respect to \( \psi_1 \) in the Hamiltonian [34], so that
\[ H^{(1)} = 0, \]
which is achieved by fixing the Lagrange multiplier
\[ \lambda(r) = \left( -\frac{\nabla^2}{2m} + U \right) \eta(r) + \int \Phi(r - r')|\eta(r')|^2 \, dr', \]
The second-order term is
\[ H^{(2)} = \int \psi_1^\dagger(r) \left( -\frac{\nabla^2}{2m} + U - \mu_1 \right) \psi_1(r) \, dr + \int \Phi(r - r') \left[ |\eta(r')|^2 \psi_1^\dagger(r') \psi_1(r) + \eta^*(r) \eta(r') \psi_1^\dagger(r') \psi_1(r) \right. \]
\[ + \frac{1}{2} \eta(r) \eta^*(r') \psi_1^\dagger(r') \psi_1(r) \psi_1(r') \eta^*(r) \left] \, dr \, dr'. \]
The third-order term reads as
\[ H^{(3)} = \int \Phi(r - r') \left[ \eta^*(r) \psi_1^\dagger(r') \psi_1(r) \psi_1(r') \eta(r) \right. \]
\[ + \psi_1^\dagger(r) \psi_1^\dagger(r') \psi_1(r) \psi_1(r') \eta(r) \left] \, dr \, dr'. \]
And the fourth-order term becomes
\[ H^{(4)} = \frac{1}{2} \int \psi_1^\dagger(r) \psi_1^\dagger(r') \Phi(r - r') \psi_1(r') \psi_1(r) \, dr \, dr'. \]
The densities of condensed and uncondensed particles are
\[ \rho_0(r) \equiv |\eta(r)|^2, \quad \rho_1(r) \equiv \langle \psi_1^\dagger(r) \psi_1(r) \rangle. \]
The numbers of condensed and uncondensed particles are given by the integrals
\[ N_0 = \int \rho_0(r) \, dr, \quad N_1 = \int \rho_1(r) \, dr. \]
Respectively, the total particle density is
\[ \rho(r) = \rho_0(r) + \rho_1(r), \]
defining the total number of particles
\[ N = \int \rho(r) \, dr = N_0 + N_1. \]
In equilibrium, the condensate function does not depend on time and is real,
\[ \eta(r, t) = \eta(r) = \eta^*(r). \]
And, since
\[ \frac{\partial}{\partial t} \langle \psi_1^\dagger(r, t) \psi_1(r, t) \rangle = 0, \]
from equation (2.20) it follows that the correlation functions
\[ \langle \psi_1^\dagger(r) \psi_1(r') \rangle = \langle \psi_1^\dagger(r') \psi_1(r) \rangle, \]
\[ \langle \psi_1(r) \psi_1(r') \rangle = \langle \psi_1^\dagger(r') \psi_1(r) \rangle, \]
\[ \langle \psi_1^\dagger(r) \psi_1(r) \psi_1(r') \psi_1(r') \rangle = \langle \psi_1^\dagger(r') \psi_1(r') \psi_1(r) \psi_1(r) \rangle \]
are also real, provided all operators \( \psi_1 \) are taken at the same time \( t \).

### 2.3. Condensate function

The evolution equation for the condensate function is given by equation (2.18). This equation, with the notation for the single-particle density matrix
\[ \rho_1(r, r') \equiv \langle \psi_1^\dagger(r') \psi_1(r) \rangle, \]
the anomalous average
\[ \sigma_1(r, r') \equiv \langle \psi_1^\dagger(r') \psi_1(r) \rangle, \]
and for the anomalous average
\[ \xi(r, r') \equiv \langle \psi_1^\dagger(r') \psi_1(r) \psi_1(r') \psi_1(r) \rangle, \]
takes the form
\[ i \frac{\partial}{\partial t} \eta(r) \equiv \left( -\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(r) \]
\[ + \int \Phi(r - r') \left[ \rho(r') \eta(r) + \rho_1(r, r') \eta(r) + \sigma_1(r, r') \eta^*(r') + \xi(r, r') \right] \, dr'. \]
In equilibrium,
\[ \frac{\partial}{\partial t} \eta(r) = 0, \]
which yields the equation
\[ \mu_0 \eta(r) \equiv \left( -\frac{\nabla^2}{2m} + U \right) \eta(r) \]
\[ + \int \Phi(r - r') \left[ \rho(r') \eta(r) + \rho_1(r, r') \eta(r) + \sigma_1(r, r') \eta^*(r') + \xi(r, r') \right] \, dr'. \]
For a uniform system, without external potentials, the condensate function turns into a constant
\[ \eta(r) = \eta = \sqrt{\rho_0} \quad (U = 0). \]
The particle density is also a constant \( \rho(r) = \rho \), and equation (2.35) reduces to the equation
\[ \mu_0 \eta = \rho \Phi_0 \eta + \int \Phi(r) \left[ \rho_1(r, 0) \eta + \sigma_1(r, 0) \eta^* + \xi(r, 0) \right] \, dr, \]
in which
\[ \Phi_0 \equiv \int \Phi(r) \, dr, \]
assuming that the interaction potential is integrable.

In the Fock space $\mathcal{F}(\psi_1)$, generated by the field operator $\psi_1$, the vacuum state is defined by the requirement

$$\psi_1(r,t)|\eta\rangle = 0,$$  \hspace{1cm} (2.37)

from which it follows that the state $|\eta\rangle$ is the coherent state with respect to the filed operator $\psi$, since

$$\hat{\psi}(r,t)|\eta\rangle = \eta(r,t)|\eta\rangle.$$  \hspace{1cm} (2.38)

Thus, the condensate function has the meaning of the coherent state [29, 30].

The vacuum state $|\eta\rangle$ of the Fock space $\mathcal{F}(\psi_1)$ is the eigenstate of the grand Hamiltonian (2.21),

$$H|\eta\rangle = H^{(0)}|\eta\rangle,$$  \hspace{1cm} (2.39)

with $H^{(0)}$ being the eigenvalue.

It is important to stress that the Fock space $\mathcal{F}(\psi_1)$, where the gauge symmetry is broken, is principally different from the Fock space $\mathcal{F}(\psi)$, without gauge symmetry breaking, generated by the field operator $\psi$ for which the Bogolubov shift is not applicable. In the Fock space $\mathcal{F}(\psi)$, without the symmetry breaking, the Hamiltonian $H[\psi]$ has the same form (2.1), but its eigenstates, given by the eigenproblem

$$H[\psi]|n\rangle = E_n|n\rangle,$$

are different from the state $|\eta\rangle$. The latter is not an eigenstate of $H[\psi]$. Actually, the Fock spaces $\mathcal{F}(\psi_1)$ and $\mathcal{F}(\psi)$ are orthogonal in thermodynamic limit [30, 35]. So, the states $|n\rangle$, pertaining to $\mathcal{F}(\psi)$, and $|\eta\rangle$, pertaining to the orthogonal Fock space $\mathcal{F}(\psi_1)$, are also orthogonal.

Averaging equation (2.18) over the vacuum coherent state $|\eta\rangle$ yields the equation for the vacuum coherent field

$$\frac{i}{\hbar}\frac{\partial}{\partial t} \eta(r,t) = \left(-\frac{\nabla^2}{2m} + U - \mu_0\right) \eta(r,t) + \int \Phi(r-r')|\eta(r',t)\rangle^2|\eta(r,t)\rangle \, dr'.$$  \hspace{1cm} (2.40)

As is evident, the equation for the vacuum coherent field (2.40) differs from the equation (2.34) for the condensate function that is a coherent field, but, generally, not the vacuum coherent field. Equation (2.40) is a particular case of (2.34), where there are no uncondensed particles, so that $\rho_1$, $\sigma_1$, as well as $\xi$, are zero.

One often confuses equation (2.40) for the vacuum coherent field with mean-filed approximation. This is not correct. The mean-field approximation for a Bose-condensed system is the Hartree–Fock–Bogolubov approximation, where $\xi$ is zero, but $\rho_1$ and $\sigma_1$ are not [29, 30].

By its mathematical structure, the vacuum coherent field equation (2.40) is the nonlinear Schrödinger (NLS) equation. First, equation (2.40) was advanced by Bogolubov [36] in his well known Lectures on Quantum Statistics published in 1949 and then republished numerous times (e.g. [31, 32]). Solutions to this equation have been studied in many papers starting from [37–43].

2.4. Mean-field approximation

The mean-field approximation for a system with Bose–Einstein condensate is the Hartree–Fock–Bogolubov (HFB) approximation, whose details are thoroughly expounded in [29, 30]. In this approximation, Hamiltonian (2.21) becomes

$$H_{\text{HFB}} = H_{\text{HFB}}^0 + \int \psi_{1\dagger}(r) \left(-\frac{\nabla^2}{2m} + U - \mu_1\right) \psi_1(r) \, dr$$

$$+ \int \Phi(r-r') \left[\rho(r')\psi_{1\dagger}(r)\psi_1(r) + \rho(r', r')\psi_{1\dagger}(r)\psi_1(r)\right] \, drdr',$$  \hspace{1cm} (2.41)

where the first term is

$$E_{\text{HFB}} = H^{(0)} - \frac{1}{2} \int \Phi(r-r') |\rho_1(r)\rho_1(r')|$$

$$+ |\rho_1(r, r')|^2 + |\sigma_1(r, r')|^2 \, drdr',$$  \hspace{1cm} (2.42)

with the notations

$$\rho(r, r') \equiv \eta(r)\eta^*(r') + \rho_1(r, r')$$  \hspace{1cm} (2.43)

and

$$\sigma(r, r') \equiv \eta(r)\eta^*(r') + \sigma_1(r, r').$$  \hspace{1cm} (2.44)

The condensate-function equation (2.34) in the Hartree–Fock–Bogolubov approximation reads as

$$i \frac{\partial}{\partial t} \eta(r) = \left(-\frac{\nabla^2}{2m} + U - \mu_0\right) \eta(r)$$

$$+ \int \Phi(r-r') |\rho(r')\eta(r) + \rho_1(r, r')\eta(r') + \sigma_1(r, r')\eta^*(r')| \, dr'.$$  \hspace{1cm} (2.45)

Here, generally, the quantities $\rho_1$ and $\sigma_1$ are not zero.

In equilibrium, this equation reduces to the equation

$$\mu_0 \eta(r) = \left(-\frac{\nabla^2}{2m} + U\right) \eta(r)$$

$$+ \int \Phi(r-r') |\rho(r')\eta(r) + \rho_1(r, r')\eta(r') + \sigma_1(r, r')\eta^*(r')| \, dr'.$$  \hspace{1cm} (2.46)

For a uniform system, when $U = 0$, the latter equation becomes

$$\mu_0 = \rho \Phi_0 + \int \Phi(r) [\rho_1(r, 0) + \sigma_1(r, 0)] \, dr.$$  \hspace{1cm} (2.47)

The Hamiltonian (2.41) can be diagonalized by means of the Bogolubov canonical transformations

$$\psi_1(r) = \sum_k [b_k u_k(r) + b_k^\dagger v_k(r)]$$  \hspace{1cm} (2.48)

and
where \( k \) is a multi-index. Since the field operators \( \psi_1 \), as well as \( b_k \), obey the Bose-Einstein statistics, we have the equations
\[
\begin{align*}
\sum_k [u_k(r)u_k^*(r') - v_k^*(r)v_k(r')] &= \delta(r-r'), \\
\sum_k [u_k(r)v_k^*(r') - v_k(r)u_k(r')] &= 0,
\end{align*}
\]
and
\[
\begin{align*}
\int [u_k^*(r)\psi_p(r) - v_k^*(r)\psi_p(r)] \, dr &= \delta_{kp}, \\
\int [u_k(r)v_p(r) - v_k(r)\psi_p(r)] \, dr &= 0.
\end{align*}
\]

For convenience, we introduce the notations
\[
\omega(r, r') = \left[ -\frac{\nabla^2}{2m} + U(r) - \mu_1 + \int \Phi(r-r')\rho(r') \, dr' \right] \delta(r-r')
\]
and
\[
\Delta(r-r') \equiv \Phi(r-r')\sigma(r, r').
\]
Hamiltonian (2.41) is diagonalized under the Bogolubov equations
\[
\int [\omega(r, r')u_k(r') + \Delta(r-r')v_k(r')] \, dr' = \varepsilon_k u_k(r),
\]
\[
\int [\omega^*(r, r')v_k^*(r') + \Delta^*(r-r')u_k(r')] \, dr' = -\varepsilon_k v_k(r).
\]
As a result, Hamiltonian (2.41) reduces to the Bogolubov form
\[
H_B = E_B + \sum_k \varepsilon_k b_k^\dagger b_k,
\]
in which
\[
E_B = E_{\text{HFB}} - \sum_k \varepsilon_k \int |v_k(r)|^2 \, dr.
\]

2.5. Uniform system
In the absence of external potentials, the system is uniform, and the field operator can be expanded over plane waves,
\[
\psi_1(r) = \frac{1}{\sqrt{V}} \sum_{k \neq 0} a_k e^{ik \cdot r},
\]
with \( V \) being the system volume (or quantization volume). Assuming that the interaction potential can be Fourier-transformed, one has
\[
\Phi(r) = \frac{1}{V} \sum_k \Phi_k e^{ik \cdot r}, \quad \Phi_k = \int \Phi(r) e^{-ik \cdot r} \, dr.
\]
The long-wave limit of the Fourier transform, defined as
\[
\lim_{k \to 0} \Phi_k = \int \lim_{k \to 0} \Phi(r) e^{-ik \cdot r} \, dr,
\]
gives the limiting value
\[
\Phi_0 = \lim_{k \to 0} \Phi_k = \int \Phi(r) \, dr.
\]
Conditions, imposed on the interaction potential, allowing for the existence of its Fourier transform are discussed in [44].

The single-particle density matrix becomes
\[
\rho_1(r, r') = \frac{1}{V} \sum_{k \neq 0} n_k e^{ik \cdot (r-r')},
\]
where
\[
n_k = \langle a_k^\dagger a_k \rangle \quad (2.65)
\]
is the momentum distribution of particles. The anomalous matrix reads as
\[
\sigma_1(r, r') = \frac{1}{V} \sum_{k \neq 0} \sigma_k e^{i k \cdot (r-r')},
\]
with the anomalous average
\[
\sigma_k = \langle a_k a_{-k} \rangle. \quad (2.67)
\]
Recall that the absolute value of the diagonal element \( |\sigma_1(r)| \) describes the density of pair-correlated particles. Hence \( |\sigma_k| \) has the meaning of the momentum distribution of pair-correlated particles [30].

For a uniform system, the diagonal elements of the single-particle density matrix,
\[
\rho_1 \equiv \rho_1(r, r) = \frac{1}{V} \sum_{k \neq 0} n_k, \quad (2.68)
\]
and of the anomalous matrix,
\[
\sigma_1 \equiv \sigma_1(r, r) = \frac{1}{V} \sum_{k \neq 0} \sigma_k, \quad (2.69)
\]
do not depend on spatial variables. The total density is a constant
\[
\rho = \rho_0 + \rho_1 \quad (\rho_0 \equiv |\eta|^2). \quad (2.70)
\]
Passing to Fourier transforms in the Bogolubov equation (2.54), we get
\[
\omega_k = \frac{k^2}{2m} + \rho \Phi_0 + \rho_0 \Phi_k + \frac{1}{V} \sum_{p \neq 0} n_p \Phi_{k+p} - \mu_1
\]  
and
\[
\Delta_k = \rho_0 \Phi_k + \frac{1}{V} \sum_{p \neq 0} \sigma_p \Phi_{k+p}.
\]  
(2.72)

This yields the spectrum of collective excitations
\[
\varepsilon_k = \sqrt{\omega_k^2 - \Delta_k^2}.
\]  
(2.73)

The momentum distribution (2.65) becomes
\[
n_k = \frac{\omega_k}{2\varepsilon_k} \coth \left( \frac{\varepsilon_k}{2T} \right) - \frac{1}{2},
\]  
(2.74)

and the anomalous average (2.67) is
\[
\sigma_k = -\frac{\Delta_k}{2\omega_k} \coth \left( \frac{\varepsilon_k}{2T} \right).
\]  
(2.75)

Here $T$ is temperature. Notice that $n_k$ and $\sigma_k$ are connected by the relation
\[
\sigma_k = -\frac{\Delta_k}{2\omega_k} \left( 1 + 2n_k \right).
\]

The condensate chemical potential (2.47) becomes
\[
\mu_0 = \rho \Phi_0 + \frac{1}{V} \sum_{k \neq 0} (n_k + \sigma_k) \Phi_k.
\]  
(2.76)

The condition for Bose condensate existence [17, 18, 30] tells us that in thermodynamic limit
\[
\lim_{k \to 0} \frac{n_k}{N} \propto \frac{1}{N} \rightarrow 0 \quad (n_k \geq 0, \ N \rightarrow \infty).
\]

This implies the condition
\[
\lim_{k \to 0} \varepsilon_k = 0 \quad (\varepsilon_k \geq 0).
\]  
(2.77)

In particular, from (2.74) it is seen that
\[
n_k \simeq \frac{T \omega_k}{\varepsilon_k} \quad (\varepsilon_k \rightarrow 0),
\]
where
\[
\omega_0 = \rho_0 \Phi_0 + \frac{1}{V} \sum_{p \neq 0} \sigma_p \Phi_p.
\]

Therefore
\[
\lim_{k \to 0} \varepsilon_k \propto \frac{1}{\sqrt{N}} \rightarrow 0 \quad (N \rightarrow \infty).
\]

A gapless spectrum of collective excitations in a system with global gauge symmetry breaking, agreeing with condition (2.77), is also required by the Hugenholtz-Pines [45] and Bogolubov [32] theorems. Equating $\varepsilon_k$ to zero at $k = 0$ results in the expression
\[
\mu_1 = \rho \Phi_0 + \frac{1}{V} \sum_{k \neq 0} (n_k - \sigma_k) \Phi_k.
\]  
(2.78)

Then equation (2.71) reduces to
\[
\omega_k = \frac{k^2}{2m} + \rho_0 \Phi_k + \frac{1}{V} \sum_{p \neq 0} (n_p \Phi_{k+p} - n_p \Phi_p + \sigma_p \Phi_p).
\]  
(2.79)

The spectrum of collective excitations (2.73) is defined by the equation
\[
\varepsilon_k^2 = \left[ \frac{k^2}{2m} + \frac{1}{V} \sum_{p \neq 0} (n_p - \sigma_p) (\Phi_{k+p} - \Phi_p) \right] \times \left\{ \frac{k^2}{2m} + 2\rho_0 \Phi_k + \frac{1}{V} \sum_{p \neq 0} [(n_p + \sigma_p) \Phi_{k+p} - (n_p - \sigma_p) \Phi_p] \right\}.
\]  
(2.80)

It is important to stress that the anomalous average $\sigma_k$ is either zero or not together with the condensate density. Thus if $\sigma_k \rightarrow 0$, then, according to (2.75), we have $\Delta_k \rightarrow 0$. Then (2.72) gives $\rho_0 \rightarrow 0$. That is, the assumption that the anomalous average is zero is equivalent to stating that there is no condensate in the system,
\[
\rho_0 = 0 \quad (\sigma_k = 0).
\]  
(2.81)

To simplify the above formulas, it is possible to make the approximation that can be called the central-peak approximation [44]. Taking into account that $n_p$ and $\sigma_p$ are maximal at $p = 0$, we may write
\[
\sum_{p} n_p \Phi_{k+p} \simeq \Phi_k \sum_{p} n_p, \quad \sum_{p} \sigma_p \Phi_{k+p} \simeq \Phi_k \sum_{p} \sigma_p.
\]  
(2.82)

Of course, this approximation is sensible provided that it does not result in unphysical divergences that cannot be regularized.

Then the chemical potentials (2.76) and (2.78) reduce to the form
\[
\mu_0 = (\rho + \rho_1 + \sigma_1) \Phi_0, \quad \mu_1 = (\rho + \rho_1 - \sigma_1) \Phi_0.
\]  
(2.83)

Equations (2.79) and (2.72) become
\[
\omega_k = \frac{k^2}{2m} + \rho \Phi_k - (\rho_1 - \sigma_1) \Phi_0, \quad \Delta_k = (\rho_0 + \sigma_1) \Phi_k.
\]  
(2.84)

And for the spectrum of collective excitations in (2.80), we obtain
\[
\varepsilon_k^2 = \left[ \frac{k^2}{2m} + (\rho_1 - \sigma_1) (\Phi_k - \Phi_0) \right] \times \left\{ \frac{k^2}{2m} + (\rho_0 + \rho_1 + \sigma_1) \Phi_k - (\rho_1 - \sigma_1) \Phi_0 \right\}.
\]  
(2.85)

2.6. Thermodynamic characteristics

The grand thermodynamic potential
\[
\Omega = -T \ln \text{Tr} \ e^{-\beta H} \quad (\beta T = 1)
\]  
(2.86)

defines the pressure
\[
p = -\frac{\Omega}{V} = -\frac{T}{V} \ln \text{Tr} \ e^{-\beta H}.
\]  
(2.87)
The latter equation is termed the equation of state. In the HFB approximation, one has

\[ \Omega = E_B + T \sum_k \ln \left(1 - e^{-\beta \epsilon_k}\right), \]  

(2.88)

where

\[ E_B = -\frac{1}{2} N \rho \Phi_0 - \rho_0 \sum_p (n_p + \sigma_p) \Phi_p \]

\[ -\frac{1}{2V} \sum_{kp} (n_k \sigma_k + \sigma_k \sigma_p) \Phi_{k+p} + \frac{1}{2} \sum_k (\epsilon_k - \omega_k). \]

(2.89)

Employing the central-peak approximation (2.82) gives

\[ E_B = -\frac{1}{2} V \Phi_0 \left[ \rho^2 + 2 \rho_0 (\rho_1 + \sigma_1) + \rho_1^2 + \sigma_1^2 \right] + \frac{1}{2} \sum_k (\epsilon_k - \omega_k). \]

(2.90)

The average of the grand Hamiltonian

\[ \langle H \rangle = \langle \hat{H} \rangle - \mu_0 N_0 - \mu_1 N_1 \]

(2.91)

can also be written as

\[ \langle H \rangle = \langle \hat{H} \rangle - \mu N, \]

(2.92)

which defines the system chemical potential

\[ \mu = \mu_0 n_0 + \mu_1 n_1, \]

(2.93)

in which the condensate fraction and the fraction of uncondensed particles are

\[ n_0 \equiv \frac{N_0}{N}, \quad n_1 \equiv \frac{N_1}{N}. \]

(2.94)

In the HFB approximation, the chemical potential reads as

\[ \mu = \rho \Phi_0 + \frac{1}{V} \sum_{k \neq 0} [n_k + (n_0 - n_1) \sigma] \epsilon_k. \]

(2.95)

And the central-peak approximation (2.82) gives

\[ \mu = \rho \Phi_0 [1 + n_1 (1 - \sigma) + n_0 \sigma], \]

where \( \sigma \equiv \sigma_1 / \rho. \)

### 2.7 Local-density approximation

When the external potential varies slowly in space (for details see reviews [18, 30]), one can extend the use of the formalism by assuming that the dependence on the spatial variable comes from the slowly varying local density. Then the local density of uncondensed particles reads as

\[ \rho_1 (r) = \frac{1}{V} \sum_{k \neq 0} n_k (r) \]

(2.96)

and the local anomalous average is

\[ \sigma_1 (r) = \frac{1}{V} \sum_{k \neq 0} \sigma_k (r). \]

(2.97)

In the HFB approximation, one has

\[ n_k (r) = \frac{\omega_k (r)}{2 \epsilon_k (r)} \coth \left[ \frac{\epsilon_k (r)}{2T} \right] - \frac{1}{2} \]

(2.98)
Summation over momentum, as usual, can be replaced by integrals. So, the density of uncondensed particles (2.96) can be written as
\[ \rho_1(\mathbf{r}) = \int n_k(\mathbf{r}) \frac{dk}{(2\pi)^3} \] (2.111)
and the anomalous average (2.97) as
\[ \sigma_1(\mathbf{r}) = \int \sigma_k(\mathbf{r}) \frac{dk}{(2\pi)^3}. \] (2.112)

The Fourier transform of the interaction potential is invariant with respect to the momentum inversion, \( \Phi_{-\mathbf{k}} = \Phi_{\mathbf{k}} \). But the interactions can be anisotropic. So the long-wave behavior of \( \Phi_{\mathbf{k}} \), generally, looks like
\[ \Phi_{\mathbf{k}} \approx \Phi_0 + \frac{1}{2} A_k k^2 \quad (k \to 0), \] (2.113)
where \( A_k \) is caused by the anisotropy of the interactions and is not expandable in powers of \( k \). Then the long-wave limit of spectrum, given by (2.110), reads as
\[ \varepsilon_k^2(\mathbf{r}) \approx c_k^2(\mathbf{r}) k^2 \]
\[ + \{1 + [\rho_1(\mathbf{r}) - \sigma_1(\mathbf{r})] m A_k\} \{1 + [\rho_0(\mathbf{r}) + \rho_1(\mathbf{r}) + \sigma_1(\mathbf{r})] m A_k\} \left( \frac{k^2}{2m} \right)^2. \] (2.114)
with the sound velocity defined by the equation
\[ c_k^2(\mathbf{r}) = \frac{\Phi_0}{m} [\rho_0(\mathbf{r}) + \sigma_1(\mathbf{r})] \{1 + [\rho_1(\mathbf{r}) - \sigma_1(\mathbf{r})] A_k\}. \] (2.115)

2.8. Grand potential

In the local-density approximation, the grand thermodynamic potential
\[ \Omega = - \int p(\mathbf{r}) \, d\mathbf{r} \] (2.116)
is the integral over the local pressure
\[ p(\mathbf{r}) = -E_B(\mathbf{r}) - T \int \ln[1 - \exp\{-\beta \varepsilon_k(\mathbf{r})\}] \frac{dk}{(2\pi)^3}, \] (2.117)
where
\[ E_B(\mathbf{r}) = -\frac{1}{2} \Phi_0 \{\rho^2(\mathbf{r}) - 2\rho_0(\mathbf{r})[\rho_1(\mathbf{r}) + \sigma_1(\mathbf{r})] + \rho_1^2(\mathbf{r}) + \sigma_1^2(\mathbf{r})\} \]
\[ + \frac{1}{2} \int [\varepsilon_k(\mathbf{r}) - \omega_k(\mathbf{r})] \frac{dk}{(2\pi)^3}. \] (2.118)
With the notation
\[ E_B = \int E_B(\mathbf{r}) \, d\mathbf{r}, \] (2.119)
the system internal energy is
\[ E = \langle H \rangle = \langle H \rangle + \mu N. \] (2.121)
The average of the grand Hamiltonian reads as
\[ \langle H \rangle = E_B + \int \varepsilon_k(\mathbf{r}) \pi_k(\mathbf{r}) \frac{dk}{(2\pi)^3} \, d\mathbf{r}. \] (2.122)
where
\[ \pi_k(\mathbf{r}) = \{\exp\{\beta \varepsilon_k(\mathbf{r})\} - 1\}^{-1}. \] (2.123)
The system chemical potential becomes
\[ \mu = \mu_0 n_0 + \frac{1}{N} \int \mu_1(\mathbf{r}) \rho_1(\mathbf{r}) \, d\mathbf{r}. \] (2.124)
The fractions of condensed and uncondensed particles are
\[ n_0 = \frac{1}{N} \int \rho_0(\mathbf{r}) \, d\mathbf{r}, \quad n_1 = \frac{1}{N} \int \rho_1(\mathbf{r}) \, d\mathbf{r}. \] (2.125)
respectively.

2.9. Bogolubov approximation

At very low temperature and asymptotically weak interactions, almost all particles are Bose-condensed. In that case, the contribution of uncondensed particles can be neglected, which means that \( \rho_1 \) and \( \sigma_1 \) are negligibly small, as compared to the density of condensed particles \( \rho_0 \sim \rho \). Neglecting in spectrum (2.106) the terms containing \( n_p \) and \( \sigma_p \) yields the Bogolubov form of the spectrum
\[ \varepsilon_k(\mathbf{r}) = \left( \rho(\mathbf{r}) \frac{\Phi_0}{m} k^2 + \left( \frac{k^2}{2m} \right)^2 \right)^{1/2}. \] (2.126)
The spectrum long-wave limit is described by the equation
\[ \varepsilon_k^2(\mathbf{r}) \approx c^2(\mathbf{r}) k^2 + [1 + 2\rho(\mathbf{r}) m A_k] \left( \frac{k^2}{2m} \right)^2, \] (2.127)
with the sound velocity
\[ c(\mathbf{r}) = \sqrt{\rho(\mathbf{r}) \frac{\Phi_0}{m}} \] (2.128)
If the interaction potential is anisotropic, then, in the Bogolubov approximation, spectrum (2.126) is also anisotropic. However the sound velocity (2.128) is isotropic.
Neglecting \( \rho_1 \) and \( \sigma_1 \) in the condensate-function equation (2.45) results in the vacuum coherent-field equation (2.40). Hence, the latter can be interpreted as the Bogolubov approximation of the condensate-function equation.
In the Thomas–Fermi approximation, where the kinetic energy is neglected, the condensate-function equation (2.40) becomes
\[ \left[ U(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \rho_0(\mathbf{r}') \, d\mathbf{r}' \right] \eta(\mathbf{r}) = \mu_0 \eta(\mathbf{r}). \]
For nonzero \( \eta \), this reduces to the equality
\[
\int \Phi(r - r') \rho_0(r') \, dr' = \mu_0 - U(r). \tag{2.129}
\]

The latter, together with the normalization
\[
\int \rho_0(r) \, dr = N_0, \quad \rho_0(r) \equiv |\eta(r)|^2,
\]
defines the condensate density and the chemical potential. If the Thomas–Fermi approximation is not involved, then the chemical potential can be represented as
\[
\mu_0 = \frac{1}{N} \int \eta^*(r) \left[ -\frac{\nabla^2}{2m} + U(r) \right] \eta(r) \, dr + \int \Phi(r - r') \rho_0(r) \rho_0(r') \, drdr'. \tag{2.130}
\]

### 2.10. Stability conditions

As follows from equation (2.128), the sound velocity is defined, provided the interaction potential is effectively repulsive, such that
\[
\Phi_0 \equiv \int \Phi(r) \, dr > 0. \tag{2.131}
\]

This requirement is valid for uniform systems and large traps with a slowly varying trapping potential, when the local-density approximation is applicable. Generally, finite traps can confine atoms with attractive interactions, if the number of atoms is limited by a critical number [3–5, 30].

The interaction potential is to be integrable, so that
\[
\left| \int \Phi(r) \, dr \right| < \infty. \tag{2.132}
\]

If the interaction potential of bare particles is not integrable, it is necessary to take account of particle correlations and use an integrable pseudopotential [46].

The general condition of thermodynamic stability requires that the fluctuations of extensive observable quantities be thermodynamically normal [7, 17, 18, 29, 30]. This implies that, if \( \hat{A} \) is the operator of an extensive observable, then its variance has to satisfy the condition
\[
0 \leq \frac{\text{var}(\hat{A})}{N} < \infty, \tag{2.133}
\]

in which
\[
\text{var}(\hat{A}) = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2.
\]

For instance, particle fluctuations are to be thermodynamically normal,
\[
0 \leq \frac{\text{var}(\hat{N})}{N} < \infty, \tag{2.134}
\]

where
\[
\hat{N} = \int \hat{\psi}^\dagger(t) \hat{\psi}(r) \, dr.
\]

The variance of the number-of-particle operator, can be represented in the form
\[
\text{var}(\hat{N}) = N + \int \rho(r) \rho(r') [g(r, r') - 1] \, drdr', \tag{2.135}
\]

with the pair correlation function
\[
g(r, r') \equiv \frac{\langle \hat{\psi}^\dagger(r) \hat{\psi}^\dagger(r') \hat{\psi}(r') \hat{\psi}(r) \rangle}{\rho(r) \rho(r')}, \tag{2.136}
\]

in which
\[
\rho(r) = \rho_0(r) + \rho_1(r).
\]

In the HFB approximation, the Hamiltonian terms of fourth order with respect to the field operators \( \psi_1 \), are reduced to the terms of second order with respect to these operators. In that sense, the HFB approximation can be called an approximation of second order. Therefore the expressions of higher orders may be not well defined in this approximation and can be omitted. Thus, omitting the terms of fourth order, with respect to \( \psi_1 \), in the pair correlation function, we obtain
\[
\frac{\text{var}(\hat{N})}{N} = 1 + \frac{2}{N} \int \rho(r) \lim_{k \to 0} [n_k(r) + \sigma_k(r)] \, dr. \tag{2.137}
\]

The details can be found in [17, 18, 30].

According to (2.102),
\[
\omega^2_\pi(r) = \Delta^2_\pi(r) + \varepsilon_\pi^2(r). \tag{2.138}
\]

We also know that in the long-wave limit \( k \to 0 \) the spectrum is gapless, with \( \varepsilon_\pi \to 0 \). Then for small \( \varepsilon_\pi \), such that
\[
\varepsilon_\pi(r) \ll |\Delta_\pi(r)|, \tag{2.139}
\]
equation (2.98) gives
\[
n_k(r) \simeq \frac{T \Delta_k(r)}{\varepsilon^2_k(r)} + \frac{\Delta_k(r)}{12T} + \frac{T}{2 \Delta_k(r)} - \frac{1}{2}, \tag{2.140}
\]

while equation (2.99) yields
\[
\sigma_k(r) \simeq -\frac{T \Delta_k(r)}{\varepsilon^2_k(r)} - \frac{\Delta_k(r)}{12T}. \tag{2.141}
\]

From here, we find
\[
\lim_{k \to 0} [n_k(r) + \sigma_k(r)] = \frac{1}{2} \left[ \frac{T}{\Delta(r)} - 1 \right], \tag{2.142}
\]

where
\[
\Delta(r) \equiv \lim_{k \to 0} \Delta_k(r) = \rho_0(r) \Phi_0 + \int \sigma_p(r) \Phi_p \frac{dp}{(2\pi)^3}. \tag{2.143}
\]

In the central-peak approximation (2.82), this simplifies to
\[
\Delta(r) = \rho_0(r) + \sigma_1(r) \Phi_0. \tag{2.144}
\]

In this way, we obtain
\[
\frac{\text{var}(\hat{N})}{N} = \frac{T}{N} \int \rho(r) \Delta(r) \, dr. \tag{2.145}
\]

To be non-negative and finite, this expression requires that \( \Phi_0 \) be nonzero and positive. It is also important to notice that the anomalous average cannot be omitted, otherwise the integral (2.137) becomes divergent.
2.11. Superfluid density

Superfluidity is defined as dissipationless flow of a fluid. The fluid motion with velocity \( \mathbf{v} \) can be initiated by the velocity boost

\[
B_\mathbf{v} = e^{i \mathbf{v} \cdot \mathbf{r}}.
\]

(2.146)

The field operator for a moving system is

\[
\hat{\psi}_\mathbf{v}(\mathbf{r}) = B_\mathbf{v} \hat{\psi}(\mathbf{r}).
\]

The momentum density operator for a moving system becomes

\[
\hat{\mathbf{P}}_\mathbf{v}(\mathbf{r}) = \hat{\mathbf{v}}^\dagger(\mathbf{r}) \hat{\mathbf{P}}_\mathbf{v}(\mathbf{r}) \hat{\mathbf{v}}(\mathbf{r}) = \hat{\mathbf{P}}(\mathbf{r}) + m \mathbf{v} \hat{\mathbf{v}}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}),
\]

where

\[
\frac{\partial}{\partial \mathbf{v}} = \hat{\mathbf{v}}^\dagger(\mathbf{r}) \hat{\mathbf{P}}_\mathbf{v}(\mathbf{r}) \hat{\mathbf{v}}(\mathbf{r}).
\]

(2.147)

The energy Hamiltonian becomes

\[
\hat{H}_\mathbf{v} = \hat{H}[\hat{\psi}] = \hat{H} + \int \hat{\mathbf{v}}^\dagger(\mathbf{r}) \left( \mathbf{v} \cdot \hat{\mathbf{P}} + \frac{m \mathbf{v}^2}{2} \right) \hat{\psi}(\mathbf{r}) \, d\mathbf{r}.
\]

Using the equality

\[
\langle \hat{A}_\mathbf{v} \rangle_{\mathbf{v}} = \text{Tr} \hat{\rho}_\mathbf{v} \hat{A}_\mathbf{v}, \quad \hat{\rho}_\mathbf{v} = \frac{\exp(-\beta \hat{H}_\mathbf{v})}{\text{Tr} \exp(-\beta \hat{H}_\mathbf{v})},
\]

(2.148)

The superfluid fraction is defined as

\[
\frac{n_s}{ns} \equiv \lim_{\mathbf{v} \to 0} \frac{\frac{\partial}{\partial \mathbf{v}} \cdot (\hat{\mathbf{P}}_\mathbf{v})}{\frac{\partial}{\partial \mathbf{v}} \cdot \hat{\mathbf{P}}_\mathbf{v}}.
\]

(2.149)

defining the local superfluid density

\[
\rho_s(\mathbf{r}) = n_s(\mathbf{r}) \rho(\mathbf{r}).
\]

Then the latter takes the form

\[
\rho_s(\mathbf{r}) = \rho(\mathbf{r}) - \frac{2Q(\mathbf{r})}{Td},
\]

with the dissipated heat density

\[
Q(\mathbf{r}) = \frac{1}{2m} \text{cov}(\hat{\mathbf{P}}(\mathbf{r}), \hat{\mathbf{P}}(\mathbf{r})),
\]

in which

\[
\text{cov}(\hat{A}, \hat{B}) \equiv \frac{1}{2} \langle \hat{A} \hat{B} + \hat{B} \hat{A} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle.
\]

In three-dimensional space, employing the HFB and local-density approximations, we have

\[
Q(\mathbf{r}) = \int \frac{k^2}{2m} \left[ n_k(\mathbf{r}) + n_k^2(\mathbf{r}) - \sigma_k^2(\mathbf{r}) \right] \frac{k}{(2\pi)^3}.
\]

Using the equality

\[
n_k(\mathbf{r}) + n_k^2(\mathbf{r}) - \sigma_k^2(\mathbf{r}) = \frac{1}{4 \sinh^2[\beta \varepsilon_k(\mathbf{r})/2]},
\]

this can be rewritten as

\[
Q(\mathbf{r}) = \frac{1}{8m} \int \frac{k^2}{\sinh^2[\beta \varepsilon_k(\mathbf{r})/2]} \frac{k}{(2\pi)^3}.
\]

The local quantities are connected to the global ones by the relations

\[
n_s = \frac{1}{N} \int \rho_s(\mathbf{r}) \, d\mathbf{r}, \quad Q = \frac{1}{N} \int Q(\mathbf{r}) \, d\mathbf{r}.
\]

It is worth stressing that the expressions for the superfluid fraction (2.147) and superfluid density (2.150) are valid for any direction of the boost velocity and for any system, isotropic or anisotropic. In all the cases, these quantities, as is evident, are scalars.

2.12. Optical lattices

Optical lattices are formed by interfering laser beams creating standing waves [11, 13, 14, 17] or by magnetic fields [47]. A lattice, with the lattice vector

\[
\mathbf{a} = \left\{ a_\alpha = \frac{\lambda_\alpha}{2} : \alpha = 1, 2, \ldots, d \right\},
\]

where \( d \) is space dimensionality, can be created by the laser wave vector

\[
\mathbf{k}_0 = \left\{ k_0^\alpha = \frac{2\pi}{\lambda_\alpha} = \frac{\pi}{a_\alpha} \right\}.
\]

The typical lattice potential has the form

\[
V_\mathbf{k}(\mathbf{r}) = \sum_{\alpha=1}^d V_\alpha \sin^2(k_0^\alpha r_\alpha).
\]

(2.151)
The effective lattice depth is characterized by the parameter

\[ V_0 \equiv \frac{1}{d} \sum_{\alpha=1}^{d} V_\alpha. \]  

(2.152)

Depending on the balance between the lattice depth and the recoil energy

\[ E_R \equiv \frac{k_0^2}{2m} \left( k_0^2 \equiv |k_0|^2 \right), \]  

(2.153)

atoms can be either localized in the vicinity of a lattice site or delocalized, moving through the whole system. The single-atom Hamiltonian is

\[ \hat{H}(r) = -\nabla^2 r + V_L (r) + U(r), \]  

(2.154)

where \( U(r) \) is an additional, say trapping, potential superimposed on the lattice potential.

The field operators can be expanded over Wannier functions (2.155), we meet the following matrix elements: the local field at the \( j \)th lattice site

\[ H_{jj}^{nn} \equiv \int w_n^*(r - \mathbf{a}_j) \hat{H}(r) w_n(r - \mathbf{a}_j) \, d\mathbf{r}, \]  

(2.156)

the tunneling matrix

\[ J_{ij}^{nn} \equiv -\int w_n^*(r - \mathbf{a}_i) \hat{H}(r) w_n(r - \mathbf{a}_j) \, d\mathbf{r}, \]  

(2.157)

with \( i \neq j \), and the interaction matrix

\[ U_{jijj}^{nn} \equiv \int w_n^*(r - \mathbf{a}_j) w_n^*(r' - \mathbf{a}_j) \hat{\Phi}(r - r') \times w_n(r' - \mathbf{a}_i) w_n(r - \mathbf{a}_i) \, d\mathbf{r} d\mathbf{r}'. \]  

(2.158)

Then the energy Hamiltonian takes the form

\[ \hat{H} = -\sum_{i\neq j} \sum_{mn} J_{ij}^{mn} \hat{c}^\dagger_m \hat{c}^\dagger_n \hat{c}_n \hat{c}_m + \sum_j \sum_{mn} H_{jj}^{nn} \hat{c}^\dagger_j \hat{c}_j + \frac{1}{2} \sum_{\langle j \rangle} \sum_{\langle n \rangle} U_{jijj}^{nn} \hat{c}^\dagger_{nj} \hat{c}^\dagger_{n\bar{j}} \hat{c}_{n\bar{j}} \hat{c}_{nj}. \]  

(2.159)

One usually considers the single-band approximation, keeping in mind the lowest band and omitting the band index, which is equivalent to the use of the expansion

\[ \hat{\psi}(r) = \sum_j \hat{c}_j \psi_j(r - \mathbf{a}_j), \]  

instead of expansion (2.155). The single-site interaction energy is denoted as \( U_j \equiv U_{jijj} \). And the two-site interaction potential, including both the direct as well as exchange interactions, is written as

\[ U_{ij} \equiv U_{jijj} + U_{ijij}. \]  

Then Hamiltonian (2.159) simplifies to the extended Hubbard model

\[ \hat{H} = -\sum_{\langle i \rangle} \sum_{\langle n \rangle} J_{ij}^{nn} \hat{c}^\dagger_n \hat{c}^\dagger_n \hat{c}_n \hat{c}_n + \frac{1}{2} \sum_{\langle i \rangle} \sum_{\langle n \rangle} U_{ij}^{nn} \hat{c}^\dagger_n \hat{c}^\dagger_n \hat{c}_n \hat{c}_n. \]  

(2.160)

One often considers the tunneling only between the nearest neighbors. In the case of an ideal lattice, the values \( h_j \) and \( U_j \) do not depend on the lattice index.

Note that, instead of expanding the field operators over Wannier functions, one could expand them over Bloch functions, thus deriving a different representation for the system Hamiltonian [17, 49]. But the Hubbard form is more convenient for treating localized particles.

### 2.13. Condensate in lattice

Let the lattice, loaded with \( N \) atoms, have \( N_L \) lattice sites, so that the filling factor be

\[ \nu \equiv \frac{N}{N_L}. \]  

(2.161)

Accomplishing the Bogolubov shift \( \hat{\psi} = \eta + \psi_1 \) and comparing it with the expansion over Wannier functions (2.155), we get the Wannier expansion for the condensate function

\[ \eta(r) = \sqrt{\frac{N_0}{N_L}} \sum_j w_0(r - \mathbf{a}_j) \]  

(2.162)

and for the field operator of uncondensed atoms

\[ \psi_1(r) = \sum_{nj} c_{nj} w_n(r - \mathbf{a}_j). \]  

(2.163)

The Wannier function \( w_0 \) is assumed to pertain to the lowest band. In this way,

\[ \hat{c}_{nj} = \sqrt{\frac{N_0}{N_L}} \delta_{n0} + c_{nj}. \]  

(2.164)

The condition of orthogonality of \( \eta \) and \( \psi_1 \) yields the equation

\[ \sum_j c_{0j} = 0, \]  

(2.165)

which gives

\[ \sum_j \hat{c}_{0j} = \sqrt{N_0N_L}. \]  

(2.166)

And condition (2.5) implies

\[ \langle c_{nj} \rangle = 0, \]  

(2.167)

which results in the order parameter

\[ \langle \hat{c}_{nj} \rangle = \sqrt{\frac{N_0}{N_L}} \delta_{n0}. \]  

(2.168)

In the single-band approximation, instead of (2.164), we have

\[ \hat{c}_j = \sqrt{m_0} + c_j, \quad \left( n_0 \equiv \frac{N_0}{N} \right). \]  

(2.169)
The site operators have to satisfy the conditions
\[
\frac{1}{N_L} \sum_j \hat{c}_j = \sqrt{\nu} n_0, \quad \sum_j c_j = 0, \\
\langle \hat{c}_j \rangle = \sqrt{\nu} n_0, \quad \langle c_j \rangle = 0.
\] (2.170)

2.14. Lattice Hamiltonian

Substituting into the grand Hamiltonian the expansion of field operators (2.155), we shall limit ourselves by the single-band approximation. The symmetry \( U_j = U_R \) and \( J_j = J_R \) will be used, which is evident for real Wannier functions.

Using the Wannier representation for the number-of-particle operators gives
\[
N_0 = \nu n_0 N_L, \quad N_1 = \sum_j c_j^\dagger c_j.
\] (2.171)

Operator (2.10), removing the linear in \( \psi_1 \) terms, reads as
\[
\hat{\Lambda} = \sum_j \left( \lambda_j c_j^\dagger + \lambda_j^* c_j \right),
\] (2.172)

with
\[
\lambda_j \equiv \int \lambda(r) w^\ast(r - a_j) \, dr.
\]

The grand Hamiltonian (2.15) is the sum
\[
H = H^{(0)} + H^{(2)} + H^{(3)} + H^{(4)},
\] (2.173)
similar to (2.21), where the terms are distinguished by the order with respect to the operators \( c_j \). The term, containing no such operators, is
\[
H^{(0)} = \nu n_0 \left( \sum_j h_j - \sum_{i \neq j} J_{ij} \right) - \mu \omega N_0 + \frac{(\nu n_0)^2}{2} \left( \sum_j U_j + \sum_{i \neq j} U_{ij} \right).
\] (2.174)
The first-order term is canceled by setting
\[
\lambda_j = \sqrt{\nu n_0} \left( \sum_j h_j - \sum_{i \neq j} J_{ij} \right) + (\nu n_0)^{1/2} \left( \sum_j U_j + \sum_{i \neq j} U_{ij} \right),
\]
which gives \( H^{(1)} = 0 \). The second-order term is
\[
H^{(2)} = -\sum_{i \neq j} U_{ij} c_i c_j + \frac{1}{2} \sum_j (h_j - \mu) c_j^\dagger c_j + \frac{\nu n_0}{2} \sum_j U_j \left( 4 c_j^\dagger c_j + c_j^\dagger c_j + c_j c_j^\dagger + c_j^\dagger c_j \right) + \frac{\nu n_0}{2} \sum_{i \neq j} U_{ij} \left( 2 c_i^\dagger c_j + 2 c_j^\dagger c_i + c_i^\dagger c_i^\dagger + c_i c_i^\dagger \right).
\] (2.175)
The third-order term reads as
\[
H^{(3)} = \sqrt{\nu n_0} \sum_j U_j \left( c_j c_j^\dagger + c_j^\dagger c_j \right) + \sqrt{\nu n_0} \sum_{i \neq j} U_{ij} \left( c_i c_i^\dagger + c_i^\dagger c_i \right).
\] (2.176)
And the fourth-order term becomes
\[
H^{(4)} = \frac{1}{2} \sum_j U_j \left( c_j c_j^\dagger + c_j^\dagger c_j \right) + \frac{1}{2} \left( c_j^\dagger c_j^\dagger + c_j c_j \right).
\] (2.177)

For an ideal lattice, it is convenient to resort to the Fourier transform
\[
c_j = \frac{1}{\sqrt{N_L}} \sum_k a_k e^{i k a_j}, \quad a_k = \frac{1}{\sqrt{N_L}} \sum_j c_j e^{-i k a_j}.
\]

In view of conditions (2.170), one has
\[
a_0 = \frac{1}{\sqrt{N_L}} \sum_j c_j = 0. \quad \text{(2.178)}
\]
The evolution equations for the operators \( c_j \) are
\[
i \frac{\partial c_j}{\partial t} = [c_j, H] = \frac{\delta H}{\delta c_j^\dagger} \quad \text{and} \quad i \frac{\partial c_j^\dagger}{\partial t} = [c_j^\dagger, H] = -\frac{\delta H}{\delta c_j}.
\]

From the latter equation, in equilibrium, when
\[
\frac{\partial}{\partial t} \langle c_j^\dagger c_j \rangle = 0,
\]
we have the relations
\[
\langle c_j^\dagger c_j \rangle = \langle c_j^\dagger c_j \rangle^\ast, \\
\langle c_j c_j \rangle = \langle c_j^\dagger c_j \rangle^\ast, \\
\langle c_j^\dagger c_j \rangle = \langle c_j c_j \rangle^\ast
\]
where the operators \( c_j \) are taken at the same moment of time. These relations mean that in equilibrium the corresponding correlation functions are real.

In equilibrium, we also have
\[
\frac{\delta H}{\delta n_0} = 0. \quad \text{(2.179)}
\]

This leads to the expression for the condensate chemical potential
\[
\mu_0 = \frac{1}{N_L} \left( \sum_j h_j - \sum_{i \neq j} J_{ij} \right) + \frac{\nu n_0}{N_L} \left( \sum_j U_j + \sum_{i \neq j} U_{ij} \right) + \frac{1}{N_L} \sum_j U_j \left( 2 c_j^\dagger c_j + c_j^\dagger c_j + c_j c_j^\dagger \right) + \frac{1}{\sqrt{\nu n_0} N_L} \sum_j U_j \left( c_j c_j^\dagger + c_j^\dagger c_j \right).
\] (2.180)

2.15. Rotating systems

The study of superfluid systems often requires to consider system rotation. Then one can treat the system either in the laboratory frame at rest or in the rotating frame, where the system is immovable. It is usually convenient to treat the system in
the rotating frame involving the transformation from the laboratory frame to the noninertial rotating frame [50–52].

Let the spatial variable in the laboratory frame at rest be \( \mathbf{r} = \{x, y, z\} = \{r_\alpha\} \). The system is assumed to rotate counter-clockwise around the axis \( \mathbf{e}_z \). In the rotating frame, where the system is immovable, the spatial variable is denoted by \( \mathbf{x} = \{x_1, x_2, x_3\} = \{x_\alpha\} \), with \( \alpha = 1, 2, 3 \). And let the rotation angle between the axes \( x \) and \( x_1 \) be denoted by \( \varphi = \varphi(t) \). The transformation from the frame at rest to the rotating frame is realized by the transformation matrix

\[
R(\varphi) = \begin{pmatrix}
\cos \varphi & -\sin \varphi & 0 \\
\sin \varphi & \cos \varphi & 0 \\
0 & 0 & 1
\end{pmatrix},
\]

so that

\[
\begin{pmatrix}
x_1 \\
x_2 \\
x_3
\end{pmatrix} = R(\varphi) \begin{pmatrix}
x \\
y \\
z
\end{pmatrix},
\]

or explicitly

\[
x_1 = x \cos \varphi - y \sin \varphi, \quad x_2 = x \sin \varphi + y \cos \varphi, \quad x_3 = z.
\]

The inverse rotation matrix is

\[
R^{-1}(\varphi) = R(-\varphi) = \begin{pmatrix}
\cos \varphi & \sin \varphi & 0 \\
-\sin \varphi & \cos \varphi & 0 \\
0 & 0 & 1
\end{pmatrix},
\]

which gives

\[
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix} = R^{-1}(\varphi) \begin{pmatrix}
x_1 \\
x_2 \\
x_3
\end{pmatrix},
\]

or explicitly

\[
x = x_1 \cos \varphi + x_2 \sin \varphi, \quad y = -x_1 \sin \varphi + x_2 \cos \varphi, \quad z = x_3.
\]

Let the orthonormal right-handed triad in the laboratory frame be denoted as \( \mathbf{e}_\alpha \), and the orthonormal right-handed triad rotating with angular velocity \( \Omega = \Omega(t) \) be \( \mathbf{e}_\alpha(t) \), with the initial condition \( \mathbf{e}_\alpha(0) = \mathbf{e}_\alpha \). The angular velocity is connected with the rotation angle by the integral

\[
\varphi(t) = \int_0^t \Omega(t') \, dt'.
\]

The rotating triad satisfies the equation

\[
\frac{d}{dt} \mathbf{e}_\alpha(t) = \Omega \times \mathbf{e}_\alpha(t),
\]

with \( \Omega = \Omega \mathbf{e}_z \). Any spatial vector \( \mathbf{r} \) can be represented either in the laboratory frame or in the rotating frame, respectively, as

\[
\mathbf{r} = \sum_\alpha r_\alpha \mathbf{e}_\alpha = \sum_\alpha x_\alpha \mathbf{e}_\alpha(t).
\]

The variables in the rotating frame, spatial \( x_\alpha \) and temporal \( \tau \), are connected with the variables of the laboratory frame \( r_\alpha \) and \( t \) by the equations

\[
x_\alpha = \mathbf{r} \cdot \mathbf{e}_\alpha(t), \quad \tau = t.
\]
where $\hat{T}$ denotes time ordering, which transforms the wave function in the laboratory frame into the wave function in the rotating frame

$$\Psi(x, \tau) = \hat{U}^+ \psi(r, \tau).$$  \hfill (2.193)

Then, substituting $\psi = \hat{U}\psi$ into equation (2.187) gives equation (2.189), with the effective Hamiltonian

$$\hat{H}_{\text{eff}} = \hat{U}^+ \hat{H} \hat{U} - i \hat{U}^+ \frac{\partial \hat{U}}{\partial \tau}. \hfill (2.194)$$

Since

$$\hat{U}^+ \hat{H}(r, \theta) \hat{U} = \hat{H}(x, \tau) \hfill (2.195)$$

and

$$-i \hat{U}^+ \frac{\partial \hat{U}}{\partial \tau} = -\hat{\Omega} \cdot \hat{L}(x), \hfill (2.196)$$

the effective Hamiltonian takes the same form as in (2.190).

These considerations are straightforwardly generalized to a many-particle system with the Hamiltonian in the laboratory frame

$$\hat{H} = \int \psi^\dagger(\mathbf{r}) \hat{H}(\mathbf{r}, \theta) \psi(\mathbf{r}) \, \text{d} \mathbf{r} + \frac{1}{2} \int \psi^\dagger(\mathbf{r}) \hat{V}(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}) \psi(\mathbf{r}') \, \text{d} \mathbf{r} \text{d} \mathbf{r}'. \hfill (2.197)$$

In the rotating frame, we obtain

$$\hat{H}_{\text{rot}} = \hat{H} - \hat{\Omega} \cdot \hat{L}, \hfill (2.198)$$

with the angular momentum operator

$$\hat{L} = \int \psi^\dagger(\mathbf{r}) \hat{L}(\mathbf{r}) \psi(\mathbf{r}) \, \text{d} \mathbf{r}, \hfill (2.199)$$

where $\hat{L}(\mathbf{r}) = \mathbf{r} \times \hat{\mathbf{p}}$.

Note that in the integrals entering (2.198) and (2.199), the variable of integration $\mathbf{x}$ is replaced by $\mathbf{r}$.

When the rotation axis is $\mathbf{e}_z$, then the angular momentum operator $\hat{L}(\mathbf{r})$ reduces to

$$\hat{L}_z(\mathbf{r}) = -i \frac{\partial}{\partial \varphi} \left( \Omega = \Omega \mathbf{e}_z \right), \hfill (2.200)$$

where $\varphi$ is the angle in the cylindrical system of coordinates.

### 3. Dipolar interaction potentials

#### 3.1. Scattering lengths

An important class of nonlocal interactions includes dipolar interactions. Dipolar interactions arise between atoms or molecules possessing electric, $d_0$, or magnetic, $\mu_0$, dipoles. Similarly to local atomic interactions that are described by a scattering length $a_s$, the strength of dipolar interactions can be characterized by an effective dipolar scattering length, or just dipolar length

$$a_D \equiv \begin{cases} 
\frac{m d_0^2}{\hbar^2}, & \text{electric dipoles} \\
\frac{m \mu_0^2}{\hbar^2}, & \text{magnetic dipoles}
\end{cases}$$

The value of electric dipoles is measured in Debye units $D$,

$$1D = 10^{-18} \text{ erg G}^{-1} \left( 1 \text{ G}^2 = 1 \text{ erg cm}^{-3} \right),$$

while that of magnetic dipoles, in Bohr magnetons $\mu_B$,

$$\mu_B = 0.927 \times 10^{-20} \text{ erg G}^{-1}.$$ 

So that the relation holds:

$$1D = 107.8282 \mu_B.$$ 

The scattering length of local interactions, generally, depends on the value of the dipoles of scattered particles, $a_s = a_s(d_0)$. Scattering lengths are often expressed in units of the Bohr radius $a_B = 0.529177 \times 10^{-8} \text{ cm}$.

An atom of $^{87}\text{Rb}$, with mass $m = 1.443 \times 10^{-22} \text{ g}$, has the magnetic moment $\mu_0 = 0.5 \mu_B$ and the dipolar length

$$a_D = 2.79 \times 10^{-9} \text{ cm} = 0.527 a_B.$$ 

An atom of $^{52}\text{Cr}$, with $m = 0.863 \times 10^{-22} \text{ g}$, possesses the magnetic moment $\mu_0 = 6 \mu_B$ and the dipolar length

$$a_D = 2.4 \times 10^{-7} \text{ cm} = 45.4 a_B.$$ 

An atom of $^{168}\text{Er}$, with $m = 2.777 \times 10^{-22} \text{ g}$, has the magnetic moment $\mu_0 = 7 \mu_B$ and the dipolar length

$$a_D = 1.052 \times 10^{-6} \text{ cm} = 199 a_B.$$ 

An atom of $^{164}\text{Dy}$, with $m = 2.698 \times 10^{-22} \text{ g}$, possesses the magnetic moment $\mu_0 = 10 \mu_B$ and the dipolar length

$$a_D = 2.087 \times 10^{-6} \text{ cm} = 395 a_B.$$ 

Polar molecules and Rydberg atoms can have electric dipole moments $d_0 \sim (0.1-10) D$ and the dipolar lengths $a_D \sim (10^{-4} - 10^{-2}) \text{ cm}$. More details can be found in reviews [20–25].

There also exist hyperfine dipolar interactions between electrons of an atom and protons of a nucleus, which is modeled by a local form. The effective scattering length of such local hyperfine interactions is

$$a_H = \frac{m \mu_0 \hbar}{4 \mu_0},$$

where $\mu_0 = 1.411 \times 10^{-23} \text{ erg G}^{-1}$ is the proton magnetic moment and $\mu_e = 0.928 \times 10^{-20} \text{ erg G}^{-1}$ is the electron magnetic moment. Thus for $^{87}\text{Rb}$, one has $a_H = 1.699 \times 10^{-11} \text{ cm}$, which is much smaller than $a_D = 2.79 \times 10^{-9} \text{ cm}$.

#### 3.2. Interaction potentials

Generally, interactions between atoms, or molecules, contain several terms. There exists the local, or contact, interaction

$$\Phi_{\text{loc}}(\mathbf{r}) = 4\pi \hbar^2 a_s \delta(\mathbf{r}), \hfill (3.1)$$

described by the scattering length $a_s$ that, strictly speaking, also depends on the dipole moment. There is the hyperfine interaction

$$A(\mathbf{r}) = \frac{8\pi}{3} \mu_n \cdot \mu_0 \delta(\mathbf{r}), \hfill (3.2)$$
in which
\[ \vec{\mu}_p = h\gamma_p \vec{I}, \quad \vec{\mu}_e = -h\gamma_e \vec{S}, \]
are the proton and electron magnetic moments, \( \gamma_p \) and \( \gamma_e \) are the proton and electron gromagnetic ratios, and \( \vec{I} \) and \( \vec{S} \) are the proton and electron spins, respectively. So that the hyperfine interaction can be written as
\[ A(r) = \frac{8\pi}{3} \hbar^2 \gamma_p \gamma_e \vec{I} \cdot \vec{S} \delta(r). \]
The hyperfine interactions are rather small. Thus
\[ \frac{8\pi}{3} |\vec{\mu}_p| |\vec{\mu}_e| = 1.097 \times 10^{-42} \text{ erg cm}^3. \]
This should be compared with the factor \( 4\pi\hbar^2 a_s/m \) in the interaction potential (3.1). For instance, the scattering length of \( ^8\text{Rb} \) is \( a_s = 103a_B = 0.545 \times 10^{-6} \text{ cm}, \) which gives
\[ 4\pi\hbar^2 a_s/m = 0.883 \times 10^{-37} \text{ erg cm}^3. \]

Similarly, one can consider electric hyperfine interactions [53].

In what follows, all contact interactions are assumed to be combined and characterized by an effective scattering length \( a_s \), in general, depending on dipole moments.

One often needs to use Fourier transforms of interaction potentials. Thus for the local interaction potential, one has
\[ \Phi^\text{loc}_k \equiv \int \Phi_{\text{loc}}(r)e^{-i k \cdot r} \, dr, \] (3.3)
which gives
\[ \Phi^\text{loc}_k = 4\pi\hbar^2 a_s/m. \] (3.4)

Note that the sufficient condition for the existence of the Fourier transform of a potential \( \Phi(r) \), being a function of bounded variation, is its absolute integrability,
\[ \int |\Phi(r)| \, dr < \infty, \] (3.5)
which is called the Dirichlet theorem [54].

The dipole–dipole interaction between two dipoles is given by the potential
\[ D(r) = \frac{1}{r^3} \left[ (\vec{d}_1 \cdot \vec{d}_2) - 3(\vec{d}_1 \cdot \vec{n})(\vec{d}_2 \cdot \vec{n}) \right], \] (3.6)
in which
\[ r \equiv |\vec{r}_2 - \vec{r}_1|, \quad \vec{n} \equiv \frac{\vec{r}_2 - \vec{r}_1}{r}, \quad r \equiv |\vec{r}|. \]
For concreteness, we write here electric dipoles \( \vec{d} \), keeping in mind that the same formulas are valid for magnetic dipoles \( \vec{j} \). If all dipoles are polarized in one direction \( \vec{e}_d \) and have the same absolute dipole moment, so that
\[ \vec{d}_1 = d_0 \vec{e}_d \quad (d_0 \equiv |\vec{d}_1|), \]
then the interaction potential becomes
\[ D(r) = \frac{d_0^2}{r^3} \left( 1 - 3 \cos^2 \vartheta \right) \left( \cos \vartheta \equiv \frac{\vec{r} \cdot \vec{e}_d}{r} \right). \] (3.7)
The Fourier transform of potential (3.6),
\[ D_k \equiv \int D(r)e^{-i k \cdot r} \, dr, \] (3.8)
reads as
\[ D_k = \frac{4\pi}{3} \left[ \frac{3(\vec{d}_1 \cdot \vec{k})(\vec{d}_2 \cdot \vec{k})}{k^2} - (\vec{d}_1 \cdot \vec{d}_2) \right], \] (3.9)
with \( k \equiv |\vec{k}|. \) And the Fourier transform of potential (3.7) for polarized dipoles is
\[ D_k = \frac{4\pi}{3} d_0^2 \left( 3 \cos^2 \vartheta_k - 1 \right) \left( \cos \vartheta \equiv \vartheta \right) \] (3.10)

However, Fourier transforms (3.9) and (3.10), as is seen, are not defined for \( k \to 0 \) as well as for \( k \to \infty. \) This happens because the dipole–dipole interaction potential is not absolutely integrable, that is, does not satisfy the Dirichlet theorem and condition (3.5). Really, in three dimensions,
\[ \int |D(r)| \, dr \sim d_0^2 \lim_{b \to 0} \lim_{R \to \infty} \frac{R}{b} \to \infty. \]
While in one and two dimensions,
\[ \int |D(r)| \, dr \sim d_0^2 \lim_{b \to 0} b^{d-3} \to \infty \quad (d = 1, 2). \]
This means that the Fourier transform for the dipole–dipole interaction potential is not well defined.

### 3.3. Regularized potential

In order to have a well defined Fourier transform, the dipole–dipole interaction potential needs to be regularized. In dimensions one and two, it is sufficient to regularize the potential only at short distance. But in three dimensions, it is necessary to regularize it both at short and at long-range distance.

The physical origin of such a regularization is quite clear. The dipole–dipole interaction potential (3.6) is written for point-like particles, while real atoms and molecules have finite sizes. Hence form (3.6) is meaningful only for \( r \) larger than a short distance \( b \) of the order of the size of the interacting particles. And at long-range distance, there exists particle screening attenuating the bare interaction. Therefore the regularized dipolar potential can be written as [44]
\[ D(r, b, \kappa) = \Theta(r - b)D(r)e^{-\kappa r}, \] (3.11)
where \( \Theta(r) \) is the unit-step function and the screening parameter \( \kappa \) defines the screening radius \( r_s = 1/\kappa. \)

The dipolar potential (3.11) is absolutely integrable, hence enjoys a well defined Fourier transform
\[ D_k(b, \kappa) \equiv \int D(r, b, \kappa)e^{-i k \cdot r} \, dr. \] (3.12)
Keeping in mind the case of polarized dipoles in three dimensions, we have
\[ D_k(b, \kappa) = D_k I_k(b, \kappa), \] (3.13)
where \( D_k \) is given by (3.10) and
The Fourier transform of the interaction potential (3.23) can be written in the form
\[
\Phi_k = \Phi_0 + f_k,
\]  
with the notation
\[
f_k \equiv D_k(b, \zeta) = D_k I_k(b, \zeta) = D_k J(q, \zeta).  
\]  
The spectrum of collective excitations can be found by using the formulas of the previous section 2. Taking into account that \( f_k \to 0 \) as \( k \to 0 \), from (2.110) we find
\[
\varepsilon_k = \left[ \frac{k^2}{2m} + (\rho_0 + \sigma_1) f_k \right] \left[ \frac{k^2}{2m} + 2(\rho_0 + \sigma_1) \Phi_0 + (2\rho_0 + \rho_1 + \sigma_1) f_k \right].
\]  
In the local-density approximation, the quantities \( \rho_0, \rho_1 \), and \( \sigma_1 \) are functions of \( r \). The long-wave limit, in view of the asymptotic form
\[
f_k \simeq \frac{1 + \zeta b}{5 \zeta^2 c^2} D_k k^2 \quad (k \to 0),
\]  
results in the phonon spectrum
\[
\varepsilon_k \simeq c_k k \quad (k \to 0),
\]  
with the anisotropic sound velocity given by the equation
\[
c_k^2 = (\rho_0 + \sigma_1) \frac{\Phi_0}{m} \left[ 1 + (\rho_0 + \sigma_1) \frac{2m(1 + \zeta b)}{5 \zeta^2 c^2} D_k \right].
\]  

3.5. Bogolubov approximation

The Bogolubov approximation is applicable for low temperatures and very weak interactions, when it is admissible to neglect both \( \rho_1 \) and \( \sigma_1 \), as compared to \( \rho_0 \sim \rho \). Recall that omitting \( \sigma_1 \) but keeping \( \rho_1 \) would be principally wrong, since these quantities are of the same order of magnitude [17, 18, 30, 34, 55].

In the Bogolubov approximation, spectrum (3.28) reduces to
\[
\varepsilon_k = \sqrt{\frac{\rho}{m} (\Phi_0 + f_k) k^2 + \left( \frac{k^2}{2m} \right)^2}.
\]  
The spectrum is anisotropic because of the presence of the dipolar part \( f_k \). In the long-wave limit, the spectrum is phononic,
\[
\varepsilon_k \simeq c_0 k \quad (k \to 0),
\]  
with the isotropic sound velocity
\[
c_B \equiv \sqrt{\frac{\rho}{m} \Phi_0} = \sqrt{\frac{4\pi \rho \mu_0}{m}}.
\]  
Note that there is no the so-called phonon instability in the long-wave limit, which would arise if the screening would be neglected.

The balance between the dipolar interactions, with the effective strength \( 4\pi \mu_0^2/3 \), and the local interaction, characterized by \( \Phi_0 \), is measured by the parameter

\[

I_k(b, \zeta) = 9kb \int_1^\infty \left[ \frac{\sin(kbx)}{(kbx)^2} - \frac{\cos(kbx)}{(kbx)^3} - \frac{\sin(kbx)}{3(kbx)^2} \right] e^{-\zeta x} dx.
\]  
(3.14)

We may notice that integral (3.14), actually, depends on two parameters,
\[
q \equiv kb, \quad \zeta \equiv \frac{\alpha}{\rho}.
\]  
(3.15)

So that it can be rewritten as
\[
I_k(b, \zeta) = J(q, \zeta)
\]  
through the integral
\[
J(q, \zeta) = 9q \int_1^\infty \left[ \frac{\sin(qx)}{(qx)^2} - \frac{\cos(qx)}{(qx)^3} - \frac{\sin(qx)}{3(qx)^2} \right] e^{-\zeta x} dx.
\]  
(3.16)

At small \( q \), we have
\[
J(q, \zeta) \simeq \frac{(1 + \zeta) e^{-\zeta}}{5_2^2} q^2 \quad (q \to 0),
\]  
(3.17)

which yields
\[
D_0(b, \zeta) \simeq \frac{D_k (1 + \zeta b) e^{-\zeta b}}{5_2^2} k^2 \quad (k \to 0).
\]  
(3.18)

Therefore the short-wave limit is well defined:
\[
D_0(b, \zeta) \equiv \lim_{k \to 0} D_k(b, \zeta) = 0.
\]  
(3.19)

In the opposite limit, we find
\[
J(q, \zeta) \simeq -3e^{-\zeta} \frac{\cos(q)}{q^2} \quad (q \to \infty),
\]  
(3.20)

which gives
\[
D_k(b, \zeta) \simeq -3D_k e^{-\zeta b} \frac{\cos(kb)}{(kb)^2} \quad (k \to \infty)
\]  
(3.21)

going to zero as \( k \to \infty \).

In the general case, the interaction potential is the sum of the contact interaction term and the dipolar term,
\[
\Phi(r) = 4\pi \hbar^2 \frac{\alpha}{m} \delta(r) + D(r, b, \zeta).
\]  
(3.22)

Then its Fourier transform writes as
\[
\Phi_k = 4\pi \hbar^2 \frac{\alpha}{m} + D_k(b, \zeta).
\]  
(3.23)

And the long-wave limit of the Fourier transform is
\[
\Phi_0 \equiv \lim_{k \to 0} \Phi_k = 4\pi \hbar^2 \frac{\alpha}{m}.
\]  
(3.24)

It is worth stressing that the use of an effective regularized potential is well justified and allows for the construction of a uniquely defined perturbation theory [46].

3.4. Excitation spectrum

For compactness, in this and following sections, we use the system of units with the Boltzmann constant \( k_B \) and Planck constant \( \hbar \) set to unity.
\[ \varepsilon_D = \frac{4\pi a_0^2}{3\hbar} = \frac{a_0}{3a_i} \quad (a_D \equiv m\hbar_0^2). \]

Then, keeping in mind polarized dipoles, for spectrum (3.31) we get
\[ \varepsilon_k^2 = c_i^2 [1 + \varepsilon_D (3\cos^2 \vartheta_k - 1)] J(q, \zeta) \frac{k^2}{2m} + \left( \frac{k^2}{2m} \right)^2, \]

where \( q = kb \) and \( \zeta = \pi b \).

The spectrum can be represented in a dimensionless form by employing the healing length \( \xi \) that is defined by the equality of the effective sound-wave energy \( mc^2 \), where \( c \) is sound velocity, with the effective kinetic energy \( 1/2m\xi^2 \), which, in the Bogolubov approximation, gives
\[ \xi \equiv \frac{1}{\sqrt{2mc_B}} = \frac{1}{\sqrt{8\pi/\rho a_i}}. \] (3.36)

Let us introduce the dimensionless momentum
\[ p \equiv k\xi \]
and the dimensionless spectrum
\[ \varepsilon(p) = \frac{\xi}{c_i} \varepsilon_k. \] (3.37)

Also, for short, let us use the notation
\[ J_p \equiv J(q, \zeta) \quad \left( q = \frac{b}{\xi} p \right) \]
(3.38)

defining the dipolar part of the interaction
\[ f_k = D_k J_p \quad (p = k\xi). \]

Then the dimensionless form of spectrum in (3.35) writes as
\[ \varepsilon(p) = p\sqrt{1 + \varepsilon_D(3\cos^2 \vartheta_k - 1)J_p + \frac{1}{2}p^2}, \] (3.40)

where
\[ \cos \vartheta_k \equiv \frac{p \cdot e_k}{p} \quad (p \equiv \xi k). \]

It is important to emphasize that in the long-wave limit we have
\[ \lim_{p \to 0} J_p = \lim_{q \to 0} J(q, \zeta) = \lim_{k \to 0} f_k(b, \infty) = 0, \]

provided the screening effect is taken into account, so that \( \infty \neq 0 \). But if the screening would be neglected, we would have
\[ J(q, 0) = \lim_{q \to 0} J(q, \zeta) = \frac{3}{q} (\sin q - \alpha \cos q), \]

which leads to
\[ \lim_{q \to 0} J(q, 0) = 1. \]

However then the Fourier transform (3.24) is not defined for \( k \to 0 \). Moreover, as follows from section 2, thermodynamic quantities, containing \( \Phi_0 \), such as the chemical potential, grand potential, and so on, would not be defined as scalars [44]. Therefore taking account of screening is compulsory for

\[ J_p(p) \]

having well defined thermodynamic characteristics. So, generally, we have to deal with the integral
\[ J_p = 9p \int_{\delta}^{\infty} \left[ \sin(\varphi z) - \cos(\varphi z) \right] e^{-\alpha \zeta z} \varphi z, \]
in which
\[ \delta \equiv \frac{b}{\xi}. \]

The short-range cutoff \( b \) can be treated to be of the order of the scattering length \( a_i \) that depends on the dipolar interactions [56, 57]. If the screening length is close to the healing length, then \( \alpha \xi = \xi/r_i \approx 1 \).

The integral \( J_p \) for \( \alpha \xi = 1 \) can be written in the form
\[ J_p = -3\pi \frac{1 + p^2}{2p^2} + \frac{1 + p^2}{4p^2} \left( \text{Ei}[-1 - ip\delta] - \text{Ei}[-1 + ip\delta] \right) \]

\[ + \frac{3e^{-\delta}}{2p^2} \sin(p\delta) - p(2 - \delta) \cos(p\delta), \]

where \( \text{Ei}[\cdot] \) is the exponential integral function [44]. The behavior of the integral \( J_p \), as a function of \( p \), for \( \delta = 0.1 \) and \( \alpha = 1/\xi \), is shown in figure 1.

\[ \text{Figure 1.} \quad \text{Behaviour of the integral} \ J_p \ \text{as a function of the dimensionless momentum} \ p \ \text{for} \ \delta = 0.1. \]

3.6. Roton instability

Spectrum (3.40) is anisotropic, depending on the direction of momentum with respect to the dipole polarization. When the momentum is parallel to the dipole polarization, which is denoted as
\[ \varepsilon_{||}(p) = \varepsilon(p) \quad (\vartheta_p = 0), \]

we have
\[ \varepsilon_{||}(p) = p\sqrt{1 + 2\varepsilon_D J_p + \frac{1}{2}p^2}. \] (3.42)

While when the momentum is orthogonal to the dipole polarization, which is denoted as
forces, have been considered for quasi-one-dimensional [64–67] and quasi-two-dimensional [68–70] cases. The instability develops for sufficiently strong dipolar forces [71–74], which depends on the trap shape, and can be connected with the roton instability [75].

The origin of the roton minimum is due to the attractive part of the dipolar interactions leading to the appearance of the negative term in spectrum (3.44).

The Bogolubov approximation is applicable for temperature close to zero. At finite temperature, one should consider spectrum (3.28) taking into account the density of uncondensed particles $\rho_l$ and the anomalous average $\sigma_1$. It is not allowed to neglect $\sigma_1$, while retaining $\rho_l$ since these quantities are of the same order of magnitude [17, 18, 30, 34, 55, 76]. Moreover, it is only taking into account the anomalous average $\sigma_1$ makes it possible to correctly describe the Bose–Einstein condensation as a second-order phase transition [77] and to achieve for the ground state energy and condensate density [78] good numerical agreement with Monte Carlo data [79].

Let us emphasize that, in the Bogolubov approximation, the spectrum of collective excitations (3.31), or (3.35), is anisotropic, while the sound velocity (3.33) is isotropic. This is because taking account of the screening makes zero the long-wave limit of $J_p \to 0$ as $p \to 0$. Not taking account of the screening is equivalent to setting unity instead of $J_p$. In that case, the Bogolubov sound velocity would become anisotropic, but simultaneously thermodynamic potential and other thermodynamic quantities that have to be scalars, would become explicitly dependent on the angle $\vartheta_2$, thus loosing their scalar form, which would be senseless [44]. However, in the HFB approximation, the sound velocity (3.30) is anisotropic, which requires to consider the density of uncondensed particles $\rho_l$ and the anomalous average $\sigma_1$.

3.7 Dipolar instability

Sufficiently strong dipolar interactions can lead to the instability of a Bose-condensed system [71–74, 80]. Roton instability, arising at finite momenta of excitations, is one of the possibilities. It may also happen instability, occurring at the
If $\varkappa \sim 1/\xi$ and $\varkappa b \ll 1$, then the above inequality reads as $\rho a_0 \xi^2 > 15/(16\pi)$. With the expression (3.36) for the healing length, we have $a_0/a_s > 7.5$.

Moreover, even for a positive $m_k$, such a quadratic spectrum does not satisfy the Landau criterion, hence cannot support superfluidity. Recall also that Bose–Einstein condensation is necessarily accompanied by global gauge symmetry breaking [1, 12, 17, 18, 30]. And the collective excitations in a system with global gauge symmetry breaking exhibit the phonon behavior in the long-wave limit [31, 32, 84]. That is, the quadratic spectrum contradicts the presence of Bose–Einstein condensate or, in other words, signifies the instability of the latter.

The phonon instability at $a_s \to 0$ leads to the divergence of the isothermal compressibility

$$\chi_T = \frac{1}{\rho N} \left( \frac{\partial N}{\partial \mu} \right)_T = \frac{\text{var}(N)}{\rho N T}. \quad (3.52)$$

In the local density approximation, this gives

$$\chi_T = \frac{1}{\rho N} \int \frac{\rho(r)}{\Delta(r)} \, dr, \quad (3.53)$$

where $\Delta(r)$ is defined in (2.144) and, in the Bogolubov approximation, it is

$$\Delta(r) = \rho(r) \Phi_0. \quad (3.54)$$

Then the compressibility becomes

$$\chi_T = \frac{1}{\rho^2 \Phi_0} = \frac{m}{4\pi \rho^2 a_s}. \quad (3.55)$$

As is evident, when $a_s \to 0$, the compressibility diverges.

### 3.8. Trapped atoms

In the previous sections, the system stability has been considered for either a uniform system or for a large trap with a slowly varying trapping potential, for which the local-density approximation is valid. But when atoms are confined in a trap, the trapping potential can stabilize atomic system that in the uniform case would be unstable.

Limiting the consideration by the Bogolubov approximation, we may neglect $\rho_1$ and $\sigma_1$, as compared to $\rho_0 \sim \rho$. Then the condensate function equation (2.34) reduces to the form given by the equation

$$i \frac{\partial}{\partial t} \eta(r,t) = \frac{\delta H^{(0)}}{\delta \eta^*(r,t)}, \quad (3.56)$$

which coincides with equation (2.40) for the vacuum coherent field.

The trapping potential is usually taken as the harmonic potential. For a trap with cylindrical symmetry, it reads as

$$U(r) = \frac{m}{2} \left( \omega_\perp^2 r_\perp^2 + \omega_z^2 z^2 \right), \quad (3.57)$$

where

$$\omega_\perp \equiv \omega_x = \omega_y, \quad r_\perp^2 = x^2 + y^2. \quad (3.58)$$
The geometry of the trap, characterized by the aspect ratio
\[ \alpha \equiv \frac{\omega_\perp}{\omega_\parallel} = \left( \frac{l_\perp}{l_\parallel} \right)^2, \quad (3.59) \]
with the oscillator lengths
\[ l_\perp \equiv \frac{1}{\sqrt{m\omega_\perp}}, \quad l_\parallel \equiv \frac{1}{\sqrt{m\omega_\parallel}}, \]
plays an important role for the system stability.

In equilibrium, the condensate-function equation takes the form
\[ \int \mathcal{D}(\mathbf{r} - \mathbf{r}')\rho(\mathbf{r}') \, d\mathbf{r}' = \int \mathcal{D}_k \rho_k e^{i\mathbf{k} \cdot \mathbf{r}} \frac{d\mathbf{k}}{(2\pi)^3}, \quad (3.62) \]
involving the Fourier transforms of the regularized potential
\[ \mathcal{D}(\mathbf{r}) = \int \mathcal{D}_k e^{i\mathbf{k} \cdot \mathbf{r}} \frac{d\mathbf{k}}{(2\pi)^3}, \quad \mathcal{D}_k \equiv D_k(b, \kappa), \]
and of the density
\[ \rho(\mathbf{r}) = \int \rho_k e^{i\mathbf{k} \cdot \mathbf{r}} \frac{d\mathbf{k}}{(2\pi)^3}. \]

The quantity \( \mathcal{D}_k \) tends to zero for \( k \gg 1/b \), while \( \rho_k \) quickly diminishes for \( k \gg \max_\alpha \{1/l_\alpha\} \), with \( l_\alpha \) being the effective system length in the \( \alpha \)-direction. Since \( b \) is of the order of \( a_\infty \), one usually has
\[ b \ll \min_\alpha \{l_\alpha\}. \quad (3.63) \]
In other words,
\[ \frac{1}{b} \gg \frac{1}{\min_\alpha \{l_\alpha\}} = \max_\alpha \left\{ \frac{1}{l_\alpha} \right\}. \quad (3.64) \]
This tells us that the integration in the right-hand side of (3.62) is effectively done over the momenta not much exceeding \( \max_\alpha \{1/l_\alpha\} \). Hence the finiteness of the trap plays the role of an effective regularization at large momenta or small distances. This implies that the short-range regularization by means of the cutoff \( b \) is not as important, provided no divergences arise.

On the other hand, \( \mathcal{D}(\mathbf{r}) \) diminishes for \( r \gg r_\parallel \equiv 1/\kappa \), while the density \( \rho(\mathbf{r}) \) for a finite trap quickly goes to zero for \( r \gg \max_\alpha \{l_\alpha\} \). Therefore for a small trap, with the sizes such that
\[ \max_\alpha \{l_\alpha\} \ll r_\parallel \equiv \frac{1}{\kappa}, \quad (3.65) \]
the screening is not crucial, since the trap length effectively limits the integration in the left-hand side of (3.62) or large distance. Therefore for such small traps the screening at large distance may be not necessary, since
\[ \kappa \ll \frac{1}{\max_\alpha \{l_\alpha\}} = \min_\alpha \left\{ \frac{1}{l_\alpha} \right\}. \]

The screening lengths in condensed matter are typically of ten Angstroms [85]. The healing length for atomic Bose condensate is \( \xi \sim (10^{-3}\text{–}10^{-4}) \text{ cm} \), while its typical size is of the order of \( (10^{-4}\text{–}10^{-2}) \text{ cm} \). So, the traps, whose maximal length is smaller that the screening radius, should be really small. Those calculations for trapped atoms or molecules, which do not take account of screening are valid only for small traps in the sense of condition (3.65).

### 3.9. Geometric stabilization

Recall first that a Bose-condensed gas with purely local attractive interactions, when \( a_r < 0 \) and \( a_D = 0 \), is unstable in a uniform system, but can be stabilized in a trap for the number of particles smaller that a critical number \( N_c \) depending on the shape geometry and the interaction strength. The value of the critical number can be estimated [86] from the expression
\[ N_c = \sqrt{\frac{\pi}{2}} \frac{l_\parallel l_\perp}{|a_r| (l_\perp^2 + l_\parallel^2 + l_z^2)} \quad (a_r < 0, \quad a_D = 0). \quad (3.66) \]

Similarly, the stability of a gas with contact plus dipolar interactions depends on the trap geometry and the interaction strength [71–74, 80]. One typically considers small traps in the sense of condition (3.65), which allows for the use of the not regularized dipolar potential. This potential is partially attractive. For instance, let us consider a cylindrical trap, with the cylinder axis along \( z \), filled by atoms whose dipoles are oriented along the axis \( z \). Then expression (3.7) shows that the atomic interactions in the direction of the axis \( z \) are attractive, while the interactions in the perpendicular direction are repulsive:
\[ D(\mathbf{r}) = -2 \frac{d_3^2}{r^3} \quad (\theta = 0), \]
\[ D(\mathbf{r}) = \frac{d_3^2}{r^3} \quad (\theta = \frac{\pi}{2}). \quad (3.67) \]

It is clear that the atomic clouds in pencil-shape traps, where the majority of atoms interact attractively, should be less stable than the atomic clouds inside pancake-shape traps, where the majority of atoms interact repulsively.

The energetic stability, at zero temperature and weak interactions, can be studied by looking for the minima of the energy functional.
\[
E = \int \eta^*(\mathbf{r}) \left[ -\frac{\nabla^2}{2m} + U(\mathbf{r}) \right] \eta(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \int \Phi(\mathbf{r} - \mathbf{r}') |\eta(\mathbf{r}')|^2 |\eta(\mathbf{r}')|^2 \, d\mathbf{r} d\mathbf{r}'.
\]

(3.68)

similarly to the stability analysis for different finite quantum systems [87]. Here a small trap is assumed in the sense of condition (3.65), so that the dipolar potential is not regularized. Taking the trial condensate function in the Gaussian form

\[
\eta(\mathbf{r}) = \frac{1}{\pi^{d/2}} \sqrt{\frac{N}{L_+ L_z}} \exp \left\{ -\frac{1}{2} \left( \frac{\mathbf{r}}{L_+} \right)^2 - \frac{1}{2} \left( \frac{z}{L_z} \right)^2 \right\},
\]

(3.69)
in which \(L_+\) and \(L_z\) are variational parameters describing the effective radius and length of the atomic cloud, gives the internal energy

\[
E = E_{\text{kin}} + E_r + E_{\text{int}},
\]

(3.70)
consisting of the kinetic energy

\[
E_{\text{kin}} = \frac{N}{4m} \left( \frac{2}{L_+^2} + \frac{1}{L_z^2} \right),
\]

(3.71)
potential trap energy

\[
E_r = \frac{N}{4} m \omega_\perp^2 \left( 2L_+^2 + \alpha^2 L_z^2 \right),
\]

(3.72)
and the interaction energy

\[
E_{\text{int}} = \frac{N^2 a_s}{\sqrt{2\pi} m \omega_\perp^2 L_z} \left[ 1 - \varepsilon_D F(\lambda) \right].
\]

(3.73)
Here the notations are used:

\[
F(\lambda) = \frac{1 + 2\lambda}{1 - \lambda} - \frac{3\lambda f(\lambda)}{(1 - \lambda)^{3/2}}
\]

(3.74)
and

\[
\lambda \equiv \left( \frac{L_+}{L_z} \right)^2,
\]

(3.75)
in which

\[
f(\lambda) = \begin{cases} 
\arctanh \sqrt{\lambda - 1}, & \lambda > 1 \\
\frac{1}{2} \ln \frac{1 + \sqrt{1 - \lambda}}{1 - \sqrt{1 - \lambda}}, & \lambda < 1.
\end{cases}
\]

One should not confuse the variational parameters \(L_+\) and \(L_z\) with the fixed oscillator lengths \(l_+\) and \(l_z\). Hence \(\lambda\) is different from the aspect ratio \(\alpha = (l_+/l_z)^2\).

Accomplishing the minimization with respect to the parameters \(L_+\) and \(L_z\) results in the energy \(E\) being a function of five parameters, \(m, N, \omega_\perp\), \(\alpha\), and \(\varepsilon_D\). A discussion on numerical analysis can be found in [21, 24]. Briefly speaking, the results are as follows. When \(a_s < 0\), the system is stable (metastable) for \(N < N_c\). If \(a_s > 0\), the system is stable for weak dipolar interactions with \(0 < \varepsilon_D < 1\). When the dipolar interactions are strong, such that \(\varepsilon_D > 1\), the system can be metastable for \(N < N_c\). The value of the critical number \(N_c\) depends on the trap ratio \(\alpha\) and the parameter \(\varepsilon_D\). Generally, atomic clouds in pancake-shape traps are more stable than those in pencil-shape traps, provided the polarization of dipoles is along the axis \(z\).

### 3.10. Thomas–Fermi approximation

The shape of the atomic cloud in a small trap can be found by invoking the Thomas–Fermi approximation [88, 89], when the kinetic energy can be neglected being much smaller than the interaction energy. Then equation (3.60) gives

\[
\rho(\mathbf{r}) = |\eta(\mathbf{r})|^2 = \rho(0) \left( 1 - \frac{r_+^2}{R_+^2} - \frac{z^2}{R_z^2} \right),
\]

(3.76)
which is valid in the region

\[
\frac{r_+^2}{R_+^2} + \frac{z^2}{R_z^2} \leq 1,
\]

where \(\rho(\mathbf{r})\) is non-negative, and is zero outside this region. The density in the center is

\[
\rho(0) = \frac{15N}{8\pi R_+^2 R_z}.
\]

(3.77)
The transverse and longitudinal radii, defining the effective size of the atomic cloud, are given by the equations

\[
R_+^5 = \frac{15\Phi_0 \sqrt{\lambda} N}{4\pi m \omega_\perp^2} \left\{ 1 + \varepsilon_D \left[ \frac{3\lambda f(\lambda)}{2(1 - \lambda)} - 1 \right] \right\}
\]

(3.78)
and

\[
3\sqrt{\lambda} \varepsilon_D \left[ \left( 1 + \frac{\alpha^2}{2} \right) F(\lambda) \frac{1}{1 - \lambda} + (\varepsilon_D - 1)(\lambda - \alpha^2) = 0, \right.
\]

(3.79)
where

\[
\lambda \equiv \left( \frac{R_+}{R_z} \right)^2, \quad \alpha \equiv \left( \frac{l_+}{l_z} \right)^2.
\]

(3.80)
But the critical number \(N_c\) cannot be found in this approximation.

### 3.11. Quantum ferrofluid

A system of atomic or molecular dipoles is somewhat analogous to a collection of nanosize ferromagnetic particles forming colloidal suspensions [90]. Therefore dipolar atomic and molecular systems can be called quantum ferrofluids [91]. The properties of such systems can be governed in a wide diapason. The \(s\)-wave scattering length can be varied by Feshbach resonance, so that the magnetic dipole–dipole interactions can become comparable in strength with the contact interaction. Moreover, it is possible to create a purely dipolar quantum gas, reducing the scattering length \(a_s\) to zero [92]. Such a dipolar gas can be stable in a pancake trap, provided the number of particles is smaller than the critical number \(N_c\) and temperature is close to zero. Dipolar gas in a pancake trap can be stable (metastable) even for a weak attractive contact interaction with \(a_s < 0\), when \(N < N_c\) and \(T = 0\) [92]. However thermal fluctuations make this gas unstable [93].

An interesting question is: What happens with the strongly dipolar gas, with \(\varepsilon_D \geq 1\) and \(a_s \geq 0\), after it becomes unstable? Experiments with \(^{165}\)Dy demonstrated that after the system looses stability it forms a metastable state with one
[94, 95] or several [96, 97] self-bound small droplets, whose lifetime being of order (0.01–0.1) s. Monte Carlo simulations [98, 99] confirmed the formation of self-bound droplets of dipolar quantum gas of trapped ¹⁶⁴Dy atoms brought to the regime of instability. When the number of droplets increases, they form ordered arrays, reminiscent of the Rosensweig instability of classical ferrofluids in an external magnetic field [90]. Theoretically, the appearance of the metastable droplets of dipolar gas can be explained by taking account of Lee–Huang–Yang corrections [100, 101]. Recall that the Lee–Huang–Yang corrections are contained in the self-consistent mean-field theory [17, 18, 30, 34, 77, 102]. These corrections are just the limiting case of a small gas parameter $\rho^{1/3} a_s$ of this theory.

The system of dipolar bosons, with increasing density or interaction strength, can also crystallize in three [103, 104] as well as in two [105] dimensions, similarly to classical fluids.

Typical size of trapped Bose–Einstein condensates is of the order of $(10^{-4}–10^{-2})$ cm. This makes it difficult to get a good resolution of an absorption image in situ. Therefore one usually observes absorption images of the atomic cloud after some time of free expansion from the trap, when the trapping potential has been switched off. The free expansion is described by rescaling the characteristic length of the cloud by time-dependent factors [89, 106].

In nonequilibrium classical ferrofluids, there can exist solitonic excitations [107]. In quantum ferrofluids, three-dimensional solitons are unstable, but can arise in lower dimensional traps [108].

3.12. Magnetic induction

In the process of time-of-flight imaging, when the trapping potential is switched off, atoms fall down out of the trap due to gravity. At this stage, in addition to studying absorption images, it is admissible to get more information on the atoms by considering their fall through a magnetic coil connected to an electric circuit.

Let the electric circuit be characterized by resistance $R$, inductance $L$, and capacity $C$. Suppose the coil of the circuit has $n_c$ turns, cross-section area $A_c$, and length $l_c$, the coil axis being directed along the unit vector $\mathbf{e}_c$. If a cloud of atoms, with dipole magnetic moments $\mu_0 \mathbf{e}_d$, passes through the coil, with the number-of particle rate $N$, this moving atomic cloud induces the electromotive force

$$E_f = -\frac{4\pi c}{cl_c} \mu_0 \varepsilon_d \cdot \mathbf{e}_c N,$$

(3.81)

where $c$ is light velocity. The electromotive force generates in the electric circuit an electric current $j$ obeying the Kirchhoff equation

$$L \frac{dj}{dt} + RJ + \frac{1}{C} \int_0^t j(t') \, dt' = E_f.$$

(3.82)

The latter can be represented [109–111] in the integral form

$$j = -\mu_0 \frac{\varepsilon_d \cdot \mathbf{e}_c}{n_c A_c} \int_0^t G(t - t') \, dN(t'),$$

(3.83)

in which the transfer function

$$G(t) \equiv \left( \cos \omega' t - \frac{\gamma}{\omega'} \sin \omega' t \right) e^{-\gamma t}$$

contains the notations

$$\omega' = \sqrt{\omega^2 - \gamma^2}, \quad \omega = \frac{1}{\sqrt{LC}}, \quad \gamma = \frac{R}{2L}.$$  

Here $\omega$ is the circuit natural frequency and $\gamma$ is the circuit damping. The circuit is assumed to be of good quality, which implies that $\gamma \ll \omega$.

It is straightforward to find the electric current, when the number of atoms passing through the coil is given. For example, if the number of atoms passing through the coil is proportional to time,

$$N(t) = \Gamma t,$$

then the induced current is

$$j = -\mu_0 \frac{\varepsilon_d \cdot \mathbf{e}_c}{n_c A_c} \frac{\Gamma}{\omega} \sin(\omega t) e^{-\gamma t}.$$  

(3.84)

Measuring the current makes it possible to find the dipole magnetic moment $\mu_0$.

As another example, let us consider the case, when the number of atoms inside the coil oscillates as

$$N(t) = N_0 + \Delta N \sin(\omega t),$$

with $N_0 \geq \Delta N > 0$. If the oscillation frequency $\omega_0$ is close to the circuit natural frequency $\omega$, so that the resonance condition $|\omega - \omega_0| \ll \omega$ holds, then the induced current is

$$j = \mu_0 \frac{\varepsilon_d \cdot \mathbf{e}_c}{2n_c A_c} \frac{\Delta N \cos(\omega_0 t)}{2} \left( 1 - e^{-\gamma t} \right).$$  

(3.85)

But if $\omega_0$ is far detuned from $\omega$, then the amplitude of the induced current diminishes by the factor $\gamma^2/\omega^2$.

3.13. Optical lattices

In the presence of an optical lattice, the effective lattice Hamiltonian can be derived following the scheme of section 2.12. In the case of lattice band gaps that are much larger than any other energy scales of the system, such as the interaction strength, temperature, and Zeeman shifts, atoms remain confined in the lowest energy band of the lattice. Then, expanding the field operators over Wannier functions, according to (2.155), and considering only the lowest lattice band, we get the extended Hubbard model

$$\hat{H} = -\sum_{\langle ij \rangle} J_{ij} \hat{c}_j^\dagger \hat{c}_j + \sum_j \hat{h}_j \hat{c}_j^\dagger \hat{c}_j + \hat{H}_Z,$$

$$+ \frac{1}{2} \sum_j U_j \hat{c}_j^\dagger \hat{c}_j \hat{c}_j^\dagger \hat{c}_j + \frac{1}{2} \sum_{\langle ij \rangle} U_{ij} \hat{c}_j^\dagger \hat{c}_j \hat{c}_i^\dagger \hat{c}_i,$$

(3.86)

in which

$$J_{ij} = -\int w^*(\mathbf{r} - \mathbf{a}_i) \hat{H}^\dagger(\mathbf{r}) w(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r},$$

$$h_j = \int w^*(\mathbf{r} - \mathbf{a}_j) \hat{H}(\mathbf{r}) w(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r},$$

$$U_{ij} = \int \left( w^*(\mathbf{r} - \mathbf{a}_i) \hat{H}^\dagger(\mathbf{r}) \right) (\mathbf{r} - \mathbf{a}_j) w(\mathbf{r} - \mathbf{a}_j) \, d\mathbf{r},$$

(3.87)
where $\hat{H}(r)$ is defined in (2.154), and the matrix elements $U_{ijkl}$ are defined in (2.158), for instance

$$U_{ij} \equiv U_{ijji}, \quad U_{ij} \equiv U_{ijji} + U_{ijij}.$$  
(3.87)

where $\hat{H}(r)$ is defined in (2.154), and the matrix elements $U_{ijkl}$ are defined in (2.158), for instance

Here we consider atoms or molecules possessing magnetic moment $\mu_S$. The Zeeman term $H_Z$ takes account of the external magnetic field $B(r)$. The field operators and the operators $\hat{c}_j$, generally, are spinors with respect to some internal degrees of freedom.

The magnetic moment $\mu_0$ of an atom can be written as

$$\mu_0 = \mu_S S \quad \text{(3.89)}$$

where $\mu_S$ is the Landé factor, and $S$ is the effective atomic spin operator. Then the Zeeman energy operator reads as

$$\hat{H}_Z = -\mu_S \int \hat{\psi}^\dagger(r) B(r) \cdot S \hat{\psi}(r) \, dr.$$  
(3.90)

Introducing the notation

$$B_{ij} \equiv \int w^* (r - a_i) B(r) w(r - a_j) \, dr$$  
(3.91)

transforms the Zeeman term (3.90) to the form

$$\hat{H}_Z = -\mu_S \sum_{ij} B_{ij} \cdot \left( \hat{c}_i^\dagger S \hat{c}_j \right).$$  
(3.92)

If either the external magnetic field is slowly varying or atoms are well localized, then

$$B_{ij} = B \delta_{ij} \quad \text{(3.93)}$$

Defining the local spin operator

$$S_j \equiv \hat{c}_j^\dagger S \hat{c}_j,$$  
(3.94)

we come to the Zeeman term

$$\hat{H}_Z = -\mu_S \sum_j B_j \cdot S_j.$$  
(3.95)

A similar Hamiltonian characterizing quantum magnetism of the dipolar lattice gas of $^{52}\text{Cr}$, having spin $S = 3$, has been realized in experiment [112].

In addition to the linear Zeeman effect, there also exists the so-called quadratic Zeeman effect that can be due either to the hyperfine structure of the atom, or to alternating external electromagnetic fields. By applying off-resonance linearly polarized light, populating the internal spin states with different $m = -S, -S+1, \ldots, S$, it is possible to exert the quadratic Zeeman shift along the light polarization axis [112–115], generating the term

$$q_{Z} \sum_j (S_j^2)^2,$$

where $q_{Z}$ is independent of the constant magnetic field and the axis $z$ is assumed to be the light polarization axis. This optically induced quadratic Zeeman shift can be tailored at high resolution and rapidly adjusted using electro-optics. By employing either positive or negative detuning the sign of $q_{Z}$ can be varied.

A similar quadratic shift can be induced by a linearly polarized microwave driving field, with the driving Rabi frequency $\Omega$ and detuning $\Delta$ from a hyperfine transition, creating quadratic Zeeman effect with $q_{Z} = -\hbar \Omega^2/4\Delta$, of the order of $100 \text{a s}^{-1}$, as is demonstrated for $^{87}\text{Rb}$ [116, 117].

Low-temperature phases and stability of dipolar bosons in optical lattices have been studied in [20–25, 28, 118, 119]. Optical lattices can stabilize even a Bose gas with attractive local interactions [120].

It is worth noting that the considered above optical lattices do not take into account phonon degrees of freedom. Taking these into account may lead to the phonon instability of insulating states in optical lattices, although their lifetime can be rather long for treating such insulating optical lattices as metastable objects [121, 122].

### 3.14. Deep lattice

Atomic degrees of freedom can be separated from the spin degrees of freedom, when atoms (or molecules) are loaded into a deep optical lattice, where the number of atoms in each lattice site is fixed and atoms (or molecules) do not jump between the lattice sites. This implies that the Wannier functions are so well localized at the related lattice sites that their intersection for different sites is practically zero. As a result, the tunneling term becomes negligible,

$$J_{ij} = 0 \quad \text{(3.96)}$$

With the interaction potential (3.23), Hamiltonian (3.86) splits into the sum

$$\hat{H} = \hat{H}_a + \hat{H}_s$$  
(3.97)

of atomic and spin terms. Taking into account that, under the assumed good localization,

$$\int |w(r - a_i)|^2 |w(r - a_j)|^2 \, dr \cong 0 \quad (i \neq j),$$

for the atomic term we have

$$\hat{H}_a = \sum_j h \hat{c}_j^\dagger \hat{c}_j + \frac{1}{2} \sum_{ij} U_{ij} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_j \hat{c}_i,$$  
(3.98)

where

$$U_{ij} \equiv \Phi_0 \int |w(r - a_j)|^4 \, dr.$$  
(3.99)

The spin part is the sum of the Zeeman term and the interaction term,

$$\hat{H}_s = \hat{H}_Z + \frac{1}{2} \sum_{ij} \sum_{\alpha\beta} P_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta.$$  
(3.100)

Here

$$P_{ij}^{\alpha\beta} = \int D^{\alpha\beta}(r - r') \left[ |w(r - a_i)|^2 |w(r' - a_j)|^2 + w^*(r - a_i)w(r - a_i)w(r' - a_j)w(r' - a_j) \right] \, drdr'.$$  
(3.101)

where
In a deep lattice, the occupation number of lattice sites each lattice site is fixed, say being a parameter. The system length plays the role of an effective regularization effect, reads as

\[ H = -\mu_S \sum_j \mathbf{B}_j \cdot \mathbf{S}_j + q_2 \sum_j \langle \mathbf{S}_j \rangle^2 + \frac{1}{2} \sum_{i \neq j} \sum_{\alpha \beta} \mathcal{D}_{ij}^{\alpha \beta} S_i^\alpha S_j^\beta. \]  

(3.106)

The coefficient \( q_2 \) here is a function of the applied intensity and the detuning, but independent of the magnetic field [112–115]. For example, for \(^{52}\)Cr, that does not possess hyperfine structure, this coefficient can reach [114]

\[ q_2 \sim \pm 0.01 \mu_B G \sim \pm 10^{-2} \text{erg} \sim \pm 10^5 \text{h s}^{-1}, \]

although usually it is less than \( 100–400 \text{ h s}^{-1} \) [112]. Anyway, this is a rather large quantity comparable or even larger than the characteristic dipolar interaction energy \( \mu_B^2 S \), where \( \rho \) is the average atomic density. The mean interatomic distance in optical lattices is of the order \( a \sim (10^{-5}–10^{-4}) \text{ cm} \). Then \( \rho \sim (10^{12}–10^{15}) \text{ cm}^{-3} \). Taking \( \mu_S \sim 10 \mu_B \) yields

\[ \rho \mu_S^2 \sim (10^{-26}–10^{-23}) \text{ erg} \sim (10–10^5) \text{ h s}^{-1}. \]

Hamiltonian (3.106) has the structure similar to that of the system of magnetic nanomolecules and magnetic nanoclusters [111, 124–128], with the quadratic Zeeman term analogous to the single-site anisotropy. Therefore the spin dynamics for this Hamiltonian can be studied in the same way as in the cited papers.

To more efficiently regulate the motion of spins, it is possible to connect the sample with a resonant electric circuit creating a magnetic feedback field \( H \) described by the Kirchhoff equation

\[ \frac{dH}{dt} + 2\gamma H + \omega^2 \int_0^t H(t') \, dt' = -4\pi \eta_c \frac{dm_c}{dt}, \]  

(3.107)

in which \( \eta_c \equiv V/V_c \) is the coil filling factor, \( V \) being the sample volume, \( V_c \), the coil volume, \( \gamma \) is the circuit attenuation, \( \omega \), the circuit natural frequency, and

\[ m_c = \frac{1}{V} \sum_{j=1}^{N_c} \mu_S \langle S_j^z \rangle. \]  

(3.108)

In the presence of an external magnetic field \( B_0 \), the total magnetic field becomes

\[ B = B_0 e_z + H e_z. \]  

(3.109)
The evolution equations are written for the variables
\[ a = \frac{1}{N_c} \sum_{i=1}^{N_c} |S_i^i|^2, \quad w = \frac{1}{N_c} \sum_{i \neq j} |S_i^i S_j^j|^2, \quad s = \frac{1}{N_c} \sum_{i=1}^{N_c} |S_i|^2, \]
\[ (3.110) \]
where \( S^i \equiv S_i^i \pm i S_i^j \). The analysis of spin dynamics can be done as in papers [111, 124–128].

It is important to stress that in order to organize coherent spin motion, that is necessary for realizing fast spin reversal, the presence of the resonant electric circuit is compulsory. If this circuit is absent, then dipolar interactions destroy spin coherence and do not allow for their coherent motion [129, 130].

As a more general case, it is possible to consider a mixture of two different atomic species, with spins \( S \) and \( I \), in addition to dipolar interactions, having exchange interactions. The total spin Hamiltonian for such a mixture has the structure
\[ \hat{H} = \hat{H}_S + \hat{H}_I + \hat{H}_{SI}, \]
with the Hamiltonian for \( S \) spins
\[ \hat{H}_S = \sum_i \hat{H}_S^i + \frac{1}{2} \sum_{i \neq j} \hat{H}_{ij}^S - \mu_B \mathbf{B} \cdot \mathbf{S}_i + q_S^2 |S_i|^2, \]
and for \( I \) spins
\[ \hat{H}_I = \sum_j \hat{H}_I^j + \frac{1}{2} \sum_{i \neq j} \hat{H}_{ij}^I - \mu_I \mathbf{B} \cdot \mathbf{I}_j + q_I^2 |I_j|^2, \]
\[ \hat{H}_{IJ} = \sum_{\alpha,\beta} C_{ij}^{\alpha,\beta} I_i^\alpha I_j^\beta - 2 J_{ij} \mathbf{I}_i \cdot \mathbf{I}_j. \]

The dipolar interactions between \( S \) spins are defined in (3.105). And for \( I \) spins, the dipolar interactions are given by the dipolar tensor
\[ C_{ij}^{\alpha,\beta} = \frac{\mu_I^2}{a_{ij}^3} \left( \delta_{\alpha,\beta} - 3 n_{ij}^\alpha n_{ij}^\beta \right) \exp(-2\kappa a_{ij}). \]

Interactions between the spins of different species are described by the Hamiltonian
\[ \hat{H}_{SI} = \sum_i A \mathbf{S}_i \cdot \mathbf{I}_i + \sum_{i \neq j} A_{ij}^{\alpha,\beta} S_i^\alpha I_j^\beta, \]
with
\[ A_{ij}^{\alpha,\beta} = \frac{\mu_B h_1}{a_{ij}^3} \left( \delta_{\alpha,\beta} - 3 n_{ij}^\alpha n_{ij}^\beta \right) \exp(-2\kappa a_{ij}). \]

The transverse magnetization, entering the Kirchhoff equation (3.107) is
\[ m_x = \frac{\mu_S}{V} \sum_i |S_i|^2 + \frac{\mu_I}{V} \sum_j |I_j|^2. \]

The possibility of the efficient manipulation of spin dynamics of dipolar gases in deep optical lattices can be used for quantum information processing.

### 4. Spinor interaction potentials

#### 4.1. Hyperfine structure

Many atoms (and molecules), having a nonzero nuclear spin, exhibit hyperfine structure of their spectra [131–134]. The difference between two adjacent hyperfine Zeeman levels is caused by the influence on the nuclear spin \( I \) (total nuclear angular momentum) of the atomic electrons. The total angular momentum of an atom \( F \) is the sum
\[ F = J + I \]
of the total angular momentum of all electrons \( J \) and of the nuclear spin \( I \). The total angular momentum of electrons
\[ \mathbf{L} = \sum_j L_j, \quad \mathbf{S} = \sum_i S_i. \]

The hyperfine energy splitting is
\[ \Delta W = A_{hyp} (\mathbf{L} \cdot \mathbf{J}), \]
where \( A_{hyp} \) is the hyperfine structure constant that is usually determined from experiments. Rewriting \( \mathbf{J} \cdot \mathbf{I} \) as
\[ \mathbf{J} \cdot \mathbf{I} = \frac{1}{2} \left( \mathbf{F}^2 - \mathbf{I}^2 - \mathbf{J}^2 \right) \]
and taking into account that
\[ \mathbf{F}^2 = F(F+1), \quad \mathbf{J}^2 = J(J+1), \quad \mathbf{I}^2 = I(I+1), \]
we have
\[ \Delta W = \frac{1}{2} A_{hyp} (F(F+1) - J(J+1) - I(I+1)). \]

The total atomic angular momentum is a vector matrix
\[ \mathbf{F} = F_x e_x + F_y e_y + F_z e_z, \]
with the matrix components
\[ F_\alpha = [F_{\alpha m}^n] \quad (\alpha = x, y, z), \]
whose indices take the values \( m \equiv m_F = -F, -F+1, \ldots, F \).

The hyperfine structure of different atoms has been described in a number of publications [131–142]. The trapping of spinor atoms is accomplished in optical traps [143].

#### 4.2. Multicomponent versus fragmented

Spinor Bose gases can condense. One sometimes name spinor condensates as fragmented. This however is not correct. A spinor condensate is multicomponent.

By the definition of Pollock [144] and Nozieres and Saint James [145], a fragmented condensate is a condensate consisting of several coexisting condensates distinguished by the collective quantum index labelling the natural orbitals. The natural orbitals are the eigenfunctions of the first-order density matrix [146] satisfying the eigenproblem
\[
\int \rho(r, r') \varphi_k(r') \, dr' = n_k \varphi_k(r), \tag{4.1}
\]
where \(k\) is the multi-index of collective states and \(n_k\) is the occupation number of the \(k\)th state. It may happen that there are several collective states \(k_1, k_2, \ldots\) for which, in thermodynamic limit, one has
\[
\lim_{N \to \infty} n_{k_i}/N > 0 \quad (i = 1, 2, \ldots). \tag{4.2}
\]
Then one says that this is a fragmented condensate. If there is just a single state labelled by \(k_0\) satisfying the above limit, this corresponds to the standard case of a Bose–Einstein condensate.

A spinor gas is characterized by a spinor field operator
\[
\psi(r) = [\hat{\psi}_m(r)] \quad (m = -F, -F+1, \ldots, F),
\]
with the index \(m\) enumerating the \(2F + 1\) hyperfine components. For each of the components, it is straightforward to define the first-order density matrix
\[
\rho_m(r, r') = (\langle \hat{\psi}_m^\dagger(r') \hat{\psi}_m(r) \rangle)
\]
and to study the related eigenproblem
\[
\int \rho_m(r, r') \varphi_{nk}(r') \, dr' = n_{mk} \varphi_{nk}(r).
\]
If for an \(m\)th component there exists the limit
\[
\lim_{N \to \infty} n_{mk}/N > 0 \quad (-F \leq m \leq F),
\]
then this component is said to be condensed, with the \(n_{mk}\) number of atoms in the condensate.

The total first-order density matrix is
\[
\rho(r, r') = (\langle \hat{\psi}^\dagger(r') \hat{\psi}(r) \rangle) = \sum_m \rho_m(r, r'). \tag{4.5}
\]
But this density matrix does not satisfy eigenproblem (4.1), instead we have
\[
\sum_m \int \rho_m(r, r') \varphi_{nk}(r') \, dr' = \sum_m n_{mk} \varphi_{nk}(r),
\]
which is not an eigenproblem.

When the density matrix can be written as a sum, like in (4.5), this does not mean that there is fragmentation. In other words, using the representation
\[
\rho_m(r, r') = \sum_p n_{mp} \varphi_{mp}(r) \varphi^\dagger_{mp}(r'),
\]
we can write
\[
\int \rho(r, r') \varphi_{nk}(r') \, dr' = \sum_p n_{mp} \varphi_{mp}(r) (\varphi_{mp}, \varphi_{nk}).
\]
But this is not an eigenproblem, since the function \(\varphi_{nk}\) is not a natural orbital. Even in the simplified case, that is often met in dealing with spinor gases, when
\[
\varphi_{mp}(r) = \zeta_m \varphi_p(r), \quad (\varphi_k, \varphi_p) = \delta_{kp},
\]
we get
\[
\int \rho(r, r') \varphi_{nk}(r') \, dr' = \sum_m n_{mk} \varphi_{mk}(r) \zeta_m \zeta_n,
\]
which again is not an eigenproblem.

The core of the trouble is that the index \(m\) is not an index of a collective state for an \(N\)-particle system, but it is a single-particle index enumerating internal hyperfine states of separate atoms. Therefore spinor condensates are multicomponent, but not fragmented.

### 4.3. Spinor Hamiltonian

The Hamiltonian of a system of spinor atoms can be written [3, 26–28] as a sum of three terms
\[
\hat{H} = \hat{H}_0 + \hat{H}_Z + \hat{H}_{\text{int}}. \tag{4.6}
\]
The first term
\[
\hat{H}_0 = \int \psi^\dagger(r) \left[ -\frac{\nabla^2}{2m} + U(r) \right] \psi(r) \, dr
\]
is the single-atom Hamiltonian not containing the angular moment \(\mathbf{F}\).

The second term is the Zeeman energy operator
\[
\hat{H}_Z = \hat{H}_{ILZ} + \hat{H}_{QZ},
\]
including the linear and quadratic Zeeman effects. The linear Zeeman term is
\[
\hat{H}_{ILZ} = -\mu_F \int \psi^\dagger(r) \mathbf{B} \cdot \mathbf{F} \psi(r) \, dr,
\]
where \(\mu_F = -\mu_B g_F\), with \(g_F\) being the Landé factor. The external magnetic field, in general, can be a function of spatial and time variables, \(\mathbf{B} = \mathbf{B}(r, t)\). And the scalar product \(\mathbf{B} \cdot \mathbf{F}\) implies the matrix
\[
\mathbf{B} \cdot \mathbf{F} = \left[ \sum_{\alpha} B^\alpha F_{\alpha mn} \right].
\]

The quadratic Zeeman effect is described by the Hamiltonian
\[
\hat{H}_{QZ} = \mp \int \psi^\dagger(r) \left( \frac{\mu_F \mathbf{B} \cdot \mathbf{F}}{\Delta W(1 + 2I)} \right)^2 \psi(r) \, dr,
\]
where \(\Delta W\) is the hyperfine energy splitting. The sign minus or plus corresponds to the relative alignment (parallel or anti-parallel) of the nuclear and electronic spin projections in the considered atom.

The interaction part of the Hamiltonian
\[
\hat{H}_{\text{int}} = H_{\text{F}} + H_{\text{D}} \tag{4.11}
\]
consists of two terms describing local interactions of atoms with angular momentum \(\mathbf{F}\) and their nonlocal dipolar interactions. Keeping in mind rotationally symmetric pair collisions in the \(s\)-wave approximation, the angular momentum of the pair \(f\) is to be even [26, 27]. The latter conclusion holds both
forbosonsandfermions.Thebinarycollisionsofatoms,of
angularmomentumFeach,withthetotalangularmomentum
ofthepairf = 0, 2, . . . , 2F, arecharacterizedbytheinteraction
potential
\[\Phi_F(r) = \frac{4\pi}{m} \delta(r) \sum_f q_f \hat{P}_f,\]
(4.12)
inwhichq_f is the scattering length for collisions between
atomiwahtothetotalangularmomentumofthepairf and \(\hat{P}_f\)
isaprojectionoperatorontothestatewiththeevenangular
momentumf = 0, 2, . . . , 2F. For atoms with the angular
momentumF, there are2F+1 components corresponding
totheangularmomentumprojections\(-F, -F + 1, \ldots, F\). In
the rotationally symmetric s-wave approximation, the system
of2F + 1 components is fully described byF + 1 scattering
lengthsq_f.

The Hamiltonian of local interactions of atoms with
angularmomentumF each has the form
\[\hat{H}_F = \frac{1}{2} \sum_{klmn} \int \hat{\psi}_k^\dagger(r) \hat{\psi}_l(r) \Phi_{klmn} \hat{\psi}_m(r) \hat{\psi}_n(r) \, dr,\]
(4.13)
where \(\Phi_{klmn}\) is a matrix element of the potential (4.12).

As soon as there are nonzero angular momenta, they induce
the related dipolar interactions with the Hamiltonian
\[\hat{H}_D = \frac{\mu_s^2}{2} \sum_{klmn} \int \hat{\psi}_k^\dagger(r) \hat{\psi}_l(r') \hat{\psi}_m(r') \hat{\psi}_n(r) \hat{D}_{klmn}(r - r') \, dr'dr',\]
(4.14)
in which the regularized dipolar interactions are given by
the factor \(\hat{D}_{klmn}(r)\) that should include the short-range regular-
ization as well as long-range screening, similarly to dipolar
interactions in the previous chapter [44, 46]. As in the previ-
ous chapter, the regularized dipolar interaction potential can be
written as
\[\hat{D}_{klmn}(r) = \Theta(r - b_D) \hat{D}_{klmn}(r) \exp(-\zeta_D r),\]
(4.15)
with the appropriate short-range cutoff b_D, a long-range
screening parameter \(\zeta_D\), and the bare dipolar interaction
potential \(\hat{D}_{klmn}(r)\). The screening parameter \(\zeta_D\) can be of the order of the inverse spinor healing length
[147] \(\xi_F \sim 10^{-4}\) cm.

Since
\[\hat{D}_{klmn}(0) = 0,\]
the order of the field operators in (4.14) can be changed, so
that to get the expression
\[\hat{H}_D = \frac{\mu_s^2}{2} \sum_{klmn} \int \hat{\psi}_k^\dagger(r) \hat{\psi}_n(r) \hat{D}_{klmn}(r - r') \hat{\psi}_m(r') \hat{\psi}_l(r') \, dr'dr'.\]
The dipolar interactions are usually smaller than the local
spinor interactions.

4.4. Grand Hamiltonian

The grand Hamiltonian for a multicomponent system is
defined similarly to the case of a single-component system.
The appearance of the condensate in the mth component is
taken into account by the Bogolubov shift of the field operator
\[\hat{\psi}_m(r) = \eta_m(r) + \psi_m(r),\]
(4.16)
wheren_m is the condensate function and \(\psi_m\) is the field
operator of uncondensed atoms in the mth component. The quanti-
ties \(\eta_m\) and \(\psi_m\) are independent variables, being orthogonal to
each other,
\[\int \eta_m^*(r) \psi_m(r) \, dr = 0.\]
(4.17)
The condensate function is the order parameter for the
mth component, which requires that
\[\eta_m(r) = \langle \hat{\psi}_m(r) \rangle, \quad \langle \psi_m(r) \rangle = 0.\]
(4.18)
The number of condensed atoms in the mth component is
\[N_{0m} = \int |\eta_m(r)|^2 \, dr.\]
(4.19)
And the number of uncondensed atoms in this component is
\[N_{1m} = \langle \hat{N}_{1m} \rangle, \quad \hat{N}_{1m} = \int \psi_m^*(r) \psi_m(r) \, dr.\]
(4.20)
Condition (4.18) can be represented as the equality
\[\langle \hat{\Lambda}_m \rangle = 0,\]
(4.21)
in which the operator
\[\hat{\Lambda}_m = \int \left[ \lambda_m(r) \psi_m^*(r) + \lambda_m^* \psi_m(r) \right] \, dr\]
eliminates in the grand Hamiltonian the terms linear in the
operators \(\psi_m\).

Thus the grand Hamiltonian reads as
\[H = \hat{H} = \sum_m \left( \mu_{0m} N_{0m} + \mu_{1m} N_{1m} + \hat{\Lambda}_m \right),\]
(4.22)
where \(\mu_{0m}\) and \(\mu_{1m}\) are the Lagrange multipliers guaranteeing
the normalization conditions (4.19) and (4.20).

The condensate-function equations and the equations of
motion for the operators of uncondensed atoms are defined as
\[i \frac{\partial}{\partial t} \eta_m(r, t) = \left( \frac{\delta H}{\delta \eta_m^*(r, t)} \right), \quad i \frac{\partial}{\partial t} \psi_m(r, t) = \left( \frac{\delta H}{\delta \psi_m^*(r, t)} \right).\]
(4.23)
Not all chemical potentials \(\mu_{0m}\) and \(\mu_{1m}\) are independent.
The components are in chemical equilibrium with each other
[148], so that for the variation of the Gibbs thermodynamic
potential one has
\[\delta G = \sum_m \left( \frac{\delta G}{\delta N_{0m}} \delta N_{0m} + \frac{\delta G}{\delta N_{1m}} \delta N_{1m} \right) = 0.\]
With the equalities

\[\delta G = \sum_m \left( \frac{\delta G}{\delta N_{0m}} \delta N_{0m} + \frac{\delta G}{\delta N_{1m}} \delta N_{1m} \right) = 0.\]
\[ \mu_{m} = \frac{\delta G}{\delta N_{m}}, \quad \mu_{l} = \frac{\delta G}{\delta N_{l}}, \]

this translates into

\[ \delta G = \sum_{m} (\mu_{m0} \delta N_{m0} + \mu_{l1} \delta N_{l1}) = 0. \]

But the variation with respect to the numbers of atoms in the components assumes the constraints for the given total numbers of condensed and uncondensed atoms

\[ N_{0} = \sum_{m} N_{m0}, \quad N_{1} = \sum_{m} N_{l1}, \]

which implies that

\[ \delta N_{00} + \sum_{m \neq 0} \delta N_{m0} = 0, \quad \delta N_{10} + \sum_{m \neq 0} \delta N_{l1} = 0. \]

Thus we come to the equation

\[ \sum_{m \neq 0} (\mu_{m0} - \mu_{00}) \delta N_{m0} + (\mu_{l1} - \mu_{l0}) \delta N_{l1} = 0. \]

Another constraint for an equilibrium system is the conservation of the z-component of the angular momentum, which implies

\[ \delta N_{0m} - \delta N_{0,-m} = 0, \quad \delta N_{1m} - \delta N_{1,-m} = 0 \quad (m \neq 0). \]

Taking this into account yields

\[ \sum_{m>0} [(\mu_{m0} + \mu_{0,-m} - 2\mu_{00}) \delta N_{m0} + (\mu_{l1} + \mu_{l,-m} - 2\mu_{l0}) \delta N_{l1}] = 0. \]

From here it follows that

\[ \mu_{m0} + \mu_{0,-m} = 2\mu_{00}, \quad \mu_{l1} + \mu_{l,-m} = 2\mu_{l0} \quad (m \neq 0). \]

Additional two conditions are defined by the fixed total number of particles \( N \) in the system and by the minimization of thermodynamic potential with respect to \( N_{0} \).

### 4.5. Atoms with \( F = 1 \)

The angular momentum \( F \) for atoms with hyperfine structure is often called hyperfine spin. As an example, the hyperfine spin \( F = 1 \) has the components

\[ F' = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad F'' = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \]

\[ F' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \]

The field operator is the three-component spinor labelled by the index \( m = -1, 0, 1 \).

\[ \hat{\psi} = \begin{bmatrix} \psi_{1} \\ \psi_{0} \\ \psi_{-1} \end{bmatrix}, \quad \hat{\psi}_{m} = \psi_{m}(r, t). \]

The Hamiltonian part, corresponding to the local spinor interactions, reads as

\[ \hat{H}_{F} = \frac{1}{2} \sum_{m} \int \hat{\psi}_{m}^{\dagger}(r) \mathcal{V}_{m}^{\dagger}(r) \hat{\psi}_{m}(r) \hat{\psi}_{m}(r) \ dr, \]

\[ + \frac{1}{2} \sum_{m \neq n} \mathcal{F}_{mn}^{\dagger} \mathcal{F}_{mn}^{\dagger} \int \hat{\psi}_{m}^{\dagger}(r) \hat{\psi}_{n}^{\dagger}(r) \hat{\psi}_{m}(r) \hat{\psi}_{n}(r) \ dr, \]

where

\[ c_{0} = \frac{4\pi}{3m} (2a_{2} + a_{0}), \quad c_{2} = \frac{4\pi}{3m} (a_{2} - a_{0}). \]

Explicitly, this takes the form

\[ \hat{H}_{F} = \frac{1}{2} \int \left[ c_{0} \hat{\psi}_{0}^{\dagger}(r) \hat{\psi}_{0}(r) \hat{\psi}_{0}^{\dagger}(r) \hat{\psi}_{0}(r) + 2c_{1} \hat{\psi}_{0}^{\dagger}(r) \hat{\psi}_{1}(r) \hat{\psi}_{0}(r) \hat{\psi}_{1}(r) \right] \ dr, \]

\[ + 2(c_{0} - c_{2}) \hat{\psi}_{0}^{\dagger}(r) \hat{\psi}_{1}(r) \hat{\psi}_{0}(r) \hat{\psi}_{1}(r) + 2c_{2} \left( \hat{\psi}_{0}^{\dagger}(r) \hat{\psi}_{1}(r) \hat{\psi}_{0}(r) \hat{\psi}_{1}(r) \right) \ dr. \]

One calls the interactions ferromagnetic, when \( c_{2} < 0 \), and antiferromagnetic when \( c_{2} > 0 \).

Examples of the Bose atoms with the hyperfine angular momentum \( F = 1 \) and their scattering lengths are: lithium [27],

\[ a_{0} = 23.9a_{B}, \quad a_{2} = 6.8a_{B} \quad (^{7}\text{Li}), \]

sodium [149],

\[ a_{0} = (50.0 \pm 1.6)a_{B}, \quad a_{2} = (55.0 \pm 1.7)a_{B} \quad (^{21}\text{Na}), \]

potassium [150, 151],

\[ a_{0} = (68.5 \pm 0.7)a_{B}, \quad a_{2} = (63.5 \pm 0.6)a_{B} \quad (^{41}\text{K}), \]

and rubidium [152, 153],

\[ a_{0} = (101.8 \pm 0.2)a_{B}, \quad a_{2} = (100.4 \pm 0.1)a_{B} \quad (^{87}\text{Rb}). \]

### 4.6. Equilibrium properties

Bose–Einstein condensation of a spinor gas of sodium atoms \(^{23}\text{Na} \) with \( F = 1 \) was recently experimentally studied in [154] taking into account the linear and quadratic Zeeman effects. Dipolar interactions here can be neglected, since \( \mu_{F}^{2}/|c_{2}| = 0.007 \). Therefore the longitudinal magnetization \( M_{z} = \langle F_{z} \rangle / N \) along the external magnetic field direction is conserved by local interatomic interactions. The linear Zeeman effect thus becomes irrelevant for equilibrium states, since it is proportional to a conserved quantity. Bose–Einstein condensation was found to occur in steps, when different Zeeman components condense one at a time. The sequence of the condensation transitions essentially depends on the quadratic Zeeman energy

\[ E_{QZ} = \frac{(\mu_{F}B)^{2}}{\Delta W(1 + 2l)^{2}}. \]
Here $\mu^2/\Delta W \approx 277 h/sG^2$ [155]. For example, for $E_{QZ} \approx 56 h^{-1}$ and a highly magnetized sample, the component $m_f = +1$ condenses first at a critical temperature $T_1$, followed by the component $m_f = 0$ at a lower temperature $T_0 < T_1$. For low magnetization, the condensation sequence is reversed: first the component $m_f = 0$ condenses at $T_0$, after which the component $m_f = +1$ follows at $T_1 < T_0$. For $E_{QZ} \approx 434 h^{-1}$, there occurs only one sequence for any magnetization, with the component $m_f = +1$ condensing first and $m_f = 0$, second at a lower temperature. At the low field, when $E_{QZ} \approx 18 h^{-1}$, for high values of $M_z$, there happens the condensation of the component $m_f = -1$, while the $m_f = 0$ component remains uncondensed.

Full theoretical investigations of finite temperature properties for spinor gases seem to be absent. Starting from papers [156, 157], one usually considers the case of zero temperature and weak interactions, when all the system is assumed to be condensed. Finite temperature properties of spinor gases with $F = 1$ were discussed in [158–160] without taking into account interactions and in [161–163] neglecting anomalous averages that, however, can be crucially important for condensed systems.

The ground-state properties of spinor gases and their collective excitations at zero temperature have been studied for the angular momenta $F = 1$ ($^7$Li, $^{25}$Na, $^{41}$K, $^{87}$Rb) [156, 157, 164–178], $F = 2$ ($^{87}$Rb, $^{85}$Rb, $^{23}$Na) [152, 179, 180], and $F = 3$ ($^{52}$Cr) [181–183]. The Lee–Huang–Yang corrections to the Bogoliubov approximation for gases with $F = 1$ and $F = 2$ are considered in [184].

As an example, let us consider the ground state of $F = 1$ atoms, neglecting dipolar interactions and ignoring the linear Zeeman effect [27, 184]. Assume that the external magnetic field is directed along the axis $z$, so that the quadratic Zeeman term (4.10) can be presented as

$$\hat{H}_{QZ} = \int \bar{\psi}^\dagger(r) \mathcal{Q} B_z \mathcal{F} \hat{\psi}(r) \, dr,$$

(4.31)

with

$$\mathcal{Q} B_z = -\frac{\mu^2 B^2}{\Delta W (1 + 2 F^2)}.$$

If we assume that all atoms are condensed and use the single-mode approximation

$$\hat{\psi}(r) \approx \sqrt{\rho(r)} \hat{\xi},$$

(4.32)

where $\rho(r)$ is average density and $\hat{\xi} = [\xi_n]$ is a column normalized to unity,

$$\|\hat{\xi}\| = \sqrt{\sum_n |\xi_n|^2} = 1,$$

then, depending on the values of the parameters $c_2$ and $q_B$, there exist the following ground-state phases.

**Ferromagnetic phase**, when $|\langle \mathcal{F} \rangle | = 1$, corresponds to one of the states

$$\hat{\xi}_+ = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad \hat{\xi}_- = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad (c_2 < 0, \ q_B < 0).$$

(4.33)

**Polar phase**, longitudinal, $\hat{\xi}_0$, or transverse, $\hat{\xi}_\perp$, for which $|\langle \mathcal{F} \rangle | = 0$, is described by the states

$$\hat{\xi}_0 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad (c_2 > 0, \ q_B > 0), \quad \hat{\xi}_\perp = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad (c_2 > 0, \ q_B < 0).$$

(4.34)

This phase sometimes is named as antiferromagnetic.

**Broken-axisymmetry phase**, with the state

$$\hat{\xi} = \frac{1}{\sqrt{2}} \begin{bmatrix} \sin \theta \\ \sqrt{2} \cos \theta \\ \sin \theta \end{bmatrix} \quad (c_2 < 0, \ 0 < q_B < -2c_2 \rho),$$

(4.35)

where $\rho = N/V$ is the average atomic density.

### 4.7 Stratification of components

A spinor gas is a mixture of several components. But a system of components requires special conditions to represent a real mixture in space. If two components interact through a local potential

$$\Phi_{ij}(r) = \Phi_{ij}(\mathcal{F}), \quad \Phi_{ij} = \int \Phi_{ij}(r) \, dr,$$

(4.36)

their mixture is stable at zero temperature, provided the stability condition for the interaction strengths is valid:

$$\Phi_{ij} < \sqrt{\Phi_{ii} \Phi_{jj}} \quad (stability, \ T = 0).$$

(4.37)

where $i \neq j$. The derivation of this condition can be found, e.g. in [30].

For example, in a spinor gas with $F = 1$, there are three components labeled by $m_f = -1, 0, 1$. Consider first the two components, $m_f = 0$ and $m_f = \pm 1$, neglecting the dipolar interactions. As follows from Hamiltonian (4.30), the interaction strengths between the atoms of the $m_f = 0$ component and between the atoms of the $m_f = \pm 1$ component, respectively, are

$$\Phi_{00} = c_0, \quad \Phi_{11} = \Phi_{-1, -1} = c_0 + c_2,$$

while the interaction strength between the atoms of different components, $m_f = 0$ and $m_f = \pm 1$, is

$$\Phi_{01} = \Phi_{01} = c_0 + c_2.$$

If the system is antiferromagnetic (polar), where $c_2 > 0$, then

$$c_0 + c_2 > \sqrt{c_0(c_0 + c_2)} \quad (c_2 > 0),$$

which implies

$$\Phi_{01} > \sqrt{\Phi_{00} \Phi_{11}} \quad (stratification, \ T = 0).$$

(4.38)

Therefore such a system at zero temperature stratifies into spatially separated components $m_f = 0$ and $m_f = \pm 1$. But these components cannot be mixed in an equilibrium system.

The situation is different for the mixture of $m_f = 1$ and $m_f = -1$ components, for which the corresponding interaction strengths are

$$\Phi_{11} = \Phi_{-1, -1} = c_0 + c_2, \quad \Phi_{-11} = c_0 - c_2.$$
For a polar system, where $c_2 > 0$, one has
\[ c_0 - c_2 < c_0 + c_2 \quad (c_2 > 0), \]
meaning that
\[ \Phi_{-1} < \Phi_{11} \Phi_{-11} \quad \text{(stability, } T = 0). \quad (4.39) \]
This mixture at zero temperature is stable.

These effects have been observed for the $nF$ components of sodium, for which $c_2 > 0$ [185, 186].

At finite temperature, the stability condition reads [30] as
\[ \Phi_{ij} < \Phi_{e}\Phi_{ji} + \frac{TV}{\overline{N}N_{ij}} \Delta S_{\text{mix}} \quad (T > 0), \quad (4.40) \]
where $i \neq j$, $N_i$ is the number of atoms in the $i$th component, and
\[ \Delta S_{\text{mix}} = -N_i \ln \frac{N_i}{\overline{N}} - N_j \ln \frac{N_j}{\overline{N}} \]
is the entropy of mixing. Hence at finite temperature it is easier to mix different components.

4.8. Nonequilibrium properties

One usually considers the equations of motion of different components, neglecting the anomalous averages. For $F = 1$, this has been done in [187–195]. The evolution of the components of the spinor gas with $F = 2$ at zero temperature has been studied in [188, 194, 196–198]. Population dynamics of an $F = 1$ Bose gas was also considered for temperatures above the Bose–Einstein condensation transition [199, 200].

The process of population dynamics is dominated by the dipolar interactions of magnetic spins rather than by the spin-mixing contact potential. This is because the Hamiltonian part, containing the local hyperfine spin interactions, is invariant with respect to spin rotations and can be expressed through integrals of motion. For instance, let us consider the interaction Hamiltonian (4.28) for $F = 1$ and employ the single-mode approximation in the form
\[ \hat{\psi}_{am}(r) = \varphi(r) \hat{a}_m \quad (m = -1, 0, 1), \quad (4.41) \]
where $\hat{a}_m$ is a Bose field operator not depending on the spatial variable and $\varphi(r)$ is a spin-independent mode function normalized to one,
\[ \int |\varphi(r)|^2 \, dr = 1. \]
This form of the single-mode approximation assumes that not all atoms are condensed, since otherwise $\hat{a}_m$ could not be a Bose operator.

In terms of the operators $\hat{a}_m$, the operator of the total number of atoms is
\[ \hat{N} = \sum_m \hat{a}_m^\dagger \hat{a}_m. \quad (4.42) \]
It is possible to introduce the effective total spin operator
\[ \hat{S} \equiv \sum_{mn} \hat{a}_m^\dagger F_{mn} \hat{a}_n. \quad (4.43) \]
Explicitly, the spin components for $F = 1$ are
\[ S^+ = \sqrt{2} \left( \hat{a}_1^\dagger \hat{a}_0 + \hat{a}_0^\dagger \hat{a}_{-1} \right), \quad S^- = \sqrt{2} \left( \hat{a}_0^\dagger \hat{a}_1 + \hat{a}_{-1}^\dagger \hat{a}_{-1} \right), \quad S^z = \hat{a}_1^\dagger \hat{a}_1 - \hat{a}_{-1}^\dagger \hat{a}_{-1}, \]
where $S^\pm \equiv S^x \pm iS^y$. The spin operator satisfies the standard spin (or angular momentum) algebra, with the commutation relations
\[ [S^+, S^-] = 2S^z, \quad [S^+, S^±] = \pm S^±. \]
For the squared spin operator
\[ S^2 = S^+ S^- + (S^z)^2 - S^z, \]
on one has
\[ [S^±, S^2] = [S^+, S^2] = 0. \]
Using the commutation relations for $\hat{a}_m$, we have the equality
\[ \sum_{mnk} \hat{a}_m^\dagger F_{mn} F_{nk} \hat{a}_k = S^z S^\beta - \sum_{mnk} \hat{a}_m^\dagger \hat{a}_n F_{mn} F_{nk} \hat{a}_k. \quad (4.44) \]
Also, we use the property of the angular momentum operators
\[ \sum_k F_{mk} \cdot F_{kn} = \sum_{\alpha k} F_{mk}^\alpha F_{kn}^\alpha = F(F + 1) \hat{d}_{nm}. \quad (4.45) \]
In that way, employing the single-mode approximation (4.41), the Hamiltonian $\hat{H}_F$ in (4.28), for $F = 1$, reduces [3, 201–203] to the simple form
\[ \hat{H}_F = \frac{1}{2} \tau_0 \hat{N}(\hat{N} - 1) + \frac{1}{2} \tau_2 (S^2 - 2\hat{N}). \quad (4.46) \]
in which
\[ \tau_0 \equiv c_0 \int |\varphi(r)|^4 \, dr, \quad \tau_2 \equiv c_2 \int |\varphi(r)|^4 \, dr. \]
This Hamiltonian is expressed through the integrals of motion. It does not influence the evolution of the effective spin, since $[S, \hat{N}] = 0$. The spin evolution is governed by the dipolar interactions and the Zeeman terms. The linear Zeeman term (4.9) takes the form
\[ \hat{H}_{LZ} = -\mu F \mathbf{B}_{\text{eff}} \cdot \mathbf{S}. \quad (4.47) \]
in which
\[ \mathbf{B}_{\text{eff}} \equiv \int \mathbf{B}(r) |\varphi(r)|^2 \, dr. \quad (4.48) \]
And the quadratic Zeeman term (4.10) that can be rewritten as
\[ \hat{H}_{QZ} = QZ \int \hat{\psi}^\dagger(r) \left( \mathbf{B} \cdot \mathbf{F} \right)^2 \hat{\psi}(r) \, dr. \quad (4.49) \]
where
\[ QZ \equiv \mp \frac{\mu F^2}{\Delta W(1 + 2F)^2}, \]
becomes
\[ \hat{H}_{QZ} = QZ \sum_{mnk} \sum_{\alpha\beta} B^{\alpha\beta} \hat{a}_m^\dagger F_{mn}^\alpha \hat{a}_k. \quad (4.50) \]
with the notation
\[ B^{\alpha \beta} \equiv \int B^\alpha(r) B^\beta(r) |\varphi(r)|^2 \, dr. \]

Spinor condensates exhibit a rich variety of nonuniform spin structures, such as magnetic domains and various textures [204–208]. Different topological excitations can arise, e.g. integer and fractional vortices, monopoles, skyrmions, and knots [27, 209–211].

An interesting question is the dynamics of equilibration and thermalization of spinor gases prepared in a strongly nonequilibrium initial state. This problem is of general interest for finite quantum systems and has been reviewed in [212–214]. For spinor gases, these topics are discussed in review [27].

4.9. Optical lattices

The field operators of atoms in an optical lattice allow for the expansion in Wannier functions
\[ \hat{\psi}_m(r) = \sum_j \hat{c}_{jm} w(r - a_j), \]
(4.51)
where the single-band approximation is assumed, \( m = -F, -F+1, \ldots, F \) is the hyperfine index, \( j = 1, 2, \ldots, N_L \) is the lattice-site index, and \( a_j \) is a lattice vector. The Wannier functions are taken to be independent of the hyperfine index.

Substituting this expansion into Hamiltonian (4.6), for concreteness, we shall keep in mind atoms with the angular momentum \( F = 1 \). The related hyperfine spin is given explicitly in equation (4.26) or can be represented in the compact form through its components
\[ F_{mn}^{\alpha} = \frac{1}{\sqrt{2}} (\delta_{mn-1} + \delta_{mn+1}), \]
\[ F_{mn}^{\gamma} = \frac{1}{\sqrt{2}} (\delta_{mn-1} - \delta_{mn+1}), \quad F_{mn}^{\delta} = m \delta_{mn} \quad (m,n = -1, 0, 1). \]
(4.52)

Respectively, the ladder components are
\[ F_{mn}^{\alpha} \equiv F_{mn}^{\alpha} \pm i F_{mn}^{\gamma} = \sqrt{2} \delta_{m,n \pm 1}. \]
(4.53)

The first term, defined in equation (4.7), becomes
\[ H_0 = -\sum_{ij} \sum_m J_{ij} \hat{c}_{im}^\dagger \hat{c}_{jm} + \sum_j \sum_m h_{ij} \hat{c}_{jm}^\dagger \hat{c}_{jm}, \]
(4.54)
with the tunneling parameter
\[ J_{ij} = -\int \hat{w}^*(r - a_i) \left[ -\frac{\nabla^2}{2m} + U(r) \right] \hat{w}(r - a_j) \, dr \]
(4.55)
and the local-energy offset due to the external potential, including the lattice and confining potentials,
\[ h_{ij} = \int \hat{w}^*(r - a_i) \left[ -\frac{\nabla^2}{2m} + U(r) \right] \hat{w}(r - a_j) \, dr. \]
(4.56)

The linear Zeeman term (4.9) is
\[ H_{LZ} = -\mu_p \sum_{ij} \sum_m \hat{B}_{ij} \cdot \hat{F}_{mn} \hat{c}_{im}^\dagger \hat{c}_{jm}, \]
(4.57)
where
\[ \hat{B}_{ij} \equiv \int \hat{w}^*(r - a_i) \hat{B}(r) \hat{w}(r - a_j) \, dr. \]
(4.58)
The quadratic Zeeman term (4.10) transforms into
\[ \hat{H}_{QZ} = Q_z \sum_{ij} \sum_{mn \alpha \beta} B^{\alpha \beta}_{ij} \hat{c}_{im}^\dagger \hat{F}_{mn}^{\alpha} \hat{F}_{mk}^{\beta} \hat{c}_{jm}, \]
(4.59)
with the notation
\[ B^{\alpha \beta}_{ij} \equiv \int \hat{w}^*(r - a_i) B^\alpha(r) B^\beta(r) \hat{w}(r - a_j) \, dr. \]
(4.60)

Taking into account that the hyperfine spin-mixing interaction is short-range, it is admissible to retain in Hamiltonian (4.28) only the single-site terms, getting
\[ \hat{H}_F = \frac{\tau_0}{2} \sum_j \sum_{mn} \hat{c}_{jm}^\dagger \hat{c}_{jm} \hat{c}_{jn} \hat{c}_{jn} + \frac{\tau_2}{2} \sum_j \sum_{mn} \hat{c}_{jm}^\dagger \hat{c}_{jm} \hat{F}_{mn} \cdot \hat{F}_{mj} \hat{c}_{jm}, \]
(4.61)
where
\[ \tau_0 \equiv c_0 \int |\hat{w}(r - a_j)|^4 \, dr, \quad \tau_2 \equiv c_2 \int |\hat{w}(r - a_j)|^4 \, dr. \]
(4.62)
The dipolar Hamiltonian (4.14) takes the form
\[ \hat{H}_D = \frac{\mu_r^2}{2} \sum_{ijfg} \sum_{klmn} D_{ijfg}^{klmn} \hat{c}_{im}^\dagger \hat{c}_{jm} \hat{c}_{kn} \hat{c}_{gm}, \]
(4.63)
with the notation
\[ D_{ijfg}^{klmn} \equiv \int \hat{w}^*(r - a_i) \hat{w}^*(r' - a_f) \hat{w}(r' - a_g) \hat{w}(r - a_j) \hat{D}_{klmn}(r - r') \, dr dr'. \]
(4.64)

Depending on the lattice depth, thermodynamic parameters, and atomic interactions, the system can be in an insulating state or in superfluid state [215–218].

4.10. Insulating lattice

If the optical lattice is sufficiently deep, such that there are no jumps of atoms between different lattice sites, when \( J_{ij} = 0 \), the system is in an insulating state. Then Hamiltonian (4.54) reads as
\[ \hat{H}_0 = \sum_j \hat{h}_j \hat{n}_j, \]
(4.66)
with the operator
\[ \hat{n}_j \equiv \sum_m \hat{c}_{jm}^\dagger \hat{c}_{jm}. \]
(4.67)
for the number of atoms in a jth lattice site.

Assuming that the external magnetic field is slowly varying in space, as compared to the variation of well-localized Wannier functions, we have

$$B_j = \delta_j \mathbf{B}(a_j) \equiv \delta_j B_j.$$  \hspace{1cm} (4.68)

In particular, when the external magnetic field is constant in space, then we have the exact equality

$$\mathbf{B}_j = \delta_j \mathbf{B}\quad (\mathbf{B} = \text{const}).$$

In this case, the linear Zeeman term (4.57) can be written as

$$\hat{H}_{LZ} = -\mu_F \sum_j B_j \cdot \mathbf{S}_j,$$  \hspace{1cm} (4.69)

where the effective spin operator is

$$\mathbf{S}_j \equiv \sum_{mn} \mathbf{c}^\dagger_{jm} \mathbf{F}_{mn} \mathbf{c}_{jn}.$$  \hspace{1cm} (4.70)

Under the condition that the external magnetic field is slowly varying, as compared to the variation of Wannier functions, from notation (4.60), we find

$$B^\alpha_j = \delta_j B^\alpha \quad (\mathbf{B} = \text{const}).$$  \hspace{1cm} (4.71)

Then the quadratic Zeeman term (4.59) takes the form

$$\hat{H}_{QZ} = Qz \sum_j \sum_{mnk} (\mathbf{B}_j \cdot \mathbf{F}_{mn}) (\mathbf{B}_j \cdot \mathbf{F}_{nk}) \mathbf{c}^\dagger_{jm} \mathbf{c}_{jn}.$$  \hspace{1cm} (4.72)

Using the commutation relations of the operators $\hat{c}_{jm}$, we have the equality

$$\sum_{mnk} \mathbf{c}^\dagger_{jm} \mathbf{F}_{mn} \mathbf{F}_{nk} \mathbf{c}_{jn} \equiv \sum_{mnkl} \mathbf{c}^\dagger_{jm} \mathbf{F}_{mn} \mathbf{c}_{jn} \mathbf{F}_{nk} \mathbf{c}_{lk}.$$  \hspace{1cm} (4.73)

We may notice that the term

$$S^\alpha_j S^\beta_j = \sum_{mnkl} \mathbf{c}^\dagger_{jm} \mathbf{F}_{mn} \mathbf{F}_{nk} \mathbf{c}_{jn} \mathbf{c}_{lk}$$

describes a consecutive destruction and creation of a single atom. While the second term in the right-hand site of equality (4.73) corresponds to the simultaneous destruction and creation of a pair of atoms. Such two-particle processes are usually less important than the single-particle ones and can be neglected. For instance, if the number of atoms in a lattice site is strictly one, then $\hat{c}_{jm} \hat{c}_{jm} = 0$. In that way, for the quadratic Zeeman term, we can write

$$\hat{H}_{QZ} = Qz \sum_j (\mathbf{B}_j \cdot \mathbf{S}_j)^2,$$  \hspace{1cm} (4.75)

where

$$Qz = \mp \frac{\mu_F^2}{\Delta W (1 + 2 \ell^2)}.$$  \hspace{1cm} (4.76)

Here $\Delta W$ is the hyperfine energy splitting.

Using equality (4.72) transforms the spin-mixing Hamiltonian (4.61) to the form

$$\hat{H}_F = \frac{\mathcal{C}_0}{2} \sum_j 2 \mathbf{S}_j - \mathbf{S}_j^2),$$  \hspace{1cm} (4.77)

where

$$\mathcal{C}_0 = \sum_{ij} (S_j^2 - 2n_j).$$

The dipolar part (4.63) for a deep insulating lattice, taking into account that the dipolar potential is regularized by a short-range cutoff, because of which $D^\theta_{klmn} = 0$, can be written as

$$\hat{H}_D = \frac{\mathcal{C}_D}{2} \sum_{ijkl} D^\alpha_{ijkl} \hat{c}^\dagger_{im} \hat{c}^\dagger_{jn} \hat{c}_{kn} \hat{c}_{jl}.$$  \hspace{1cm} (4.78)

Employing the same procedure as in section 3, Hamiltonian (4.78) can be represented as

$$\hat{H}_D = \frac{1}{2} \sum_{ij} D^{\alpha\beta}_{ij} S^\alpha_j S^\beta_j,$$  \hspace{1cm} (4.79)

with the interaction potential

$$D^{\alpha\beta}(r) = \Theta(r - b_F) D^{\alpha\beta}(r) \exp(-\kappa r),$$  \hspace{1cm} (4.80)

in which

$$D^{\alpha\beta}(r) = \mu^2_F \frac{\delta_{\alpha\beta} - 3n^\alpha n^\beta}{r^3} \quad (n \equiv \frac{r}{r}).$$

For well localized atoms, potential (4.80) simplifies to the expression

$$D^{\alpha\beta}(r) = \Theta(a_{ij} - b_F) D^{\alpha\beta}_{ij} \exp(-\kappa r),$$  \hspace{1cm} (4.81)

with the dipolar tensor

$$D^{\alpha\beta}_{ij} = \frac{\mu^2_F}{a_{ij}} \left( \delta_{\alpha\beta} - 3n^\alpha n^\beta \right),$$  \hspace{1cm} (4.82)

where

$$n_{ij} = \frac{a_{ij}}{|a_{ij}|}, \quad a_{ij} = a_i - a_j.$$  

The short-range cutoff $b_F$ is of the order of the effective size of an atom, which is usually smaller than the lattice spacing. Hence the factor $\Theta(a_{ij} - b_F)$ can be omitted, being effectively taken into account by the summation with $i \neq j$. The screening parameter $\kappa r$ is of the order of the inverse spin healing length. The latter can be defined by equating the effective kinetic energy $\hbar^2/2mF^2$ with the effective potential energy of spin interactions $\mu_F^2$, which gives the spin healing length

$$\xi_F = \sqrt{2\mu_F^2}.$$  

The typical lattice spacing for optical lattices is $a \sim (10^{-5} - 10^{-4})$ cm, with the average density $\rho \sim (10^{12} - 10^{15})$ cm$^{-3}$. Assuming $\mu_F \sim 10\mu_B$ gives the typical energy $\mu_F^2 \sim (10^{-26} - 10^{-21})$ erg. Then the spin healing length is $\xi_F \sim (10^{-5} - 10^{-3})$ cm, which is close to the mean interatomic distance. Therefore taking into account the dipolar interactions of only nearest neighbors is a good approximation.
Summarizing, Hamiltonian (4.6) can be considered as being composed of three parts

$$\hat{H} = \hat{H}_{\text{L}} + \hat{H}_{\text{Z}} + \hat{H}_{\text{D}}.$$  
(4.83)

The first term \(\hat{H}_{\text{L}} = \hat{H}_0 + \hat{H}_F\),

$$\hat{H}_{\text{L}} = \sum_j \left[ \hbar \vec{n}_j + \frac{\tau_0}{2} \vec{\hat{n}}_j (\vec{\hat{n}}_j - 1) + \frac{\tau_0}{2} (\vec{S}^2_j - 2\vec{n}_j) \right],$$  
(4.84)

includes local spinor interactions. This term is invariant with respect to spin rotations and, since \([\vec{S}_j, \vec{n}_j] = [\vec{S}_j, \hat{H}_\text{L}] = 0\), it does not influence spin motion.

Spin motion is governed by the Zeeman—effect part

$$\hat{H}_{\text{Z}} = \sum_j \left[ -\mu_B \vec{B}_j \cdot \vec{S}_j + Q_z (\vec{B}_j \cdot \vec{S}_j)^2 + q_z (\vec{S}_j)^2 \right]$$  
(4.85)

and by the dipolar Hamiltonian (4.79). The Zeeman term consists of the linear Zeeman part, the quadratic Zeeman part caused by an external magnetic field and by the alternating-current quadratic Zeeman term.

The Hamiltonian similar to expression (4.83), but without the quadratic Zeeman term, has been derived in [219–222]. However, the quadratic Zeeman effect is an essential phenomenon in the physics of spinor atoms.

The alternating-current quadratic Zeeman term, due to the alternating-current Stark shift, can be induced either by applying off-resonance linearly polarized light, populating the internal spin states and exerting the quadrupole shift along the light polarization axis [112–115], or by a linearly polarized microwave driving field [116, 117, 223]. Here we assume that the light polarization axis is the axis \(z\). The coefficient \(q_z\) is independent of the non-driving magnetic field and depends only on the intensity and detuning of the quasi-resonance driving field. The alternating-field induced quadratic Zeeman shift can be tailored at high resolution and rapidly adjusted using electrooptics. By employing either positive or negative detuning the sign of \(q_z\) can be varied. The quasi-resonance quadratic Zeeman effect makes it possible to get \(q_z\) of the order \((100–10^5)\hbar s^{-1}\).

### 4.11. Spin Dynamics

Considering weak deviations of spins from their equilibrium positions, one can study such phenomena as spin echo [224] and ferromagnetic resonance [225] in spinor gases. In these studies, one usually does not take into account the quadratic Zeeman effect.

Here we shall describe how one could consider strongly nonequilibrium spin states and spin motion in the presence of the quadratic Zeeman effect. Also, we take into account the existence of a longitudinal and transverse external magnetic fields, so that the total magnetic field at site \(j\) is

$$\vec{B}_j = B_0 \hat{e}_z + H e_z.$$  
(4.86)

The transverse field can be created by a resonant magnetic coil, as in equation (3.107), which will allow for the efficient regulation of spin motion.

From the spin-operator components \(S_i^\chi\), we pass to the ladder operators using the relations

$$S_0^\chi = \frac{1}{2} (S_0^+ + S_0^-), \quad S_0^\pm = \frac{i}{2} (S_0^+ - S_0^-).$$

Then the Zeeman Hamiltonian (4.85) becomes

$$\hat{H}_{\text{Z}} = \sum_j \left\{ -\frac{\mu_B B_0}{2} \left( S_0^+ + S_0^- \right) + \left( Q_z B_0^2 + q_z (S_j)^2 \right) \right\} \left( S_j^+ S_j^- + (S_j^+)^2 + (S_j^-)^2 + S_j^+ S_j^- + (S_j^-)^2 \right)$$

$$\hat{H}_{\text{D}} = \sum_{ij} \left\{ a_{ij} (S_i^+ S_j^- - S_i^- S_j^+) + b_{ij} (S_i^+ S_j^+ - b_{ij} S_i^- S_j^-) + 2 c_{ij} S_i^+ S_j^- \right\},$$  
(4.88)

in which

$$a_{ij} = D_{ij}, \quad b_{ij} = \frac{1}{4} (D_{ij}^+ - D_{ij}^- - 2iD_{ij}^x), \quad c_{ij} = \frac{1}{2} (D_{ij}^+ - D_{ij}^-).$$

The equations of motion

$$i \frac{d}{dt} S_j^\pm = [S_j^\pm, H], \quad i \frac{d}{dt} S_j^0 = [S_j^0, H],$$

are derived by employing the commutation relations

$$[S_i^+, S_j^-] = 2 \delta_{ij}, \quad [S_i^-, S_j^+] = 2 \delta_{ij}.$$  
(4.89)

Recall that in the Hamiltonian (4.83) only the Zeeman (4.87) and dipolar (4.88) terms contribute to the equations of motion, since the spin-mixing part \(\hat{H}_{\text{L}}\) commutes with the spin operator.

In what follows, we shall need the notations for the Zeeman frequency

$$\omega_0 \equiv -\mu_B B_0 > 0$$  
(4.89)

and for the quadratic Zeeman parameter

$$D \equiv Q_z B_0^2 + q_z.$$  
(4.90)

Dipolar interactions enter the evolution equations through the local fluctuating fields

$$\xi_D \equiv \sum_j \left( a_{ij} S_j^+ + c_{ij} S_j^- + c_{ij} S_j^0 \right)$$  
(4.91)

and

$$\varphi_D \equiv \sum_j \left\{ a_{ij} S_j^- - 2c_{ij} S_j^0 - 2b_{ij} S_j^+ \right\}.$$  
(4.92)
Here the index $j$ runs over all lattice sites. The self-interaction term is zero because the dipolar interaction potential is regularized, such that $D_{ij} = 0$.

Since for a macroscopic sample, for which boundary effects are negligible,
\[ \sum_j D_{ij}^\beta = 0, \]
we have
\[ \sum_j a_{ij} = \sum_j b_{ij} = \sum_j c_{ij} = 0. \]

Therefore, assuming that the average $\langle S_i^\alpha \rangle$ does not depend on the site index $j$, we see that the fluctuating dipolar fields on the average are zero centered,
\[ \langle \xi_D \rangle = \langle \varphi_D \rangle = 0. \]

Also, we define the effective force
\[ f \equiv -i(\mu t^H + \varphi_D). \tag{4.93} \]

Finally, we come to the Heisenberg equations of motion for the ladder operator,
\[ \frac{dS_j^\alpha}{dt} = -i(\omega_0 + \xi_D)S_j^- + fS_j^\alpha - iD(S_j^\alpha S_j^\alpha + S_j^- S_j^-) + \frac{i}{2} Q_z H^2 \left[ (S_j^+ + S_j^-)S_j^\alpha + S_j^\alpha (S_j^+ + S_j^-) \right] - \frac{i}{2} Q_z B_0 H \left[ S_j^\alpha S_j^- + S_j^- S_j^\alpha - 4(S_j^\alpha)^2 + 2(S_j^-)^2 \right], \tag{4.94} \]
and for the $z$-component of the spin operator,
\[ \frac{dS_j^z}{dt} = -\frac{1}{2}(f^+ S_j^- + f S_j^0) + \frac{i}{2} Q_z H^2 \left[ (S_j^-)^2 - (S_j^0)^2 \right] + \frac{i}{2} Q_z B_0 H \left[ (S_j^- - S_j^0)S_j^0 + S_j^0 (S_j^- - S_j^0) \right]. \tag{4.95} \]

The equation for $S_j^\alpha$ follows from the Hermitian conjugation of equation (4.94).

### 4.12. Stochastic quantization

Averaging the equations of motion (4.94) and (4.95), we consider the following functions: the transition function
\[ u \equiv \frac{1}{SN_L} \sum_{j=1}^{N_L} \langle S_j^\alpha \rangle, \tag{4.96} \]
describing the mean spin rotation of the transverse spin component, the coherence intensity
\[ w \equiv \frac{1}{SN_L(N_L - 1)} \sum_{i \neq j} \langle S_i^\alpha S_j^\alpha \rangle, \tag{4.97} \]
showing the level of coherence in the spin motion, and the spin polarization
\[ s \equiv \frac{1}{SN_L} \sum_{j=1}^{N_L} \langle S_j^0 \rangle, \tag{4.98} \]
defining the average magnetic polarization per atom. Here $S$ implies the maximal eigenvalue of $S_j^\alpha$.

In the process of averaging the equations of motion, there is the necessity of decoupling the spin-spin correlation functions. The natural decoupling seems to be the mean-field approximation
\[ \langle S_i^\alpha S_j^\alpha \rangle = \langle S_i^\alpha \rangle \langle S_j^\alpha \rangle \quad (i \neq j). \tag{4.99} \]

There are, however, some problems when using this decoupling. The first problem is that decoupling (4.99) can be used for different lattice sites, but it is not valid for coinciding sites, if $S$ is arbitrary. This is because there happen such expressions
\[ S_i^\alpha S_j^\beta + S_j^\beta S_i^\alpha = 0 \quad \left( S = \frac{1}{2} \right), \]
that become zero for $S = 1/2$. The general decoupling, taking into account this case reads [111, 124, 226] as
\[ \langle S_i^\alpha S_j^\beta + S_j^\beta S_i^\alpha \rangle = \left( 2 - \frac{1}{S} \right) \langle S_i^\alpha \rangle \langle S_j^\beta \rangle. \tag{4.100} \]

This decoupling correctly interpolates between the quantum case of $S = 1/2$ and $S \to \infty$, when spins behave classically.

The other problem is that the mean-field approximation is actually a semi-classical approximation that can be employed for treating the coherent spin motion, although it does not correctly describe the initial quantum stage of spin motion, when coherence has not been imposed on the system. In the semi-classical approximation, there is no spin motion at all, if the initial transverse projection is zero, that is, when $u(0) = 0$. Thus the semi-classical approximation cannot characterize the development of coherence and hence, to correctly define the delay time for the start of the coherent stage of motion. This problem can be overcome by using the stochastic quantization [109–111, 124, 226], when the local fluctuating fields (4.91) and (4.92) are treated as stochastic variables. Note that field (4.91) is real, while (4.92) is complex. These variables are assumed to be zero-centered and representing white noise, so that their mutual correlations are given by the stochastic averaging
\[ \langle \langle \xi_D(t) \rangle \rangle = \langle \langle \varphi_D(t) \rangle \rangle = 0, \quad \langle \langle \xi_D(t) \xi_D(t') \rangle \rangle = 2\gamma_3 \delta(t - t'), \]
\[ \langle \langle \xi_D(t) \varphi_D(t') \rangle \rangle = \langle \langle \varphi_D(t) \varphi_D(t') \rangle \rangle = 0, \quad \langle \langle \varphi_D(t) \varphi_D(t') \rangle \rangle = 2\gamma_2 \delta(t - t'). \tag{4.101} \]

Here $\gamma_3$ is the attenuation caused by fluctuating dipolar fields, hence it is of the order of $\rho\mu^2 S$.

To take into account spin correlations above the mean field, we introduce the transverse attenuation $\gamma_2 = \rho\mu^2 \sqrt{S(S + 1)}$ that is defined in the second-order perturbation theory [227]. Generally, there also exists the longitudinal attenuation $\gamma_1$ that comes about because the Zeeman energy can be transferred to other degrees of freedom.

In the equations of motion, the quadratic Zeeman parameter (4.90) plays the role of an effective anisotropy shifting the Zeeman frequency to the quantity
\[ \omega_z \equiv \omega_0 + \omega_2 S, \quad \omega_2 \equiv (2S - 1)D. \tag{4.102} \]
Finally, we obtain the equation for the transition function,
\[ \frac{du}{dt} = -i(\omega_s + \xi_d - i\gamma_2)u + f_s + i(2S-1)Q_zB_0F(u^* + u)s \]
\[ + \frac{i}{2}(2S-1)Q_zB_0F(u^* + u)s - \frac{i}{2}(2S-1)Q_zB_0H(w - 2x^2 + u^2), \]  
(4.103)
coherence intensity,
\[ \frac{dw}{dt} = -2\gamma_2w + (u^*f + f^*u)s \]
\[ + \frac{i}{2}(2S-1)Q_zB_0F[(u^*)^2 - (u^2)]s + i(2S-1)Q_zB_0H(u^* - u)s^2, \]
(4.104)
and for the spin polarization,
\[ \frac{dx}{dt} = -\frac{1}{2}(u^*f + f^*u) \]
\[ + \frac{i}{4}(2S-1)Q_zB_0F[(u^2 - (u^2)]s + i(2S-1)Q_zB_0H(u - u^*)s - \gamma(x - s_\infty), \]
(4.105)
where \( s_\infty \) is the equilibrium spin polarization.

These equations are to be complemented by the definition of the transverse magnetic field \( H \). Here we keep in mind that the field \( H \) is a resonator feedback field created by a resonant magnetic coil surrounding the sample. Then the equation for \( H \) follows from the Kirchhoff equation giving \([109–111, 122, 124, 226]\)
\[ \frac{dH}{dt} + 2\gamma H + \omega^2 \int_0^t \int_0^t H(t') dt' = -4\pi\eta \frac{dm_s}{dt}, \]  
(4.106)
where \( \gamma \) is the resonator attenuation, \( \omega \) is the resonator natural frequency, \( \eta_c = V/V_c \) is the coil filling factor and
\[ m_s = \frac{\mu_0}{V} \sum_j (S^j). \]  
(4.107)

The equation for \( H \) can be represented in the integral form
\[ H = -4\pi\eta \int_0^t \int_0^t G(t' - t') \tilde{m}_s(t') dt', \]  
(4.108)
with the source
\[ \tilde{m}_s = \frac{1}{2} \rho \mu_0 S \frac{d}{dt} (u^* + u) \]  
(4.109)
and the transfer function
\[ G(t) = \left[ \cos(\omega t) - \frac{\gamma}{\omega} \sin(\omega t) \right] \exp(-\gamma t), \]
where
\[ \omega \equiv \sqrt{\omega^2 - \gamma^2}. \]

The effective interaction energy of the feedback field \( H \) with the sample is proportional to the parameter
\[ \gamma_0 \equiv \pi\eta_c \rho^2 \mu_0^2 S. \]  
(4.110)

### 4.13. Scale separation

The efficient coupling of an electric circuit with the sample occurs only in the resonant case, when the natural frequency of the circuit is tuned close to the Zeeman frequency of spins,
\[ \frac{\Delta}{\omega} \ll 1 \quad (\Delta \equiv \omega - \omega_0). \]  
(4.111)
The quadratic Zeeman effect shifts the effective frequency to the value \( (4.102)\). In order not to spoil the above quasi-resonance condition, this quadratic shift should be small, such that
\[ |A| \ll 1 \quad (A \equiv \frac{\omega D}{\omega_0}). \]  
(4.112)
All attenuations are to be small as compared to the Zeeman frequency,
\[ \frac{\gamma}{\omega_0} \ll 1, \quad \frac{\gamma_0}{\omega_0} \ll 1, \quad \frac{\gamma_1}{\omega_0} \ll 1, \quad \frac{\gamma_2}{\omega_0} \ll 1. \]  
(4.113)
And the quadratic Zeeman effect is assumed not to destroy the resonance situation, so that the inequalities
\[ \frac{Q_zH^2}{\omega_0} \ll 1, \quad \frac{Q_zB_0H}{\omega_0} \ll 1. \]  
(4.114)
are valid.

Under these conditions, equation \( (4.108) \) can be solved by the iterative procedure starting with \( u \propto \exp(-\omega_s t) \). After one iteration, we find
\[ \mu_i H = i (uX - X^* u^*), \]  
(4.115)
with the coupling function
\[ X = \gamma_0 \gamma \left[ \frac{1 - \exp(-i(\omega - \omega_0)t - \gamma t)}{\gamma + i(\omega - \omega_0)} + \frac{1 - \exp(-i(\omega + \omega_0)t - \gamma t)}{\gamma - i(\omega + \omega_0)} \right]. \]  
(4.116)

The first, resonant, term here prevails over the second, nonresonant one, because of which
\[ X \equiv \gamma_0 \omega_t \frac{1 - \exp(-i\Delta_s t - \gamma t)}{\gamma + i\Delta_s}, \]  
(4.117)
where the dynamic detuning
\[ \Delta_s \equiv \omega - \omega_s = \omega - \omega_0(1 + As) \]  
(4.118)
is defined.

Introducing the dimensionless coupling parameter
\[ g \equiv \frac{\gamma_0 \omega_0}{\gamma \omega_2}, \]  
(4.119)
we can represent the real part of the coupling function as
\[ \alpha \equiv \operatorname{Re} X = g \frac{\gamma_0 \omega_0}{\gamma} \frac{1}{\gamma + \Delta_s} \left[ 1 - \frac{\cos(\Delta_s t) - \Delta_s}{\gamma} \sin(\Delta_s t) \right] e^{-\gamma t} \]  
(4.120)
and the imaginary part as
\[ \beta \equiv \operatorname{Im} X = -g \frac{\gamma_0 \omega_0}{\gamma} \frac{1}{\gamma + \Delta_s} \left[ 1 - \frac{\cos(\Delta_s t) + \Delta_s}{\gamma} \sin(\Delta_s t) \right] e^{-\gamma t} \]  
(4.121)
The ratio of the imaginary part to the real part is \( \beta / \alpha \sim \Delta_s / \gamma \).

Substituting the feedback field (4.115) into equation (4.103) yields the form
\[
\frac{du}{dt} = -i\Omega u - i\varphi_D s - i\xi_D u,
\] (4.122)
in which
\[
\Omega = \omega_S - i(\gamma_2 - X_S) - \frac{1}{2}(2S - 1) \frac{Q_S}{\mu_F^2} (2|X|^2 - X^2) \omega_S
\]
and in quantum information processing.

Equations (4.111) to (4.114), the functional variable \( u \) is to be treated as fast while the variables \( w \) and \( s \) as slow. Then we can employ the scale separation approach \cite{110, 111, 226, 228–231}. Following this approach, we solve equation (4.122) for the fast variable, keeping there the slow variables as integrals of motion, which gives
\[
u = \nu_0 \exp \left\{ -i\Omega t - i \int_0^t \xi_D(t') \, dt' \right\}
- i \int_0^t \varphi_D(t') \exp \left\{ -i\Omega(t - t') - i \int_{t'}^t \xi_D(t'') \, dt'' \right\} \, dt'.
\] (4.123)
Then the solution for the fast variable, together with the expression for the feedback field, is substituted into the equations for the slow variables, whose right-hand sides are averaged over time and over the stochastic variables \( \xi_D \) and \( \varphi_D \), which yields the equations for the guiding centers. Thus we come to the equation for the coherence intensity
\[
\frac{dw}{dt} = -2\gamma_2 w + 2\alpha ws + 2\gamma_3 s^2
+ 2(2S - 1) \frac{Q_S}{\mu_F^2} \alpha_\beta w^2 s - 2(2S - 1) \frac{Q_S B_0}{\mu_F} \alpha_\omega s^2,
\] (4.124)
and for the spin polarization
\[
\frac{ds}{dt} = -\alpha w - \gamma_3 s
- (2S - 1) \frac{Q_S}{\mu_F^2} \alpha_\beta w^2 + (2S - 1) \frac{Q_S B_0}{\mu_F} \alpha_\omega s - \gamma_1 (s - s_\infty).
\] (4.125)

Equations (4.124) and (4.125) characterize spin dynamics that can be regulated by choosing the appropriate system parameters. The motion of spins also produces electromagnetic radiation \cite{109, 111, 129, 130, 232–235} that, however, is rather small. The main advantage in the feasibility of regulating the spin dynamics is that this can be used in spintronics and in quantum information processing.

### 4.14. Spin waves

Dipolar interactions, in the presence of nonzero magnetization and an external magnetic field can support spin waves \cite{111, 221, 226}. Spin waves correspond to small fluctuations of spins, which can be characterized by presenting the spin operators as
\[
S_j^\alpha = \langle S_j^\alpha \rangle + \delta S_j^\alpha.
\] (4.126)

Let us consider the initial stage of spin dynamics, when the feedback field has not yet being formed, \( H = 0 \), and spins, being polarized, have not yet started rotation, so that
\[
\langle S_j^\alpha \rangle = 0,
\]
\[
\langle S_j^\alpha \rangle \neq 0.
\] (4.127)

Assuming that the averages \( \langle S_j^\alpha \rangle \) do not depend on the index \( j \), we have
\[
\xi_D = \sum_j \left( a_j \delta S_j^+ + c_j \delta S_j^- + c_j^* \delta S_j^- \right),
\]
\[
\varphi_D = \sum_j \left( \frac{a_j}{2} \delta S_j^- - 2b_j \delta S_j^- - 2c_j \delta S_j^- \right).
\]

Substituting representation (4.126) into the spin equations of motion (4.94) and (4.95), and linearizing the latter with respect to small deviations, we get the equations for the spin deviations
\[
\frac{d}{dt} S_j^- = -i\omega_j S_j^- - i\varphi_D S_j^-,
\]
\[
\frac{d}{dt} S_j^- = 0,
\] (4.128)
where we take into account that \( \delta S_j^\alpha = S_j^\alpha \). With the initial condition \( \delta S_j^\alpha(0) = 0 \), it follows that \( \delta S_j^\alpha(t) = 0 \). Then
\[
\xi_D = \sum_j \left( c_j \delta S_j^+ + c_j^* \delta S_j^- \right),
\]
\[
\varphi_D = \sum_j \left( \frac{a_j}{2} \delta S_j^- - 2b_j \delta S_j^+ \right).
\]

Introduce the Fourier transforms for the dipolar interaction parameters
\[
a_{ij} = \frac{1}{N_L} \sum_k a_k e^{ik \cdot r_i},
\]
\[
b_{ij} = \frac{1}{N_L} \sum_k b_k e^{ik \cdot r_i},
\] (4.129)
and for the spin operators
\[
S_j^\pm = \sum_k S_k^\pm e^{i\pm k \cdot r_j},
\] (4.130)
where we use the notation \( r_j \) for the lattice vectors instead of \( \mathbf{a}_j \) in order not to confuse with the dipolar parameter \( a_{ij} \).

Then equation (4.128) yields
\[
\frac{d}{dt} S_k^- = -iA_k S_k^- + iB_k S_k^+,
\] (4.131)
where
\[
A_k \equiv \omega_k + \frac{a_k}{2} \langle S_j^\alpha \rangle,
\]
\[
B_k \equiv 2b_k \langle S_j^\alpha \rangle.
\] (4.132)

Looking for the solution in the form
\[
S_k^- = u_k e^{-i\omega_k t} + v_k e^{i\omega_k t},
\]
we obtain the spectrum of spin waves
\[
\omega_k = \sqrt{A_k^2 - |B_k|^2}.
\] (4.133)

In the long-wave limit \( k \to 0 \), the spectrum enjoys the typical of spin waves quadratic dependence on momentum,
\( \omega_k \simeq |\omega| \left[ 1 - \langle S_j \rangle \sum_{\langle j \rangle} \frac{a_{ij} \cdot (k \cdot r_{ij})^2}{\omega} \right] . \) (4.134)

Here the summation is over the nearest neighbours.

The spectrum is stable, provided that \( |A_k| > |B_k| \), which implies the inequality
\[
|\omega_0 + \left( \frac{\omega_0}{\epsilon} + \frac{\alpha_k}{2} \right) \langle S_j \rangle | > 2 |B_k \langle S_j \rangle |.
\] (4.135)

Hence, under sufficiently strong external magnetic field and nonzero spin polarization, the spectrum of spin waves is well defined.

### 4.15. Influence of Tunneling

In the previous sections, we have considered well defined isolating states in an optical lattice, when the tunneling term can be neglected. Now our aim is to take into account the influence of this term, considering an almost insulating state slightly perturbed by weak tunneling of atoms. If the tunneling is not negligible, then boson tunneling processes induce effective interactions between spins \([236–238]\).

Let us consider the case, when the lower energy hyperfine manifold has 3 magnetic sublevels, so that the total moment corresponds to spin \( S = 1 \). The Hamiltonian part, including tunneling and the interaction term \( H_I \) defined in equation (4.77) reads as
\[
\tilde{H} = -J \sum_{\langle j \rangle} \sum_m \hat{c}_{im} \hat{c}^\dagger_{jm} + H_I , \] (4.136)

where the summation is over the nearest neighbours. The interaction parameters are given in equation (4.62) and the tunneling parameter \( J \) can be found from equation (4.55).

The usual expression for the optical lattice potential in \( d \) dimensions is
\[
U(r) = \sum_{\alpha=1}^{d} V_{\alpha} \sin^2 \left( k_{\alpha}^0 r_\alpha \right) \left( k_{\alpha}^0 = \frac{\pi}{a_{\alpha}} \right). \] (4.137)

To form an insulating state, the lattice potential depth has to be essentially larger than the recoil energy
\[
E_R \equiv \frac{1}{2m} \left( \frac{1}{d} \sum_{\alpha=1}^{d} \frac{\pi^2}{a_{\alpha}^2} \right). \] (4.138)

For a cubic \( d \)-dimensional lattice, for which \( V_{\alpha} = V_0 \) and the recoil energy is
\[
E_R = \frac{\pi^2}{2ma^2} \left( a_{\alpha} = a, \right)
\]

there should be \( E_R/V_0 \ll 1 \).

For an insulating state, one can resort to the tight-binding approximation treating the well localized Wannier functions as Gaussians. Then from equation (4.55) for a cubic lattice, we find \([17, 121]\) the tunneling parameter
\[
J = \frac{d}{4} \left( \pi^2 - 4 \right) V_0 \exp \left( -\frac{dn^2}{4} \sqrt{\frac{V_0}{E_R}} \right). \] (4.139)

And for the integral entering the interaction parameters, we have
\[
\int |w(r)|^4 \, dr = \left( \frac{\pi}{2} \right)^{d/2} \frac{1}{a^d} \left( \frac{V_0}{E_R} \right)^{d/4} .
\]

Then these parameters in three dimensions take the form
\[
\bar{c}_0 = \sqrt{8\pi} \frac{3}{3} \left( \frac{a_0 + 2a_2}{a} \right) E_R \left( \frac{V_0}{E_R} \right)^{3/4} , \]
\[
\bar{c}_2 = \sqrt{8\pi} \frac{3}{3} \left( \frac{a_2 - a_0}{a} \right) E_R \left( \frac{V_0}{E_R} \right)^{3/4} . \] (4.140)

Respectively, for \( d = 3 \), the tunneling parameter is
\[
J = \frac{3}{4} \left( \pi^2 - 4 \right) V_0 \exp \left( -\frac{3\pi^2}{4} \sqrt{\frac{V_0}{E_R}} \right) . \] (4.141)

Let us consider the Mott state with odd number of atoms per lattice site, when the filling factor can be written as
\[
\nu \equiv \frac{N}{N_L} = 2n + 1 \quad (n = 0, 1, 2, \ldots). \] (4.142)

The tunneling is assumed to be weak, such that
\[
J\nu \ll \sqrt{\bar{c}_0 \bar{c}_2} . \] (4.143)

The effective spin Hamiltonian, valid for any odd number of atoms per site \( \nu \), in the limit of small tunneling between sites, can be found in the second order perturbation theory with respect to the tunneling parameter \([236]\), resulting in the Hamiltonian
\[
\tilde{H} = -J_0 - J_1 \sum_{\langle j \rangle} \langle S_i \cdot S_j \rangle - J_2 \sum_{\langle j \rangle} \langle S_i \cdot S_j \rangle^2 , \] (4.144)

in which
\[
J_0 \frac{J_1}{J_2} = \frac{4(15 + 20n + 8n^2)}{45(\bar{c}_0 + \bar{c}_2)} - \frac{4(1 + n)(3 + 2n)}{9(\bar{c}_0 + 2\bar{c}_2)} + \frac{128(5 + 2n)}{225(\bar{c}_0 + 4\bar{c}_2)} , \]
\[
J_1 \frac{J_1}{J_2} = \frac{2(15 + 20n + 8n^2)}{15(\bar{c}_0 + \bar{c}_2)} - \frac{16(5 + 2n)n}{75(\bar{c}_0 + 2\bar{c}_2)} , \]
\[
J_2 \frac{J_1}{J_2} = \frac{2(15 + 20n + 8n^2)}{45(\bar{c}_0 + \bar{c}_2)} + \frac{4(1 + n)(3 + 2n)}{9(\bar{c}_0 + 2\bar{c}_2)} + \frac{4(5 + 2n)n}{225(\bar{c}_0 + 4\bar{c}_2)} . \]

In the case of one atom per lattice site, when \( \nu = 1 \) and \( n = 0 \), one has
\[
J_0 \frac{J_1}{J_2} = \frac{4}{3(\bar{c}_0 + \bar{c}_2)} - \frac{4}{3(\bar{c}_0 + 2\bar{c}_2)} + \frac{128}{45(\bar{c}_0 + 4\bar{c}_2)} , \]
\[
J_1 \frac{J_1}{J_2} = \frac{2}{\bar{c}_0 + \bar{c}_2} , \quad J_2 \frac{J_1}{J_2} = \frac{2}{3(\bar{c}_0 + \bar{c}_2)} + \frac{4}{3(\bar{c}_0 - 2\bar{c}_2)} . \]

In the general case, the total effective spin Hamiltonian for \( S = 1 \) and odd filling factor, omitting the constant terms but taking account of the Zeeman and dipolar terms becomes
\[
\tilde{H} = -J_1 \sum_{\langle j \rangle} \langle S_i \cdot S_j \rangle - J_2 \sum_{\langle j \rangle} \langle S_i \cdot S_j \rangle^2 + H_Z + \tilde{H}_D . \] (4.145)
The first two terms here describe effective spin interactions induced by atomic tunneling. These terms can noticeably influence spin dynamics. Thermodynamics of the system with Hamiltonian (4.145) can also strongly differ from that characterized by the usual Heisenberg interaction [239].

5. Conclusion

The paper reviews the main properties of bosonic atoms and molecules interacting through nonlocal interaction potentials, such as the dipolar potential, and also through spinor potentials. The specific points of the present review, distinguishing it from the previous review articles are as follows.

The emphasis is not on briefly listing the numerous properties of the considered systems, but rather on concentrating on the main of these properties, with thoroughly explaining the methods of their description.

The necessity of regularizing the dipolar interaction potential is emphasized. Without this regularization, one often comes to unphysical conclusions, when thermodynamic quantities, such as chemical potential, free energy, and internal energy become not scalars, which is certainly meaningless.

A special attention is paid to the derivation of effective spin Hamiltonians for dipolar and spinor atomic systems. Methods of regulating spin motion are discussed. The possibility for such an efficient manipulation of spin dynamics is important for applications in spintronics and quantum information processing.

Acknowledgments

The author is grateful for discussions and friendly support to V S Bagnato and E P Yukalova.

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