Conserving and gapless approximations for an inhomogeneous Bose gas at finite temperatures

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We derive and discuss the equations of motion for the condensate and its fluctuations for a dilute, weakly interacting Bose gas in an external potential within the self-consistent Hartree-Fock-Bogoliubov (HFB) approximation. Account is taken of the depletion of the condensate and the anomalous Bose correlations, which are important at finite temperatures. We give a critical analysis of the self-consistent HFB approximation in terms of the Hohenberg-Martin classification of approximations (conserving vs gapless) and point out that the Popov approximation to the full HFB gives a gapless single-particle spectrum at all temperatures. The Beliaev second-order approximation is discussed as the spectrum generated by functional differentiation of the HFB single-particle Green's function. We emphasize that the problem of determining the excitation spectrum of a Bose-condensed gas (homogeneous or inhomogeneous) is difficult because of the need to satisfy several different constraints.

I. INTRODUCTION

The recent observation[1] of Bose condensation in atomic gases trapped in an external potential well has focused attention on the excitation spectrum of an inhomogeneous weakly interacting Bose-condensed gas at finite temperatures. Until very recently, this excitation spectrum was only addressed indirectly in the course of calculating[2,3] the local density $n(\mathbf{r})$ and local condensate density $n_c(\mathbf{r})$.

The excitation spectrum of a Bose system is very dependent on the subtle dynamical correlations induced by the Bose condensate.[4] In particular, one must calculate the single-particle and density-fluctuation spectrum in a consistent manner to ensure that they are identical, as they must be in a Bose-condensed system. In general, self-energy energy approximations which lead to a single-particle spectrum without an energy gap in the long-wavelength limit are not consistent with a density-fluctuation spectrum which satisfies conservation laws (or the corresponding sum rules).

A major purpose of this paper is to point out that a useful way of understanding various approximations for the excitations in a spatially nonuniform Bose gas is provided by the kind of analysis developed in the early 1960's for a spatially uniform Bose gas and codified in the well-known paper by Hohenberg and Martin.[4] It is based on distinguishing ''conserving'' vs ''gapless'' approximations and the key role played by the Hugenholtz-Pines theorem.

We use this classification to examine the equations of motion for a nonuniform condensate and its excited states in the finite-temperature Hartree-Fock-Bogoliubov (HFB) approximation, as well as simpler approximations discussed in the literature. An approximate version of the HFB due to Popov[5,6] gives a simple gapless approximation for the single-particle spectrum below the transition (we do not discuss the critical region very near $T_{\rm BE}$) but also reduces to the $T=0$ Bogoliubov approximation discussed by Fetter[7] for a nonuniform gas. We also sketch the procedure[4,8] for using the HFB approximation for the single-particle self-energies to generate by functional differentiation a density-fluctuation spectrum which is gapless in the long-wavelength limit. This can be shown to be identical to Beliaev's second-order approximation for the single-particle spectrum[9] at all temperatures.

The emphasis in this paper is on the formal structure of various kinds of approximations and how to assess their validity, using the HFB approximation as a specific example. Our results in (8) and (23) should provide a platform for future numerical calculations of the HFB excitation spectrum of an inhomogeneous Bose gas at $T\neq 0$, of the kind recently discussed by Edwards *et al.*[10] and Fetter[11] using the Bogoliubov approximation at $T=0$.[7] However, as we emphasize in the final section, the question of what are the ''correct'' excitations in a dilute weakly interacting Bose gas at finite temperatures is not a simple one. It requires the full apparatus of many-body theory.

II. HARTREE-FOCK-BOGOLIUBOV APPROXIMATION

Our starting point is the exact Heisenberg equation of motion[12,13] for the Bose field operator $\hat{\psi}(\mathbf{r})$

$$i\frac{\partial\hat{\psi}(\mathbf{r},t)}{\partial t}=\left(-\frac{\nabla^2}{2m}+U_{\rm ex}(\mathbf{r})-\mu\right)\hat{\psi}(\mathbf{r},t)+g\,\hat{\psi}^{\dagger}(\mathbf{r},t)\,\hat{\psi}(\mathbf{r},t)\,\hat{\psi}(\mathbf{r},t), \tag{1}$$

where we have assumed a short-range interaction $v(\mathbf{r}-\mathbf{r}')=g\,\delta(\mathbf{r}-\mathbf{r}')$ between the atoms. (In the s-wave approximation, which is adequate for the very dilute gases of interest, one has $g=4\pi a/m$.) We assume the atoms are trapped in a static external potential $U_{\rm ex}(\mathbf{r})$. Separating out the condensate part in the usual fashion,[9,12] we have

$$\hat{\psi}(\mathbf{r},t)=\Phi(\mathbf{r})+\tilde{\psi}(\mathbf{r},t), \tag{2}$$

where $\Phi(\mathbf{r})\equiv\langle\hat{\psi}(\mathbf{r},t)\rangle=\langle\hat{\psi}(\mathbf{r})\rangle$ plays the role of a spatially varying macroscopic Bose field. The thermal average in (2) and elsewhere is the usual anomalous average appropriate to a Bose broken symmetry.[4] Using (2), the interaction term in (1) can be written out in the form

$$\hat{\psi}^\dagger\hat{\psi}\hat{\psi}=|\Phi|^2\Phi+2|\Phi|^2\tilde{\psi}+\Phi^2\tilde{\psi}^\dagger+\Phi^*\tilde{\psi}\tilde{\psi}+2\Phi\tilde{\psi}^\dagger\tilde{\psi}+\tilde{\psi}^\dagger\tilde{\psi}\tilde{\psi}. \tag{3}$$

We treat the last term in (3) in the self-consistent mean-field approximation, namely

$$\tilde{\psi}^\dagger(\mathbf{r},t)\tilde{\psi}(\mathbf{r},t)\tilde{\psi}(\mathbf{r},t)\simeq 2\langle\tilde{\psi}^\dagger(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle\tilde{\psi}(\mathbf{r},t)+\langle\tilde{\psi}(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle\tilde{\psi}^\dagger(\mathbf{r},t), \tag{4}$$

and then (3) reduces to

$$\begin{aligned}\hat{\psi}^\dagger(\mathbf{r},t)\hat{\psi}(\mathbf{r},t)\hat{\psi}(\mathbf{r},t)=&|\Phi(r)|^2\Phi(\mathbf{r})\\&+2[|\Phi(\mathbf{r})|^2+\langle\tilde{\psi}^\dagger(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle]\tilde{\psi}(\mathbf{r},t)\\&+[\Phi^2(\mathbf{r})+\langle\tilde{\psi}(\mathbf{r})\tilde{\psi}(\mathbf{r}\rangle]\tilde{\psi}^\dagger(\mathbf{r},t)\\&+2\Phi(\mathbf{r})\tilde{\psi}^\dagger(\mathbf{r},t)\tilde{\psi}(\mathbf{r},t)\\&+\Phi^*(\mathbf{r})\tilde{\psi}(\mathbf{r},t)\tilde{\psi}(\mathbf{r},t).\end{aligned} \tag{5}$$

For the zero-range interaction we are considering, the Hartree and Fock (exchange) terms are identical. This is the origin of the factor of 2 in (4), (5) and subsequent equations.

The time independent, spatially inhomogeneous Bose order parameter $\Phi(\mathbf{r})$ is given directly by taking an average over (1),

$$\left(-\frac{\nabla^2}{2m}+U_{\rm ex}(\mathbf{r})-\mu\right)\Phi(\mathbf{r})+g\langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle=0. \tag{6}$$

The time dependence cancels out in the last term using the cyclic invariance of the trace. Taking the anomalous average of (5), the linear terms in $\tilde{\psi}(\mathbf{r},t)$ vanish since $\langle\tilde{\psi}(\mathbf{r},t)\rangle=\langle\tilde{\psi}(\mathbf{r})\rangle=0$ and we are left with

$$\langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle=|\Phi(\mathbf{r})|^2\Phi(\mathbf{r})+2\Phi(\mathbf{r})\langle\tilde{\psi}^\dagger(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle+\Phi^*(\mathbf{r})\langle\tilde{\psi}(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle. \tag{7}$$

Using this in (6), we find

$$\left(-\frac{\nabla^2}{2m}+U_{\rm ex}(\mathbf{r})-\mu\right)\Phi(\mathbf{r})+g[n_c(\mathbf{r})+2\tilde{n}(\mathbf{r})]\Phi(\mathbf{r})+g\tilde{m}(\mathbf{r})\Phi^*(\mathbf{r})=0, \tag{8}$$

where we have introduced the local densities:

$$\begin{aligned}n_c(\mathbf{r})&\equiv|\Phi(\mathbf{r})|^2,\\\tilde{n}(\mathbf{r})&\equiv\langle\tilde{\psi}^\dagger(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle,\\\tilde{m}(\mathbf{r})&\equiv\langle\tilde{\psi}(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle.\end{aligned} \tag{9}$$

We note that (8) only reduces to a closed (nonlinear) equation for $\Phi(\mathbf{r})$ when both $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$ are neglected (i.e., in the Bogoliubov approximation.[7]) In the case of a spatially uniform Bose gas $[U_{\rm ex}(\mathbf{r})\to 0]$, all the functions in (9) become constant, independent of position.

The excitations of the condensate are described by $\tilde{\psi}(\mathbf{r},t)$ in (2) and are given by the exact equation of motion

$$i\frac{\partial\tilde{\psi}(\mathbf{r},t)}{\partial t}=\left[-\frac{\nabla^2}{2m}+U_{\rm ex}(\mathbf{r})-\mu\right]\tilde{\psi}(\mathbf{r},t)+g[\hat{\psi}^\dagger(\mathbf{r},t)\hat{\psi}(\mathbf{r},t)\hat{\psi}(\mathbf{r},t)-\langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle]. \tag{10}$$

This follows from subtracting (6) from (1). Consistent with our mean-field derivation of (8), the quadratic terms in the last line of (5) are treated in a mean-field approximation, i.e., we use

$$\begin{aligned}\tilde{\psi}^\dagger(\mathbf{r},t)\tilde{\psi}(\mathbf{r},t)&\simeq\langle\tilde{\psi}^\dagger(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle,\\\tilde{\psi}(\mathbf{r},t)\tilde{\psi}(\mathbf{r},t)&\simeq\langle\tilde{\psi}(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle.\end{aligned} \tag{11}$$

With (11), the last term in (10) is given by

$$\hat{\psi}^\dagger(\mathbf{r},t)\hat{\psi}(\mathbf{r},t)\hat{\psi}(\mathbf{r},t)-\langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle\simeq 2\langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle\tilde{\psi}(\mathbf{r},t)+\langle\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle\tilde{\psi}^\dagger(\mathbf{r},t). \tag{12}$$

Using (12), (10) reduces to

$$i\frac{\partial\tilde{\psi}(\mathbf{r},t)}{\partial t}=\left(-\frac{\nabla^2}{2m}+U_{\rm ex}(\mathbf{r})-\mu\right)\tilde{\psi}(\mathbf{r},t)+2gn(\mathbf{r})\tilde{\psi}(\mathbf{r},t)+gm(\mathbf{r})\tilde{\psi}^\dagger(\mathbf{r},t), \tag{13}$$

where the self-consistent densities are defined by [see (9)]

$$n(\mathbf{r})\equiv\langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle=|\Phi(\mathbf{r})|^2+\langle\tilde{\psi}^\dagger(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle\equiv n_c(\mathbf{r})+\tilde{n}(\mathbf{r}), \tag{14}$$

$$m(\mathbf{r})\equiv\langle\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle=\Phi^2(\mathbf{r})+\langle\tilde{\psi}(\mathbf{r})\tilde{\psi}(\mathbf{r})\rangle\equiv\Phi^2(\mathbf{r})+\tilde{m}(\mathbf{r}). \tag{15}$$

One can easily derive the analogous equation of motion for $\tilde{\psi}^\dagger(\mathbf{r},t)$.

The coupled equations of motions given by (8) and (13) correspond to the Hartree-Fock-Bogoliubov (HFB) approximation. One can derive the same or similar results[3] by a variety of ways but the above approach has the advantage when one is interested in the excitations since it is easy to relate these equations of motion to a more general Green's functions[4,8,9] formulation discussed in Sec. III.

The preceding derivation of (8) and (13) is equivalent to the grand canonical Hamiltonian

$$\hat{K}\equiv\hat{H}-\mu\hat{N}=\int d\mathbf{r}\hat{\psi}^\dagger(\mathbf{r})\left[-\frac{\nabla^2}{2m}+U_{\rm ex}(\mathbf{r})-\mu\right]\hat{\psi}(\mathbf{r})+\frac{g}{2}\int d\mathbf{r}\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}) \tag{16}$$

being treated using a self-consistent quadratic approximation. Expanding the field operators in this expression using (2), one finds after a little algebra[14]

$$\hat{K}_{\rm HFB}=\int d\mathbf{r}\Phi^*(\mathbf{r})\left[\hat{T}(\mathbf{r})+\frac{1}{2}gn_c(\mathbf{r})\right]\Phi(\mathbf{r}) + \int d\mathbf{r}\tilde{\psi}^\dagger(\mathbf{r})\hat{\mathscr{L}}\tilde{\psi}(\mathbf{r})+\frac{g}{2}\int d\mathbf{r}m(\mathbf{r})\tilde{\psi}^\dagger(\mathbf{r})\tilde{\psi}^\dagger(\mathbf{r}) + \frac{g}{2}\int d\mathbf{r}m^*(\mathbf{r})\tilde{\psi}(\mathbf{r})\tilde{\psi}(\mathbf{r}), \tag{17}$$

where $\hat{\mathscr{L}}\equiv\hat{T}(\mathbf{r})+2gn(\mathbf{r})$, with

$$\hat{T}(\mathbf{r})\equiv-\frac{\nabla^2}{2m}+U_{\rm ex}(\mathbf{r})-\mu. \tag{18}$$

The coefficients of the linear terms in $\tilde{\psi},\tilde{\psi}^\dagger$ in (17) can be shown to vanish by using the fact that $\Phi(\mathbf{r})$ is given by the solution of (8). In going from (16) to (17), the *only* approximation involves how we treat the terms cubic and quartic in $\tilde{\psi}$ and $\tilde{\psi}^\dagger$, namely (all quantities depend on $\mathbf{r}$)

$$\hat{K}_3\equiv g\int d\mathbf{r}[\Phi^*\tilde{\psi}^\dagger\tilde{\psi}\tilde{\psi}+\Phi\tilde{\psi}^\dagger\tilde{\psi}^\dagger\tilde{\psi}] \simeq g\int d\mathbf{r}[2\tilde{n}\Phi^*+\tilde{m}^*\Phi]\tilde{\psi} + g\int d\mathbf{r}[2\tilde{n}\Phi+\tilde{m}\Phi^*]\tilde{\psi}^\dagger, \tag{19}$$

$$\hat{K}_4\equiv\frac{g}{2}\int d\mathbf{r}\tilde{\psi}^\dagger\tilde{\psi}^\dagger\tilde{\psi}\tilde{\psi}\simeq\frac{g}{2}\int d\mathbf{r}[4\tilde{n}\tilde{\psi}^\dagger\tilde{\psi}+\tilde{m}^*\tilde{\psi}\tilde{\psi}+\tilde{m}\tilde{\psi}^\dagger\tilde{\psi}^\dagger]. \tag{20}$$

That is, within the HFB mean-field approximation, $\hat{K}_3$ is linear in $\tilde{\psi},\tilde{\psi}^\dagger$ while $\hat{K}_4$ is quadratic in $\tilde{\psi},\tilde{\psi}^\dagger$. We note that the coefficients in (19) and (20) involve either $\tilde{n}(\mathbf{r})$ or $\tilde{m}(\mathbf{r})$.

One can easily diagonalize (17) by using the linear transformation

$$\tilde{\psi}(\mathbf{r})=\sum_j\,(u_j(\mathbf{r})\hat{\alpha}_j-v_j^*(r)\hat{\alpha}_j^\dagger), \qquad \tilde{\psi}^\dagger(r)=\sum_j\,(u_j^*(\mathbf{r})\hat{\alpha}_j^\dagger-v_j(r)\hat{\alpha}_j), \tag{21}$$

where $\hat{\alpha}_j$ and $\hat{\alpha}_j^\dagger$ are annihilation and creation operators satisfying the usual Bose commutation relations. One can show that (17) reduces to[15]

$$\hat{K}_{\rm HFB}=\int d\mathbf{r}\Phi^*(\mathbf{r})\left[\hat{T}(\mathbf{r})+\frac{1}{2}g|\Phi(\mathbf{r})|^2\right]\Phi(\mathbf{r}) -\sum_j\,E_j\int d\mathbf{r}|v_j(\mathbf{r})|^2+\sum_j\,E_j\hat{\alpha}_j^\dagger\hat{\alpha}_j, \tag{22}$$

if the c-number functions $u_j(\mathbf{r})$ and $v_j(\mathbf{r})$ are given by the solutions of the coupled HFB eigenvalue equations

$$\hat{\mathscr{L}}u_j(\mathbf{r})-gm(\mathbf{r})v_j(\mathbf{r})=E_ju_j(r), \qquad \hat{\mathscr{L}}v_j(\mathbf{r})-gm^*(\mathbf{r})u_j(\mathbf{r})=-E_jv_j(r). \tag{23}$$

Here the operator $\hat{\mathscr{L}}$ is defined before (18) and $m(\mathbf{r})$ is defined in (15). One can also derive the same results working directly with the equation of motion (13) and its Hermitian conjugate. In particular, one may easily verify that

$$\tilde{\psi}(\mathbf{r},t)=\sum_j\,[u_j(\mathbf{r})\hat{\alpha}_je^{-iE_jt}-v_j^*(\mathbf{r})\hat{\alpha}_j^\dagger e^{iE_jt}], \qquad \tilde{\psi}^\dagger(\mathbf{r},t)=\sum_j\,[u_j^*(r)\hat{\alpha}_j^\dagger e^{iE_jt}-v_j(\mathbf{r})\hat{\alpha}_je^{-iE_jt}], \tag{24}$$

solves (13) (and its adjoint) if u_j, v_j, and E_j satisfy the generalized "Bogoliubov" equations given in (23). The results in (22) and (23) effectively reduce the problem to a gas of noninteracting Bose quasiparticles with an energy spectrum given by E_j.

We note that with (21), one easily can derive expressions for $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$ in (9) in terms of the self-consistent solutions of the coupled equations (23), namely

$$\tilde{n}(\mathbf{r})=\sum_j\,\{[|u_i(\mathbf{r})|^2+|v_j(\mathbf{r})|^2]N_0(E_j)+|v_j(r)|^2\}, \qquad \tilde{m}(\mathbf{r})=-\sum_j\,u_j(\mathbf{r})v_j^*(\mathbf{r})[2N_0(E_j)+1], \tag{25}$$

where $N_0(E)$ is the Bose distribution for the quasiparticle excitations

$$\langle\hat{\alpha}_j^\dagger\hat{\alpha}_j\rangle_{\rm HFB}=\frac{1}{e^{\beta E_j}-1}\equiv N_0(E_j). \tag{26}$$

One must solve the coupled HFB equations (23) and the condensate equation (8) using self-consistent values of $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$, given by (25), and $n_c(\mathbf{r})\equiv|\Phi(\mathbf{r})|^2$. Computationally, solving this set of coupled equations is similar to solving the simpler $T=0$ Bogoliubov approximation.[7,10,11] The major difference is that (8) is no longer a closed equation for $\Phi(\mathbf{r})$ but involves the self-consistent diagonal and off-diagonal densities, $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$. The latter depend on the excited states given by the solutions of the self-consistent coupled equations in (23).

It is useful to summarize how one would solve the HFB equations given by (8) and (23), for a given anisotropic parabolic potential-well trap and temperature:

(a) First calculate $n_0(\mathbf{r})=|\Phi(\mathbf{r})|^2$ and $\tilde{n}(\mathbf{r})$ for a noninteracting gas ($g=0$). In this case, the off-diagonal correlation function $\tilde{m}(\mathbf{r})=0$.

(b) Use these noninteracting gas results in (23) to solve for u_j, v_j, and E_j. With these excited states, one can calculate $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$ from (25) and use these in (8) to find $\Phi(\mathbf{r})$.

(c) Iterate the above procedure to self-consistency.

Before discussing the implications and validity of (8) and (13), it is useful to relate these results to simpler approximations given in the literature on inhomogeneous dilute Bose

gases. We recall that (13) and its adjoint are equivalent to (23) and (24). If we set both $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$ to zero, (8) reduces to the well-known Gross-Pitaevskii approximation, where $\Phi(\mathbf{r})$ is given by a closed nonlinear Schrödinger equation.[16] Neglecting $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$ in (13) or (23) leads to the standard Bogoliubov approximation. This simplified version of Eqs. (8) and (13) has been derived and discussed in detail by Fetter[7] (see also Refs. 10 and 11). Since one is ignoring the noncondensate atoms ($\tilde{n}=0$), this approximation is only appropriate at $T\simeq 0$, where most of the atoms are in the condensate ($n_c \simeq n$). Note that in the Bogoliubov approximation, the cubic terms ($\hat{K}_3$) and quartic terms ($\hat{K}_4$) in (19) and (20) are omitted completely.

The next level of approximating (8) and (23) would be to keep $\tilde{n}(\mathbf{r})$ but neglect the anomalous density $\tilde{m}(\mathbf{r})$ as being small compared to both $\tilde{n}(\mathbf{r})$ and $n_0(\mathbf{r})$. This approximation has been used by Popov[5] (in a homogeneous gas) to discuss the finite-temperature region close to the Bose-Einstein transition. This Popov approximation[6] formally reduces to the Bogoliubov approximation at $T=0$, where $\tilde{n}$ also becomes negligible. As we shall see in Sec. III, it leads to a gapless spectrum, in contrast with the full HFB. Thus omitting $\tilde{m}(\mathbf{r})$ but calculating $\tilde{n}(\mathbf{r})$ in a self-consistent way seems to give a reasonable first approximation for the excitation spectrum in Bose gases at *all* temperatures.

The calculation of $\tilde{n}(\mathbf{r})$ and $n_c(\mathbf{r})$ given by Goldman *et al.*[2] involved equations equivalent to (8) with $\tilde{m}(\mathbf{r})=0$ and to (23) with $m(\mathbf{r})=0$. This somewhat *ad hoc* approximation is equivalent to putting $v_j(\mathbf{r})=0$ in (23). This simplified version of (23) has been justified in Refs. 2 and 3 as being adequate for the purpose of calculating $\tilde{n}(\mathbf{r})$ and $n_0(\mathbf{r})$ at temperatures just below $T_{\rm BE}$, even if it does not lead to a very good approximation for the excitation spectrum.

III. CONSERVING VS GAPLESS APPROXIMATIONS

We now turn to a discussion of the HFB equations given by (8) and (13). The general problem of finding the excitation frequencies in a homogeneous weakly interacting Bose-condensed gas was exhaustively studied and various approximations were classified in a famous paper by Hohenberg and Martin (see, in particular, Sec. VI of Ref. 4). Any approximation put forward in the study of an inhomogeneous Bose gas can be usefully analyzed by examining its implications in the corresponding homogeneous case.

For interacting Bose-condensed systems, it is convenient to formulate the discussion in terms of Green's functions.[4,12] A key role is played by the 2×2 matrix single-particle Green's function, defined as

$$G_1(1,1')=-i\langle T\hat{\Psi}(1)\hat{\Psi}^\dagger(1')\rangle, \tag{27}$$

where

$$\hat{\Psi}(1)\equiv\begin{pmatrix}\hat{\psi}(1)\\ \hat{\psi}^\dagger(1)\end{pmatrix};\quad \Psi^\dagger(1)\equiv(\hat{\psi}^\dagger(1),\psi(1)) \tag{28}$$

and 1 represents $\mathbf{r},t$. Writing out the 2×2 matrix in (27) explicitly, we have

$$G_{\alpha\beta}(1,1')=-\begin{pmatrix} i\langle T\hat{\psi}(1)\hat{\psi}^\dagger(1')\rangle & i\langle T\hat{\psi}(1)\hat{\psi}(1')\rangle \\ i\langle T\hat{\psi}^\dagger(1)\hat{\psi}^\dagger(1')\rangle & i\langle T\hat{\psi}^\dagger(1)\hat{\psi}(1')\rangle\end{pmatrix}. \tag{29}$$

Separating out the Bose condensate part of the field operator as in (2), (29) naturally splits into two parts

$$G_{\alpha\beta}(1,1')=\tilde{G}_{\alpha\beta}(1,1')+G_{(1/2)\alpha}(1)G^\dagger_{(1/2)\beta}(1'), \tag{30}$$

where the condensate Green's function is described by

$$\hat{G}_{1/2}(1)\equiv\sqrt{-i}\langle\hat{\Psi}(1)\rangle=\sqrt{-i}\begin{pmatrix}\Phi(1)\\ \Phi^*(1)\end{pmatrix} \tag{31}$$

$$\hat{G}^\dagger_{1/2}(1)\equiv\sqrt{-i}\langle\hat{\Psi}^\dagger(1)\rangle=\sqrt{-i}(\Phi^*(1),\Phi(1)), \tag{32}$$

and $\tilde{G}_{\alpha\beta}(1,1')$ is identical to (29) except that it involves the noncondensate part of the field operators ($\tilde{\psi}$ and $\tilde{\psi}^\dagger$). The signature of a Bose-condensed interacting system is the appearance of anomalous correlation functions such as $\Phi(1)=\langle\hat{\psi}(1)\rangle$ and $\tilde{G}_{12}(1,1')=-i\langle T\tilde{\psi}(1)\tilde{\psi}(1')\rangle$.

A very convenient way of generating the equations of motion for $\tilde{G}_1(1,1')$ and $\hat{G}_{1/2}(1)$ is to use functional differentiation with respect to external fields.[4] For homogeneous systems in thermal equilibrium, it is customary to set these generating fields to zero at the end of the calculation. However, in the context of the newly observed Bose-condensed gases,[1] these external fields are of direct physical relevance, playing the role of the static external trapping potential as well as time-dependent external perturbations.[10,11] In this regard, the general formalism developed in Ref. 4 is particularly useful. The general equations of motion for $\tilde{G}_1(1,1')$ and $\hat{G}_{1/2}(1)$ are given by (2.6) and (2.7) of Ref. 8. If we only include a *static* external potential, the equation of motion for $\tilde{G}_1(1,1')$ is

$$\left[i\tau^{(3)}_{\alpha\beta}\frac{\partial}{\partial t}-\hat{T}(\mathbf{r})\delta_{\alpha\beta}\right]\tilde{G}_{\beta\alpha'}(1,1')$$

$$=\delta(1-1')\delta_{\alpha\alpha'}+\Sigma_{\alpha\beta}(1,\overline{2})\tilde{G}_{\beta\alpha'}(\overline{2},1'), \tag{33}$$

where $\tau^{(3)}=\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)$ and the single-particle operator $\hat{T}(\mathbf{r})$ is defined in (18). Here, repeated Greek indices are summed and a bar represents the usual integration over $\mathbf{r},t$. This Dyson-Beliaev equations in (33) for the single-particle Green's functions in a Bose-condensed system depends on the 2×2 matrix self-energy $\Sigma_{\alpha\beta}(1,1')$ in addition to the chemical potential μ. The analogous equation of motion for the two components of $\hat{G}_{1/2}$ is given by (for a static external field)

$$-\hat{T}(\mathbf{r})G_{1/2\alpha}(\mathbf{r})=\sqrt{-i}\,\eta_\alpha(\mathbf{r}). \tag{34}$$

Here we have introduced the condensate "source function" $\eta_\alpha(\mathbf{r})$, which itself is a functional of $\hat{G}_{1/2}$ and $\tilde{G}_1$. Writing (34) more explicitly, it corresponds to

$$\left[-\frac{\nabla^2}{2m}+U_{\rm ex}(\mathbf{r})-\mu\right]\Phi(\mathbf{r})=-\eta_1(\mathbf{r}). \tag{35}$$

One can now define what a "conserving" approximation is, namely that there exists a functional $\Phi[\hat{G}_{1/2},\tilde{G}_1]$ of the correlation functions $\hat{G}_{1/2}$ and $\tilde{G}_1$ such that the self-energy and the condensate source functions are given by

$$\frac{\delta\Phi[\hat{G}_{1/2},\tilde{G}_1]}{\delta\tilde{G}_1(1,1')}=\hat{\Sigma}(1,1'),$$
$$\frac{1}{2\sqrt{-i}}\frac{\delta\Phi[\hat{G}_{1/2},\tilde{G}_1]}{\delta\hat{G}^{\dagger}_{1/2}(1)}=\hat{\eta}(1). \tag{36}$$

Martin and De Dominicis[17] have proven that if such a functional Φ exists, the two-particle Green's functions generated by functional differentiation of $G_1(1,1')$ [given by (29) – (32)] with respect to a time-dependent, spatially varying external field are *guaranteed* to satisfy the usual conservation laws.[18] The HFB approximation discussed in Sec. II can be shown to be an example of such a conserving approximation. Using Eq. (6.42) of Ref. 4, one can easily verify that

$$\hat{\Sigma}_{\rm HFB}(1,1')=g\begin{pmatrix}2n(\mathbf{r}) & m(\mathbf{r})\\ m^*(\mathbf{r}) & 2n(\mathbf{r})\end{pmatrix}\delta(1-1') \tag{37}$$

and

$$\hat{\eta}_{\rm HFB}(1)=g\begin{pmatrix}n(\mathbf{r})+\tilde{n}(\mathbf{r}), & \tilde{m}(\mathbf{r})\\ \tilde{m}^*(\mathbf{r}), & n(\mathbf{r})+\tilde{n}(\mathbf{r})\end{pmatrix}\begin{pmatrix}\Phi(\mathbf{r})\\ \Phi^*(\mathbf{r})\end{pmatrix}. \tag{38}$$

When substituted into (33) and (34), one finds results equivalent to (23) and (8), respectively. This HFB approximation is often called the Girardeau-Arnowitt approximation in the Bose gas literature.[4] Solving (33) using (37), we arrive at the coupled equations for $\tilde{G}_{11}$ and $\tilde{G}_{21}$,

$$\left[i\frac{\partial}{\partial t}-\hat{T}(\mathbf{r})-2gn(\mathbf{r})\right]\tilde{G}_{11}(1,1')-gm(\mathbf{r})\tilde{G}_{21}(1,1')=\delta(1-1'),$$
$$\left[-i\frac{\partial}{\partial t}-\hat{T}(\mathbf{r})-2gn(\mathbf{r})\right]\tilde{G}_{21}(1,1')-gm^*(\mathbf{r})\tilde{G}_{11}(1,1')=0. \tag{39}$$

This is the HFB generalization of the Bogoliubov approximation, the latter being given by (55.22) and (55.24) of Fetter and Walecka[12] for inhomogeneous systems. As expected, the structure of (39) is identical to (23).

The problem with a conserving approximation is that while the two-particle Green's functions [such as the density-response function $\chi_{nn}(1,1')$] are guaranteed to have a spectrum consistent with conservation laws such as the equation of continuity,[18] the single-particle spectrum of $\tilde{G}_1(1,1')$ which one starts with may have unphysical features. In particular, one is not ensured of a gapless spectrum for long-wavelength excitations. In homogeneous systems, such a gapless spectrum of $\tilde{G}_1(1,1')$ is guaranteed if the self-energies satisfy the Hugenholtz-Pines (HP) theorem, namely[4,19]

$$\mu=\Sigma_{11}(\mathbf{q}=0,\omega=0)-\Sigma_{12}(\mathbf{q}=0,\omega=0). \tag{40}$$

More generally, it can be proven that this theorem will be satisfied if the self-energies can be generated from the condensate source function according to[4]

$$\sqrt{-i}\frac{\delta\hat{\eta}(1)}{\delta\hat{G}_{1/2}(1')}=\hat{\Sigma}(1,1'). \tag{41}$$

Here $\hat{\eta}(1)$ is an explicit functional of $\hat{G}_{1/2}$ and implicitly through the dependence of $\tilde{G}_1$ on $\hat{G}_{1/2}$. Approximations for the self-energy consistent with (41) are referred to as "gapless" approximations. The HFB approximation for $\hat{\eta}(1)$ and $\hat{\Sigma}(1,1')$ do *not* satisfy (41), and as a consequence the HFB spectrum of $\tilde{G}_1(1,1')$ has a quasiparticle spectrum with a gap in the limit of long wavelengths.[4] In contrast, the simple Bogoliubov approximation[12] is a gapless approximation, as is the Beliaev second-order approximation.[9] Figures 4 and 5 of Ref. 4 give a convenient summary of conserving and gapless approximation for uniform Bose gases.

We can illustrate the above somewhat formal discussion by considering the HFB approximation for a uniform system [$U_{\rm ex}(\mathbf{r})\to 0$]. Using (38) in (35), or equivalently (8), we have [since $\Phi(\mathbf{r})=$ const]

$$-\mu\Phi+g(n+\tilde{n})\Phi+\tilde{m}\Phi^*=0, \tag{42}$$

and hence the HFB gives the following result for the chemical potential:[8]

$$\mu=g(n+\tilde{n}+\tilde{m}). \tag{43}$$

For a homogeneous system, where we have $\tilde{G}_{\alpha\beta}(1,1')=\tilde{G}_{\alpha\beta}(1-1')$, one can solve (39) by Fourier transformation.[14] The poles of $\tilde{G}_{\alpha\beta}(\mathbf{k},\omega)$ are easily found to be given by

$$E_k^2=\left(\frac{k^2}{2m}-\mu+2gn\right)^2-(gm)^2. \tag{44}$$

Making use of the HFB chemical potential μ given by (43), one sees that there is a finite energy gap at $k=0$,

$$E^2_{k=0}=g^2[n_c-\tilde{m}]^2-g^2[n_c+\tilde{m}]^2=4g^2|\tilde{m}|n_c, \tag{45}$$

where we recall that $\tilde{m}$ is negative [see (25)]. Clearly the HFB does not satisfy the HP theorem (40), since the latter relation gives

$$\mu=2gn-gm=g(n+\tilde{n}-\tilde{m}), \tag{46}$$

which differs from the HFB result in (43). Using (46) in (44) gives a gapless spectrum but this procedure is *ad hoc*. One is using a chemical potential which is not consistent with the equation of motion for $\hat{G}_{1/2}(1)$ or, equivalently, $\Phi(\mathbf{r})$.

At the end of Sec. II, we introduced several approximate versions of the HFB results. We can now discuss these approximations in terms of the excitation spectrum they lead to in the homogeneous case:

(a) "Bogoliubov" corresponds to setting $\tilde{m}=\tilde{n}=0$. Both (43) and (46) reduce to the same result $\mu=gn_c$ and hence the single-particle excitations are gapless. This is valid at zero temperature.

(b) "Popov" corresponds to setting $\tilde{m}=0$ but keeping $\tilde{n}$ finite. Both (43) and (46) reduce to $\mu=2gn-gn_c$ and hence the excitations are gapless. As discussed at the end of Sec. II, this gives a good approximation at all temperatures, with a phonon velocity $(gn_c(T)/m)^{1/2}$.

(c) In Goldman *et al.*,[2] the off-diagonal self-energies in (37) involving $m(\mathbf{r})$ are neglected but only $\tilde{m}(\mathbf{r})$ is neglected in the source term (38). The result is that (44)

reduces to $E_k = k^2/2m - \mu + 2gn$, while (43) reduces to $\mu = gn + g\tilde{n} = 2gn - gn_c$. Thus one obtains a spectrum $E_k = k^2/2m + gn_c$ with an energy gap. This approximation can be used for calculating $\tilde{n}$ and other thermodynamic quantities near $T_{\rm BE}$, where the thermally significant excitations have a large enough momentum that the spectrum $E_k = k^2/2m + gn_c$ is adequate.[20]

In the Popov approximation to the HFB [in which the anomalous density $\tilde{m}(r)$ is omitted], there is a special solution of the generalized Bogoliubov equations (23) corresponding to $u_0(\mathbf{r}) = v_0(\mathbf{r}) = \Phi(\mathbf{r})$ with $E_0 = 0$, where $\Phi(\mathbf{r})$ is a solution of (8) with $\tilde{m}(\mathbf{r}) = 0$. As with the simpler Bogoliubov approximation discussed by Fetter,[7,11] one sees in this case that the condensate wave function $\Phi(\mathbf{r})$ plays the role of the zero-energy single-particle mode and the fluctuations of the condensate associated with $\tilde{\psi}$ are described by all the higher energy modes $(E_i > 0)$. In contrast, within the full HFB, there is no zero energy solution of (23) corresponding to the solution $\Phi(\mathbf{r})$ of (8).

As we have noted above, conserving approximations for $\tilde{G}_1(1,1')$ and $\hat{G}_{1/2}(1)$ such as the HFB can be used to generate two-particle Green's functions which are guaranteed to satisfy conservation laws and related sum rules[4,17,18] and thus will lead to a gapless density-fluctuation spectrum. In addition, we recall that in the presence of a Bose broken symmetry, the single-particle and density-fluctuation correlation functions exhibit the same poles.[19] This fundamental feature holds for both uniform and nonuniform Bose systems, as can be seen, for example, from Eq. (6.38) of Hohenberg and Martin.[4] Thus by using the HFB single-particle matrix Green's function G_1 to generate the density-response function by functional differentiation, one is effectively generating an ''improved'' single-particle spectrum which will be gapless. In particular, as discussed on pp. 350–351 of Ref. 4, the HFB G_1 generates a density-response function which is found to be identical to Beliaev's second-order single-particle spectrum.[9] In the uniform case, this equivalence has been formally proven at *all* temperatures in a Bose-condensed gas by Cheung and Griffin (see Sec. IV of Ref. 8). The fact that this new spectrum is gapless follows from the fact that the Beliaev self-energies satisfy the HP relation in (40), with μ being given by the HFB result in (43).

The above procedure shows that the excitations given by the Beliaev second-order approximation is the correct generalization on the HFB excitation spectra. Such calculations involve evaluating the various bubble or polarization diagrams [see Eq. (2.30) of Ref. 8] which involve products of two HFB single-particle propagators $\tilde{G}_1$. However, at temperatures close enough to $T_{\rm BE}$, it is adequate to evaluate these polarization bubble diagrams using a simple particle-like spectrum such as used in Refs. 2 and 20.

Within a variational calculation, Bijlsma and Stoof[21] have recently obtained (for a uniform system) the equivalent of the Popov approximation as defined above, but with g replaced by the many-body t matrix calculated at finite temperature in the ladder diagram approximation. This extension and its relation to the full Beliaev second-order approximation will be discussed elsewhere.[22]

IV. CONCLUSIONS

Within the full Hartree-Fock-Bogoliubov approximation, we have given a simple derivation of the coupled equations of motion for the condensate $\Phi(\mathbf{r})$ and its excited states, as given by (8) and (23), respectively. In contrast with previous work which was variational in nature,[2,3] our derivation in Sec. II works directly with a mean-field approximation for the equation of motion for the condensate (Φ) and noncondensate $(\tilde{\psi})$ parts of the quantum field operator. This brings out the physics involved most clearly and has the advantage that one can make contact with the more general Green's function formulation[4,8] discussed in Sec. III. The self-consistent HFB has, of course, the advantage of being derivable variationally and thus the total energy is minimized even if the HFB excitations have certain deficiencies.

Because of the dynamical correlations induced by the Bose-broken symmetry, a consistent theory of excitations is surprisingly difficult to formulate even in a dilute Bose gas. This is already shown when one tries to improve the ''gapless'' Bogoliubov approximation by working with the ''conserving'' Hartree-Fock-Bogoliubov (HFB) approximation which is not ''gapless.'' Hohenberg and Martin[4] (HM) give a systematic discussion of this problem, introducing a classification of different approximations. In the present paper, we have emphasized the usefulness of the HM classification when dealing with inhomogeneous atomic Bose gases in an external potential well.[1] We have used it to examine the single-particle spectrum predicted by the full HFB,[3] as well as various simplifications of it which have been used in the literature.[2,5,7] In addition, the HFB has a special significance since it can be used to generate a density-response function by functional differentiation which turns out to have the same spectrum as the Beliaev second-order approximation[9] for the single-particle Green's functions at all temperatures below $T_{\rm BE}$.[8]

The reason that finding the ''correct'' excitation spectrum of a Bose-condensed gas is complicated is because it is difficult to simultaneously satisfy different requirements within a given approximation. The Hohenberg-Martin classification scheme we have used in Sec. III of this paper does not solve the problem of finding an approximation which is manifestly *both* gapless and consistent with conservation laws. An alternative approach which addresses this problem is based on the dielectric formalism (for a review, see Sec. 5.1 of Ref. 19). This is a diagrammatic procedure which builds in the close connection between the single-particle and density-response functions so that their excitation spectra are identical, with the conservation laws being incorporated through generalized Ward identities. This formalism[23] cuts across the HM classification and gives a procedure for choosing approximations which yield both a gapless elementary-excitation spectrum and response functions consistent with conservation laws (sum rules). In a future publication, we hope to discuss inhomogeneous Bose gases using this dielectric formalism approach.[23,19]

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