Comparison of gapless mean-field theories for trapped Bose-Einstein condensates

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We present two gapless mean-field theories for trapped Bose-Einstein condensates, and compare them to the better known Hartree-Fock-Bogoliubov (HFB)-Popov approach. The proposed theories are based on suitable inclusion of the simplest anomalous average of the Bose field operator. This leads to an effective interaction between two atoms which is both temperature and density dependent, as opposed to the HFB-Popov approach, for which it is constant. These theories are compared to the HFB-Popov approach for a trapped one-dimensional condensate of 2000 atoms. The density profiles and excitation frequencies of the proposed theories differ from the corresponding HFB-Popov ones by at most a few percent. [S1050-2947(98)12109-1]

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I. INTRODUCTION

The theoretical description of trapped Bose-Einstein condensed gases has so far relied heavily on the Hartree-Fock-Bogoliubov (HFB) mean-field approximation [1–3]. This theory takes account of the mean fields of both condensed and excited atoms, as well as the lowest order (or pair) anomalous average of the Bose field operator. This represents pair correlations between atoms and becomes crucial in the case of net attractive interactions (in which case it may lead to a competing BCS-like phase transition, as discussed in Ref. [4]). However, a limitation of the HFB approach was clear from the early days of its use, when it was shown that the theory predicted a gap in the single-particle excitation spectrum of homogeneous gases [2], in violation of Goldstone's theorem [5]. The simplest way to overcome this limitation of the HFB approach is to make the so-called Popov approximation [6–8], in which the anomalous average does not explicitly appear. The fact that the HFB-Popov theory is gapless (see, e.g., Ref. [8]) implies that it can be considered a better theory for the elementary excitations of Bose-Einstein condensates than the full HFB approach. The HFB-Popov theory has therefore been employed in a variety of calculations [9–11]. Indeed, the frequencies of elementary excitations calculated via the HFB-Popov theory are in excellent agreement with the experiments of Jin *et al.* [12] at reasonably low temperatures.

At higher temperatures, however, ($T>0.6T_c$, where T_c is the transition temperature), the theory appears to deviate from experimental results [10]. This is probably due to the inherent limitations of the HFB-Popov theory, namely, (i) it assumes that the condensate moves through a static thermal cloud [13–16], and (ii) it does not take into account the full effects of the medium on the interatomic collisions. Zaremba, Griffin, and Nikuni [17] discussed how to go beyond the approximation of a static thermal cloud and treat the coupled dynamics of condensed and excited atoms under the assumption of local thermodynamic equilibrium for the excited states. However, one would not expect this approach to be valid for the experiments of Ref. [12], where the thermal cloud is rather dilute.

In this paper we address the second of the above limitations of the HFB-Popov theory, and take into account some of the effects of the medium on the atomic collisions. As already argued elsewhere [13,14], the HFB-Popov theory does not deal adequately with the fact that collisions are taking place in the presence of other condensed and excited atoms. This has two effects on the colliding atoms: (i) the intermediate collisional states may be occupied, leading to a modification of the scattering amplitude via bosonic enhancement; and (ii) the spectrum of initial, intermediate, and final states is altered (i.e., the atoms participating in the collisions are not bare atoms, but dressed ones, or quasiparticles). The medium therefore modifies the effective interaction experienced by a pair of colliding atoms from its value in vacuum. The latter is often termed the two-body T matrix, and, for low-energy scattering, can be well approximated by the contact potential $V(\mathbf{r}-\mathbf{r}')=U_0\delta(\mathbf{r}-\mathbf{r}')$, where U_0 is given in terms of the binary s-wave scattering length a by $U_0=4\pi\hbar^2a/m$ [18]. However, the atomic interactions in the condensate cannot be completely described by this contact potential [19], because the scattering length is determined experimentally in dilute atomic gases in the absence of condensation [20]. Nonetheless, at $T=0$, these many-body effects are small, as they depend on the parameter n_0a^3, where n_0 is the condensate density [21].

The effects of the medium on a colliding pair lead to the replacement of the two-body T matrix by the many-body T matrix. A detailed discussion of the two-body and many-body T matrices, and their respective domains of validity, can be found in Refs. [13,14,22,23]. In this paper we propose (and briefly motivate) two novel mean-field theories which employ an approximation for the many-body T matrix, and therefore take part of the effects discussed above into account[1]. This is achieved by consideration of the anomalous averages of the Bose field operator, which leads to a gener-

[1]The issue of a generalized gapless theory has also been addressed in the early literature in a variety of approaches [24]. However, such methods have not yet facilitated explicit numerical results for condensate densities and excitation frequencies, and are harder to link to the more familiar HFB formalism.

alized effective interaction that is both temperature and density dependent. This effective interaction is shown to be consistent with analytical expressions in the homogeneous limit [13,23]. The predictions of the proposed theories are compared to those of other more elementary approaches (and in particular to the HFB-Popov theory) for trapped one-dimensional (1D) Bose-condensed assemblies of 2000 atoms. The modifications which are introduced over the HFB-Popov theory are found to be of the order of a few percent.

This paper is structured as follows: Secs. II and III describe and motivate the two mean-field theories. The numerical implementation of these theories in 1D systems is discussed in Sec. IV. The subsequent two sections analyze the predictions of the various theories and compare them to those of the HFB-Popov theory, with the main results summarized in Sec. VII. Finally, the Appendix establishes the link between our expression for the effective interaction in trapped gases, and known analytical results for the homogeneous gas.

II. GAPLESS MEAN-FIELD THEORIES

The self-consistent equations discussed in this paper can all be summarized by the generalized eigenvalue problem

$$\left\{ -\frac{\hbar^2\nabla_{\mathbf{r}}^2}{2m} + V_{\rm trap}(\mathbf{r}) - \mu + \tilde{U}_{\rm con}(\mathbf{r})|\psi(\mathbf{r})|^2 + 2\tilde{U}_{\rm exc}(\mathbf{r})\tilde{n}(\mathbf{r}) \right\} \psi(\mathbf{r}) = 0, \tag{1}$$

$$\hat{\mathcal{L}}(\mathbf{r})u_j(\mathbf{r}) + \tilde{U}_{\rm con}(\mathbf{r})\psi^2(\mathbf{r})v_j(\mathbf{r}) = \hbar\omega_j u_j(\mathbf{r}), \tag{2}$$

$$\hat{\mathcal{L}}(\mathbf{r})v_j(\mathbf{r}) + \tilde{U}_{\rm con}(\mathbf{r})[\psi^*(\mathbf{r})]^2 u_j(\mathbf{r}) = -\hbar\omega_j v_j(\mathbf{r}). \tag{3}$$

In these equations, the condensate wave function is denoted by $\psi(\mathbf{r})$, μ represents the chemical potential of the assembly, $u_j(\mathbf{r})$ and $v_j(\mathbf{r})$ are the usual Bogoliubov functions [25], and the Hermitian operator $\hat{\mathcal{L}}$ is defined by

$$\hat{\mathcal{L}}(\mathbf{r}) = -\frac{\hbar^2\nabla_{\mathbf{r}}^2}{2m} + V_{\rm trap}(\mathbf{r}) - \mu + 2\tilde{U}_{\rm con}(\mathbf{r})|\psi(\mathbf{r})|^2 + 2\tilde{U}_{\rm exc}(\mathbf{r})\tilde{n}(\mathbf{r}). \tag{4}$$

To model the interactions between trapped atoms in the most general manner, we have allowed them to interact with each other via different effective interactions, depending on whether they are both in the condensate [$\tilde{U}_{\rm con}(\mathbf{r})$] or not [$\tilde{U}_{\rm exc}(\mathbf{r})$]. The physical justification for such a distinction will be discussed shortly. The quantity $\tilde{n}(\mathbf{r})$ appearing in Eqs. (1)–(4) corresponds to the density profile of excited atoms, and is to be determined self-consistently [9] by a transformation to the quasiparticle basis [i.e., via Eq. (7)].

The above set of self-consistent equations is gapless, irrespective of the choice of potentials $\tilde{U}_{\rm con}(\mathbf{r})$ and $\tilde{U}_{\rm exc}(\mathbf{r})$ [26]. This follows from the fact that Eqs. (1)–(4) support a zero-frequency mode with $[u_0(\mathbf{r}), v_0(\mathbf{r})] = [\psi(\mathbf{r}), -\psi^*(\mathbf{r})]$. The three different theories to be compared in this paper (including the HFB-Popov theory) form special cases of the above set of equations, depending on the choice of $\tilde{U}_{\rm con}(\mathbf{r})$ and $\tilde{U}_{\rm exc}(\mathbf{r})$, as outlined below.

(i) The HFB-Popov theory corresponds to $\tilde{U}_{\rm con}(\mathbf{r}) = \tilde{U}_{\rm exc}(\mathbf{r}) = U_0$, where $U_0 = 4\pi\hbar^2 a/m$ is the usual dilute Bose gas effective interaction strength.

(ii) The first gapless theory ($G1$) is defined by $\tilde{U}_{\rm con}(\mathbf{r}) = \tilde{U}(\mathbf{r})$ and $\tilde{U}_{\rm exc}(\mathbf{r}) = U_0$, where $\tilde{U}(\mathbf{r}) = U_0[1 + \tilde{m}(\mathbf{r})/\psi^2(\mathbf{r})]$ and $\tilde{m}(\mathbf{r})$ represents the pair anomalous average [defined in Eq. (8)].

(iii) The second gapless theory ($G2$) is defined by $\tilde{U}_{\rm con}(\mathbf{r}) = \tilde{U}_{\rm exc}(\mathbf{r}) = \tilde{U}(\mathbf{r})$, with $\tilde{U}(\mathbf{r})$ as above.

We point out that both the $G1$ and $G2$ theories extend beyond the HFB approximation, and we shall show that they correspond to the two extreme approximations for the momentum dependence of the many-body T matrix. We also note that the full HFB theory cannot be written in the (gapless) form of Eqs. (1)–(4), because it does not treat all condensate-condensate interactions consistently [27]. In Sec. II we briefly discuss the physical origin of the theories described above.

III. MOTIVATION OF PROPOSED MEAN-FIELD THEORIES

The effective interaction $\tilde{U}(\mathbf{r})$ employed in both the $G1$ and $G2$ theories arises naturally in the time-independent Gross-Pitaevskii equation (QPE) for the condensate mean field $\psi(\mathbf{r})$. In the usual form of the HFB theory (see, e.g., Ref. [8]) based on the contact interaction $V(\mathbf{r}-\mathbf{r}') = U_0\delta(\mathbf{r}-\mathbf{r}')$, the condensate wave function is determined by

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V_{\rm trap}(\mathbf{r}) - \mu \right)\psi(\mathbf{r}) + U_0[|\psi(\mathbf{r})|^2 + 2\tilde{n}(\mathbf{r})]\psi(\mathbf{r}) + U_0\tilde{m}(\mathbf{r})\psi^*(\mathbf{r}) = 0, \tag{5}$$

with $\psi(\mathbf{r})$ normalized to the total number of condensate particles, i.e., $\int d\mathbf{r}|\psi(\mathbf{r})|^2 = N_0$. The first term in Eq. (5) describes the 'free' evolution of the condensate mean field in a confining potential $V_{\rm trap}(\mathbf{r})$. The two terms in the square brackets, correspond, respectively, to collisions between two atoms in the condensate and between an atom in the condensate and an excited one. The final term (neglected in the HFB-Popov approximation) contains the effect of the simplest anomalous average of the Bose field, which represents pair correlations between atoms.

These pair correlations modify the scattering of two condensate atoms, producing an effective interatomic potential [14,23]. In the simplest approximation, this potential is given by the two-body T matrix, itself conventionally approximated by $U_0\delta(\mathbf{r}-\mathbf{r}')$ [18]. The next level of approximation corresponds to the inclusion of many-body effects, which are introduced by $\tilde{m}(\mathbf{r})$. The form of the effective interaction in this case can be seen by grouping the final term of Eq. (5) with the expression $U_0|\psi(\mathbf{r})|^2\psi(\mathbf{r})$, which gives

$$U_0[|\psi(\mathbf{r})|^2\psi(\mathbf{r})+\tilde{m}(\mathbf{r})\psi^*(\mathbf{r})]=U_0\left[1+\frac{\tilde{m}(\mathbf{r})}{\psi^2(\mathbf{r})}\right]|\psi(\mathbf{r})|^2\psi(\mathbf{r})$$

$$=\tilde{U}(\mathbf{r})|\psi(\mathbf{r})|^2\psi(\mathbf{r}) \qquad (6)$$

Hence $\tilde{U}(\mathbf{r})$ can be thought of as an approximation to the full many-body interaction potential between two condensate atoms in the presence of the condensate and excited-state mean fields.

The Appendix shows that for a homogeneous gas, our definition of the effective interaction $\tilde{U}(\mathbf{r})$ is equivalent to the zero-energy, zero-momentum limit of the many-body T matrix if one includes the effect of the mean field on the spectrum of the intermediate states in a collision but not on the propagator. This avoids difficulties associated with infrared divergences in the theory [13]. $\tilde{U}(\mathbf{r})$ is therefore the natural extension of the existing homogeneous treatments [13,23] to the case of trapped gases. It is nonetheless an approximation of the many-body T matrix, and we believe that full calculations should be possible for trapped gases in the near future.

Our discussion so far shows that $\tilde{m}(\mathbf{r})$ upgrades the effective interaction between two atoms to the many-body T matrix. However, in view of Eq. (5), this effective interaction only appears rigorously in the interactions between two condensate atoms. To obtain an effective interaction in collisions between condensed and excited atoms in a rigorous manner, one must deal explicitly with correlations of three particles [28], which requires a treatment beyond the usual mean-field approach [assumed in Eq. (5)] [14]. To a first approximation [and in the same manner as for $\tilde{m}(\mathbf{r})$] such three-particle correlations lead to the introduction of the two-body T matrix in the condensate–excited-state interactions. At the next level of approximation they produce additional terms in Eq. (5), which correspond to many-body effects (i.e., a many-body T matrix) in the interactions between condensed and excited atoms [29].

The two theories discussed in this paper differ in how the condensate–excited-state interactions are approximated. In the low-momentum regime, many-body effects are important. Since we expect the interaction between condensed and excited atoms to be the same as that between two condensate atoms, this leads to the use of $\tilde{U}(\mathbf{r})$ to describe all interactions, thus motivating the $G2$ theory. However, in the limit of high relative momenta the condensate–excited-state interactions are best described by the two-body T matrix since many-body effects die out in this regime [26,23]. This motivates the $G1$ theory, in which the condensate-condensate interactions are modeled by $\tilde{U}(\mathbf{r})$, whereas the condensate-excited state interactions are described in terms of U_0. Having discussed the origin of the various theories, let us now briefly describe their numerical implementation.

IV. SELF-CONSISTENT NUMERICAL ANALYSIS

Equations (1)–(3) form a set of nonlinear eigenvalue problems which must be solved self-consistently. The numerical procedure for doing this has been explicitly reported in the literature [9,10] and can be summarized in the following steps

(i) Solve Eqs. (1)–(3) in the zero-temperature limit of $\tilde{n}(\mathbf{r})=\tilde{m}(\mathbf{r})=0$, which also implies that $\tilde{U}(\mathbf{r})=U_0$. One thus obtains an initial value for the condensate wave function $\psi(\mathbf{r})$, as well as the quasiparticle functions $u_j(\mathbf{r})$ and $v_j(\mathbf{r})$ (which are henceforth treated as real quantities).

(ii) Calculate $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$ by transforming to a quasiparticle basis [see Eqs. (7) and (8)].

(iii) Resolve Eqs. (1)–(3) using the new values of $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$, and iterate to convergence.

The excited-state density $\tilde{n}(\mathbf{r})$ and the pair anomalous average $\tilde{m}(\mathbf{r})$ can be calculated by a Bogoliubov transformation [30] to quasiparticle basis, yielding the well-known expressions

$$\tilde{n}(\mathbf{r})=\sum_j \{[|u_j(\mathbf{r})|^2+|v_j(\mathbf{r})|^2]N_Q(E_j)+|v_j(\mathbf{r})|^2\}, \quad (7)$$

$$\tilde{m}(\mathbf{r})=\sum_j u_j(\mathbf{r})v_j^*(\mathbf{r})[2N_Q(E_j)+1], \qquad (8)$$

where the quasiparticle populations $N_Q(E_j)$ are given by the Bose-Einstein distribution $N_Q(E_j)=1/(e^{\beta E_j}-1)$, with $\beta=1/k_BT$. The expression for $\tilde{m}(\mathbf{r})$ is ultraviolet divergent, which is a consequence of the use of a contact approximation to describe the two-body T matrix rather than the full pseudopotential given in Ref. [18]. However, it is known that the effect of using the full pseudopotential is to remove this divergence [21,31,32], and this justifies our renormalization of $\tilde{m}(\mathbf{r})$ by the subtraction of the high-energy part. The excited-state density is calculated using a small basis set for the strongly coupled low-lying states, and treating all states above this as an ideal gas. The error this involves can be determined by repeating the simulations using a larger basis set. In one dimension we find that 40 basis states is sufficient for a good description of the system even at temperatures above critical.

The form of the interaction potential $\tilde{U}(\mathbf{r})$ of Eq. (6) can lead to numerical difficulties in a trap, since the condensate wave function $\psi(\mathbf{r})$ becomes small away from the center. We therefore compute with a modified form of the interaction potential given by $\tilde{U}(\mathbf{r})=U_0((1+\tilde{m}G)/[\epsilon+\psi^2G])$ where ϵ is a small parameter of the order of 10^{-2}. Our results are independent of the value of ϵ, as has been confirmed by performing simulations using various different (small) values. This is to be expected since physical results depend on the properties of the system in the region of condensation, i.e., near the center of the trap, where ϵ is indeed negligible in comparison to the condensate wave function.

In three dimensions, the U_0 which appears in $\tilde{U}(\mathbf{r})$ is related to the s-wave scattering length via the usual expression $U_0=4\pi\hbar^2a/m$. In one dimension, however, U_0 is simply a measure of the strength of the interactions relative to the spacing of the energy levels in the trap. It has dimensions of energy times length and in our simulations we used a value of $U_0/\hbar\omega x_{\rm osc}=10$, which corresponds to strong interactions. Here ω is the trap frequency, m is the mass of an

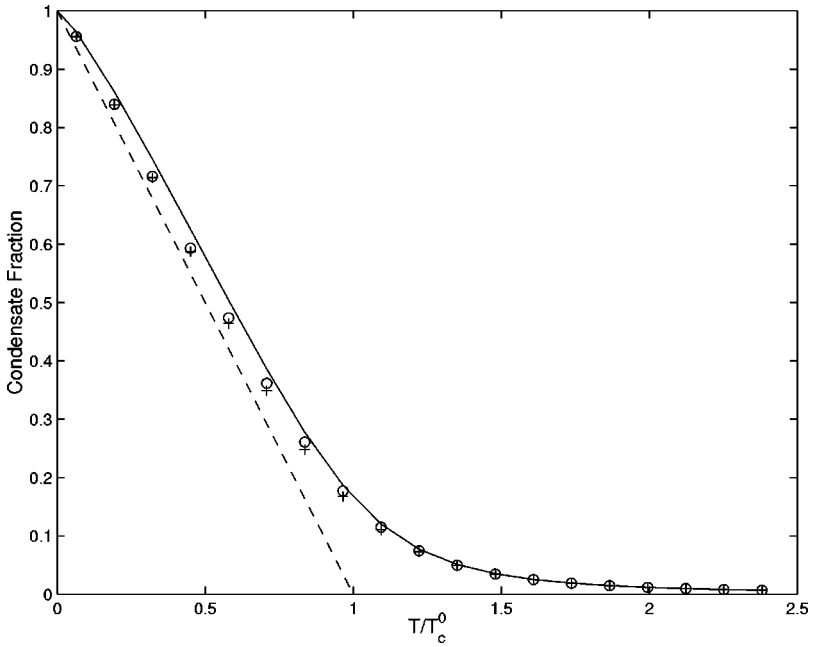

FIG. 1. This figure shows the condensate fraction as a function of temperature for a trapped assembly of 2000 atoms. The solid line corresponds to the noninteracting limit, whereas ○ and + respectively, correspond to the interacting HFB-Popov and $G2$ models. The $G1$ predictions coincide with those of the HFB-Popov model on the scale of this plot (see also Fig. 4). The dotted line gives the condensate fraction for a noninteracting gas of a very large number of atoms using a formula given in Ref. [33]. Comparison with the other curves clearly shows that the effects of interactions on the condensate fraction are much smaller than the finite number effects.

atom, and $x_{\rm osc}=\sqrt{\hbar/2m\omega}$ is the oscillator length unit which sets the scale of length for the system. The value for the interaction strength was chosen so that the effects of our theories would be clearly visible.

Finally we should mention that at high temperatures the eigenvalue μ which appears in the GPE cannot be taken to be the true chemical potential if there is a constraint on the total number of particles in the system. Thus we use a Bose distribution of the form $N_Q(E_j)=1/(e^{(\beta E_j-\delta\mu)}-1)$, where $\delta\mu$ is the difference between the true chemical potential and the eigenvalue appearing in the GPE and is of order $1/N_0$. The μ which appears in Eq. (4) is still given by the eigenvalue of the GPE, however, since the calculation of the quasiparticle energies is really a calculation of their energies relative to the condensate. This correction is necessary if the numerical procedure is to be consistent with the way one calculates the statistical properties of an ideal gas for a fixed number of particles. It is more significant in one dimension than in three because of the more rapid decrease of the condensate population with temperature.

Having discussed the numerical techniques, we now turn to the interpretation of the predictions of the $G1$ and $G2$ theories and their comparison to the HFB-Popov theory. We shall see that as far as density profiles or excitation frequencies are concerned, the predictions of the $G1$ theory lie remarkably close to those of the HFB-Popov theory. The deviation of the $G2$ theory from the HFB-Popov theory is more significant, but is still only of order a few percent.

V. RESULTS IN TRAPPED ONE-DIMENSIONAL CONDENSATES

A. Condensate fraction and critical temperature

Let us first discuss the temperature dependence of the condensate fraction and the importance of interactions in a trapped 1D Bose condensate. Since we have a finite number of atoms, the transition point is smeared out and shifted relative to the large number limit. Although these are very small effects in three dimensions, they are much more noticeable in one dimension [33]. In this section, we examine the further modifications imposed on the transition temperature by the addition of interactions. We find that the presence of interactions has only a small effect on the 1D transition temperature (see Fig. 1). In three dimensions, such a shift (albeit small) has been measured in anisotropic condensates with repulsive interactions [34]. These experiments indicate a lower transition temperature, in agreement with theoretical predictions [35]. This can be understood as follows: the presence of repulsive interactions leads to atoms being repelled from the center of the trap, where their density is highest. This corresponds to a reduction in the phase-space density, so to reach the critical value required for Bose-Einstein condensation (BEC) the system must be cooled to a lower temperature than an ideal Bose gas [36]. Furthermore, once the system has undergone BEC, the repulsive interactions will lead to a lower condensate fraction at any given temperature than for an ideal gas.

These features are shown clearly in Fig. 1, where the condensate fraction is plotted as a function of temperature for the case of an ideal Bose gas, as well as for the three interacting models discussed earlier: HFB-Popov (denoted by ○), $G1$ (coinciding with the HFB-Popov theory), and $G2$ (+). In Fig. 1 (and subsequent figures), the temperature is expressed in dimensionless units of T/T_c^0 where T_c^0 is defined by $N=(k_bT_c^0/\hbar\omega)\log(2k_bT_c^0/\hbar\omega)$. This result for the critical temperature in a 1D trap applies to the limit $N\to\infty$, and is derived in Ref. [33]. Note that this is not the usual thermodynamic limit in which $N\to\infty$ with $N\omega$ held constant, both because BEC cannot occur in one dimension in this limit and

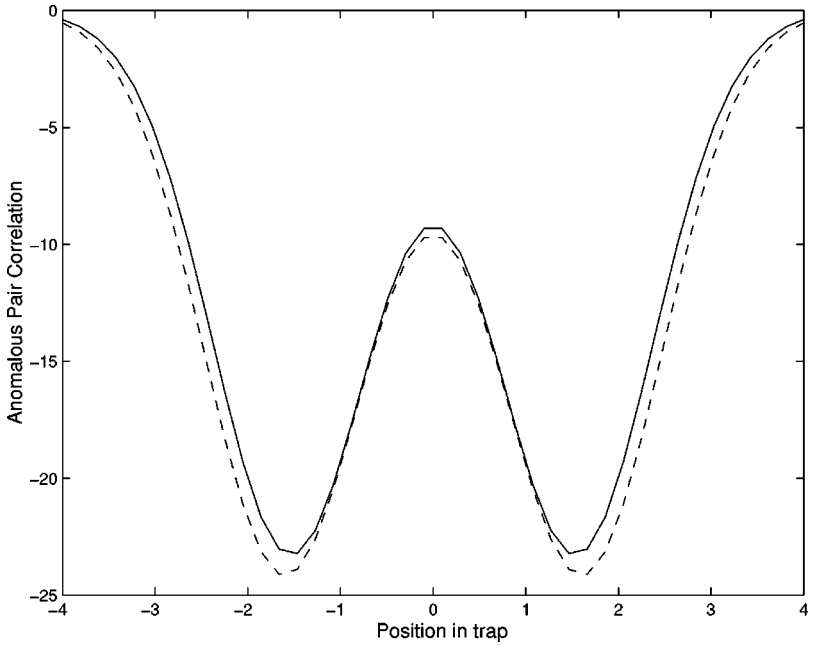

FIG. 2. ''Density profile'' of the anomalous pair average $\tilde{m}(\mathbf{r})$ at $T/T_c^0=0.58$ in both the $G1$ (solid line) and $G2$ (dashed) theories. The position in the trap is in units of $x_{\rm osc}$, and the anomalous average is in units of $1/x_{\rm osc}$, where the harmonic-oscillator length unit is $x_{\rm osc}=\sqrt{\hbar/2m\omega}$.

because it is not the appropriate limit for current experiments (see Ref. [33]). Of course a transition temperature is not precisely defined in a finite system [37], but T_c^0 sets the scale for the appearance of a condensate, and for the case of 2000 atoms it is given by $(k_b T_c^0/\hbar\omega)=310.91$. The ideal Bose gas results shown in Fig. 1 are the exact results for an assembly of 2000 atoms (solid line), based on the analysis of Ketterle and van Druten [33]. These are accurately reproduced by our numerical routine.

Figure 1 confirms that repulsive interactions lower the transition point, and shows clearly that these modifications are negligible in comparison to the finite number effects. As a result, there is no significant difference in the temperature dependence of the condensate fraction between the $G1$, $G2$, and HFB-Popov theories. In particular, the predictions of the $G1$ and HFB-Popov theories cannot be distinguished on the scale of Fig. 1. Nonetheless, both the $G1$ and $G2$ theories predict a slightly smaller condensate fraction than the HFB-Popov theory, which may come as a surprise to the reader, given that $\tilde{U}(\mathbf{r})$ is always locally smaller than U_0 (see subsequent Fig. 3). Indeed, if this generalized effective interaction were *constant* (i.e., position independent) and less than U_0, both the $G1$ and $G2$ plots would lie between the ideal gas and HFB-Popov curves. However, as shown more explicitly below, the net effect of $\tilde{U}(\mathbf{r})$ is to push atoms away from the center of the trap and out of the condensate (in comparison to the HFB-Popov theory). Thus, both of the theories yield a lower value for the total number of condensate atoms at a given temperature, with the correction from the HFB-Popov theory being largest in the $G2$ theory.

B. Position-dependent effective interaction $\tilde{U}(\mathbf{r})$

Modifications from the HFB-Popov theory in both the $G1$ and $G2$ theories are due to the many-body effective interaction $\tilde{U}(\mathbf{r})$ which has been introduced. A physical understanding of these modifications therefore requires a knowledge of the form of this interaction strength. The important feature in both these theories is the explicit appearance of $\tilde{m}(\mathbf{r})$. The ''density profile'' of $\tilde{m}(\mathbf{r})$ at $T/T_c^0=0.58$ is plotted in Fig. 2 for both the $G1$ and $G2$ theories. It is found to be predominantly negative, and slightly larger in magnitude in the $G2$ theory than in the $G1$ theory. This leads to a marginally smaller effective interaction $\tilde{U}(\mathbf{r})$ in the case of the $G2$ theory, with the difference between $\tilde{U}(\mathbf{r})$ in the two theories increasing with increasing temperature. This is clearly displayed in Fig. 3, where the value of $\tilde{U}(\mathbf{r})$ near the trap center is plotted for both theories and a range of temperatures. $\tilde{U}(\mathbf{r})$ varies strongly within the trap, experiencing a local maximum at the trap center, where the condensate density reaches its peak. At large distances from the trap center it reduces asymptotically to the dilute Bose gas U_0, as would be expected for interactions in the absence of condensation. We have also examined the effect of different scattering lengths by varying the nonlinearity in our 1D NLSE. This led to the anticipated result that smaller scattering lengths generate effective interactions which deviate less from the conventional U_0.

C. Density profiles of trapped atoms

Having discussed the form of $\tilde{U}(\mathbf{r})$, we can now compare the density profiles of the trapped atoms (both condensed and excited) for a fixed temperature, as predicted by the $G1$, $G2$, and HFB-Popov theories, and the ideal Bose gas. The detailed atomic profiles of condensed and excited atoms are illustrated in Figs. 4(a) and 4(b) at a temperature $T/T_c^0=0.58$, for which there are (see Fig. 1) approximately equal numbers of atoms in the condensate and excited states.

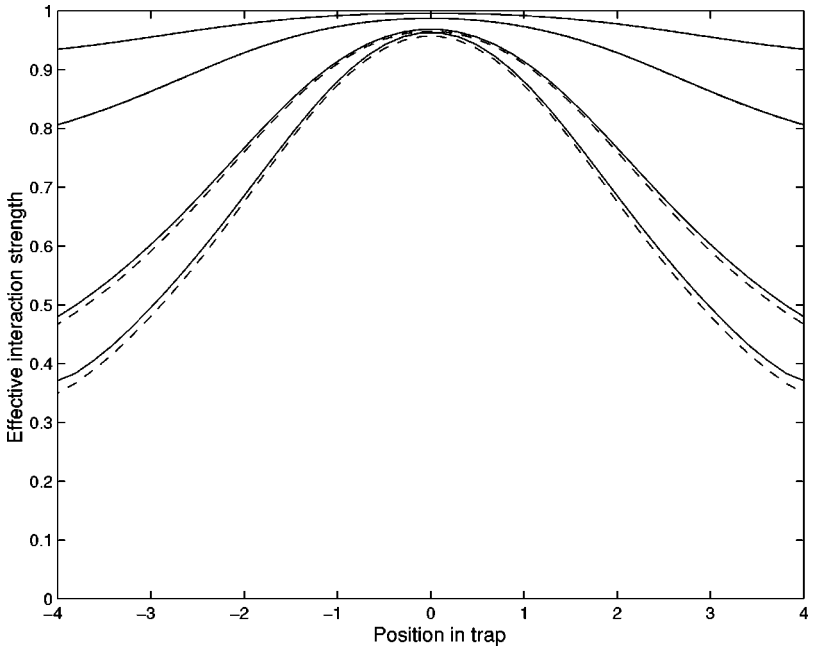

FIG. 3. Variation of the effective interaction $\tilde{U}(\mathbf{r})$ (in units of U_0) near the center of the trap. The position in the trap is given in units of the oscillator length $x_{\rm osc}$. The solid lines correspond to the $G1$ predictions, and the dashed lines to the corresponding values in the $G2$ theory. The curves shown correspond to different temperatures ($T/T_c^0 = 0.06,\ 0.19,\ 0.58$, and 0.84), with temperature increasing with the lower curves. The predictions of the $G1$ and $G2$ theories are indistinguishable in the low-temperature region (top two curves).

Figure 4(a) shows clearly that repulsive interactions cause condensate atoms to be repelled from the center of the trap where their density is highest, i.e., the corresponding wave function spreads out relative to the noninteracting case. The particular interaction model chosen has an additional (but much smaller) effect, with the corresponding wave function for the $G1$ and $G2$ theories, respectively, spreading further from the ideal case than the HFB-Popov theory. This leads to an associated change in the profile of excited atoms, as plotted (over the region of appreciable condensation) in Fig. 4(b). In both cases [Figs. 4(a) and 4(b)], we note that the main qualitative differences from the HFB-Popov theory arise in the $G2$ theory with the $G1$ theory leading to very minor modifications. This is readily understood by noting that the condensate–excited-state interactions are given by $\tilde{U}(\mathbf{r})$ in the $G2$ theory and by U_0 in the $G1$ and HFB-Popov theories. Since $\tilde{U}(\mathbf{r}) < U_0$ everywhere in the trap (and particularly in the region of large excited state density) the energy price associated with excited atoms is less in the $G2$ theory than in either the $G1$ or HFB-Popov theories. As a result there are fewer atoms in the condensate at any given temperature in the $G2$ theory (see Fig. 1) and so the condensate density at the center is lower and the excited state density is higher (Fig. 4).

D. Temperature dependence of $\tilde{U}(\mathbf{r})$ at the trap center

Another issue worth examining is the temperature dependence of the generalized effective interaction $\tilde{U}(\mathbf{r})$ at the center of the trap in both the $G1$ and $G2$ interacting models. This is plotted in Fig. 5, which shows that as the temperature increases $\tilde{U}_0(r=0)$ decreases in the low-temperature regime, reaches a minimum around the transition point, and then increases again in the region of negligible condensation. This can be understood as follows: In the low-temperature region, the pair anomalous average is negligible and produces no significant modification of the effective interaction from the dilute Bose gas strength U_0. As the temperature increases, however, the anomalous average becomes increasingly negative, and reaches a peak near the critical temperature, since at that point the fluctuations of the BEC order parameter are maximized. Simultaneously the condensate density decreases so that the effective interaction $\tilde{U}_0(r) = U_0[1+\tilde{m}(\mathbf{r})/\psi^2(\mathbf{r})]|$ becomes progressively smaller. As the temperature is further increased beyond the critical point, the system asymptotically approaches the normal (uncondensed) phase, for which the anomalous average vanishes and the effective interaction of a dilute atomic gas is known to be accurately determined by U_0.

In the homogeneous limit, it is well known that the zero-energy, zero-momentum limit of the many-body T matrix vanishes exactly at the transition temperature [13,23,38,39], which is characteristic of a second-order phase transition [40]. This feature is reproduced by the definition of our effective many-body interaction $\tilde{U}(\mathbf{r})$ of Eq. (6), since the homogeneous limit of $\tilde{U}(\mathbf{r})$ corresponds precisely to the zero-energy, zero-momentum limit of the many-body T matrix, as shown in the Appendix. However, for trapped condensates we must consider the fact that collisions do not occur precisely at zero momentum. In this case, our expression for $\tilde{U}(\mathbf{r})$ predicts a decrease of the effective interaction (with respect to the value in vacuum, or U_0) of the order of 4–5 %, with the lower prediction being made by the G2 theory. The fact that this decrease is much less significant than the homogeneous case should not come as a surprise, since it is already well documented that a treatment of trapped gases as locally homogeneous breaks down in a very small region

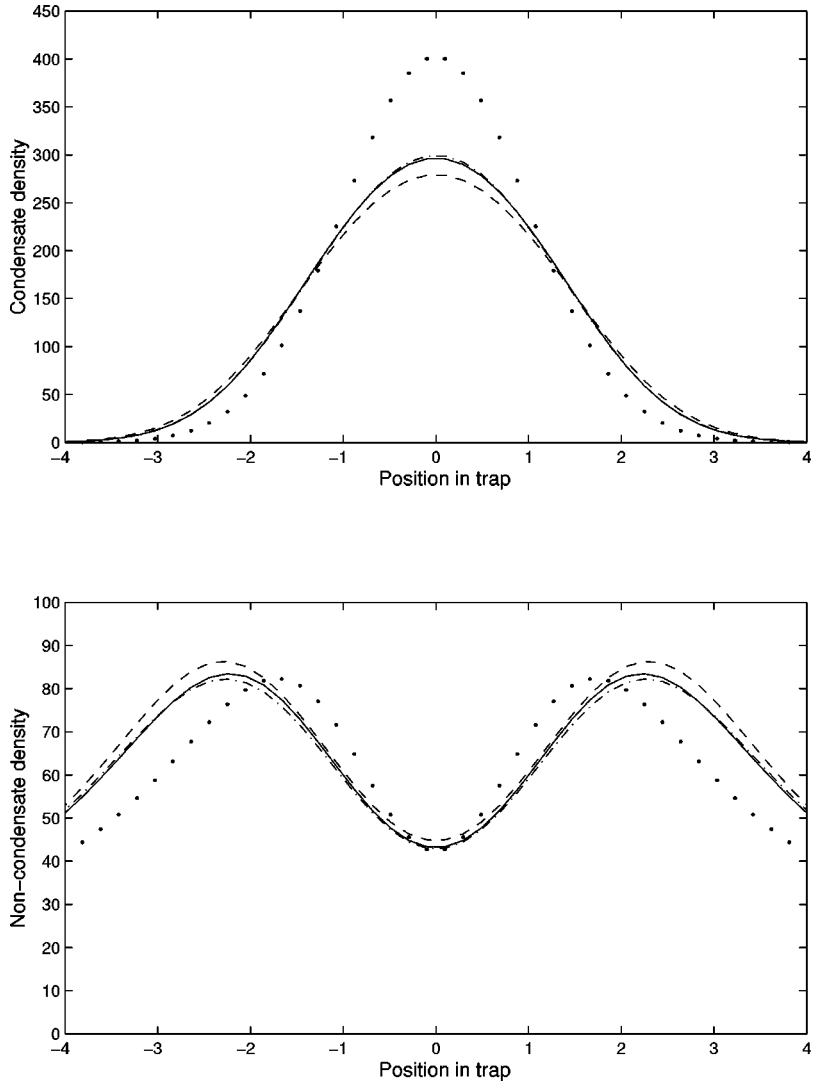

FIG. 4. Atomic density profiles (in units of $1/x_{\mathrm{osc}}$) in the region of appreciable condensation at $T/T_c^0 = 0.58$. The position in the trap is given in units of the oscillator length x_{osc}. (a) shows the condensate, and (b) the noncondensate profiles. These are shown within the HFB-Popov (dash-dotted line), $G1$ (solid), and $G2$ (dashed) approximations. The dotted lines show the corresponding results in the absence of interactions. The total density is obtained from the sum of these two figures and has a maximum at the center of the trap as expected.

near the transition temperature, when the correlation length becomes infinite [22].

VI. FREQUENCIES OF ELEMENTARY EXCITATIONS IN ONE DIMENSION

Possibly the simplest way to compare theories with experiment in the case of trapped Bose-Einstein condensates is to consider the frequencies of elementary excitations. In this section we compare the predictions of the $G1$, $G2$, and HFB-Popov theories for the temperature dependence of these frequencies for 1D inhomogeneous Bose-Einstein condensates.

A. Numerical consistency of the $G1$, $G2$, and HFB-Popov theories

As mentioned earlier, a gapless theory should have a solution with precisely zero excitation energy, and this is the case for all the theories considered here. Numerically, the code employed reproduces this zero frequency mode to order 10^{-14}, which acts as a useful first consistency test. A much more interesting question is whether any of the theories considered satisfy the generalized Kohn theorem for parabolic confinement [41]. This states that the partially Bose-condensed system should have a mode of oscillation corresponding to the rigid motion of the entire system (i.e., condensate and excited atoms), at a frequency which is exactly the same as the lowest excitation in the noninteracting limit (i.e., 1 in harmonic-oscillator units). We have found this theorem to be only approximately satisfied by the theories presented here (to within 12% by the HFB-Popov theory, 10% by the $G1$ theory and 5% by the $G2$ theory). Furthermore, the $G2$ theory is found to reach the anticipated value asymptotically much faster with increasing temperature than the other two theories.

However, a complete theory of elementary excitations should recover this mode exactly, as opposed to the approximate behavior found here. The reason why these theories do not exactly satisfy the Kohn theorem, is that they do not consistently treat the dynamics of both condensed and excited atoms [9,10,13–17], as the condensate is assumed to

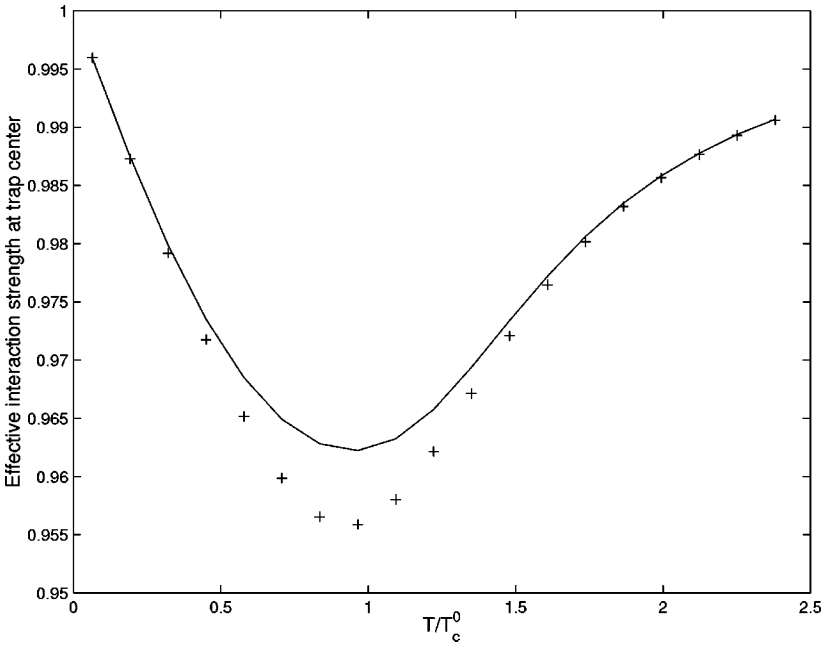

FIG. 5. This figure shows the behavior of $\tilde{U}(\mathbf{r})$ (in units of U_0) at the center of the trap, as a function of temperature. $\tilde{U}_0(r=0)$ acquires its minimum value near the transition temperature for both the $G1$ (solid line) and $G2$ (+) theories. Note that the variation from the value of the dilute Bose gas U_0 is minimal in comparison to the complete vanishing of the interaction anticipated for a homogeneous system.

move in a static thermal cloud. For the Kohn theorem to be completely satisfied, one must take into account the dynamics of the thermal cloud. This was done in Ref. [17] by means of a kinetic theory based on the assumption of local thermodynamic equilibrium for the excited states. This is a reasonable assumption for those experimentally available condensates which are sufficiently dense for the collisional mean free path to be much smaller than the typical atomic de Broglie wavelength, leading to rapid local equilibration of the system. Nonetheless, such an approach is not expected to be of much use in the case of very dilute condensates such as those of Ref. [12]. One should not be too discouraged, however, if the Kohn theorem is only approximately satisfied, because this need not necessarily have a large effect on the excitation frequencies of other modes [42]. This appears reasonable since the low-temperature predictions of the HFB-Popov theory agree with experimental data [12] within the few percent experimental uncertainty [10].

B. Temperature dependence of excitation frequencies

Possibly the most important result of this paper, is the temperature dependence of the excitation frequencies of the low-lying modes, which is shown in Fig. 6. The $G1$ predictions are denoted by the solid line, and are found to be very similar to those of the HFB-Popov theory (denoted by ○). The predictions of the $G2$ theory, on the other hand, are significantly different from the other two theories for a wide range of temperatures. In fact, the $G2$ theory is only compatible with the $G1$ and HFB-Popov theories in the limits of low and high temperature. In the former case, this is because the appreciable condensation means that the effect of the excited atoms and the anomalous average is negligible; thus all theories tend to the same value. In the limit of high temperatures ($T \gg T_c^0$) the condensate density is greatly reduced, and all theories should tend to the noninteracting limit, given by the dash-dotted line of Fig. 6. This is already well satisfied for $T \sim O(2T_c^0)$.

There are two interesting qualitative differences between the $G2$ theory and the other two theories over the important intermediate temperature region (roughly $0.2 < T/T_c^0 < 2$) which we would like to comment on: First, the $G2$ theory predicts a much weaker temperature dependence of the excitation frequencies for temperatures $T < T_c^0$. Second, the excitation frequencies predicted by both the $G1$ and HFB-Popov theories overshoot the noninteracting ones, before approaching them asymptotically, whereas in the $G2$ theory, the noninteracting limit is reached asymptotically from below. The significance (if any) of this overshoot is yet to be determined, but it is interesting to note that this overshoot occurs roughly at the transition temperature.

The dashed lines of Fig. 6 correspond to the predictions of zero-temperature theory [i.e., Eq. (1) with $\tilde{n}(\mathbf{r}) = \tilde{m}(\mathbf{r}) = 0$], using a condensate population determined[2] from Fig. 1. The predictions of such a theory are only meaningful at low temperatures, where they are found to be in good agreement with the HFB-Popov theory. However, the difference between these predictions and the other theories at higher temperatures provides an indication of the importance of interactions between condensed and excited atoms.

VII. DISCUSSION

In this paper we have presented two gapless mean-field theories, which we have compared to the conventional HFB-

[2]Here we have used the HFB-Popov curve for condensate population as a function of temperature, although use of the corresponding curves for the other interacting models leads to negligible differences.

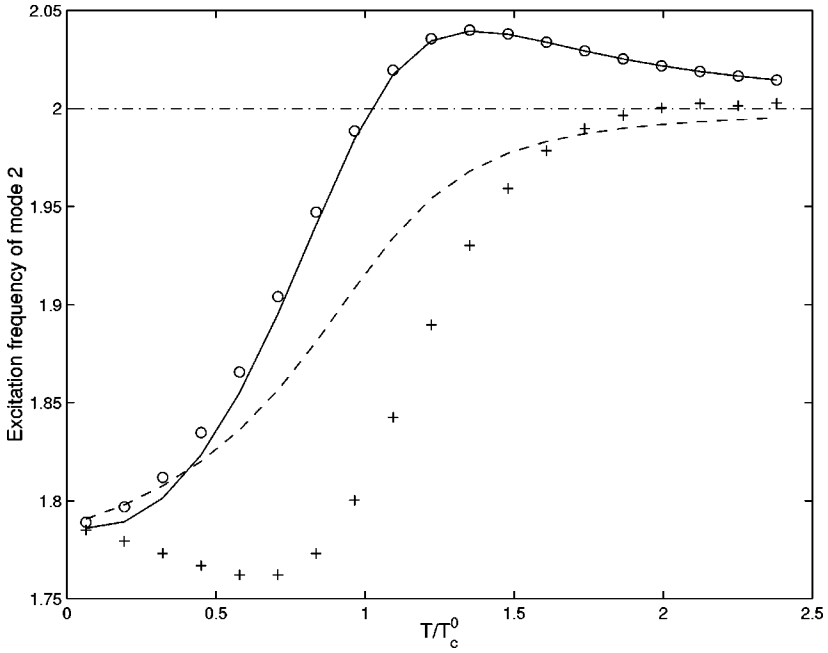

FIG. 6. Temperature dependence of the excitation frequency of mode 2 (breathing mode) for a variety of theoretical treatments. Frequencies are measured in units of the trap frequency. The $G1$ predictions (solid line) lie very close to those of the HFB-Popov theory ($\bigcirc$), whereas the $G2$ results ($+$) reveal a significantly different qualitative behavior from the aforementioned theories for most of the interesting temperature range. The $G2$ predictions are seen to be almost temperature independent at low temperatures, and do not overshoot the frequencies of the noninteracting gas (dash-dotted line), unlike the $G1$ and HFB-Popov predictions. The dashed line corresponds to the predictions of zero-temperature theory, evaluated for numbers of condensate atoms determined from the HFB-Popov curve of Fig. 1 (see text). A similar behavior is observed in the other low-lying modes of excitation for all the above theories.

Popov approach. We believe this to be the first numerical calculation of excitation frequencies for a trapped gas beyond the HFB-Popov and HFB methods. The interesting features of these theories arise from the effect of the medium on the colliding atoms, and are taken into account using an effective many-body interaction. These theories differ from each other in their treatment of interactions involving excited states which are approximated either by the high-momentum limit of the many-body T matrix ($G1$) or by the low-momentum limit ($G2$). These represent the two extreme approximations for the many-body T matrix, and one might expect a complete treatment of the interactions to lie between these two theories. All theories considered in this paper (including the HFB-Popov theory) treat the thermal cloud statically, thus yielding an inherent limitation.

The expression we have used for the low-momentum limit of the many-body T matrix in the inhomogeneous case is given by the $\tilde{U}(\mathbf{r})$ of Eq. (6). This is a function of both the s-wave scattering length and the anomalous average $\tilde{m}(\mathbf{r})$, and is therefore both density and temperature dependent, as opposed to the constant effective interaction $U_0 = (4\pi\hbar^2 a)/m$ of the HFB-Popov theory. In addition, we have shown that $\tilde{U}(\mathbf{r})$ is consistent with an explicit expression for the homogeneous many-body T matrix in the zero-energy, zero-momentum limit [13,23], suggesting that our approach is a natural extension of these homogeneous treatments to the case of a trapping potential. Such a statement is further justified by the fact that our theory is in agreement with the requirements recently laid forward by Giorgini [16] for a mean-field theory beyond the HFB-Popov theory.

The main effect of employing $\tilde{U}(\mathbf{r})$ in both the $G1$ and $G2$ theories is to push atoms toward the edges of the trap and out of the condensate. This in turn influences the frequencies of elementary excitations of the condensed system. In one dimension, we find that quantities of interest (e.g., condensate fraction, atomic density profiles, and excitation frequencies) predicted by the $G1$ theory are effectively identical to the predictions of the HFB-Popov theory. In contrast there is significantly different behavior for the $G2$ theory, especially in the frequencies of the elementary excitations. This is because interactions involving excited states are treated differently in the $G2$ theory as compared with both $G1$ and HFB-Popov theories. The extent of the deviation of the $G2$ theory from both the $G1$ and HFB-Popov theories may be somewhat surprising. Nonetheless, this may well be needed to explain the experimental observations in small trapped assemblies, if one accepts the initial measurements of excitation frequencies reported in Ref. [12]. Preliminary results [43] of the $G2$ theory for the anisotropic 3D condensates of this experiment indicate very good agreement with experimental data in one of the modes of oscillation (quadrupole mode), whereas the agreement in the other mode deviates even further from experiment than the HFB-Popov predictions. Clearly, a lot of work remains to be done on this issue.

ACKNOWLEDGMENTS

We are indebted to H. T. C. Stoof for stimulating discussions and, in particular, for pointing out to us that a gapless theory can be obtained even if the interactions involving excited atoms are treated by a different effective interaction to the collisions between two condensed atoms. We would also

like to thank R. J. Dodd, D. A. W. Hutchinson, and M. Rusch.

APPENDIX: THE MANY-BODY *T* MATRIX IN THE HOMOGENEOUS LIMIT

In this appendix we show that the effective interaction $\tilde{U}(\mathbf{r})=U_0[1+\tilde{m}(\mathbf{r})/\psi^2(\mathbf{r})]$ of Eq. (6) is a valid approximation to the many-body T matrix. This is achieved by proving the equivalence of $\tilde{U}(\mathbf{r})$ to the homogeneous many-body T matrix (denoted here by $\tilde{\Gamma}_0$ as in [13]) in the zero-energy, zero-momentum limit.

It was shown in Refs. [13,23] that $\tilde{\Gamma}_0$ is related to the zero-momentum limit of the vacuum scattering amplitude U_0 via

$$\tilde{\Gamma}_0=\frac{U_0}{1+\alpha(T)U_0}, \tag{A1}$$

where $\alpha(T)$ depends both on the energies of the intermediate states in a collision and on propagator factors for these states. Explicit expressions for $\alpha(T)$ can be obtained [13,23] by ignoring the infrared-divergent contributions. Here we follow the notation of Ref. [13], which gives

$$\alpha(T)=\int\frac{d^3\mathbf{k}}{(2\pi)^3}\left(\frac{1}{2E_k}\coth\frac{\beta E_k}{2}-\frac{1}{2\epsilon_k}\right), \tag{A2}$$

where the term $-(1/2\epsilon_k)$ is required to remove ultraviolet divergences arising from the integration over all momenta. In this equation ϵ_k is the bare particle energy, and E_k corresponds to the quasiparticle energy given by

$$E_k=\sqrt{\epsilon_k^2+2n_0\tilde{\Gamma}_0\epsilon_k}, \tag{A3}$$

where n_0 is the condensate density. $\tilde{\Gamma}_0$ rather than U_0 appears in this expression since the numerical procedure is made self-consistent.

We can now rewrite the expression for $\alpha(T)$ of Eq. (A2) by noting that $\coth(\beta E_k/2)=(e^{\beta E_k}+1)/(e^{\beta E_k}-1)=2N(E_k)+1$, where $N(E_k)=[e^{\beta E_k}-1]^{-1}$ is the Bose-Einstein distribution. Thus, writing Eq. (A1) as $\tilde{\Gamma}_0=U_0[1-\alpha(T)\tilde{\Gamma}_0]$, we obtain

$$\tilde{\Gamma}_0=U_0\left[1-\tilde{\Gamma}_0\int\frac{d^3\mathbf{k}}{(2\pi)^3}\left(\frac{2N(E_k)+1}{2E_k}-\frac{1}{2\epsilon_k}\right)\right]. \tag{A4}$$

Let us now show that the homogeneous limit of $\tilde{U}(\mathbf{r})$ yields exactly the same relation as Eq. (A4). To do this, we require the homogeneous expression for $\tilde{m}(\mathbf{r})$ which, after the subtraction of the ultraviolet divergent part[3], is given by

$$\tilde{m}(\mathbf{r})=\tilde{m}=\int\frac{d^3\mathbf{k}}{(2\pi)^3}(u_kv_k[2N(E_k)+1]-\lim_{k\to\infty}u_kv_k), \tag{A5}$$

where u_k and v_k are the Bogoliubov transformation factors expressed as [44]

$$u_k=\left[\frac{E_k+\epsilon_k+n_0\tilde{\Gamma}_0}{2E_k}\right]^{1/2},\quad v_k=-\left[\frac{\epsilon_k+n_0\tilde{\Gamma}_0-E_k}{2E_k}\right]^{1/2}. \tag{A6}$$

$\tilde{\Gamma}_0$ rather than U_0 appears in these expressions [as in the quasiparticle energies of Eq. (A3)], since they are evaluated self-consistently. A simple calculation then gives $u_kv_k=-n_0\tilde{\Gamma}_0/2E_k$, enabling us to write $\tilde{m}$ as

$$\tilde{m}=-n_0\tilde{\Gamma}_0\int\frac{d^3\mathbf{k}}{(2\pi)^3}\left(\frac{2N(E_k)+1}{2E_k}-\frac{1}{2\epsilon_k}\right). \tag{A7}$$

Since $n_0=\psi^2$, comparison with Eq. (A4) clearly shows that

$$\tilde{\Gamma}_0=U_0\left[1+\frac{\tilde{m}}{\psi^2}\right], \tag{A8}$$

which is the result we set out to prove.

Since the expression for $\alpha(T)$ of Eq. (A2) does not include the infrared divergent contribution, it has the same form both above and below T_c [13]. This means that although $\tilde{\Gamma}_0$ takes into account the modification of the energy spectrum produced by the mean field, the propagators appearing in the many-body T matrix are unperturbed ones. Hence Eq. (A8) corresponds formally to the zero-energy, zero-momentum limit of the homogeneous many-body T matrix which takes into account the modification imposed by the medium on the energy spectrum, but not on the propagators, as argued in the text. This is expected to be a very good approximation for most temperatures, except for a very small region near $T=0$ [23].

[3]This subtraction can be justified as follows: we have argued that $\tilde{m}(\mathbf{r})$ modifies the effective interation between two condensate atoms, replacing the bare interatomic potential with the scattering matrix. However, the contact potential $U_0\delta(\mathbf{r}-\mathbf{r}')$ which appears in our equations is actually an approximation of the two-body T matrix rather than to the bare interatomic potential [this is because the s-wave scattering length which appears in U_0 is measured by observing the effect of (complete) collisions in the absence of condensation]. Thus the perturbative part of $\tilde{m}(\mathbf{r})$ is implicitly present in the use of the contact potential, and to avoid double counting we must renormalize $\tilde{m}(\mathbf{r})$ by subtracting it.

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