

Self-consistent calculation of the coupling constant in the Gross-Pitaevskii equation

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A method is proposed for a self-consistent evaluation of the coupling constant in the Gross-Pitaevskii equation without involving a pseudopotential replacement. A renormalization of the coupling constant occurs due to medium effects and the trapping potential, e.g., in quasi-1D or quasi-2D systems. It is shown that a simplified version of the Hartree-Fock-Bogoliubov approximation leads to a variational problem for both the condensate and a two-body wave function describing the behavior of a pair of bosons in the Bose-Einstein condensate. The resulting coupled equations are free of unphysical divergences. Particular cases of this scheme that admit analytical estimations are considered and compared to the literature. In addition to the well-known cases of low-dimensional trapping, crossover regimes can be studied. The values of the kinetic, interaction, external, and release energies in low dimensions are also evaluated and contributions due to short-range correlations are found to be substantial.

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I. INTRODUCTION

The Gross-Pitaevskii (GP) equation [1] is a powerful tool for describing most of the physical properties of Bose-Einstein condensates of trapped alkali atoms (see reviews [2–5]). In the GP approach, the ground state energy of a trapped dilute Bose gas of atoms of mass m is the functional

$$E = \int d\mathbf{r} \left[\frac{\hbar^2}{2m} |\nabla \phi|^2 + V_{\text{ext}}(\mathbf{r}) |\phi|^2 + \frac{g}{2} |\phi|^4 \right], \quad (1)$$

of the order parameter $\phi = \phi(\mathbf{r}) = \langle \hat{\Psi}(\mathbf{r}) \rangle$, where $\hat{\Psi}(\mathbf{r})$ is the bosonic field operator and $V_{\text{ext}}(\mathbf{r})$ is an external trapping potential. The coupling constant g in the GP functional (1) is intimately related to the density expansion of the energy of the homogeneous Bose gas. Indeed, in the homogeneous case Eq. (1) yields $E/N = gn/2$ where $n = N/V \approx |\phi|^2$ is the 3D density. This expression should be equal to the known first term in the density expansion $E/N = 2\pi\hbar^2 a n/m$ in three dimensions [6,7]. With a being the 3D scattering length, the coupling constant $g = 4\pi\hbar^2 a/m$ coincides with the zero momentum limit of the scattering amplitude, the two-body T -matrix, for two particles scattering in a vacuum. This standard approach based on the low-density expansion of the homogeneous gas neglects the influence of inhomogeneous trapping potentials which may require a renormalization of the coupling constant.

The situation is more complicated for two dimensional Bose gases, which can be regarded as the limiting case of a 3D gas with a highly inhomogeneous trapping potential. Kolomeisky *et al.* [8] proposed that the form (1) of the energy functional is still valid. However, in this case the coupling constant becomes dependent on the local density. Indeed, Schick's result for the energy $E/N = 2\pi\hbar^2 n_{2D} / [-m \ln(n_{2D} a_{2D}^2)]$ of a dilute 2D Bose gas [9] leads to the coupling constant $g = 4\pi\hbar^2 / (-m \ln|\phi|^2 a_{2D}^2)$ [8] and further corrections were derived in Refs. [10–13]. Here, n_{2D} and a_{2D} denote the two-dimensional density and scattering length, re-

spectively. This generalization can be understood as a local density approximation, which yields consistent energy values in the homogeneous and inhomogeneous cases but does not reveal the nature of the additional nonlinearity in the GP equation. Moreover, it is not clear what the nonlinearity should be in the crossover regimes from 2D to 3D and from 1D to 3D. A mathematically rigorous justification of the GP functional [14] is of importance but hardly can help us in this situation.

The purpose of the present paper is to show how a density-dependent renormalized coupling constant emerges naturally in a simplified Hartree-Fock-Bogoliubov (HFB) approximation starting from the bare interaction potential $V(r)$. To this end, we derive generalized GP equations where the order parameter is coupled to the pair wave function of two bosons in the condensate. The latter has already been discussed in detail in Refs. [13,15–17]. The generalized GP equations permit us to consider interaction potentials with a hard core directly without the δ -function replacement by accurately accounting for the short-range spatial correlations of the particles. These correlations become essential in low dimensions since the Born approximation for two scattering particles fails at small momenta (see, e.g., Ref. [19], Sec. 45). We note that the correct treatment of the short-range correlations is also possible within the Jastrow[20] and the Faddeev-Yakubovsky [21] approaches.

It is well known that the original HFB scheme leads to an artificial gap in the spectrum [22,23]. Moreover, this scheme in conjunction with the δ -function replacement has an ultraviolet divergence [7,24]. These problems then have to be cured by further approximations as classified by Griffin [25]. Alternatively, complicated renormalization procedures [26,27] or pseudopotentials [28,29] have been suggested. In this paper we will discuss a novel approximation derived from the full HFB scheme where the use of the bare two-body potential provides an implicit renormalization, and the ultraviolet divergences are avoided. We will discuss the excitation spectrum and show that it is gapless in a reasonable approximation.

Low dimensional Bose systems are not only of general theoretical interest but also find the attention of current experimental exploration [30–33]. In these experiments, the low dimensional condensate is realized by highly anisotropic 3D trapping potentials when the single-particle energy-level spacing in the tightly confined dimensions exceeds the interaction energy between atoms $\hbar\omega_{\rho,z} \gtrsim \mu$. Here the frequencies are associated with the axially symmetric harmonic potential, and μ is the part of the chemical potential coming from the particle interaction, which is of order of the mean interaction energy per particle. This criterion takes the form $l_{\rho,z} \lesssim \xi$ in terms of the coherence length $\xi = \hbar / \sqrt{\mu m}$ [34] and the radial (axial) harmonic oscillator length $l_{\rho,z} = \sqrt{\hbar / (m\omega_{\rho,z})}$.

Theoretically, the 2D regime $l_z \langle \langle \xi, l_\rho \rangle \rangle \xi$ was investigated in detail by Petrov, Holzmann, and Shlyapnikov [35]. The coupling constant was assumed to be the T -matrix of two particles scattering in the harmonic trap with $l_\rho = \infty$ at the energy of relative motion $E = 2\mu$. An additional nonlinearity is introduced, since the local value of μ depends on the density and the coupling constant in a self-consistent way. In this regime, the motion of particles is confined in z -direction to zero-point oscillation. This implies that the order parameter can be represented in the form $\phi(x, y, z) = \phi_0(z)\phi(x, y)$, where $\phi_0(z)$ is the ground state of the 1D harmonic oscillator and $\phi(x, y)$ is governed by the two dimensional GP equation resulting from the functional (1) in two dimensions. So, in this regime, the behaviour of the condensate in x - y plane is the same as in the “pure” 2D case with the 2D scattering length written in terms of the length l_z of the tight confinement [35].

An improved many body T -matrix theory was developed by Stoof and co-workers [36] in order to describe not only the homogeneous low-dimensional Bose gases but also the crossover from 3D to lower dimensions. The coupling constant in the inhomogeneous case is represented by the local value of the T -matrix, which depends on the local value of the chemical potential. The local T -matrix approximation was also used in Ref. [37] and the microscopic approach of Ref. [38]. Thus, one can say, slightly simplifying the situation, that the common method of evaluating of the coupling constant in the above works is to determine first the T -matrix from the corresponding two-body Schrödinger equation supposing that the motion of the particles is infinite in some directions, and after that to replace the coupling constant by the local value of the T -matrix. In this paper we offer a method beyond the local T -matrix approximation. The coupling constant is determined self-consistently for a given 3D geometry from a unified variational scheme. As a result, we obtain a nonlocal term in the energy functional, which can be of practical importance if the external potential varies on the scale of the interaction potential. This may be realized, e.g., for condensates of loosely-bound molecules in tight or strongly oscillating potentials like optical lattices. We expect experiments to enter this regime in the near future as both atomic condensates in optical lattices [31,39] and molecular condensates [40–42] are currently under intense experimental investigation.

As a starting point of our approach we assume that we have a Bose-Einstein condensate or quasicondensate with a

well-defined order parameter. Long-range fluctuations of the phase, which become important for many physical properties in low-dimensional traps [43], are beyond the scope of our scheme. They can be studied by means of the approaches of Refs. [35,36,44,45]. Also the strongly-interacting fermionized regime of the Tonks-Girardeau gas [32], which was studied in Ref. [46], cannot be described with the methods of this paper. However, we note that our scheme, within its accuracy, is simple and physically transparent and able to reproduce not only the value of the coupling constant in 1D [47] and 2D [35] regimes but also to describe the 3D-2D and 3D-1D crossovers. Furthermore, it allows us to calculate directly the correct values of the kinetic and interaction energies of bosons in the trap, which are *not* given by the first and the third terms, respectively, in the GP functional (1) [48].

The paper is organized as follows. In Sec. II we derive the generalized GP functional and corresponding equations from a simplified HFB approximation. In Sec. III, a few specific cases are considered that admit analytical estimations, including the homogeneous and inhomogeneous Bose gases in low dimensions. In Sec. IV we calculate the values of various contributions in the energy. In particular, the release energy of the low dimensional gases is estimated. In Sec. V we derive a useful virial theorem and a relation between the chemical potential and different parts of the energy functional. The eigenfunctions of the two-body density matrix and a relation between the normal and anomalous averages are obtained within the HFB approximation in Appendices A and B, respectively.

II. GENERALIZED GROSS-PITAIEVSKII EQUATIONS

A. Failure of standard GP approach

In the standard approach [2–5], the equilibrium value of the order parameter ϕ is determined by minimization of the GP functional (1) with the constraint of particle-number conservation $\delta(E - \mu'N) / \delta\phi^*(\mathbf{r}) = 0$. Here $N \approx N_0$ is the number of particles and the chemical potential μ' appears as a Lagrange multiplier. Introducing for later convenience $\mu = \mu' - E_0$ as the chemical potential due to interaction where E_0 is the ground state energy of a noninteracting particle, we arrive at

$$(E_0 + \mu)\phi = -\frac{\hbar^2}{2m}\nabla^2\phi + V_{\text{ext}}(\mathbf{r})\phi + g|\phi|^2\phi. \quad (2)$$

The simplicity of this derivation is based on the simple form of the GP energy functional (1), where the effects of the binary interparticle interactions has been reduced to a single parameter given by the coupling constant. In order to determine the constant self-consistently, it should be examined carefully how the interaction term $(g/2)|\phi|^4$ appears in the GP functional (1).

In a general many-body system with binary interactions, the expectation value of the interaction energy is a functional of the *two-body* density matrix $\langle \hat{\Psi}^\dagger(x_1)\hat{\Psi}^\dagger(x_2)\hat{\Psi}(x'_2)\hat{\Psi}(x'_1) \rangle$. For a pairwise interaction potential $V(x_1, x_2) = V(\mathbf{r}_1 - \mathbf{r}_2, \sigma_1, \sigma_2)$ we thus obtain [19,49]

$$E_{\text{int}} = \left\langle \frac{1}{2} \sum_{i \neq j} V(x_i, x_j) \right\rangle = \frac{1}{2} \int dx_1 dx_2 V(x_1, x_2) \times \langle \hat{\Psi}^\dagger(x_1) \hat{\Psi}^\dagger(x_2) \hat{\Psi}(x_2) \hat{\Psi}(x_1) \rangle, \quad (3)$$

where $x=(\mathbf{r}, \sigma)$ stands for the coordinate and spin or sort indices of a particle, respectively, and $\int dx \cdots = \sum_\sigma \int d\mathbf{r} \cdots$. The kinetic energy and the energy of interaction with an external field are determined by the one-body matrix $\langle \hat{\Psi}^\dagger(x) \hat{\Psi}(x') \rangle$

$$E_{\text{kin}} = \left\langle \sum_i \frac{p_i^2}{2m} \right\rangle = -\frac{\hbar^2}{2m} \int dx \nabla_x^2 \langle \hat{\Psi}^\dagger(x') \hat{\Psi}(x) \rangle \Big|_{x'=x}, \quad (4)$$

$$E_{\text{ext}} = \left\langle \sum_i V_{\text{ext}}(x_i) \right\rangle = \int dx V_{\text{ext}}(x) \langle \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \rangle. \quad (5)$$

The behavior of the one- and two-body matrices is easy to understand in the dilute limit, when the condensate depletion $(N-N_0)/N$ is small. We note that the number of bosons in the condensate N_0 is defined as the macroscopic eigenvalue of the one-body density matrix $\langle \hat{\Psi}^\dagger(x) \hat{\Psi}(x') \rangle$, that is $\int dx' \langle \hat{\Psi}^\dagger(x') \hat{\Psi}(x) \rangle \phi_0(x') = N_0 \phi_0(x)$. The field operator can be expanded in the complete orthonormal set of eigenfunctions of the one-body matrix $\hat{\Psi}(x) = \hat{a}_0 \phi_0(x) + \sum'_\nu \hat{a}_\nu \phi_\nu(x)$, where the sum \sum'_ν means $\sum_{\nu \neq 0}$ and $\int dx |\phi_\nu(x)|^2 = 1$. Appearance of the Bose-Einstein condensate implies the macroscopic occupation of N_0 , i.e., the ratio N_0/N remains finite in the thermodynamic limit. Following Bogoliubov [6,50] we now replace the condensate operators by c -numbers $\hat{a}_0^\dagger = \hat{a}_0 \approx \sqrt{N_0}$ and represent the Bose field operator in the form $\hat{\Psi}(x) = \phi(x) + \hat{\vartheta}(x)$ [51]. Here $\phi(x) = \sqrt{N_0} \phi_0(x)$ is the c -number part, and $\hat{\vartheta}(x) = \sum'_\nu \hat{a}_\nu \phi_\nu(x)$ the operator part, for which we have $\langle \hat{\Psi}(x) \rangle = \phi(x)$ and $\langle \hat{\vartheta}(x) \rangle = 0$. Thus, the order parameter is nothing else but the non-normalized eigenfunction of the one-body density matrix.

In the original approach of Gross and Pitaevskii, the simplest mean-field approximation is used when the operator part is completely neglected: $\hat{\Psi}(x) \approx \phi(x)$ and $\hat{\Psi}^\dagger(x) \approx \phi^*(x)$. Assuming additionally that the order parameter does not change significantly at the distances of order of the radius R_e of the interaction potential, we obtain the GP energy functional (1) for spinless bosons from Eqs. (3)–(5) with the coupling constant

$$g \approx g_B \equiv \int d\mathbf{r} V(r). \quad (6)$$

This coupling constant can be identified with the two-body scattering amplitude at zero momentum in the Born approximation. The validity of the GP approach with the coupling constant g_B of Eq. (6) is certainly linked to the validity condition of the Born approximation at zero momentum that the potential $V(r)$ be small and integrable.

Of the two assumptions mentioned above, namely the slow spatial variation of the order parameter and the validity of the Born approximation, the former is usually fulfilled as the healing length $\xi = \hbar / \sqrt{\mu m}$ as a lower bound of the length scale of the order parameter [3,4] is usually much larger than the effective range of the interaction. The latter assumption, however, is clearly not fulfilled for experiments with cold atomic gases as their interactions are of the hard-core type.

The validity of the GP approach can be extended to such systems by an argument attributed to Landau [6,16]. He noted that at extremely low energies, as predominant in the dilute-gas BEC, the scattering properties are completely determined by only one single parameter, which is the 3D s -wave scattering length a . This allows us to replace the Born approximation for the scattering amplitude g_B by its exact value $g = 4\pi\hbar^2 a/m$, which can be found from the two-body Schrödinger equation even for hard-core potentials. This indirect argument, however, cannot be used in one or two dimensions as there is no such simple relation between the integral in Eq. (6) and the scattering amplitude as we have in three dimensions. Furthermore the Born series for the scattering amplitude diverges for small momenta in two dimensions and below (see, e.g., Ref. [19], Sec. 45).

B. Pair wave function in a medium

The above described deficiencies of the naive GP approach may be remedied by accounting for the two-particle scattering processes explicitly. Within the HFB scheme this is possible through certain correlations introduced by the fluctuation operators $\hat{\vartheta}$. In order to see the relation between the two-particle scattering process and the correlation functions mentioned above it is useful to introduce the concept of a two-body or *pair wave function in the medium* of other particles [15,50]. The pair wave functions in the medium of the many body system are defined as eigenfunctions of the two-body density matrix, as discussed in detail in Appendix A. They should be distinguished from the two-body wave functions in the vacuum, which relate to a system of two particles. For the latter we will use the superscript (0) .

Let us suppose that we know the exact eigenfunctions of the two-body density matrix. Then we can expect for the dilute gas, where low-momentum two-body processes dominate the behavior of the system, that the pair wave functions in the medium should be very close [15] to the two-body wave functions in the vacuum, which are the solutions of the two-body Schrödinger equation. This physical assumption was used to obtain the density expansions for the 3D [16,17] and 2D [13] homogeneous Bose gases in a very simple manner. However, various approximations in the many-body theory can break this relation.

C. A simplified HFB scheme

Within the HFB approximation for the homogeneous Bose gas, all eigenfunctions of the two-body density matrix except for one are plane waves and are thus treated in the Born approximation as shown in Appendix A. This is an obvious drawback of the HFB scheme. It turns out that the

two-body wave function that is not a plane wave is proportional to the anomalous average

$$\varphi(x_1, x_2) \equiv \langle \hat{\Psi}(x_1) \hat{\Psi}(x_2) \rangle \quad (7)$$

and corresponds to the macroscopic eigenvalue $N_0(N_0-1)$ in the limit of large N . It is the pair wave function that describes the two-particle scattering process in the medium of the Bose-Einstein condensate [15,52]. Thus we can go beyond the Born approximation in the framework of the HFB method by keeping only the contribution of the anomalous average $\langle \hat{\Psi}(x_1) \hat{\Psi}(x_2) \rangle$ and neglecting the contribution of the other wave functions in the two-body density matrix. Due to small condensate depletion $(N-N_0)/N \ll 1$, one can expect that the contribution of only this eigenfunction will be sufficient for obtaining the coupling constant in the GP equation. In this simplified version of the HFB approximation we set

$$\langle \hat{\Psi}^\dagger(x_1) \hat{\Psi}^\dagger(x_2) \hat{\Psi}(x'_2) \hat{\Psi}(x'_1) \rangle \approx \varphi^*(x_1, x_2) \varphi(x'_1, x'_2). \quad (8)$$

Extracting the c -number part of the field operator, the anomalous averages can be rewritten as

$$\varphi(x_1, x_2) = \phi(x_1) \phi(x_2) + \psi(x_1, x_2), \quad (9)$$

where we introduced the notation $\psi(x_1, x_2) \equiv \langle \hat{\psi}(x_1) \hat{\psi}(x_2) \rangle$ for the anomalous two-boson correlation function associated with the scattering part of the two-body wave function. The functions $\varphi(x_1, x_2)$ and $\psi(x_1, x_2)$ are symmetric with respect to permutation of x_1 and x_2 due to the commutation relations for the Bose field operators.

For the one-body density matrix we find $\langle \hat{\Psi}^\dagger(x) \hat{\Psi}(x') \rangle = \phi^*(x) \phi(x') + \langle \hat{\psi}^\dagger(x) \hat{\psi}(x') \rangle$. We note that the normal $\langle \hat{\psi}^\dagger(x) \hat{\psi}(x') \rangle$ and anomalous $\langle \hat{\psi}(x) \hat{\psi}(x') \rangle$ averages are not independent quantities as discussed in Appendix B and Refs. [16,17]. Within the Hartree-Fock-Bogoliubov scheme, the relations between them appear as a specific property of the HFB ground state (the quasiparticle vacuum) and do not contain parameters of the Hamiltonian in explicit form. We will use the approximate relation (B20), which leads to

$$\langle \hat{\Psi}^\dagger(x) \hat{\Psi}(x') \rangle = \phi^*(x) \phi(x') + \int dx_2 \psi^*(x, x_2) \psi(x_2, x'). \quad (10)$$

With the help of Eqs. (8)–(10) we rewrite Eqs. (3)–(5) in terms of the anomalous averages

$$E_{\text{int}} = \frac{1}{2} \int dx_1 dx_2 V(x_1, x_2) |\varphi(x_1, x_2)|^2, \quad (11)$$

$$E_{\text{ext}} = \frac{1}{2} \int dx_1 dx_2 [V_{\text{ext}}(x_1) + V_{\text{ext}}(x_2)] |\psi(x_1, x_2)|^2 + \int dx_1 V_{\text{ext}}(x_1) |\phi(x_1)|^2, \quad (12)$$

$$E_{\text{kin}} = \frac{1}{2} \int dx_1 dx_2 \psi^*(x_1, x_2) (\hat{T}_1 + \hat{T}_2) \psi(x_1, x_2) + \int dx_1 \phi^*(x_1) \hat{T}_1 \phi(x_1), \quad (13)$$

where $\hat{T}_j = -\hbar^2 \nabla_j^2 / (2m)$ and $j=1, 2$. The total number of particles is related directly to the one-body matrix: $N = \int dx \langle \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \rangle$. With Eq. (10) we find

$$N = \int dx_1 |\phi(x_1)|^2 + \int dx_1 dx_2 |\psi(x_1, x_2)|^2. \quad (14)$$

The current approximations are useful for a variational scheme where the functions $\phi(x_1)$ and $\psi(x_1, x_2)$ are determined by minimization of the total energy with the constraint $N = \text{const}$. Using the Lagrange method, we obtain the conditions $\delta E / \delta \phi(x_1) = \delta E / \delta \phi^*(x_1) = \delta E / \delta \psi(x_1, x_2) = \delta E / \delta \psi^*(x_1, x_2) = 0$ for the energy functional

$$E[\{\phi, \psi, \mu'\}] = E_{\text{kin}} + E_{\text{ext}} + E_{\text{int}} - \mu'(N - \mathcal{N}), \quad (15)$$

given by Eqs. (11)–(14). Here $\mu' = \mu + E_0$ is the chemical potential and $\mathcal{N} = \langle \hat{N} \rangle$ is the average number of particles, i.e., the left-hand side (LHS) of Eq. (14) at the equilibrium values of the functions ϕ and ψ corresponding to the minimum (ground state) of the functional (15). Note that the variation $\delta \psi(x_1, x_2)$ is symmetric under the permutation of x_1 and x_2 , so, the equation $\int dx_1 dx_2 g(x_1, x_2) \delta \psi(x_1, x_2) = 0$ leads to $g(x_1, x_2) + g(x_2, x_1) = 0$ for arbitrary functions $g(x_1, x_2)$.

This variational procedure yields the following system of equations for the one- and two-body functions $\phi(x_1)$ and $\varphi(x_1, x_2)$, respectively,

$$\mathcal{L}_1 \phi(x_1) + \int dx_2 \phi^*(x_2) V(x_1, x_2) \varphi(x_1, x_2) = 0, \quad (16)$$

$$(\mathcal{L}_1 + \mathcal{L}_2) \psi(x_1, x_2) + V(x_1, x_2) \varphi(x_1, x_2) = 0, \quad (17)$$

where the operators \mathcal{L}_1 and \mathcal{L}_2 stand for

$$\mathcal{L}_j = -\hbar^2 \nabla_j^2 / (2m) - \mu - E_0 + V_{\text{ext}}(x_j), \quad j=1, 2,$$

and ϕ , φ and ψ are simply related by Eq. (9). Due to this relation, Eq. (16) is nonlinear with respect to ϕ and can be associated with the GP equation. Equation (17) is the analogue of the two-particle Schrödinger equation and is linear with respect to φ , though not uniform. The obtained system of two equations allows us to determine the coupling constant self-consistently. A specific feature of Eq. (16) is the *nonlocal* nature of the last term, which can play a role when the radius of the interacting potential becomes of the order of the characteristic length of the anisotropic trapping potential in some direction, say, $R_e \sim l_z \ll \xi$, or if the trapping potential has a strongly oscillating contribution with the scale of the order of R_e . At the same time, Eqs. (16) and (17) indeed reduce to the GP equation with the 3D coupling constant $g = 4\pi\hbar^2 a/m$ in the limit $R_e \ll \xi \ll l_x, l_y, l_z$ as will be shown in Sec. III B 1.

When the external potential becomes independent of some coordinate, say z , particles can move freely in

z-direction and we should impose the boundary conditions that follow from Bogoliubov's principle of correlation weakening [50]:

$$\langle \hat{\Psi}(x)\hat{\Psi}(x') \rangle \approx \langle \hat{\Psi}(x) \rangle \langle \hat{\Psi}(x') \rangle \text{ when } |z - z'| \rightarrow \infty.$$

Physically, this implies that the function $\psi(x_1, x_2) = \langle \hat{\vartheta}(x_1)\hat{\vartheta}(x_2) \rangle$ vanishes at the spatial distances of order of the coherence (healing) length, $|\mathbf{r}_1 - \mathbf{r}_2| \gtrsim \xi$.

A time-dependent generalization of Eqs. (16) and (17) can in principle be derived from the equations of motion of the field operators. Here, however, we will not elaborate the full derivation but instead present a simple argument that leads to a useful time-dependent scheme. In the case of a time-independent Hamiltonian, it can be easily seen that the GP order parameter depends on time as

$$\begin{aligned} \phi(x, t) &= \langle N - 1 | \hat{\Psi}(x, t) | N \rangle = \phi(x) \exp[-i(E_N - E_{N-1})t/\hbar] \\ &= \phi(x) \exp[-i\mu' t/\hbar]. \end{aligned}$$

Here, $|N\rangle$ and E_N are the ground state and energy of N bosons, respectively. By analogy, we find $\psi(x_1, x_2, t) = \psi(x_1, x_2) \exp[-i2\mu' t/\hbar]$ and $\varphi(x_1, x_2, t) = \varphi(x_1, x_2) \exp[-i2\mu' t/\hbar]$. We now argue that the chemical potential in Eqs. (16) and (17) arises due to time derivatives, which leads to the obvious generalization

$$i\hbar \frac{\partial}{\partial t} \phi(x_1, t) = \hat{H}_1 \phi(x_1, t) + E_{\text{nl}}(x_1, t), \quad (18)$$

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \varphi(x_1, x_2, t) &= [\hat{H}_1 + \hat{H}_2 + V(x_1, x_2)] \varphi(x_1, x_2, t) \\ &+ \phi(x_1, t) E_{\text{nl}}(x_2, t) + \phi(x_2, t) E_{\text{nl}}(x_1, t), \end{aligned} \quad (19)$$

where we denote

$$\hat{H}_j = -\frac{\hbar^2 \nabla_j^2}{2m} + V_{\text{ext}}(x_j, t), \quad j = 1, 2,$$

$$E_{\text{nl}}(x, t) = \int dy \phi^*(y, t) V(x, y) \varphi(x, y, t).$$

The functions $\phi = \langle \hat{\Psi}(x, t) \rangle$ and $\varphi = \langle \hat{\Psi}(x_1, t) \hat{\Psi}(x_2, t) \rangle$ are normalized as $\int dx |\phi(x, t)|^2 = N_0$ and $\int dx_1 dx_2 |\varphi(x_1, x_2, t)|^2 = N_0(N_0 - 1) \approx N_0^2$, respectively. The time-dependent generalized GP equations (18) and (19) become the ordinary one- and two-body Schrödinger equations, respectively, in the limit $\xi \gg l_x, l_y, l_z$ when we can neglect all the nonlinear terms, which are responsible for many-body effects. Therefore they are of slightly more general validity than the stationary equations (16) and (17), which imply a large particle number, since $E_N - E_{N-2} \approx 2(E_N - E_{N-1}) \approx 2\mu'$ is valid only for $N \gg 1$. We notice that the time-dependent equations similar to those of (18) and (19) were derived in [67] by the method of non-commutative cumulants.

D. Properties and limits of validity

The time-dependent equations (18) and (19) give access to the elementary excitation spectrum. At the moment we cannot prove the gaplessness of the spectrum in the most general case, but we can solve for the excitation energies approximately. With the ansatz $\varphi(\mathbf{r}_1, \mathbf{r}_2, t) = \phi(\mathbf{r}_1, t) \phi(\mathbf{r}_2, t) [1 + \psi(r)/n_0]$, we obtain the Bogoliubov excitation energy $\omega_k = \sqrt{T_k^2 + 2n_0 U(k) T_k}$ with the k -dependent scattering amplitude $U(k)$ (for the notations see Sec. III A). This form of the spectrum for a singular two-particle interaction was proposed without derivation by Bogoliubov in Ref. [6]. For small k we can replace $U(k=0) = 4\pi\hbar^2 a/m$ and obtain the usual (gapless) Bogoliubov dispersion. The additional features in the obtained spectrum at medium and high energies reflect the structure of the interaction potential neglected in the standard GP approach and present a clear advantage of our extended scheme. As a consequence, we can expect that Levinson's theorem for quasiparticle scattering [53] will be modified.

Let us discuss limits of validity of the generalized GP equations (16) and (17). First, we imply that the Bose-Einstein condensate (or quasicondensate in low dimensions, see Sec. III B) is developed strongly. This means that $r_0 \ll \xi$, where r_0 is an average distance between bosons [3,4]. Second, the above derivation can be applied only to the short-range interaction potentials that decrease at least as fast as $V(r) \sim 1/r^{\varepsilon+D}$ for $r \rightarrow \infty$, where D is dimension and $\varepsilon > 0$ [16,17]. For a long-range interaction like Coulomb repulsion, the approximation (8) works badly. Third, the approximations (8) and (B20) are insufficient to describe the long-range behavior of the normal $\langle \hat{\vartheta}^\dagger(x_1) \hat{\vartheta}(x_2) \rangle$ and anomalous $\langle \hat{\vartheta}(x_1) \hat{\vartheta}(x_2) \rangle$ correlation functions, which are governed by Bogoliubov's "1/q²" theorem [50,54,55]. According to this theorem, the above correlation functions should decay as $1/|\mathbf{r}_1 - \mathbf{r}_2|^2$ when $|\mathbf{r}_1 - \mathbf{r}_2| \gtrsim \xi$ at zero temperature if the Bose-Einstein condensate exists. Our scheme gives $1/|\mathbf{r}_1 - \mathbf{r}_2|$ decay, as we show in Sec. III A. However, we stress that *the long-range behavior is not needed for obtaining the coupling constant*, since the integral in Eq. (16) contains the anomalous correlation function multiplied by the short-range potential $V(x_1, x_2)$ with the characteristic radius $R_e \lesssim \xi$. Since the developed scheme describes well only the short-range behaviour of $\psi(x_1, x_2)$ for $|\mathbf{r}_1 - \mathbf{r}_2| \lesssim \xi$, the integration in the last term of Eq. (14) should be restricted to this region

$$N = \int dx_1 |\phi(x_1)|^2 + \int_{|\mathbf{r}_1 - \mathbf{r}_2| \leq \xi} dx_1 dx_2 |\psi(x_1, x_2)|^2, \quad (20)$$

otherwise we obtain formally divergent term. This modification of the original scheme, however, does not change the working equations (16)–(19) in the region $|\mathbf{r}_1 - \mathbf{r}_2| \leq \xi$, which is of sole interest for our purposes. We stress that Eq. (20) is really needed only when minimizing the energy functional (15) directly. Furthermore, if we obtain the solutions of Eqs. (16) and (17) as functions of the chemical potential in the grand canonical ensemble, then the condition (14) or (20) can be employed without the second term at all in order to rewrite the answer in terms of the total number of particles in

the canonical ensemble, owing to small condensate depletion.

Note that the standard HFB approximation can be obtained by using the variational scheme if, first, one substitutes Eqs. (3)–(5) into the energy functional (15), second, employ the restrictions Eqs. (B18) and (B19), and third, retain all additional terms missing in Eq. (8), where the three- and four-boson averages of $\hat{\psi}$ and $\hat{\psi}^\dagger$ ought to be evaluated by means of the Wick's theorem and, consequently, the three-boson averages vanish.

III. EXAMPLES

In this section we restrict ourselves to spinless bosons with an isotropic short-range interaction $V=V(r)$, where $r=|\mathbf{r}_1-\mathbf{r}_2|$. Even after this simplification, the solution of the generalized GP equations (16) and (17) remains a rather complex problem. Nevertheless, in a number of specific limiting cases we are able to obtain analytic results.

A. The homogeneous case

Let us investigate Eqs. (16) and (17) in three and two dimensions for the homogeneous Bose gas. In the homogeneous case $V_{\text{ext}}=0$, hence we have $\psi=\psi(r)$, $E_0=0$, and Eq. (16) gives the trivial solution $\phi=\sqrt{n_0}=\text{const}$. In this subsection, we use the common notation n_0 for the condensate density in both 2D and 3D cases. Thus, Eqs. (16) and (17) read

$$\mu = \int d\mathbf{r} V(r) [n_0 + \psi(r)],$$

$$2\mu\psi(r) = -\frac{\hbar^2}{m}\nabla^2\psi(r) + V(r)[n_0 + \psi(r)],$$

and $\psi(r)\rightarrow 0$ for $r\rightarrow\infty$ in accordance with Bogoliubov's principle of correlation weakening. Taking the Fourier transformation of the last equation, we obtain

$$\mu = n_0 U(0), \quad (21)$$

$$\frac{\psi(k)}{n_0} = -\text{P} \frac{U(k)}{2(T_k - \mu)}, \quad (22)$$

where we denote $U(k) = \int d\mathbf{r} V(r) e^{-i\mathbf{k}\cdot\mathbf{r}} [1 + \psi(r)/n_0]$, $T_k = \hbar^2 k^2 / (2m)$, and the symbol P stands for the principle value of the associated integral. The latter appears as a natural regularization for the singular denominator in the RHS of Eq. (22) and implies that the scattering part of the two-body wave function $\psi(k)$ is real and corresponds to a standing wave. Note that another regularization, such as the standard replacement $k \rightarrow k \pm i\epsilon$, leads to the same results in the leading order at small densities. Within the more accurate method [16,17], we obtain the same equation as Eq. (22) but with the Bogoliubov denominator $2\sqrt{T_k^2 + 2n_0 U(k) T_k}$. The latter provides the correct values of both the short- and long-range behavior of the correlator $\psi(r) = \langle \hat{\psi}(\mathbf{r}) \hat{\psi}(0) \rangle$ [which is the Fourier transform of $\psi(k)$], while Eq. (22) provides only the short-range behavior. Indeed, in the 3D case we have $\psi(r)$

$\sim \cos(\sqrt{2}r/\xi)/r$ at $r \gtrsim \xi$ (see below) but not $\psi(r) \sim 1/r^2$ as it should be.

Equation (22) can be rewritten in the Lippmann-Schwinger form with the help of the Fourier transformation. By using the familiar property of Fourier transformation $\int d\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}} g(\mathbf{k}) f(\mathbf{k}) / (2\pi)^D = \int d\mathbf{r}' f(\mathbf{r}') g(\mathbf{r}-\mathbf{r}')$ (here D is the dimension), we obtain the equation for $\varphi(r) = n_0 + \psi(r)$

$$\varphi(r) = n_0 + \int d\mathbf{r}' V(r') \varphi(r') G(|\mathbf{r}-\mathbf{r}'|), \quad (23)$$

where the Green function is introduced

$$G(r) = -\text{P} \int \frac{d\mathbf{k}}{(2\pi)^D} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{2(T_k - \mu)}. \quad (24)$$

In the dilute limit, when the average distance between particles is much less than the coherence length, the wave function $\varphi(r)/n_0$, describing the behavior of two particles in the condensate, should be proportional [15,56] to the s -wave function $\varphi^{(0)}(r)$, which corresponds to relative motion of two particles with zero momentum and obeys the two-body Schrödinger equation in the center-of-mass system

$$-(\hbar^2/m)\nabla^2\varphi^{(0)}(r) + V(r)\varphi^{(0)}(r) = 0. \quad (25)$$

In the 3D case, the coefficient of proportionality is equal to unity [6] in the leading order with respect to the density, provided the following boundary conditions are imposed: first $|\varphi_{3D}^{(0)}(r)| < \infty$ at $r=0$ and second, $\varphi_{3D}^{(0)}(r) \rightarrow 1 - a/r$ for $r \rightarrow \infty$. In the developed formalism, this can be easily inferred from the obtained equation (23). Indeed, direct integration in Eq. (24) gives $G_{3D}(r) = -m \cos(\sqrt{2}r/\xi) / (4\pi\hbar^2 r)$, and, hence, $G_{3D}(r) \approx -m / (4\pi\hbar^2 r)$ when $r \lesssim \xi$. Thus we have $\varphi(r) \approx n_0 \varphi_{3D}^{(0)}(r)$ within this region, and integration of Eq. (25) yields $U(0) = 4\pi\hbar^2 a/m$. For the dilute gas we have also $n_0 \approx n$, and Eq. (21) leads to the familiar expression for the chemical potential $\mu \approx 4\pi\hbar^2 n a/m$.

In the 2D case, the low-energy behavior of the 2D Green's function (24) is easily calculated: $G_{2D}(r) \approx m / (2\pi\hbar^2) \ln[e^\gamma r / (\sqrt{2}\xi)]$ when $r \lesssim \xi$. Then it is not difficult to see from Eq. (23) that, first, $\varphi(r)/n_0$ obeys the 2D Schrödinger equation (25), and, second, its asymptotics for $r \rightarrow \infty$ is

$$\varphi(r)/n_0 \rightarrow 1 + \ln[e^\gamma r / (\sqrt{2}\xi)] m U(0) / (2\pi\hbar^2). \quad (26)$$

Hence, due to linearity of Eq. (25), the solution for $\varphi(r)$ should be proportional to the wavefunction $\varphi_{2D}^{(0)}(r)$ that obeys the 2D Schrödinger equation (25) with the following boundary conditions: first $|\varphi_{2D}^{(0)}(r)| < \infty$ at $r=0$ second, $\varphi_{2D}^{(0)}(r) \rightarrow \ln(r/a_{2D})$ for $r \rightarrow \infty$. The latter equation can be considered as the definition of the 2D scattering length [57]. Note that in the case of hard disks, a_{2D} coincides with the radius of the disks. It is convenient to introduce the dimensionless parameter u by the relation $U(0) = 4\pi\hbar^2 u/m$, such that u is the dimensionless scattering amplitude for two bosons in a medium of other bosons. By comparing the asymptotics (26) with that of $\varphi_{2D}^{(0)}(r)$, we derive

$$\begin{aligned} \varphi(r) &= 2un_0\varphi_{2D}^{(0)}(r), \\ -\ln(a_{2D}/\xi) &= 1/(2u) + \ln(e^\gamma/\sqrt{2}). \end{aligned} \quad (27)$$

With the help of Eq. (21) and the definition of ξ (see above), the relation (27) becomes a self-consistent equation for u

$$1/u + \ln u = -\ln(n_{2D}a_{2D}^2 2\pi) - 2\gamma, \quad (28)$$

where we neglect the condensate depletion in the leading order, putting $n_0 \approx n_{2D}$. By means of the latter approximation, the expression (21) takes the form

$$\mu = 4\pi\hbar^2 n_{2D} u / m. \quad (29)$$

Thus, the 2D chemical potential is given by Eqs. (28) and (29), which lead to the density expansion

$$\begin{aligned} \mu &= \frac{4\pi\hbar^2 n_{2D}}{m} \left(-\frac{1}{\ln(n_{2D}a_{2D}^2)} + \frac{1}{\ln^2(n_{2D}a_{2D}^2)} \right. \\ &\quad \left. \times \ln \left[-\frac{1}{\ln(n_{2D}a_{2D}^2)} \right] + \dots \right). \end{aligned} \quad (30)$$

Equations (28) and (29) are in agreement with the results of Refs. [10–12] and with the more accurate scheme of Ref. [13], which yields the correction for the chemical potential

$$\mu = (4\pi\hbar^2 n_{2D}/m)(u + u^2 + \dots). \quad (31)$$

Here, u is given by the more exact relation

$$1/u + \ln u = -\ln(n_{2D}a_{2D}^2 \pi) - 2\gamma, \quad (32)$$

where $\gamma=0.5772\dots$ is the Euler constant. By means of this relation, one can rewrite Eq. (31) in terms of the gas parameter $n_{2D}a_{2D}^2$ and obtain three more terms in the expansion (30). Note that Eq. (32) differs from Eq. (28) by a numerical factor under the logarithm, which is essential only for obtaining these additional terms but not the terms given by relation (30).

B. The inhomogeneous case

1. The Gross-Pitaevskii regime

First of all, we should verify that the equations obtained in Sec. II lead to the standard GP scheme in the case $R_e \ll \xi \ll l$, where l is the characteristic length of an isotropic trap. In this regime, one can expect that the pair wave function $\varphi(\mathbf{r}_1, \mathbf{r}_2)$ is very close to that obtained in the homogeneous case, with the difference that the density is spatially dependent now. So, we put by definition $\varphi(\mathbf{r}_1, \mathbf{r}_2) = \phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\tilde{\varphi}(\mathbf{r}_1, \mathbf{r}_2)$ and $\psi(\mathbf{r}_1, \mathbf{r}_2) = \phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\tilde{\psi}(\mathbf{r}_1, \mathbf{r}_2)$, and, hence, $\tilde{\varphi}(\mathbf{r}_1, \mathbf{r}_2) = 1 + \tilde{\psi}(\mathbf{r}_1, \mathbf{r}_2)$ by Eq. (9). Substituting those expressions into Eqs. (16) and (17) yields

$$\begin{aligned} &\left[-\frac{\hbar^2}{2m}\nabla_1^2 - \mu - E_0 + V_{\text{ext}}(\mathbf{r}_1) \right] \phi(\mathbf{r}_1) + \phi(\mathbf{r}_1) |\phi(\mathbf{r}_1)|^2 \\ &\quad \times \int d\mathbf{r}_2 V(|\mathbf{r}_1 - \mathbf{r}_2|) \tilde{\varphi}(\mathbf{r}_1, \mathbf{r}_2) = 0, \end{aligned} \quad (33)$$

$$\begin{aligned} &-\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2)\tilde{\psi}(\mathbf{r}_1, \mathbf{r}_2) + V(\mathbf{r}_1 - \mathbf{r}_2)\tilde{\varphi}(\mathbf{r}_1, \mathbf{r}_2) \\ &= [f(\mathbf{r}_1) + f(\mathbf{r}_2)]\tilde{\psi}(\mathbf{r}_1, \mathbf{r}_2), \end{aligned} \quad (34)$$

where we use the condition $R_e \ll \xi$ in the first equation and introduce the notation

$$f(\mathbf{r}) = \int d\mathbf{r}' |\phi(\mathbf{r}')|^2 V(\mathbf{r} - \mathbf{r}') \tilde{\varphi}(\mathbf{r}, \mathbf{r}') + \frac{\hbar^2}{m} \frac{\nabla_{\mathbf{r}} \phi(\mathbf{r})}{\phi(\mathbf{r})} \cdot \nabla_{\mathbf{r}}, \quad (35)$$

with the last term being a differential operator. Since $\varphi(\mathbf{r}_1, \mathbf{r}_2) \approx \phi(\mathbf{r}_1)\phi(\mathbf{r}_2)$ at the distances of order of the correlation length, we have $\tilde{\varphi}(\mathbf{r}_1, \mathbf{r}_2) \approx 1$ at these distances. Consequently, the LHS of Eq. (34) remains finite when the density tends to zero, while the RHS becomes small. Indeed, the first term of Eq. (35) is of order of $\hbar^2 a n / m$. The second term is less than $\hbar^2 / (m\xi^2)$ because the characteristic scale of the order parameter cannot be smaller than ξ in the case $\xi \ll l$ and the same applies to $\tilde{\psi}$. Hence, in the leading order we can completely neglect the RHS of Eq. (34), which leads to the standard Schrödinger equation (25) for $\tilde{\varphi}$. Thus, we come to the approximation

$$\varphi(\mathbf{r}_1, \mathbf{r}_2) \approx \phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\varphi_{3D}^{(0)}(r). \quad (36)$$

Using the well-known relation for the 3D scattering length

$$4\pi\hbar^2 a / m = \int d^3r V(r)\varphi_{3D}^{(0)}(r), \quad (37)$$

we can rewrite Eq. (33) in the standard GP form with the coupling constant $g = 4\pi\hbar^2 a / m$. Note that, nevertheless, the equilibrium value of the energy (15) differs from that of the GP value (1) by the terms arising from the condensate depletion because the second term in the RHS of Eq. (10) is not equal to zero. We will discuss these corrections to the energy in Secs. IV and V.

2. 2D regime

Here we consider the Bose gas confined only in z direction by the trapping potential $V_{\text{ext}} = V_{\text{ext}}(z)$. The system is homogeneous in the x - y plane and assumed to be infinitely large. Physically this means that the x - y size of the system is much larger than the characteristic radius of the trapping potential $l_z \equiv \sqrt{\hbar/(m\omega_z)}$. The order parameter ϕ now becomes independent of x and y , and the two-body function depends on the relative distance $\rho = |\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2|$ between points $\boldsymbol{\rho}_1 = (x_1, y_1)$ and $\boldsymbol{\rho}_2 = (x_2, y_2)$, so $\varphi(\mathbf{r}_1, \mathbf{r}_2) = \varphi(z_1, z_2, \rho)$. The 2D regime is provided by the condition $l_z \ll \xi$. Moreover, the condition $R_e \ll \xi$ is fulfilled in most experiments. As was discussed in Sec. I the density profile is then governed by the ground state solution $\phi_0(z)$ of the one-particle Schrödinger equation

$$[-\hbar^2\nabla^2/(2m) - E_0 + V_{\text{ext}}(z)]\phi_0(z) = 0,$$

because the second term in Eq. (16) can be treated as a small correction. Thus, we can put in the leading order $\phi(z) \approx \sqrt{n_{2D}}\phi_0(z)$; $\phi_0(z)$ is normalized to unity. By analogy with

standard perturbation theory, the chemical potential, as the first correction to E_0 , can be found with the unperturbed eigenfunction ϕ_0 . So, multiplying Eq. (16) by $\phi_0(z_1)$ and integrating by z_1 yield

$$\mu = n_{2D} \int d\boldsymbol{\rho} \widetilde{U}(\boldsymbol{\rho}), \quad (38)$$

where by definition

$$\begin{aligned} \widetilde{U}(\boldsymbol{\rho}) \equiv & \int dz_1 dz_2 V(\sqrt{\rho^2 + (z_1 - z_2)^2}) \\ & \times \varphi(z_1, z_2, \rho) \phi_0(z_1) \phi_0(z_2) / n_{2D}. \end{aligned} \quad (39)$$

In the same manner, one can multiply Eq. (17) by $\phi_0(z_1) \phi_0(z_2)$ and carry out the integration by z_1 and z_2 , which results in the equation

$$2[\hbar^2 \nabla_\rho^2 / (2m) + \mu] \widetilde{\psi}(\boldsymbol{\rho}) = \widetilde{U}(\boldsymbol{\rho}) \quad (40)$$

for the function

$$\widetilde{\psi}(\boldsymbol{\rho}) = \int dz_1 dz_2 \psi(z_1, z_2, \rho) \phi_0(z_1) \phi_0(z_2) / n_{2D}. \quad (41)$$

Thus, we arrive at the system of equations (38) and (40), which coincides with that of Eqs. (21) and (22) in homogeneous case if we put $U(k) = \int d\boldsymbol{\rho} \widetilde{U}(\boldsymbol{\rho}) e^{-i\mathbf{k}\cdot\boldsymbol{\rho}}$ and perform the Fourier transformation of Eq. (40). By the same method as in Sec. III A, we obtain the asymptotics for sufficiently large ρ [physically, for $R_e \ll \rho \ll \xi$, when only the first term dominates in Eq. (40)]

$$\widetilde{\varphi}(\rho) \approx 1 + \ln[e^{\gamma} \rho / (\sqrt{2} \xi)] m \mu / (2 \pi \hbar^2 n_{2D}), \quad (42)$$

where by definition

$$\widetilde{\varphi}(\rho) = \int dz_1 dz_2 \varphi(z_1, z_2, \rho) \phi_0(z_1) \phi_0(z_2) / n_{2D} = 1 + \widetilde{\psi}(\rho). \quad (43)$$

The latter relation is due to Eqs. (9) and (41).

In order to obtain the chemical potential in terms of the 3D scattering length a and the length l_z of the trapping potential, we use the following approximation: [58]

$$\varphi(z_1, z_2, \rho) = C \varphi_{3D}^{(0)}(r) n_{2D} \phi_0(z_1) \phi_0(z_2) \quad (44)$$

in the region $r \ll l_z \ll \xi$, where $r = \sqrt{\rho^2 + (z_1 - z_2)^2}$, and $\varphi_{3D}^{(0)}(r)$ denotes the 3D solution of the Schrödinger equation (25) with asymptotics for $r \gg R_e$

$$\varphi_{3D}^{(0)}(r) \approx 1 - a/r. \quad (45)$$

Here the crucial point is that the constant $C \neq 1$, which determines the 2D behavior of the system. If we substitute Eq. (44) into Eq. (43) and take the integral, we arrive at a new expression for $\widetilde{\varphi}(\rho)$. This should be expanded with respect to the dimensionless variable ρ/l_z and compared with Eq. (42). Since the main contribution in that integral comes from the asymptotics (45), one can use it instead of the function $\varphi_{3D}^{(0)}(r)$ itself. By performing this procedure for the harmonic

trapping potential with $\phi_0(z) = \exp[-z^2/(2l_z^2)]/\sqrt{l_z \sqrt{\pi}}$, we have

$$\widetilde{\varphi}(\rho) \approx C + \frac{2Ca}{l_z \sqrt{2\pi}} \ln[e^{\gamma/2} \rho / (2\sqrt{2} l_z)].$$

Comparing this relation with Eq. (42) yields

$$C = \sqrt{2\pi} l_z u / a, \quad (46)$$

and the chemical potential is given by Eq. (29) with the dimensionless parameter u obeying the equation

$$1/u + \ln u = \sqrt{2\pi} l_z / a - \gamma - \ln(16\pi n_{2D} l_z^2). \quad (47)$$

This result for μ is well consistent with relations (38) and (39). Indeed, substitution of Eq. (44) with constant (46) into Eq. (39) leads to Eq. (29) provided that the relation (37) is employed in conjunction with the approximation $\exp[-(z_1 - z_2)^2/(2l_z^2)] \approx 1$ due to the integration with the short-range potential with $R_e \ll l_z$. In the leading order at small 2D densities, expressions (29) and (47) result in

$$\mu = \frac{4\pi \hbar^2 n_{2D}}{m} \frac{1}{\sqrt{2\pi} l_z / a - \gamma - \ln(16\pi n_{2D} l_z^2)}. \quad (48)$$

This differs from the result [35] of Petrov, Holzmann, and Shlyapnikov only by the additional numerical term $-\gamma - \ln 2 = -1.2703\dots$ in the denominator. We note that the healing length in two dimensions takes the form $\xi = 1/\sqrt{4\pi n_{2D} u}$, which differs from that in three dimensions $\xi = 1/\sqrt{4\pi n a}$. Due to the criterion $1/\sqrt{n_{2D}} \ll \xi$, the obtained results relate to sufficiently small densities, for which $u \ll 1$.

3. 1D regime

Contrary to the 3D and 2D nonideal Bose gases, there is no Bose-Einstein condensate in one dimension [10,59] in the thermodynamic limit, because the long-wave fluctuations of the phase break the off-diagonal long-range order. Nevertheless, one can speak about the quasicondensate [44] if a size of the 1D system is sufficiently small. Indeed, at zero temperature the phase fluctuations are suppressed if $\ln(L_z/\xi) \ll n_{1D} \xi$ [44,45], which can be fulfilled only at finite number of particles. Here L_z stands for the size in z direction.

All calculations concerning the 1D quasicondensate in the case $R_e \ll l_\rho \ll \xi$ can be done in complete analogy with the 2D inhomogeneous Bose gas considered in the previous subsection. The gas is strongly confined in the x - y plane by the harmonic trapping potential in $V_{\text{ext}} = m\omega_\rho^2 \rho^2/2$ with the length $l_\rho = \sqrt{\hbar/(m\omega_\rho)}$, and remains homogeneous in z direction. In the regime involved, we can put $\phi(\rho) = \sqrt{n_{1D}} \phi_0(\rho)$, $\phi_0(\rho) = \exp[-\rho^2/(2l_\rho^2)]/l_\rho \sqrt{\pi}$ is the ground state solution of the one-particle Schrödinger equation with the energy $E_0 = \hbar\omega_\rho$. Reasoning by analogy with Sec. III B 2, we obtain

$$\mu = n_{1D} \int dz \widetilde{U}(z), \quad (49)$$

where we introduce the even function $\widetilde{U}(z) = \widetilde{U}(-z)$

$$\begin{aligned} \widetilde{U}(z) = & \int d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2 V(\sqrt{(\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2)^2 + z^2}) \\ & \times \varphi(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2, z) \phi_0(\rho_1) \phi_0(\rho_2) / n_{1D}. \end{aligned}$$

The 1D analogue of Eq. (40) is the equation

$$2 \left[\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + \mu \right] \widetilde{\psi}(z) = \widetilde{U}(z) \quad (50)$$

for the function

$$\widetilde{\psi}(z) = \int d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2 \psi(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2, z) \phi_0(\rho_1) \phi_0(\rho_2) / n_{1D}.$$

Equation (50) can be rewritten in the Lippmann-Schwinger form at $\mu \rightarrow 0$ (see discussion in Sec. III A)

$$\widetilde{\varphi}(z) = 1 + (m/\hbar^2) \int dz' \widetilde{U}(z') |z - z'|/2 \quad (51)$$

for the function $\widetilde{\varphi}(z)$, defining as

$$\widetilde{\varphi}(z) = \int d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2 \varphi(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2, z) \phi_0(\rho_1) \phi_0(\rho_2) / n_{1D}. \quad (52)$$

Equations (49) and (51) give the asymptotics for $R_c \ll z \ll \xi$

$$\widetilde{\varphi}(z) \simeq 1 + m\mu|z|/(2n_{1D}\hbar^2). \quad (53)$$

On the other hand, in the region $r \ll l_p \ll \xi$ we can use the analogue of Eq. (44)

$$\varphi(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2, z) = C \varphi_{3D}^{(0)}(r) n_{1D} \phi_0(\rho_1) \phi_0(\rho_2), \quad (54)$$

which leads to the asymptotics after the integration in Eq. (52)

$$\widetilde{\varphi}(z) \simeq C - C(\sqrt{\pi/2} - |z|/l) a / l_p. \quad (55)$$

Comparing Eqs. (53) and (55) yields

$$C = 1/(1 - \sqrt{\pi/2} a / l_p), \quad (56)$$

$$\mu = \frac{2\hbar^2 n_{1D} a}{m l_p^2} \frac{1}{1 - \sqrt{\pi/2} a / l_p}, \quad (57)$$

which differs from Olshanii's result [47] through the numerical factors $\sqrt{\pi} = 1.772\dots$ in the denominator instead of the constant 1.4603... introduced by him. We note that in the paper [47] $a_{\perp} = \sqrt{2\hbar/(m\omega_{\rho})} = \sqrt{2}l_p$ in our notation. One can see that the criteria of applicability of the obtained results $l_p \ll \xi$ and $1/n_{1D} \ll \xi$ impose the following restriction on the 1D density:

$$\frac{a}{l_p^2} \ll n_{1D} \ll \frac{1}{a}, \quad (58)$$

since $\xi \simeq l_p / \sqrt{2an_{1D}}$ in one dimension.

IV. THE KINETIC, INTERACTION, AND EXTERNAL FIELD ENERGY OF THE TRAPPED BOSE GAS

The simplest method for obtaining the values of the interaction energy (3), the kinetic energy (4), and the energy of

interaction with an external field (5), is to apply the variational theorem. The latter can be formulated in general as follows. If a function $f(x)$ obeys the functional equation

$$\delta F[\{f(x)\}, \lambda] / \delta f(x) = 0 \quad (59)$$

with the functional F depending on the function $f(x)$ and the parameter λ , then the solution of Eq. (59) $f(x) = f_0(x, \lambda)$ is also dependent on λ . Nevertheless, when calculating the derivative of the stationary value of the functional with respect to λ , we can take into consideration only the explicit dependence on this parameter

$$dF[\{f_0(x, \lambda)\}, \lambda] / d\lambda = \delta F[\{f_0(x, \lambda)\}, \lambda] / \delta \lambda. \quad (60)$$

This is obvious due to Eq. (59).

The variational theorem (60) is still valid if the functional contains two or more functions. In our case, the functions can be associated with $\phi(x_1)$ and $\psi(x_1, x_2)$ involved in the energy functional (15). Considering \mathcal{N} as the parameter of the variational theorem, we come to the standard thermodynamic relation $\partial E / \partial \mathcal{N} = \mu' = \mu + E_0$. One can rewrite this derivative in terms of the energy per particle $\varepsilon = E/N$ and the density of particles $\partial E / \partial \mathcal{N} = \partial(\varepsilon n) / \partial n$, which gives the relation $\varepsilon = (1/n) \int_0^n dn' \mu(n') + E_0$. Then relations (29) and (47) lead to

$$\varepsilon_{2D} \simeq 2\pi\hbar^2 n_{2D} u / m + \frac{\hbar^2}{2ml_z^2}, \quad (61)$$

with u given by Eq. (47). In the same manner, we obtain from Eq. (57) [60]

$$\varepsilon_{1D} = \frac{\hbar^2 n_{1D} a}{m l_p^2} \frac{1}{1 - \sqrt{\pi/2} a / l_p} + \frac{\hbar^2}{ml_p^2}. \quad (62)$$

Equations (61) and (62) give us the equilibrium value of the energy (15) per particle in the 2D and 1D cases, respectively. In order to calculate the interaction energy with the help of the variational theorem, one can replace $V \rightarrow \lambda V$ and differentiate ε with respect to λ at $\lambda = 1$. All we need to know is the derivative of the 3D scattering length, which reads [16,61]

$$\lambda \frac{\partial a}{\partial \lambda} = m \frac{\partial a}{\partial m} = \frac{m}{4\pi\hbar^2} \int d^3r [\varphi_{3D}^{(0)}(r)]^2 \lambda V(r). \quad (63)$$

It is convenient to introduce one more characteristic length [16], the positive parameter b ,

$$b = a - \lambda \left. \frac{\partial a}{\partial \lambda} \right|_{\lambda=1} = \frac{1}{4\pi} \int d^3r |\nabla \varphi_{3D}^{(0)}(r)|^2.$$

So, we have

$$\varepsilon_{2Dint} \simeq \frac{2\pi\hbar^2 n_{2D}}{m} u^2 \frac{\sqrt{2\pi} l_z}{a} \left(1 - \frac{b}{a} \right), \quad (64)$$

$$\varepsilon_{1Dint} \simeq \frac{\hbar^2 n_{1D} a}{m l_p^2} \left(1 - \frac{b}{a} \right), \quad (65)$$

where we use the approximation $u^2/(1-u) \simeq u^2$ in Eq. (64) and restrict ourselves by the leading order in Eq. (65).

With the same method, replacing $V_{\text{ext}} \rightarrow \lambda V_{\text{ext}}$ (which is equivalent to $l \rightarrow l/\sqrt[4]{\lambda}$) and differentiating, we arrive at the external energy per particle

$$\varepsilon_{2\text{Dext}} \approx \frac{2\pi\hbar^2 n_{2\text{D}} u^2}{m} \frac{1}{4} \left(\frac{\sqrt{2\pi} l_z}{a} - 2 \right) + \frac{\hbar^2}{4ml_z^2}, \quad (66)$$

$$\varepsilon_{1\text{Dext}} \approx \frac{\hbar^2 n_{1\text{D}} a}{2m l_\rho^2} + \frac{\hbar^2}{2ml_\rho^2}. \quad (67)$$

In the same manner, we have $\varepsilon_{\text{kin}} = -m\partial\varepsilon/\partial m$, which leads to

$$\varepsilon_{2\text{Dkin}} \approx \frac{2\pi\hbar^2 n_{2\text{D}} u}{m} - \frac{2\pi\hbar^2 n_{2\text{D}} u^2}{m} \left[\frac{1}{4} \left(\frac{\sqrt{2\pi} l_z}{a} - 2 \right) + \frac{\sqrt{2\pi} l_z}{a} \left(1 - \frac{b}{a} \right) \right] + \frac{\hbar^2}{4ml_z^2}, \quad (68)$$

$$\varepsilon_{1\text{Dkin}} \approx \frac{\hbar^2 n_{1\text{D}} b}{m l_\rho^2} - \frac{\hbar^2 n_{1\text{D}} a}{2m l_\rho^2} + \frac{\hbar^2}{2ml_\rho^2}. \quad (69)$$

One can see that sum of the kinetic, external and interaction energies equals to the total energy, as it should be. Note that the developed formalism allows us to calculate the interaction energy directly, starting from the expression (11) and using Eq. (37), since we have the analytic expressions (44), (46), (54), and (56) for the short-range behavior of the anomalous average.

We note that the ratio b/a need not be small. In particular, it is of order of ten for the realistic interaction potentials of alkali atoms [48]. We stress that the term with the length b appears in the mean interaction energy by virtue of the short-range two-body correlations at the distances of order of a and in the mean kinetic energy by sufficiently large momenta of order of $p \gtrsim \hbar/a$ in the momentum distribution. In the static structure factor, this region is rather difficult to be measured experimentally. The density expansion method gives the value of the release energy that is defined as *sum* of the interaction and kinetic energies

$$\varepsilon_{2\text{Drel}} \approx \frac{2\pi\hbar^2 n_{2\text{D}} u}{m} - \frac{2\pi\hbar^2 n_{2\text{D}} u^2}{m} \frac{1}{4} \left(\frac{\sqrt{2\pi} l_z}{a} - 2 \right) + \frac{\hbar^2}{4ml_z^2}, \quad (70)$$

$$\varepsilon_{1\text{Drel}} \approx \frac{\hbar^2 n_{1\text{D}} a}{2m l_\rho^2} + \frac{\hbar^2}{2ml_\rho^2}. \quad (71)$$

As one can see, the parameter b is canceled and not involved in the values of the release energy. Let us compare the values of the release (70) and (71) and total energy (61) and (62). The energy of zero-point oscillation is involved in the release energy with the factor 1/2, as it should be for the harmonic trap. The other terms would coincide in the standard GP approach, but we have obvious difference due to accounting for the noncondensate contribution. In principle, the obtained corrections should be measurable in experiments.

V. VIRIAL THEOREM

The virial theorem can be obtained immediately from the energy functional (15) if we consider its variation in vicinity of the stationary state (ground state) with respect to the scaling transformation of the ground state functions ϕ_0 and ψ_0 , obeying the generalized GP equations (16) and (17). Namely, we substitute into Eq. (15) the functions $\phi(\mathbf{r}_1) = \alpha^{3/2} \phi_0(\alpha \mathbf{r}_1)$ and $\psi(\mathbf{r}_1) = \alpha^3 \psi_0(\alpha \mathbf{r}_1, \alpha \mathbf{r}_1)$. Replacing the variables in the integrals $\mathbf{r}_1 \rightarrow \alpha \mathbf{r}_1$ and $\mathbf{r}_2 \rightarrow \alpha \mathbf{r}_2$, we notice that, first, the last term in the functional equals to zero for any α , and, second, the other terms can be written in terms of its stationary values

$$E(\alpha) = \alpha^2 E_{\text{kin}} + E_{\text{ext}}/\alpha^2 + E_{\text{int}}[V(r/\alpha)]. \quad (72)$$

Since the variation of the functional should be zero for any small variations of the functions, we have $dE/d\alpha = 0$ at $\alpha = 1$, which leads to

$$2E_{\text{kin}} - 2E_{\text{ext}} + E_{\text{int}}[-rV'(r)] = 0, \quad (73)$$

where the terms are given by Eqs. (11)–(13). The value of the last term corresponds to the interaction energy with the potential $-rV'(r) = -rdV(r)/dr$. In the case of the GP approximation (36), one can simplify the last item in Eq. (73) by means of Eq. (37) and relation [6]

$$\frac{4\pi\hbar^2 a}{m} = - \int_0^\infty dr 4\pi r^2 [\varphi^{(0)}(r)]^2 \left(2V(r) + r \frac{dV(r)}{dr} \right).$$

The result takes a form

$$\begin{aligned} E_{\text{int}} &\approx \frac{1}{2} \int d\mathbf{R} |\phi(\mathbf{R})|^4 \int d\mathbf{r} [-rV'(r)] [\varphi_{3\text{D}}^{(0)}(r)]^2 \\ &= \frac{2\pi\hbar^2}{m} (3a - 2b) \int d\mathbf{R} |\phi(\mathbf{R})|^4. \end{aligned} \quad (74)$$

If the potential is of the weak-coupling type [18], one can neglect $b \ll a$ and arrive at the virial theorem obtained for the δ -function interaction potential [3].

If the system is homogeneous in the x - y plane (the 2D Bose gas of Sec. III B 2) or in the z direction (the 1D Bose gas of Sec. III B 3), it can be considered as confined by infinite walls in associated directions. Then one should be careful when deriving the virial theorem from Eq. (72), as all its terms relate to the density $n_{2\text{D}}/\alpha^2$ or $n_{1\text{D}}/\alpha$ for the 2D or 1D Bose gas, respectively. For this reason, we come to

$$2n_{2\text{D}} \frac{\partial \varepsilon_{2\text{D}}}{\partial n_{2\text{D}}} = 2\varepsilon_{2\text{Dkin}} - 2\varepsilon_{2\text{Dext}} + \varepsilon_{2\text{Dint}}[-rV'(r)], \quad (75)$$

$$n_{1\text{D}} \frac{\partial \varepsilon_{1\text{D}}}{\partial n_{1\text{D}}} = 2\varepsilon_{1\text{Dkin}} - 2\varepsilon_{1\text{Dext}} + \varepsilon_{1\text{Dint}}[-rV'(r)]. \quad (76)$$

The interaction term in these equations can be easily calculated by analogy with Eq. (74) but using Eqs. (44) and (54), respectively. It is not difficult to be convinced with the help of Eqs. (61) and (62) that the virial theorems (75) and (76) are fulfilled.

One can also find a relation between the chemical potential and the various parts of the energy. Let us multiply Eq. (16) by $\phi(x_1)$ and integrate over x_1 , and multiply Eq. (17) by $\psi(x_1, x_2)$ and also integrate over x_1 and x_2 . Summing the obtained expressions yields

$$N\mu = E_{\text{kin1}} + 2E_{\text{kin2}} + E_{\text{ext1}} + 2E_{\text{ext2}} + 2E_{\text{int}}. \quad (77)$$

Here, E_{ext1} and E_{kin1} are the condensate contributions in the external and kinetic energies given by the last terms in Eqs. (12) and (13), respectively, and E_{ext2} and E_{kin2} are associated with the noncondensate contributions, given by the residual parts of these equations. One can easily see that the relation (77) is fulfilled with E_{ext1} and E_{kin1} corresponding to the last terms in Eqs. (66)–(69) for the 2D and 1D Bose gases, respectively. One can notice that E_{kin2} could be negative for the 1D Bose gas, if $b < a/2$ [see the first two terms in Eq. (69)]. Certainly, this is not a drawback of Eqs. (16) and (17) it is but due to the choice of ansatz $\phi(\rho) = \sqrt{n_{1D}}\phi_0(\rho)$, which leads to overestimation of the quasicondensate contribution E_{kin1} in the 1D kinetic energy. Indeed, the Gaussian profile $n_{1D}|\phi_0(\rho)|^2$ relates to the *total* density of the 1D gas $\langle \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}) \rangle$ but not to the “quasicondensate component” $|\phi(\rho)|^2$. The latter is difficult to define accurately in the 1D case, since there is no eigenvalue of the one-body density matrix that is proportional to the total number of particles. Nevertheless, we stress that the total value of $E_{1D\text{kin}}$ is positive, and the results (65), (67), and (69) look quite reasonable.

VI. CONCLUSIONS

The main result of this paper are the generalized GP equations in the time-dependent (18) and (19) and stationary form (16) and (17), which allow us to determine the interaction term self-consistently for interaction potentials even containing a hard core. The method, which can be used for homogeneous, strongly inhomogeneous quasi-low-dimensional, and crossover regimes was derived within a general HFB framework.

The HFB method is a mean-field approximation, which generally works well only for weak-coupling potentials [18]. In order to extend the HFB scheme to hard-core potentials, the bare interaction potential is usually replaced by a renormalized pseudopotential $V(r) \rightarrow (4\pi\hbar^2/m)\delta^3(\mathbf{r})$. However, such a replacement leads to an ultraviolet divergence and incorrect treatment of short-range correlations of the particles. We have shown that the appropriate renormalization can be obtained *within* the HFB scheme if, from the two-body density matrix, only the anomalous correlation function $\varphi(x_1, x_2) = \langle \hat{\Psi}(x_1)\hat{\Psi}(x_2) \rangle$ is retained. The anomalous correlation function can be interpreted as the wave function of two bosons in the condensate. Its short-range behavior is described well in the proposed scheme at the cost of losing the correct description of the long-range behavior. However, long-range correlations are not needed for deriving the nonlinear term in the generalized GP approach, which instead is determined by short-range correlations. Methods which can describe both the short- and long-range correlations accu-

rately were discussed in Refs. [13,16,17,24], but these methods are appropriate only for the homogeneous Bose gas. The method proposed in this paper was shown to work as well in inhomogeneous situations. Cigar (quasi-1D) and pancake (quasi-2D) geometries were considered as examples. Furthermore, it was shown that the contribution of short-range correlations to the kinetic and release energies of a tightly trapped gas can be calculated within this scheme and that they are substantial. Interesting future applications of the proposed method may include the modification of the nonlinearity in quasi-1D waveguides [62,63] and molecular Bose condensates in optical lattices.

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APPENDIX A: TWO-BODY WAVE FUNCTIONS IN THE HARTREE-FOCK-BOGOLIUBOV APPROXIMATION

In general, the two-body density matrix can be expanded in a complete set of its eigenfunctions

$$\begin{aligned} \langle \hat{\Psi}^\dagger(x_1)\hat{\Psi}^\dagger(x_2)\hat{\Psi}(x'_2)\hat{\Psi}(x'_1) \rangle &= \sum_{\nu,\mu} N_{\nu,\mu} \varphi_{\nu,\mu}^*(x_1, x_2) \\ &\times \varphi_{\nu,\mu}(x'_1, x'_2). \end{aligned} \quad (A1)$$

The eigenfunctions can be called two-body or pair wave functions. If they are normalized to unity, it follows from Eq. (A1) that $\int dx_1 dx_2 \langle \hat{\Psi}^\dagger(x_1)\hat{\Psi}^\dagger(x_2)\hat{\Psi}(x_2)\hat{\Psi}(x_1) \rangle = N(N-1) = \sum_{\nu,\mu} N_{\nu,\mu}$, i.e., the sum of all $N_{\nu,\mu}$ is the total number of pairs. Therefore, the non-negative quantity $N_{\nu,\mu}$ can be interpreted as the mean number of the pairs in the state (ν, μ) , any pair being doubly taken.

Let us consider the homogeneous spinless Bose gas in the HFB approximation [22,25]. Within that approximation, the two-body wave functions can be easily calculated [15]. The statistical average of any product of quantum operators $\hat{\vartheta}$ and $\hat{\vartheta}^\dagger$ can be calculated with the Wick–Bloch–De Dominicis theorem [64], since the Hamiltonian is approximated by a *quadratic form* of the Bose operators $\hat{\alpha}_{\mathbf{p}}^\dagger$ and $\hat{\alpha}_{\mathbf{p}}$ connected with initial operators $\hat{a}_{\mathbf{p}}^\dagger$ and $\hat{a}_{\mathbf{p}}$ by the canonical Bogoliubov transformations (see Appendix). Extracting the *c*-number part $\hat{\Psi} = \sqrt{n_0} + \hat{\vartheta}$ and $\hat{\Psi}^\dagger = \sqrt{n_0} + \hat{\vartheta}^\dagger$ and using that theorem, one can rewrite the four-boson average in the form

$$\begin{aligned} &\left\langle \hat{\Psi}^\dagger\left(\mathbf{R} + \frac{\mathbf{r}}{2}\right)\hat{\Psi}^\dagger\left(\mathbf{R} - \frac{\mathbf{r}}{2}\right)\hat{\Psi}\left(\mathbf{R}' - \frac{\mathbf{r}'}{2}\right)\hat{\Psi}\left(\mathbf{R}' + \frac{\mathbf{r}'}{2}\right) \right\rangle \\ &= n_0^2 \bar{\varphi}^*(r)\bar{\varphi}(r') + \int d^3p d^3q \left[2n_0 \delta(\mathbf{q}/2 - \mathbf{p}) \frac{n(\mathbf{q})}{(2\pi)^3} \right. \\ &\quad \left. + \frac{n(\mathbf{q}/2 + \mathbf{p})n(\mathbf{q}/2 - \mathbf{p})}{(2\pi)^3} \right] \sqrt{2} \cos(\mathbf{p} \cdot \mathbf{r}) \sqrt{2} \cos(\mathbf{p} \cdot \mathbf{r}') \\ &\quad \times \exp[i\mathbf{q} \cdot (\mathbf{R}' - \mathbf{R})], \end{aligned} \quad (A2)$$

where we put by definition $\bar{\varphi}(r) = 1 + \langle \hat{\vartheta}(\mathbf{R} + \mathbf{r}/2)\hat{\vartheta}(\mathbf{R}$

$-\mathbf{r}/2\rangle/n_0$. Because the expansion (A2) is written in the thermodynamic limit, the sum in Eq. (A1) becomes an integral. The Bose-Einstein condensate manifests itself in presence of δ -functions in this integral (note that the first term in the RHS can be included in the integral with the help of the δ -functions). By comparing the representation (A1) with that of Eq. (A2), one can conclude the following.

(i) The quantum numbers of the pair wave functions are the relative momentum $\nu=\mathbf{p}$ and the center-of-mass (total) momentum $\mu=\mathbf{q}$ of two particles; all these functions belong to continuous spectrum and thus describe the scattering of two bosons in the medium of the other bosons.

(ii) The maximum eigenvalue $N_0(N_0-1)\approx N_0^2$ with $\mathbf{p}=\mathbf{q}=0$ corresponds to the state of two particles in the condensate; its normalized eigenfunction $\widehat{\varphi}(\mathbf{r})/V$ can be interpreted as a pair wave function of the condensate-condensate type. Thus, the anomalous average $\langle\widehat{\vartheta}(\mathbf{r})\widehat{\vartheta}(0)\rangle$ can be associated with the scattering part of the two-body wave function of the bosons in the condensate [15]; in particular, it is responsible for the short-range spatial correlations of two bosons in the Bose-Einstein condensate.

(iii) The other macroscopic eigenvalues $2N_0n_q$ with $\mathbf{q}=\pm 2\mathbf{p}$ correspond to the two-body states with one particle in the condensate and another one beyond the condensate; its eigenfunctions $\sqrt{2}\cos(\mathbf{q}\cdot\mathbf{r}/2)\exp[i\mathbf{q}\cdot\mathbf{R}]/V$ are of the condensate-noncondensate type [66]. The residuary nonmacroscopic eigenvalues $n(\mathbf{q}/2+\mathbf{p})n(\mathbf{q}/2-\mathbf{p})$ are related to the noncondensate-noncondensate pairs with the two-body wave functions $\sqrt{2}\cos(\mathbf{p}\cdot\mathbf{r})\exp[i\mathbf{q}\cdot\mathbf{R}]/V$.

Note that the wave function of the condensate-condensate type is not reduced to a product of two one-body wave functions in the condensate, which equal to $1/\sqrt{V}$ for the homogeneous Bose gas. This is obvious, as particles in the Bose-Einstein condensate interact with each other and with the other particles beyond the condensate. Another important point is that all the other two-body wave functions are symmetrized plane waves (consistent with the Born approximation) in the framework of the HFB method. This is evidently a disadvantage of the HFB scheme. As a consequence, we always arrive at divergences for a hard-core potential when evaluating the contribution of the condensate-noncondensate and noncondensate-noncondensate wave functions in the interaction energy (3). At the same time, the contribution of the condensate-condensate “channel” should be finite in the interaction energy provided the anomalous averages are calculated in a self-consistent manner. The generalization of the expansion (A2) beyond the HFB approach and more detailed discussions can be found in Ref. [15]. The pair wave function method of Ref. [15] was generalized to the inhomogeneous systems in Ref. [68].

APPENDIX B: RELATION BETWEEN THE NORMAL AND ANOMALOUS TWO-BOSON AVERAGES

Let us establish a relation between the normal $\langle\widehat{\vartheta}^\dagger(x_1)\widehat{\vartheta}(x_2)\rangle$ and the anomalous average $\langle\widehat{\vartheta}(x_1)\widehat{\vartheta}(x_2)\rangle$ for the vacuum state, which describes the behavior of the N -body system at zero temperature, in the framework of the

Hartree-Fock-Bogoliubov method. We remember that the vacuum state $|0\rangle$ is defined as $\alpha_\nu|0\rangle=0$ for any $\nu\neq 0$, here the quasiparticle creation and destruction operators $\widehat{\alpha}_\nu^\dagger$ and $\widehat{\alpha}_\nu$ can be introduced through the Bogoliubov transformation ($f\neq 0$)

$$\widehat{a}_f = \sum_\nu (u_{f\nu}\widehat{\alpha}_\nu + v_{f\nu}\widehat{\alpha}_\nu^\dagger), \quad (\text{B1})$$

$$\widehat{a}_f^\dagger = \sum_\nu (u_{f\nu}^*\widehat{\alpha}_\nu^\dagger + v_{f\nu}^*\widehat{\alpha}_\nu), \quad (\text{B2})$$

where f and ν denote discrete (multi)indices. The sum \sum'_ν means $\sum_{\nu\neq 0}$ and the Bose-operators \widehat{a}_f^\dagger and \widehat{a}_f create and destruct a particle in the eigenstate $\phi_f(x)$ of the one-body matrix $\langle\widehat{\Psi}^\dagger(x')\widehat{\Psi}(x)\rangle$

$$\int dx' \langle\widehat{\Psi}^\dagger(x')\widehat{\Psi}(x)\rangle \phi_f(x') = n_f \phi_f(x),$$

normalized as $\int dx |\phi_f(x)|^2 = 1$. Note that the set of eigenfunctions including the normalized condensate function $\phi_0(x) = \langle\widehat{\Psi}(x)\rangle/\sqrt{N_0}$ with $N_0 = n_{f=0}$ is complete and orthogonal,

$$\sum_f \phi_f^*(x) \phi_f(x') = \delta(x-x'), \quad (\text{B3})$$

$$\int dx \phi_f^*(x) \phi_{f'}(x) = \delta(f-f'), \quad (\text{B4})$$

where we define the “discrete” δ -function as

$$\delta(f) = \begin{cases} 1, & f=0, \\ 0, & f\neq 0. \end{cases}$$

From the Bose commutation relations $[\widehat{a}_f, \widehat{a}_{f'}^\dagger] = \delta(f-f')$ and $[\widehat{\alpha}_f, \widehat{\alpha}_{f'}^\dagger] = \delta(f-f')$ and Eqs. (B1) and (B2) we obtain at $f, f' \neq 0$,

$$\sum_\nu (u_{f\nu} u_{f'\nu}^* - v_{f\nu} v_{f'\nu}^*) = \delta(f-f'), \quad (\text{B5})$$

$$\sum_\nu (u_{f\nu} v_{f'\nu} - v_{f\nu} u_{f'\nu}) = 0. \quad (\text{B6})$$

By using the definition of the quasiparticle vacuum state and Eqs. (B1) and (B2), we can calculate the averages

$$F(f, f') = \langle\widehat{a}_f^\dagger \widehat{a}_{f'}\rangle = \sum_\nu v_{f\nu}^* v_{f'\nu}, \quad (\text{B7})$$

$$\Phi(f, f') = \langle\widehat{a}_f \widehat{a}_{f'}\rangle = \sum_\nu u_{f\nu} v_{f'\nu}. \quad (\text{B8})$$

Our purpose is to find the relation between the normal $F(f, f')$ and the anomalous $\Phi(f, f')$ averages for that state. In order to simplify our calculations, we rewrite Eqs. (B1) and (B2) in the matrix notations

$$\begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} = X \begin{pmatrix} \hat{\alpha} \\ \hat{\alpha}^\dagger \end{pmatrix}, \quad X = \begin{pmatrix} U & V \\ V^* & U^* \end{pmatrix}. \quad (\text{B9})$$

Here the matrix X is composed of the matrix $(U)_{ij}=u_{ij}$ and $(V)_{ij}=v_{ij}$. The columns contain the operators \hat{a}_f and \hat{a}_f^\dagger , and $\hat{\alpha}_v$ and $\hat{\alpha}_v^\dagger$, respectively. We use the standard notations for the complex conjugate $(V^*)_{ij}=v_{ij}^*$, transposed $(V^T)_{ij}=v_{ji}$, and Hermitian conjugate matrix $(V^\dagger)_{ij}=v_{ji}^*$. Then Eqs. (B7) and (B8) read

$$F = V^* V^T = F^\dagger, \quad \Phi = UV^T = \Phi^T, \quad (\text{B10})$$

and Eqs. (B5) and (B6) can be written as

$$\begin{pmatrix} U & V \\ V^* & U^* \end{pmatrix} \begin{pmatrix} U^\dagger & -V^T \\ -V^\dagger & U^T \end{pmatrix} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}, \quad (\text{B11})$$

where $\mathbb{1}$ denotes the identity matrix. Let us introduce the composed matrices

$$\sigma_3 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}, \quad \sigma_+ = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix}, \quad (\text{B12})$$

and rewrite Eq. (B11) in the form

$$X\sigma_3 X^\dagger \sigma_3 = \mathbb{1}, \quad (\text{B13})$$

where $\mathbb{1}$ stands now for the composed identity matrix, i.e., the RHS of Eq. (B11). The matrix representation (B13) is very convenient. For example, from this equation we have $X^{-1} = \sigma_3 X^\dagger \sigma_3$, and

$$\begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} = \sigma_3 X^\dagger \sigma_3 \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & -V^T \\ -V^\dagger & U^T \end{pmatrix} \begin{pmatrix} \hat{a} \\ \hat{a}^\dagger \end{pmatrix},$$

which reads in usual notations

$$\hat{\alpha}_f = \sum_v (u_{vf}^* \hat{a}_v - v_{vf} \hat{a}_v^\dagger),$$

$$\hat{\alpha}_f^\dagger = \sum_v (u_{vf} \hat{a}_v^\dagger - v_{vf}^* \hat{a}_v).$$

This equation together with the commutation relations leads to

$$\sum_v (u_{vf}^* u_{vf'} - v_{vf} v_{vf'}^*) = \delta(f - f'),$$

$$\sum_v (v_{vf} u_{vf'}^* - u_{vf}^* v_{vf'}) = 0,$$

which is nothing else but the matrix equation $X^\dagger \sigma_3 X \sigma_3 = \mathbb{1}$, resulting from Eq. (B13).

Employing the idea of Ref. [65], in which the Hartree-Fock-Bogoliubov method for Fermi systems was developed, we define the matrix K with the help of the notations (B10) and (B12)

$$K = X^\dagger \sigma_3 \sigma_+ X \sigma_3 = \begin{pmatrix} \mathbb{1} + F^* & -\Phi \\ \Phi^* & -F \end{pmatrix}.$$

Due to Eq. (B13) and the relation $(\sigma_+)^2 = \sigma_+$ we have $K^2 = K$. Rewriting the latter equation in terms of the matrix F and Φ , we obtain two independent relations

$$\Phi^* \Phi = F + F^2, \quad (\text{B14})$$

$$F^* \Phi = \Phi F, \quad (\text{B15})$$

which read in components

$$\sum_f \Phi^*(f_1, f) \Phi(f, f_2) = \sum_f F(f_1, f) F(f, f_2) + F(f_1, f_2), \quad (\text{B16})$$

$$\sum_f F(f, f_1) \Phi(f, f_2) = \sum_f \Phi(f_1, f) F(f, f_2). \quad (\text{B17})$$

By using these equations, Eqs. (B3) and (B4), and the definition $\hat{\vartheta}(x) = \sum_v \hat{a}_v \phi_v(x)$, one can rewrite Eqs. (B16) and (B17) in the coordinate representation

$$\begin{aligned} & \int dx \langle \hat{\vartheta}^\dagger(x_1) \hat{\vartheta}^\dagger(x) \rangle \langle \hat{\vartheta}(x) \hat{\vartheta}(x_2) \rangle = \langle \hat{\vartheta}^\dagger(x_1) \hat{\vartheta}(x_2) \rangle \\ & + \int dx \langle \hat{\vartheta}^\dagger(x_1) \hat{\vartheta}(x) \rangle \langle \hat{\vartheta}^\dagger(x) \hat{\vartheta}(x_2) \rangle, \quad (\text{B18}) \\ & \int dx \langle \hat{\vartheta}^\dagger(x) \hat{\vartheta}(x_1) \rangle \langle \hat{\vartheta}(x) \hat{\vartheta}(x_2) \rangle \\ & = \int dx \langle \hat{\vartheta}(x_1) \hat{\vartheta}(x) \rangle \langle \hat{\vartheta}^\dagger(x) \hat{\vartheta}(x_2) \rangle. \quad (\text{B19}) \end{aligned}$$

If the condensate depletion is small, one can neglect the second term in the RHS of Eq. (B18), which is of the next order. Thus, we obtain the expression

$$\langle \hat{\vartheta}^\dagger(x_1) \hat{\vartheta}(x_2) \rangle \approx \int dx \langle \hat{\vartheta}^\dagger(x_1) \hat{\vartheta}^\dagger(x) \rangle \langle \hat{\vartheta}(x) \hat{\vartheta}(x_2) \rangle. \quad (\text{B20})$$

Note that Eq. (B19) turns into identity in the approximation (B20), and the same is valid for Eqs. (B15) and (B17).

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