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Stability of Bose condensed atomic ^{7}Li

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We study the stability of a Bose condensate of atomic ^{7}Li in a (harmonic oscillator) magnetic trap at nonzero temperatures. In analogy to the stability criterion for a neutron star, we conjecture that the gas becomes unstable if the free energy as a function of the central density of the cloud has a local extremum which conserves the number of particles. Moreover, we show that the number of condensate particles at the point of instability decreases with increasing temperature, and that for the temperature interval considered, the normal part of the gas is stable against density fluctuations at this point. [S1050-2947(96)07312-X]

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I. INTRODUCTION

Since several groups reported evidence for Bose-Einstein condensation (BEC) in atomic gas samples of ^{87}Rb [1], ^{23}Na [2], and possibly ^{7}Li [3] last year, there has been an increased interest in this field of physics. After almost two decades, one has finally been able to verify the prediction which Bose and, in particular, Einstein launched so many years ago. This opens a totally new era regarding research on degenerate systems, and it is to be expected that there will appear many new and interesting experimental and theoretical results about the properties of Bose condensed atomic gases in the near future.

This is certainly true for the ^{87}Rb and the ^{23}Na systems, but maybe less so for the ^{7}Li system, because the experimental results on the latter gas are not yet completely understood. In contrast to the former systems where the atoms have a positive s-wave scattering length a, ^{7}Li atoms have a negative s-wave scattering length. This leads to an effectively attractive interatomic interaction, which makes the system unstable at large densities. Indeed one of us showed that a dilute, homogeneous gas of atoms with a negative s-wave scattering length a collapses to a dense (liquid or solid) state before the density is reached at which BEC is expected to occur at a given temperature [4]. Furthermore, it was shown that the BEC transition is actually preceded by a BCS-like transition to a superfluid state and that this transition also occurs in the unstable regime of the phase diagram.

However, as was pointed out by Hulet [5] and Ruprecht *et al.* [6], the situation is different if the atoms are confined by a magnetic trap. In particular, it was found that for an inhomogeneous gas cloud at zero temperature the condensate is stable at the mean-field level if the number of particles is sufficiently small, or more precisely if $N<N_{0,\max}\equiv 0.573l/|a|$, where $l=\sqrt{\hbar/m\omega}$ is the typical size of the one-particle ground state in the trap. However, quantum fluctuations cause a decay of the condensate on a time scale which is fortunately much longer than the time scales at which the experiments were performed. The same holds true at the relatively high temperatures of interest experimentally, even though the decay is now caused by thermal fluctuations [7].

However, in Ref. [7] only the stability of the condensate was discussed. Although this is an important first step, it is clearly not sufficient, because we know from the homogeneous case that also the noncondensed gas can be unstable against density fluctuations. Therefore we will consider here the stability of the complete system including condensate as well as above condensate particles. We will try to answer the question when the system as a whole becomes unstable and whether it is the condensate part or the noncondensate part which causes the instability.

In this stability analysis we cannot make use of the simple local-density approximation. The local-density approximation is only applicable in systems for which the correlation length ξ (roughly speaking the distance over which the particles influence each other) is much smaller than the typical trap size l over which the density changes and the system behaves locally homogeneous. However, close to the critical temperature the correlation length diverges, and the local-density approximation always breaks down. Nevertheless, it is valid at the spinodal point if we satisfy the condition that $k_BT/\hbar\omega \gg l/|a| \gg 1$ or equivalently $N \gg N_{0,\max}^3$ [7,8], i.e., the total number N of particles in the gas must be much larger than the third power of the maximum number of condensate particles $N_{0,\max}$. Since this amounts to $N\gg 10^9$ for the trap parameters of the Rice experiment [3], it is clear that on the basis of the local-density approximation we cannot decide if a cloud of 10^4-10^5 atoms is mechanically stable and therefore (meta)stable. On the other hand, if it were allowed to use the local density approximation at the spinodal point, we would immediately conclude that a (meta)stable condensate cannot exist.

To go beyond the local-density approximation, we will present numerical results for the free energy of the system at several temperatures. To do so, we first present in Sec. II the finite temperature theory for the inhomogeneous gas. The equations of motion that describe the gas are derived from a variational principle [8]. In analogy to the homogeneous case, we incorporate the possibility of both a BEC and a BCS transition. Subsequently we give an expression for the free energy. Since the experiments with ^{7}Li are performed at densities and temperatures such that $na\Lambda_{th}^2 \ll 1$ (where n is the density and $\Lambda_{th}=\sqrt{2\pi\hbar^2/mk_BT}$ the thermal wavelength of the atoms) and in particular even at $T\simeq T_c$, the theory can be simplified by neglecting the possible BCS pairing and using the Hartree-Fock approximation. However, in view of the fast experimental developments, it is to be expected that

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also the regime $na\Lambda_{th}^2 \gg 1$, which amounts to $T \ll T_c$, can be reached in the near future and this is why we present here the full theory including also the effects of BCS pairing. In Sec. III we then present our numerical results. In Sec. III A we discuss the zero temperature limit of the Hartree-Fock approximation and make a comparison with previous calculations. Also a thermodynamic criterion for the stability of the gas is given. In Sec. III B we proceed to nonzero temperatures. We calculate the maximum number of condensate particles as a function of temperature and pronounce upon the issue whether the condensate or the noncondensate causes the instability of the gas. The paper ends in Sec. IV with some conclusions.

II. THEORY

We start this paper with the equilibrium theory for a dilute gas of particles with mass m in an external trap potential $V_{\text{ext}}(\vec{r})$, interacting with each other through an approximately local (because $|a| \ll l$) two-body potential $V_0\delta(\vec{r})$. In the numerical calculations which follow subsequently, we will specialize to ^{7}Li atoms, which have a negative s-wave scattering length a and $V_0 < 0$. The interparticle interaction is therefore effectively attractive.

The grand-canonical Hamiltonian of the system is given by [9]

$$H = \int d\vec{r} \left\{ \psi^\dagger(\vec{r}) \left(-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\vec{r}) - \mu \right) \psi(\vec{r}) + \frac{1}{2} V_0 \psi^\dagger(\vec{r}) \psi^\dagger(\vec{r}) \psi(\vec{r}) \psi(\vec{r}) \right\}, \tag{1}$$

where μ is the chemical potential, and $\psi(\vec{r})$ and $\psi^\dagger(\vec{r})$ annihilates and creates, respectively, a particle at position $\vec{r}$. As usual, the density of particles in the system $n(\vec{r})$ is given by the grand canonical average $\langle \psi^\dagger(\vec{r})\psi(\vec{r}) \rangle$, and the total number of particles is $N = \int d\vec{r} n(\vec{r})$, which ultimately determines the chemical potential of the gas.

For particles with a positive s-wave scattering length a, the annihilation operator $\psi(\vec{r})$ has a nonvanishing expectation value below the critical temperature. By separating out this expectation value in the usual way [9], i.e.,

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \psi'(\vec{r}), \tag{2}$$

where ψ' describes the noncondensate part and $\psi_0(\vec{r}) = \langle \psi(\vec{r}) \rangle = \sqrt{n_0(\vec{r})}$ is the condensate wave function, one can derive the equations of motion for the condensate as well as the noncondensate part of the gas. However, in the case of a negative s-wave scattering length, it can be shown for the homogeneous case that the free energy as a function of the expectation value of the field operator ψ has at low temperatures a local *maximum* for some nonzero value of $\langle \psi(\vec{r}) \rangle$ and there is only a local *minimum* for $\langle \psi(\vec{r}) \rangle = 0$, which is therefore the correct value around which one has to expand [8]. As a result we must use a different order parameter to describe a phase transition due to quantum degeneracy effects, namely, the BCS-type order parameter $\langle \psi(\vec{r})\psi(\vec{r}) \rangle$. In the case of bosons, this is actually known as the Evans-Rashid order parameter.

A. Evans-Rashid transition

To derive the equations of motion that describe the gas, it is useful to determine the (exact) grand-canonical potential

$$\Omega_{ex}(T,\mu) = -k_B T \ln\{\mathrm{Tr}[\exp(-\beta H)]\}, \tag{3}$$

from which all thermodynamic quantities that we wish to know can be calculated. It is well known that if H_t is some trial Hamiltonian, and Ω_t the corresponding grand-canonical potential, we have the variational principle [10]

$$\Omega_{ex} \leq \Omega \equiv \Omega_t + \langle H - H_t \rangle_t, \tag{4}$$

where $\langle O \rangle_t$ is the expectation value of the operator O in the grand-canonical ensemble based on H_t. The trial Hamiltonian that we want to use here is given by

$$H_t = \int d\vec{r} \left\{ \psi^\dagger(\vec{r}) \left(-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\vec{r}) - \mu + \hbar\Sigma(\vec{r}) \right) \psi(\vec{r}) + \frac{1}{2}\Delta_0(\vec{r}) \psi^\dagger(\vec{r}) \psi^\dagger(\vec{r}) + \frac{1}{2}\Delta_0^*(\vec{r}) \psi(\vec{r}) \psi(\vec{r}) \right\}. \tag{5}$$

It is quadratic in the field operators and indeed has nonzero expectation values for both $\langle \psi^\dagger(\vec{r})\psi(\vec{r}) \rangle_t$ and $\langle \psi(\vec{r})\psi(\vec{r}) \rangle_t$. In this expression, the functions $\hbar\Sigma(\vec{r})$, $\Delta_0(\vec{r})$, and its complex conjugate $\Delta_0^*(\vec{r})$ are variational parameters which have to be determined by minimization of the grand-canonical potential Ω. The trial Hamiltonian has nondiagonal elements proportional to the BCS order parameter $\Delta_0(\vec{r})$ and the diagonal contribution proportional to $\hbar\Sigma(\vec{r})$ is the self-energy due to the two-body interaction.

This trial Hamiltonian can be put into the diagonal form

$$H_t = E_g + \sum_j \hbar\omega_j b_j^\dagger b_j \tag{6}$$

by applying the Bogoliubov transformation

$$\psi(\vec{r}) = \sum_j [u_j(\vec{r}) b_j + v_j^*(\vec{r}) b_j^\dagger], \tag{7a}$$

$$\psi^\dagger(\vec{r}) = \sum_j [v_j(\vec{r}) b_j + u_j^*(\vec{r}) b_j^\dagger]. \tag{7b}$$

The operators b_j and $b_j^\dagger$ are required to satisfy the usual Bose commutation relations, and therefore the functions $u_j(\vec{r})$ and $v_j(\vec{r})$ are normalized as

$$[\psi(\vec{r}), \psi^\dagger(\vec{r}\,')] = \sum_j [u_j(\vec{r}) u_j^*(\vec{r}\,') - v_j^*(\vec{r}) v_j(\vec{r}\,')] = \delta(\vec{r} - \vec{r}\,'). \tag{8}$$

Using the relations $[H_t, b_j] = -\hbar\omega_j b_j$ and $[H_t, b_j^\dagger] = \hbar\omega_j b_j^\dagger$ and substituting Eqs. (7a) and (7b) into the commutators $[H_t,\psi]$ and $[H_t,\psi^\dagger]$, it is found that $u_j(\vec{r})$ and $v_j(\vec{r})$ must be solutions to the following eigenvalue equation:

$$\begin{pmatrix} H_0+\hbar\Sigma(\vec{r})-\mu-\hbar\omega_j & \Delta_0(\vec{r}) \\ -\Delta_0^*(\vec{r}) & -H_0-\hbar\Sigma(\vec{r})+\mu-\hbar\omega_j \end{pmatrix} \times \begin{pmatrix} u_j(\vec{r}) \\ v_j(\vec{r}) \end{pmatrix} = 0, \tag{9}$$

where $H_0=-\hbar^2\nabla^2/2m+V_{\rm ext}(\vec{r})$. These coupled equations are the Bogoliubov-DeGennes equations [11]. They can be solved self-consistently once the functions $\hbar\Sigma(\vec{r})$ and $\Delta_0(\vec{r})$ are obtained from minimization of Ω and expressed in terms of $u_j(\vec{r})$ and $v_j(\vec{r})$. Furthermore the ground-state energy E_g in Eq. (6) is given by

$$E_g=\int d\vec{r}\sum_j \left\{-\hbar\omega_j|v_j(\vec{r})|^2-\frac{1}{2}\Delta_0 u_j^*(\vec{r})v_j(\vec{r}) + \frac{1}{2}\Delta_0^*(\vec{r})u_j(\vec{r})v_j^*(\vec{r})\right\}. \tag{10}$$

We now return to the calculation of the thermodynamic potential Ω. Since H_t is diagonal according to Eq. (6), it is easily verified that the first term on the right-hand side of Eq. (4) is given by

$$\Omega_t=E_g+k_BT\sum_j \ln(1-e^{-\beta\hbar\omega_j}), \tag{11}$$

whereas the second term can be rewritten, using Wick's theorem [9], as

$$\begin{aligned}\langle H-H_t\rangle_t=\int d\vec{r}\Big\{ & V_0\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t \\ & +\frac{1}{2}V_0\langle\psi^\dagger(\vec{r})\psi^\dagger(\vec{r})\rangle_t\langle\psi(\vec{r})\psi(\vec{r})\rangle_t-\hbar\Sigma(\vec{r}) \\ & \times\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t-\frac{1}{2}\Delta_0(\vec{r})\langle\psi^\dagger(\vec{r})\psi^\dagger(\vec{r})\rangle_t \\ & -\frac{1}{2}\Delta_0^*(\vec{r})\langle\psi(\vec{r})\psi(\vec{r})\rangle_t\Big\}.\end{aligned} \tag{12}$$

Substituting the Bogoliubov transformation from Eq. (7), we find that

$$\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t=\sum_j \{[|u_j(\vec{r})|^2+|v_j(\vec{r})|^2]N(\hbar\omega_j)+|v_j(\vec{r})|^2\} \tag{13}$$

and

$$\langle\psi(\vec{r})\psi(\vec{r})\rangle_t=\sum_j u_j(\vec{r})v_j^*(\vec{r})[1+2N(\hbar\omega_j)], \tag{14}$$

where the function $N(\hbar\omega_j)=\langle b_j^\dagger b_j\rangle_t=(e^{\beta\hbar\omega_j}-1)^{-1}$ is the Bose distribution function for the Bogoliubov quasiparticles.

The still unknown functions $\hbar\Sigma(\vec{r})$, $\Delta_0^*(\vec{r})$, and $\Delta_0(\vec{r})$ have to be chosen such that the functional $\Omega[\hbar\Sigma,\Delta_0,\Delta_0^*]$ is minimal, i.e.,

$$\left.\frac{\partial\Omega}{\partial\hbar\Sigma}\right|_{\Delta_0,\Delta_0^*}=\left.\frac{\partial\Omega}{\partial\Delta_0}\right|_{\hbar\Sigma,\Delta_0^*}=\left.\frac{\partial\Omega}{\partial\Delta_0^*}\right|_{\hbar\Sigma,\Delta_0}=0. \tag{15}$$

The last condition is just the complex conjugate of the second, and it suffices to consider only one of them. In the Appendix it is shown that Eq. (15) requires that

$$\hbar\Sigma(\vec{r})=2V_0\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t \tag{16}$$

and

$$\Delta_0(\vec{r})=V_0\langle\psi(\vec{r})\psi(\vec{r})\rangle_t. \tag{17}$$

As is explained in Ref. [12], to incorporate all two-body scattering processes in this many-particle system, the factor V_0 in Eq. (16) must be replaced by the many-body T-matrix $T^{\rm MB}$, but in the regime of interest where the temperature is large compared to the average interaction energy, i.e., $na\Lambda_{th}^2\ll 1$, this can be approximated by the two-body scattering matrix $T^{2B}=4\pi a\hbar^2/m$ and we find the usual Hartree-Fock contribution to the self-energy $\hbar\Sigma(\vec{r})=2n(r)T^{2B}$. In addition, Eq. (17) corresponds to the gap equation of BCS theory. Since this theory already incorporates all ladder diagrams, the factor V_0 here should not be replaced by the many-body T matrix. Collecting together all terms, we find for the thermodynamic potential

$$\Omega=E_g+k_BT\sum_j \ln(1-e^{-\beta\hbar\omega_j}) -\int d\vec{r}\left[n^2(\vec{r})T^{2B}-\frac{1}{2}\frac{|\Delta_0(\vec{r})|^2}{V_0}\right]. \tag{18}$$

From this expression the free energy of the system can be calculated directly using the thermodynamic identity $F=\Omega+\mu N$.

The equations obtained thus far are only valid when there is no Bose condensate present. However, as in the homogeneous case, it is evident that the lowest energy $\hbar\omega_0$ will go through zero at sufficiently low temperatures and at this point the corresponding one-particle ground state becomes macroscopically occupied, i.e., a Bose condensate is formed. Hence, this ground state has then to be considered explicitly.

B. Bose-Einstein condensation

We now address the changes in the above equations that are required if a Bose condensate is present. First, we consider the limit $T\rightarrow 0$, for which all particles in the system tend to occupy the ground state. In the (trial) grand-canonical ensemble

$$Z_t={\rm Tr}[\exp(-\beta H_t)]={\rm Tr}\left[\exp\left(-\beta E_g-\beta\sum_j \hbar\omega_j b_j^\dagger b_j\right)\right] \tag{19}$$

used thus far, one can calculate by standard-statistical physics methods that for any j the expectation value $\langle b_j^\dagger b_j^\dagger b_j b_j\rangle_t = \langle N_j^2\rangle_t - \langle N_j\rangle_t = 2\langle N_j\rangle_t^2$, where $\langle N_j\rangle_t = -(1/\beta)\partial \ln Z_t/\partial \hbar\omega_j = N(\hbar\omega_j)$. In fact, the factor of 2 in the self-energy Eq. (16) originates from this property. However, at zero temperature all particles will tend to the ground state and we therefore find that the fluctuations in the total number of particles are given by

$$\frac{\langle N^2\rangle - \langle N\rangle^2}{\langle N\rangle^2} = \frac{\langle N_0^2\rangle - \langle N_0\rangle^2}{\langle N_0\rangle^2} \simeq 1 + \frac{1}{\langle N_0\rangle} = 1 + \frac{1}{\langle N\rangle} \quad (20)$$

and of order $\mathcal{O}(1)$ instead of the usual $\mathcal{O}(1/\sqrt{\langle N\rangle})$. Hence the fluctuations in the particle number are as large as the average itself, which leads to the conclusion that the use of the grand-canonical ensemble does not lead to an appropriate description of the Bose condensed gas.

There are basically two ways to restrict the grand-canonical ensemble and circumvent this problem. The first one is to introduce a condensate expectation value according to $\langle b_0\rangle = \sqrt{N_0}$. Clearly, we then have $\langle N_0^2\rangle = N_0^2$, and at zero temperature we end up with $\hbar\Sigma = n_0 T^{2B}$ instead of Eq. (16). For nonzero temperatures the effect will be that the ground-state wave function satisfies Eq. (9) with $\hbar\Sigma = (2n - n_0)T^{2B}$, whereas the excited state wave functions obey the same equation except that now $\hbar\Sigma = 2nT^{2B}$. Moreover, the free-energy density now contains the term $f = \frac{1}{2}n_0^2 T^{2B}$ instead of $n_0^2 T^{2B}$ [cf. Eq. (18) and using $f = \Omega/V + \mu n$]. Thus from energy considerations, it is indeed favorable to introduce a condensate expectation value if the s-wave scattering length is positive ($T^{2B} > 0$), but this is not the case for negative a. As mentioned previously, it can be shown that the thermodynamic potential $\Omega(\langle\psi\rangle)$ is a sombrero-shaped function with extremum at $|\langle b_0\rangle| = \sqrt{N_0}$, which is, however, inverted with respect to the $\langle b_0\rangle$ plane when the scattering length a changes from positive to negative [8]. Therefore, the local minimum at $\langle b_0\rangle = \sqrt{N_0}$ that is present for $a > 0$ becomes a local maximum for $a < 0$, and the local minimum of the thermodynamic potential occurs at $\langle b_0\rangle = 0$ in the latter case. So, for a gas of ^{7}Li atoms, the use of the order parameter $\langle b_0\rangle$ appears not to be the correct way to control the fluctuations in the number of condensate particles.

The second method to restrict the condensate fluctuations is to introduce a different restricted grand-canonical ensemble according to

$$Z_t = \mathrm{Tr}[e^{-\beta H_t}] = \sum_{N_0} \mathrm{Tr}[e^{-\beta E_g - \beta\sum_j \hbar\omega_j b_j^\dagger b_j}\delta_{b_0^\dagger b_0, N_0}]$$

$$\equiv \sum_{N_0} e^{-\beta\Omega_t(\mu,N_0)}, \quad (21)$$

where

$$e^{-\beta\Omega_t(\mu,N_0)} = e^{-\beta E_g - \beta\hbar\omega_0 N_0} \prod_{j\neq 0} \exp[-\ln(1 - e^{-\beta\hbar\omega_j})].$$

From these expressions it follows that

$$\Omega_t(\mu,N_0) = E_g + \hbar\omega_0 N_0 + k_B T \sum_{j\neq 0} \ln(1 - e^{-\beta\hbar\omega_j}).$$

The total number of particles is therefore given by $N = \Sigma_j \langle N_j\rangle_t = \Sigma_j \partial\Omega_t/\partial\hbar\omega_j = N_0 + \Sigma_{j\neq 0} N(\hbar\omega_j)$. Moreover, the largest contribution to the sum over the number of condensate particles in Eq. (21) comes from a minimum in Ω_t, which implies that $N_0 = 0$ if $\hbar\omega_0 < 0$ and $0 < N_0 < \infty$ if $\hbar\omega_0 = 0$.

The expectation value $\langle N_0^2\rangle$ calculated in this restricted grand-canonical ensemble (by construction) equals $\langle N_0\rangle^2$, whereas for the other energy levels ($j \neq 0$) nothing has changed compared with the results in the original grand-canonical ensemble. In conclusion we therefore arrive at the *same* equations for the ground-state and the excited state wave functions as we had derived by the first method for a gas with positive s-wave scattering length: The ground-state wave function $(u_0(\vec{r}), v_0(\vec{r}))$ satisfies Eq. (9) with $\hbar\Sigma = [2n(\vec{r}) - n_0(\vec{r})]T^{2B}$ whereas the excited states have just $\hbar\Sigma = 2n(\vec{r})T^{2B}$. In addition, the condensate density obeys $n_0(\vec{r}) = N_0[|u_0(\vec{r})|^2 + |v_0(\vec{r})|^2] + |v_0(\vec{r})|^2$ and the total density is given by $n(\vec{r}) = n_0(\vec{r}) + \Sigma_{j\neq 0}\{N(\hbar\omega_j)[|u_j(\vec{r})|^2 + |v_j(\vec{r})|^2] + |v_j(\vec{r})|^2\}$. The change in expectation value $\langle N_j^2\rangle$ for $j = 0$ will of course also change the free energy if the system is Bose condensed. Taking this change into account, the grand-canonical potential Ω turns out to be given by Eq. (18) except that the term $j = 0$ must be excluded from the summation over states and a term $\frac{1}{2}\int d\vec{r}\, n_0^2(\vec{r})T^{2B}$ must be added. As a result, the free energy becomes

$$F = \mu \int d\vec{r}\, n(\vec{r}) + E_g + k_B T \sum_{j\neq 0} \ln(1 - e^{-\beta\hbar\omega_j})$$

$$- \int d\vec{r} \left[\left(n^2(\vec{r}) - \frac{1}{2} n_0^2(\vec{r}) \right) T^{2B} - \frac{1}{2} \frac{|\Delta_0(\vec{r})|^2}{V_0} \right]. \quad (22)$$

Note that the self-energy $\hbar\Sigma$ for the ground state contains a term $n_0(\vec{r})T^{2B}$. According to Ref. [12], the two-body scattering matrix in this term should again have been the many-body T matrix. However, at sufficiently high temperatures such that $na\Lambda_{th}^2 \ll 1$, or even in the opposite regime if the interaction energy between the atoms is smaller than the energy splitting of the one-particle states, i.e., $nT^{2B} < \hbar\omega$, the many-body T matrix T^{MB} can be approximated by T^{2B}.

C. Mechanical stability

For the homogeneous gas with effectively attractive interactions, the free-energy density satisfies $\partial f/\partial n = \mu$, and the chemical potential μ as a function of the density n becomes multivalued ($\partial^2 f/\partial n^2$ changes sign) for smaller densities than those needed for BEC. This is the instability criterium for the homogeneous system. A detailed analysis shows that in this case the BEC transition is indeed preceded by a BCS transition, but that both transitions occur in the unstable regime of the phase diagram.

However, in the Introduction we already mentioned that in an inhomogeneous system a metastable condensate can exist if the number of condensate particles is sufficiently small, i.e., $N_0 < 0.573 l/|a|$ [6]. Qualitatively this can be understood from the fact that a collapse of the condensate requires that other harmonic oscillator states need to be mixed into the wave function of the condensate. For this, energy is needed (virtually), which can be supplied by the interactions provided that the densities in the system are sufficiently high. As a result, when the density of the gas becomes so high that the system will collapse, there must be some radial unstable mode in the density fluctuations.

Systems of compact objects such as white dwarfs and neutron stars [17] can also be unstable for collapse under certain conditions. Although a compact object consists of degenerate fermions (electrons, protons, and neutrons), and furthermore time and length scales for stellar systems cannot be compared with those of the Bose condensate, the physics in both systems has interesting similarities.

Indeed, the final state of a star when it has burnt up all its nuclear fuel is a white dwarf, neutron star, or black hole, depending on its mass. Such a compact object is formed because in the final stages the star still radiates energy at the expense of gravitational energy, i.e., the system contracts. This cannot go on indefinitely, because at a certain point, the electrons and protons in the star become degenerate. This causes an extra internal pressure and the star will come to equilibrium. For a white dwarf, which has a maximum mass of 1.4 times the solar mass, this occurs at a radius of about 5000 km. In this stage the gradient of the pressure just cancels the gradient in potential energy. However, when the mass of the original star is between 1.4 and 3 times the solar mass, the gravitational force will be so strong that equilibrium can only be restored when almost all electrons and protons are squeezed together to neutrons by inverse β decay: In that case the star contracts to an even more compact neutron star with a radius of about 10 km. Above these definite maximum masses, the white dwarf and the neutron star cannot support themselves against gravitational collapse and this can lead to black hole formation. To study the stability of these systems, it is known that it is convenient to parametrize all equilibrium density profiles $n(\vec{r};n_c)$ by the central density n_c of the star and that at the point of instability the mass of the object as a function of the central density of matter n_c exhibits an extremum.

In analogy, we thus expect that in the case of a trapped atomic gas, the onset of the instability is determined by the condition $\partial F/\partial n_c = 0$ and that there exists a zero mode in the density fluctuations at this point. To see this more explicitly, we consider the free energy functional $F[n]$, which gives the free energy of the equilibrium density profile $n(\vec{r};n_c)$. As a result we have

$$F[n(\vec{r};n_c)+\delta n(\vec{r})] = F[n(\vec{r};n_c)] + \int d\vec{r}\,\mu(n_c)\,\delta n(\vec{r}) + \frac{1}{2}\int d\vec{r}\,d\vec{r}\,'\,\frac{\delta^2 F}{\delta n(\vec{r})\,\delta n(\vec{r}\,')}\bigg|_{n(\vec{r};n_c)} \delta n(\vec{r})\,\delta n(\vec{r}\,') + \cdots, \tag{23}$$

where $\mu(n_c) = \delta F/\delta n(\vec{r})|_{n(\vec{r};n_c)}$. If the central density is changed slightly, we have

$$F[n(\vec{r};n_c+\delta n_c)] = F\left[n(\vec{r};n_c) + \frac{\partial n(\vec{r};n_c)}{\partial n_c}\delta n_c + \mathcal{O}(\delta n_c^2)\right] = F[n(\vec{r};n_c)] + \int d\vec{r}\,\mu(n_c)\frac{\partial n(\vec{r};n_c)}{\partial n_c}\delta n_c + \mathcal{O}(\delta n_c^2). \tag{24}$$

We thus conclude that if $\partial F/\partial n_c = 0$, then either $\mu(n_c)=0$ or $\int d\vec{r}\,\partial n(\vec{r};n_c)/\partial n_c = 0$. The latter possibility is in general the physically relevant one because it shows that the two density profiles $n(\vec{r};n_c)$ and $n(\vec{r};n_c+\delta n_c)$ have the same total number of particles, i.e.,

$$N(n_c+\delta n_c) = \int d\vec{r}\,n(\vec{r};n_c+\delta n_c) \simeq \int d\vec{r}\,n(\vec{r};n_c) = N(n_c). \tag{25}$$

The fact that two density profiles containing the same number of particles have the same free energy up to first order indicates that there is a zero mode present. Roughly speaking, it does not cost energy to deform the first density profile continuously into the second, which indicates the threshold for instability. We therefore anticipate that the onset of instability occurs if the free energy has an extremum which conserves particle number [i.e., $\mu(n_c)\neq 0$] as a function of the central density of the gas. So, although collapse in compact objects and in a Bose condensate is caused by a different mechanism, the final criterion in both system may be, surprisingly enough, the same.

D. Hartree-Fock approximation

We have derived the equations that describe an inhomogeneous gas at nonzero temperatures. A convenient procedure to solve these equations numerically would be to start with some suitable initial distribution of particles $n(\vec{r})$ and an initial BCS order parameter $\Delta_0(\vec{r})$, and iterate the equations to self-consistency. It is, however, well known that it is rather difficult to ensure the self-consistency of $\Delta_0(\vec{r})$ [11], and furthermore that Eq. (17) contains a divergence, because the interparticle potential was approximated by a δ-function potential. For a homogeneous gas, this divergence can easily be corrected for, but in this inhomogeneous case, it is not *a priori* clear how one has to deal with it properly, although it is not difficult to convince oneself that the divergence can be canceled by calculating the molecular states of two atoms in the trap. Fortunately it is not necessary to solve these problems here because we are primarily interested in the regime $na\Lambda_{th}^2 \ll 1$, where the average energy $k_B T$ of the particles is much larger than the interaction energy and the effect of $\Delta_0(\vec{r})$ is very small. Therefore, we neglect in the following the BCS order parameter $\Delta_0(\vec{r})$, which in turn means that the functions $v_j(\vec{r})=0$. So, for the uncondensed gas, the Bogoliubov–de Gennes equation (9) then reduces to the Schrödinger equation for a particle in an effective potential $V_{\text{eff}}(\vec{r}) = V_{\text{ext}}(\vec{r}) + 2n(\vec{r})T^{2B}$,

$$\left(-\frac{\hbar^2\nabla^2}{2m}+V_{\text{ext}}(\vec{r})+2n(\vec{r})T^{2B}-\mu\right)\phi_j(\vec{r})=\hbar\omega_j\phi_j(\vec{r}) \tag{26}$$

and the free energy of the system is

$$F=\Omega+\mu N=k_BT\sum_j \ln[1-\exp(-\beta\hbar\omega_j)] -\int d\vec{r}n^2(\vec{r})T^{2B}+\mu\int d\vec{r}n(\vec{r}), \tag{27}$$

where the particle density is given by

$$n(\vec{r})=\sum_j |\phi_j(\vec{r})|^2N(\hbar\omega_j), \tag{28}$$

and the wave functions $\phi_j(\vec{r})$ are subject to the condition

$$\int d\vec{r}|\phi_j(\vec{r})|^2=1. \tag{29}$$

When the ground state is macroscopically occupied, the noncondensed particles satisfy Eq. (26) for $j\neq 0$, and the condensate wave function satisfies

$$\left(-\frac{\hbar^2\nabla^2}{2m}+V_{\text{ext}}(\vec{r})+[2n(\vec{r})-n_0(\vec{r})]T^{2B}-\mu\right)\phi_0(\vec{r}) =\hbar\omega_0\phi_0(\vec{r}), \tag{30}$$

where the condensate density is given by $n_0(\vec{r})=N_0|\phi_0(\vec{r})|^2$ and N_0 is the total number of particles in the condensate. The noncondensate density is $n'(\vec{r})=\Sigma_{j\neq 0}|\phi_j(\vec{r})|^2N(\hbar\omega_j)$, and the total density is $n(\vec{r})=n_0(\vec{r})+n'(\vec{r})$. The free energy in this case, according to Eq. (22), is given by

$$F=k_BT\sum_{j\neq 0} \ln[1-\exp(-\beta\hbar\omega_j)] -\int d\vec{r}\left[n^2(\vec{r})-\frac{1}{2}n_0^2(\vec{r})\right]T^{2B}+\mu\int d\vec{r}n(\vec{r}). \tag{31}$$

Note that for $T=0$, i.e., all particles in the ground state, Eq. (30) corresponds to the nonlinear Schrödinger equation (NLSE), studied, for example, by Ruprecht *et al.* [6] and first derived by Goldman *et al.* [14] in their pioneering work on spin-polarized atomic hydrogen. In addition, note that Bergeman [13] in his analysis uses Eq. (26) with T^{2B} replaced by $T^{2B}/2$ for both the condensate and the excited state wave functions, which corresponds to the Hartree approximation. Although this gives correct results at zero temperature, this is no longer true for nonzero temperatures because it does not properly take into account the mean-field interactions due to the noncondensate part of the gas.

III. RESULTS

At this point we have all tools available to study the stability of atomic ^{7}Li for temperatures obeying $na\Lambda_{th}^2\ll 1$. As mentioned previously, this is done numerically by solving Eq. (26) and Eq. (30) self-consistently with the total particle density $n(\vec{r})$. The gas is assumed to be confined by an isotropic harmonic oscillator potential

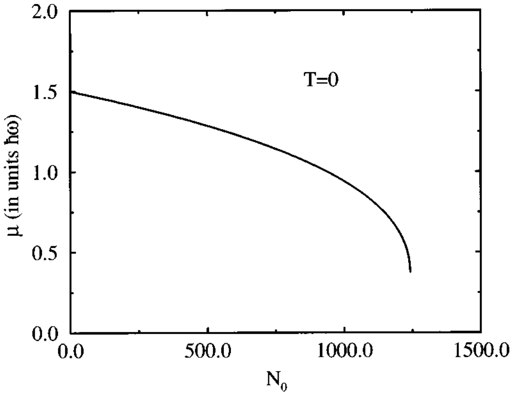

FIG. 1. Chemical potential as a function of total number of condensate particles.

$$V_{\text{ext}}(\vec{r})=\tfrac{1}{2}m\omega^2r^2,$$

where we take for ω the ''average'' $(\omega_x\omega_y\omega_z)^{1/3}$ of the (nonisotropic) trap frequencies used in the Rice experiment [3]. This results in an energy splitting of $\hbar\omega/k_B=7.1$ nK. Due to this simplification the density profile of the gas will depend only on the distance r from the center of the trap. The s-wave scattering length of ^{7}Li is $a=-27.3a_0$, where a_0 is the Bohr radius [15]. We first consider the case $T=0$ and subsequently present results for nonzero temperatures.

A. The $T=0$ case

In this section all particles are considered to be in the condensate, which is the case at zero temperature. This has already been subject to extensive research of several other papers, see for instance Refs. [6] and [16]. For a fixed number of condensate particles N_0, the lowest energy eigenvalue and wave function of the Schrödinger type equation (30) is solved by a numerical integration, and the density distribution $n(r)=n_0(r)$, the chemical potential μ, and the free energy F are determined from this solution.

In Fig. 1 we plot first of all μ as a function of N_0. If there are only a few particles in the condensate, μ is seen to be equal to $\frac{3}{2}\hbar\omega$, i.e., the ground-state energy of a particle in a harmonic oscillator. However, as N_0 increases, the effective potential $V_{\text{eff}}(r)=\frac{1}{2}m\omega^2r^2+n(r)T^{2B}$ grows deeper and deeper in a small range around the center of the trap since T^{2B} is negative, which pulls the particles more and more to the center of the trap. This decreases the value of the ground-state energy and consequently also the chemical potential. As can be seen from the figure, for $N_0>1241$, a solution cannot be found anymore, indicating that the condensate becomes unstable. The maximum number of $N_{0,\max}=1241$ corresponds well with the condition $N_{0,\max}\simeq 0.573l/|a|$ found by Ruprecht *et al.* for the appropriate trap parameters [6].

The free energy given by Eq. (31) is plotted as a function of N_0 and as a function of the central density n_c of the gas in Figs. 2 and 3, respectively. Notice that the derivative of the

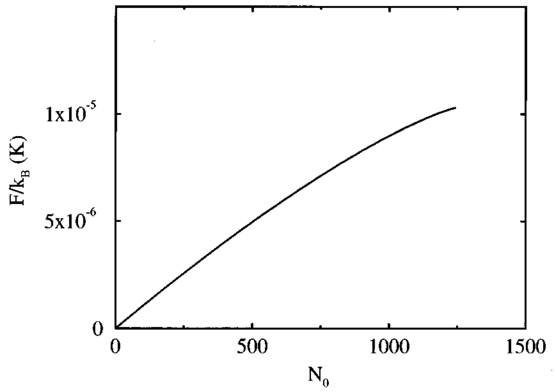

FIG. 2. Free energy as a function of total number of condensate particles.

free energy with respect to the number of condensate particles exactly reproduces the chemical potential, i.e., $\mu = \partial F/\partial N$, showing the consistency of our calculations. From Fig. 3 it follows that the free energy as a function of the central density approaches a constant (maximum) value. This is also shown in the inset of this figure. So, as anticipated in Sec. II C, the instability appears at an extremum of the free energy as a function of the central density of the gas cloud. If the density increases further, the gas will collapse to a dense state. With the theory presented above we clearly cannot describe the gas beyond this point, for we would need a theory that can describe the system also at high densities.

B. The $T \neq 0$ case

For nonzero temperatures the particles in the gas occupy the harmonic oscillator states in Eq. (26) according to the normal Bose distribution at a given chemical potential. However, if μ is increased from $-\infty$ to some value below $\frac{3}{2}\hbar\omega$, the number of particles in the ground state starts to increase dramatically, and we can only put more particles in the system by forcing them into the ground state. At this point, $\hbar\omega_0$ equals zero and the gas consists of a condensate part with density $n_0(r) = N_0|\phi_0(r)|^2$, as well as a noncondensate part with density $n'(r) = \Sigma_{j\neq 0} N(\hbar\omega_j)|\phi_j(r)|^2$. So, the calculation of the chemical potential and the free energy now consists of two parts which correspond to the use of the unrestricted and restricted grand-canonical ensemble, respectively. In the first part we increase μ from $-\infty$ to some maximum value $\mu_{\max}$, above which there are no longer any solutions. In the second part, on the other hand, we increase the number N_0 of particles in the ground state and then determine μ from the ground-state energy of the trap using that $\hbar\omega_0 = 0$. Note that in this second part the chemical potential decreases again, because the increasing density of the condensate lowers the ground-state energy. This behavior of the chemical potential explains why no solutions with $\mu > \mu_{\max}$, could be found in the calculation with the unrestricted grand-canonical ensemble. The two parts of the calculation join smoothly together within an error of the order of 1% at $\mu_{\max}$, where the condensate fraction is of the order of 5%.

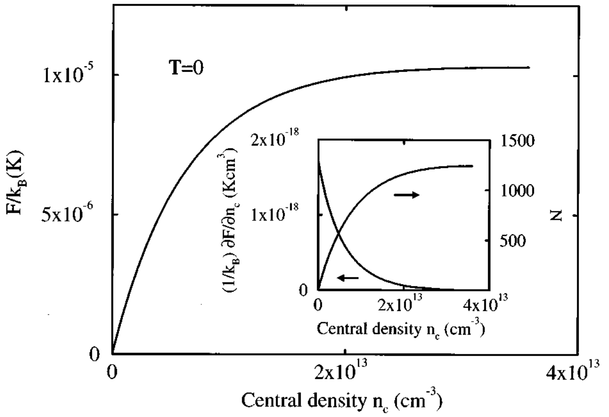

FIG. 3. Free energy as a function of the central density. The inset shows that the derivative of the free energy with respect to the central density approaches zero at the point of instability and that at this point the number of particles as a function of the central density exhibits a maximum.

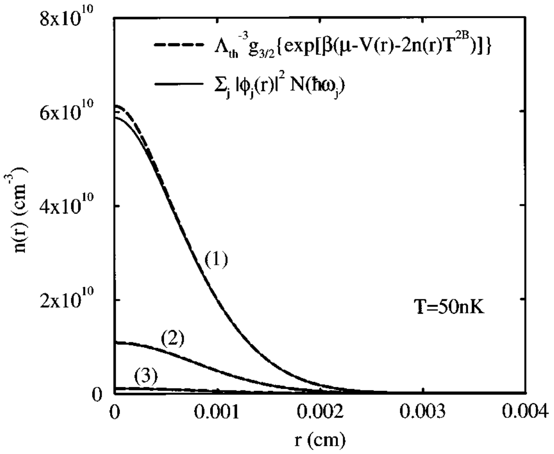

FIG. 4. Comparison between exact density and $\Lambda_{th}^{-3} g_{3/2}(\zeta)$ above the critical temperature for (1) $\mu = -\hbar\omega$, (2) $\mu = -10\hbar\omega$, and (3) $\mu = -25\hbar\omega$.

At nonzero temperatures the density profiles of the gas are determined by calculating all energy levels and corresponding eigenfunctions up to $10k_BT$. Since the ideal 3D harmonic oscillator energy levels are given by $\varepsilon_{n,l} = (2n + l + 3/2)\hbar\omega$, where n and l are integers, this corresponds to taking as many as $[1/2(10k_BT/\hbar\omega)]^2$ levels into account. Clearly, this number increases rapidly as a function of temperature. When the number of particles in the ground state is small (typically corresponding to $\mu \lesssim -\hbar\omega$), Eq. (26) was used to calculate all wave functions and Eq. (27) to calculate the free energy. For larger values of μ, the ground state was determined by Eq. (30) and the free energy by Eq. (31). To check that our results are consistent, we first compare in Fig. 4 the density profile above the critical temperature with the prediction of the local-density approximation, i.e., with

$$n(r) = 1/\Lambda_{th}^3 g_{3/2}(\exp\{\beta[\mu - V(r) - 2n(r)T^{2B}]\}).$$

The agreement is good for large and negative μ, but for $\mu \simeq -\hbar\omega$, a deviation becomes visible around the center of the trap, indicating that the critical temperature is approached.

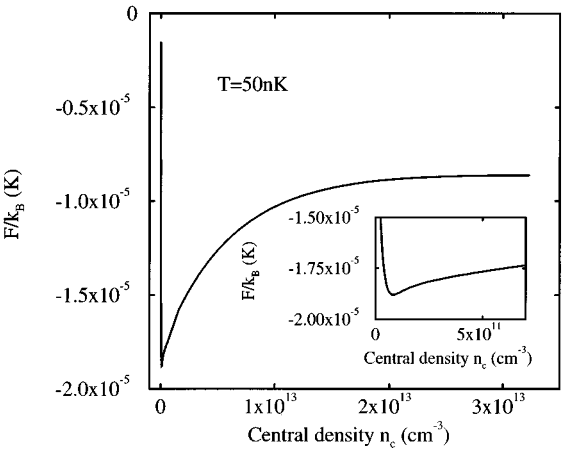

FIG. 5. Free energy as a function of the central density for $T=50$ nK.

In Figs. 5 and 6 the free energy is plotted as a function of the (total) central density of the gas at $T=50$ nK and $T=100$ nK, respectively. We again checked that $\mu=\partial F/\partial N$ as required. The inset in both figures shows a magnification of the local minimum in the free energy curve where μ goes through zero. This is not a point of instability of the system because small variations in the central density do not conserve the total number of particles. The point of instability occurs again where the free energy approaches a local maximum. Note that the maximum densities in the center of the trap that can be obtained are orders of magnitude higher then those for a homogeneous trap. In the homogeneous case, collapse occurs already at densities smaller than $n_{\rm BEC}=\zeta(3/2)/\Lambda_{th}^3\simeq 2.612/\Lambda_{th}^3$ For $T=50$ nK this corresponds to $n_{\rm BEC}=1.07\times 10^{11}$ cm^{-3}, and for $T=100$ nK we have $n_{\rm BEC}=3.04\times 10^{11}$ cm^{-3}. Note, furthermore, that the interaction term $[2n(r)-n_0(r)]T^{2B}$ in the effective potential $V_{\rm eff}(r)$ of the ground state becomes in the center of the trap as large as $n_c T^{2B}\simeq -5\hbar\omega$.

Next we take a closer look at the point of instability of the system when the temperature increases. As was pointed out before, however, the number of harmonic oscillator states which have to be taken into account to calculate the density acurately increases very rapidly and thus slows down the calculation considerably. To avoid this, for temperatures higher than 150 nK we make use of the fact that only the lowest wave functions of the harmonic oscillator states are influenced by the interaction term $2n(r)T^{2B}$ or $[2n(r)-n_0(r)]T^{2B}$ for the ground state, and the wave functions of the higher states are unaffected, although their occupation numbers change, due to the fact that μ equals the ground-state energy if there is a Bose condensate present.

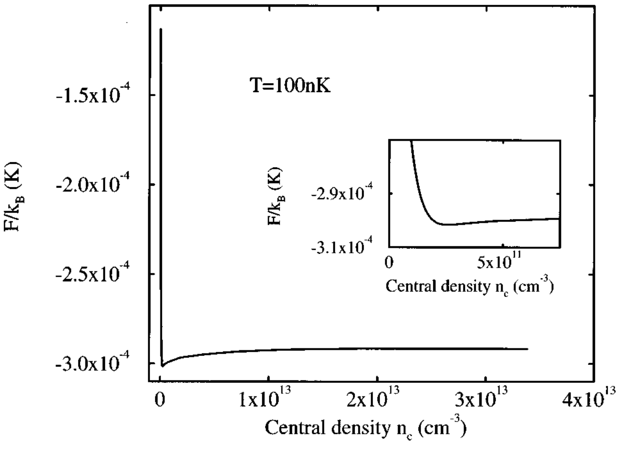

FIG. 6. Free energy as a function of the central density for $T=100$ nK.

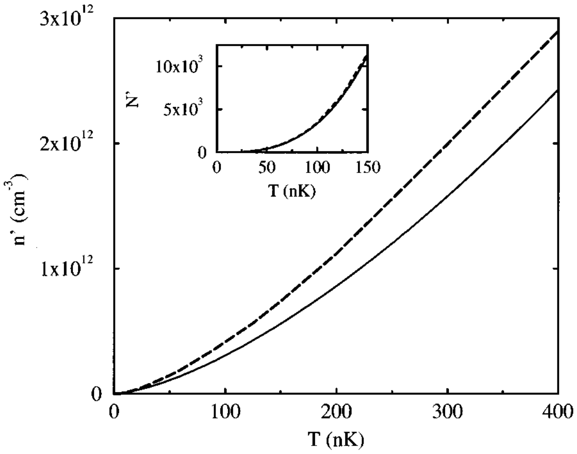

FIG. 7. Normal density $n'(0)$ in the center of the trap at the point of instability of the system (dashed line). The solid line shows $n_{\rm BEC}=2.612/\Lambda_{th}^3$ The inset shows the number of noncondensed particles as a function of temperature for the harmonic oscillator with (dashed) and without (solid) interaction, which is given by $N'=1.202(k_BT/\hbar\omega)^3$.

In Fig. 7 we plot at the point of instability the normal density of the gas in the center of the trap $n'(0)$ as a function of temperature (dashed line) and compare this with the density $n_{\rm BEC}\simeq 2.612/\Lambda_{th}^3$ (solid line) required for BEC in the homogeneous case. In the inset of the same figure, the number of noncondensed particles as a function of temperature is plotted (dashed line), and this is compared with the usual criterion for the onset of BEC in a noninteracting gas, i.e., $N_{\rm BEC}=\zeta(3)(k_BT/\hbar\omega)^3\simeq 1.202(k_BT/\hbar\omega)^3$ (solid line). As expected, the consequence of the attractive interatomic interaction is that the noncondensed particles are pulled towards the center of the trap. The solid line in Fig. 8 shows the maximum number of condensate particles as a function of temperature. Clearly, the occupation of the condensate at the point where the gas becomes unstable decreases when the temperature increases. In Ref. [7] it was argued that an increase in temperature would *not* lead to a decrease in the maximum number of condensate particles since the noncondensed density is approximately constant over the extent of the condensate wave function and therefore only shifts the effective potential $V_{\rm eff}(r)$ by a constant. If this is true, the observed decrease can only be explained by the noncondensed part of the gas becoming unstable before the condensate holds the maximum number of particles. This might also be physically reasonable because the contribution of the normal part of the gas to the total density increases everywhere and especially around the center of the trap.

In view of this we want to try to answer the question whether it is the condensate or (as in the homogeneous case)

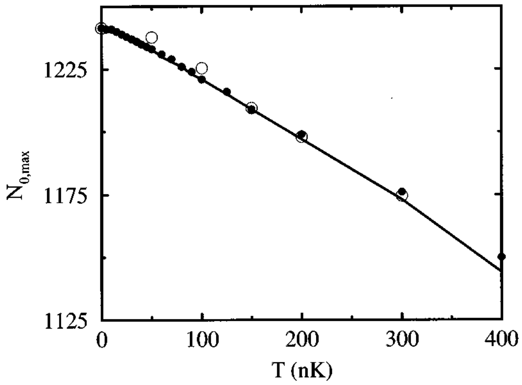

FIG. 8. Maximum number of condensate particles (solid line). The dots denote the maximum condensate at fixed normal part, and the open circles give the maximum occupation of the condensate that can be calculated from the effective oscillator strength due to the presence of the noncondensed part of the gas.

the noncondensed part of the gas which causes instability. Of course, for zero temperature the condensate becomes unstable, and we expect the same for such low temperatures that the noncondensed part is only a small fraction of the gas. For higher temperatures this might change since the number of noncondensed particles increases very rapidly as a function of temperature. To analyze this issue, we calculated in the temperature interval $0 \leqslant T \leqslant 400$ nK the density profiles of the condensate $n_0(r)$ and the normal part of the gas $n'(r)$ at the spinodal point. The condensate fraction N_0/N decreases from 1 for $T=0$ to about 0.005 for $T=400$ nK. Subsequently, we try to add particles to the condensate, and try to find a new solution to the nonlinear Schrödinger equation (30) for the increased number of condensate particles, *while keeping the noncondensate density profile fixed.*

The results are also plotted in Fig. 8: The dots in this figure denote the maximum number of particles that can be in the condensate given the noncondensate density at the temperature of interest. For temperatures $T \leqslant 50$ nK, the system becomes already unstable if only one particle is added to the condensate, from which we draw the conclusion that at this temperature it is still the condensate which renders the instability. For higher temperatures, it is possible to add a few particles to the condensate, but this appears to be the result of numerical inaccuracies in our calculation. We thus conclude that the condensate is unstable at the point of instability of the whole system.

Because of this result, we suspect that the simple argument that the maximum number of condensate particles remains constant because the noncondensed part of the gas is approximately constant over the extent of the condensate wave function, may not be sufficiently accurate in this system. The only difference in the condensate wave function at different temperatures arises due to the contribution of the term $2n'(r)T^{2B}$ to the effective potential. In Fig. 9 we plotted for $T=0$ [and consequently $n'(r)=0$] (solid lines), and for $T=300$ nK (dashed lines) the effective potential $V_{\text{eff}}(r)=1/2m\omega^2r^2+2n'(r)T^{2B}$ and the corresponding condensate densities $n_0(r)$. When $V_{\text{eff}}(r)$ for $T=300$ nK is shifted upward such that the zeros of both potentials coincide, it is clear that the normal part of the gas effectively increases the oscillator strength of the trap potential when the temperature increases. Since the maximum condensate size $N_{0,\max} \propto l/|a| \propto 1/\sqrt{\omega}$, an increase in the effective oscillator strength felt by the condensate causes a decrease in the maximum condensate size. A measure for the deviation of the effective oscillator strength from the original strength ω is given by the expression

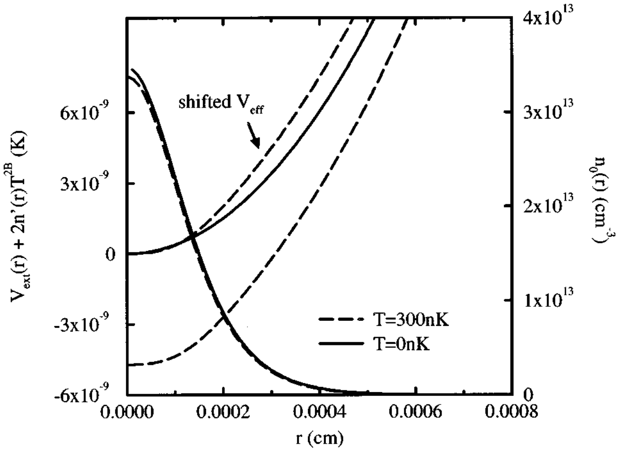

FIG. 9. Condensate density (right scale) and effective potential (left scale) for $T=0$ (solid lines) and $T=300$ nK (dashed lines).

$$\omega_{\text{eff}}^2=\omega^2\frac{\int d\vec{r}\{V_{\text{ext}}(r)+2[n'(r)-n'(0)]T^{2B}\}n_0(r)}{\int d\vec{r}V_{\text{ext}}(r)n_0(r)},$$

and for nonzero temperature we thus estimate that the maximum number of condensate particles is given by

$$N_{0,\max}(T)=N_{0,\max}(0)\sqrt{\frac{\omega}{\omega_{\text{eff}}(T)}}.$$

For $T=300$ nK this amounts to $N_{0,\max}(300)=1174.5$, which corresponds rather accurately with the value 1173 from our full calculation. For some other temperatures the maximum occupation of the condensate determined in this way is denoted in Fig. 8 by the open circles. We can conclude that the growth of the normal part of the gas occurs at the expense of the condensate when temperature increases.

IV. CONCLUSION

We performed a numerical calculation to study the stability of a Bose condensate in a trapped gas of ^{7}Li atoms at zero and nonzero temperatures. This was done by determining all quantum states for particles in a harmonic oscillator trap and interacting via two-body scattering. The proposed criterion that the gas becomes mechanically unstable when the free energy of the system as a function of the central density of the gas approaches a maximum value, is confirmed by the calculations.

For zero temperature, the maximum number of condensate particles is in agreement with previous calculations, and for nonzero temperature this number decreases considerably. This is due to the fact that the condensate experiences an effective oscillator strength due to the presence of the noncondensed part of the gas. This effective potential increases as temperature increases and therefore results in a decrease of the maximum occupation of the condensate. For the temperature interval $0\leqslant T\leqslant 400$ nK the condensed part of the gas renders the instability at the spinodal point, so in contrast to the homogeneous case, the normal part of the gas remains stable against density fluctuations.

Furthermore, from the results in Sec. III B and the discussion in Sec. II B, it can be concluded that at low temperatures it seems necessary to include also many-body effects in, e.g., the scattering length, since the average interaction nT^{2B} becomes substantially larger than the energy splitting $\hbar\omega$. To do so appears to be an important challenge for the future which is not only difficult in practice but even in principle due to the presence of infrared divergences in the theory of the dilute Bose gas [18]. Closely related to this issue is the effect of the BCS transition on the properties of the gas, which still needs to be incorporated in the numerical calculations. Once the experiments enter into this low temperature regime where $na\Lambda_{th}^2\gg 1$, it should be interesting to compare the experimental data with the mean-field analysis presented here, and to see if possible deviations can be understood by the above mentioned corrections. This is of course not only true for ^{7}Li, but also for any other atomic species with a negative scattering length such as ^{85}Rb and ^{123}Cs.

ACKNOWLEDGMENTS

We would like to thank Chris Pethick for pointing out to us the analogy between the metastable Bose condensate and compact objects and the stability criteria of the latter system. Furthermore, we thank Randy Hulet and Keith Burnett for various enlightening discussions.

APPENDIX

To calculate the minimum of the grand-canonical potential Ω of Eq. (4), it is convenient in the following to introduce a compact notation for the inner product of two states. From Eq. (8), it is found that the normalization can be rewritten as

$$\begin{aligned}1&=\int d\vec{r}[|u_j(\vec{r})|^2-|v_j(\vec{r})|^2]\\&=\int d\vec{r}(u_j^*(\vec{r}),-v_j^*(\vec{r}))\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}u_j(\vec{r})\\v_j(\vec{r})\end{pmatrix}\\&\equiv(j|1|j),\end{aligned}\tag{A1}$$

which thus defines our convention for the inner product.

We start with the derivative of Ω with respect to $\hbar\Sigma$. For simplicity we consider here only homogeneous variations of $\hbar\Sigma$. It is straightforward to generalize this to inhomogeneous variations. The same will apply later on for variations in Δ_0. The derivative $\partial\Omega/\partial\hbar\Sigma$ is given by

$$\begin{aligned}\frac{\partial\Omega}{\partial\hbar\Sigma}=&\frac{\partial E_g}{\partial\hbar\Sigma}+\sum_j N(\hbar\omega_j)\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}\\&+\int d\vec{r}\Bigg\{2T^{2B}\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t\frac{\partial\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t}{\partial\hbar\Sigma}\\&+\frac{1}{2}V_0\frac{\partial\langle\psi^\dagger(\vec{r})\psi^\dagger(\vec{r})\rangle_t}{\partial\hbar\Sigma}\langle\psi(\vec{r})\psi(\vec{r})\rangle_t\\&+\frac{1}{2}V_0\frac{\partial\langle\psi(\vec{r})\psi(\vec{r})\rangle_t}{\partial\hbar\Sigma}\langle\psi^\dagger(\vec{r})\psi^\dagger(\vec{r})\rangle_t-\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t\\&-\hbar\Sigma\frac{\partial\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t}{\partial\hbar\Sigma}-\frac{1}{2}\Delta_0(\vec{r})\frac{\partial\langle\psi^\dagger(\vec{r})\psi^\dagger(\vec{r})\rangle_t}{\partial\hbar\Sigma}\\&-\frac{1}{2}\Delta_0^*(\vec{r})\frac{\partial\langle\psi(\vec{r})\psi(\vec{r})\rangle_t}{\partial\hbar\Sigma}\Bigg\}.\end{aligned}\tag{A2}$$

Equating the whole expression to zero, and grouping together the terms proportional to the derivative of an expectation value with respect to $\hbar\Sigma$, the solution is seen to be given by Eq. (16) and Eq. (17), if we can prove that

$$\frac{\partial E_g}{\partial\hbar\Sigma}+\sum_j N(\hbar\omega_j)\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}-\int d\vec{r}\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t=0.\tag{A3}$$

This is most easily achieved by assuming that all functions $u_j(\vec{r})$, $v_j(\vec{r})$, and $\Delta_0(\vec{r})$ are real. In that case, the first term on the left reduces to

$$\frac{\partial E_g}{\partial\hbar\Sigma}=-\sum_j\left\{\int d\vec{r}\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}v_j^2(\vec{r})+\hbar\omega_j\frac{\partial}{\partial\hbar\Sigma}\int d\vec{r}v_j^2(\vec{r})\right\}.\tag{A4}$$

The derivative $\partial\hbar\omega_j/\partial\hbar\Sigma$ can be calculated by perturbing the Hamiltonian according to

$$\delta H=\begin{pmatrix}\delta\hbar\Sigma&0\\0&-\delta\hbar\Sigma\end{pmatrix}.$$

The energy shift in $\hbar\omega_j$ is then, to first order, given by

$$\delta\hbar\omega_j=(j|\delta H|j)=\int d\vec{r}[u_j^2(\vec{r})+v_j^2(\vec{r})]\delta\hbar\Sigma,$$

and therefore

$$\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}=\int d\vec{r}[u_j^2(\vec{r})+v_j^2(\vec{r})].\tag{A5}$$

Using furthermore that $\int d\vec{r}[u_j^2(\vec{r})-v_j^2(\vec{r})]=1$, it is found that

$$\int d\vec{r}v_j^2(\vec{r})=\frac{1}{2}\left(\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}-1\right),\tag{A6}$$

so Eq. (A4) can be rewritten as

$$\begin{aligned}\frac{\partial E_g}{\partial \hbar\Sigma} &= -\frac{1}{2}\sum_j \left(\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}-1\right)\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma} - \frac{1}{2}\sum_j \hbar\omega_j \frac{\partial^2\hbar\omega_j}{\partial\hbar\Sigma^2}\\ &= \sum_j \int d\vec{r}\, v_j^2(\vec{r}) + \frac{1}{2}\sum_j \left[1-\left(\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}\right)^2 - \hbar\omega_j\frac{\partial^2\hbar\omega_j}{\partial\hbar\Sigma^2}\right].\end{aligned} \tag{A7}$$

The factor between brackets is zero. This can be seen by first applying a Taylor expansion to show that the energy change $\delta\hbar\omega_j$ due to the shift $\hbar\Sigma+\delta\hbar\Sigma$ can be written as

$$\delta\hbar\omega_j = \frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}\,\delta\hbar\Sigma + \frac{1}{2}\,\frac{\partial^2\hbar\omega_j}{\partial\hbar\Sigma^2}\,(\delta\hbar\Sigma)^2 + \mathcal{O}((\delta\hbar\Sigma)^3).$$

Therefore, the last term between the brackets in Eq. (A7) can be identified with twice the second-order energy shift. Making use then of the standard expression for this second-order energy shift

$$\delta\hbar\omega_j = (j|\delta H|j) + \sum_{i\neq j}\frac{(j|\delta H|i)(i|\delta H|j)}{\hbar\omega_j-\hbar\omega_i} + \cdots, \tag{A8}$$

which still holds with our definition of the inner product, we obtain

$$\begin{aligned}&\sum_j \left[1-\left(\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}\right)^2 - \hbar\omega_j\frac{\partial^2\hbar\omega_j}{\partial\hbar\Sigma^2}\right]\\ &\quad= \sum_j \Bigg[1-\left(j\left|\frac{\partial H}{\partial\hbar\Sigma}\right|j\right)\left(j\left|\frac{\partial H}{\partial\hbar\Sigma}\right|j\right)\\ &\qquad - 2\hbar\omega_j\sum_{i\neq j}\frac{\left(j\left|\frac{\partial H}{\partial\hbar\Sigma}\right|i\right)\left(i\left|\frac{\partial H}{\partial\hbar\Sigma}\right|j\right)}{\hbar\omega_j-\hbar\omega_i}\Bigg]\\ &\quad= \sum_j \left\{1-\left(j\left|\left(\frac{\partial H}{\partial\hbar\Sigma}\right)^2\right|j\right)\right\} = 0,\end{aligned}$$

where the third line follows from the completeness of the eigenstates of the Bogoliubov–de Gennes equation and from the fact that if we write $2\hbar\omega_j = (\hbar\omega_j-\hbar\omega_i) + (\hbar\omega_j+\hbar\omega_i)$ only the antisymmetric part contributes. Finally, we also need that

$$\frac{\partial H}{\partial\hbar\Sigma} = \begin{pmatrix} 1 & 0\\ 0 & -1\end{pmatrix}.$$

Collecting all terms together we thus indeed find that [see Eq. (A3)]

$$\begin{aligned}&\frac{\partial E_g}{\partial\hbar\Sigma} + \sum_j N(\hbar\omega_j)\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma} - \int d\vec{r}\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t\\ &\quad= \int d\vec{r}\sum_j \{v_j^2(\vec{r}) + N(\hbar\omega_j)[u_j^2(\vec{r})+v_j^2(\vec{r})]\}\\ &\qquad - \int d\vec{r}\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t = 0.\end{aligned} \tag{A9}$$

At the same time the derivative of Ω with respect to Δ_0 must be zero. That this is also the case can be shown by a similar calculation. Assuming Δ_0, u_j, and v_j to be real, the equation $\partial\Omega/\partial\Delta_0=0$ reduces to

$$\frac{\partial E_g}{\partial\Delta_0} + \sum_j N(\hbar\omega_j)\frac{\partial\hbar\omega_j}{\partial\Delta_0} - \frac{1}{2}\langle\psi\psi\rangle_t - \frac{1}{2}\langle\psi^\dagger\psi^\dagger\rangle_t = 0 \tag{A10}$$

if the functions $\hbar\Sigma$ and Δ_0 are given by Eqs. (16) and (17). Using Eq. (A6), the first term on the left-hand side is equal to

$$\begin{aligned}\frac{\partial E_g}{\partial\Delta_0} &= -\sum_j \left\{\frac{\partial\hbar\omega_j}{\partial\Delta_0}\int d\vec{r}\,v_j^2(\vec{r}) + \hbar\omega_j\frac{\partial}{\partial\Delta_0}\int d\vec{r}\,v_j^2(\vec{r})\right\}\\ &= -\frac{1}{2}\sum_j \left\{\frac{\partial\hbar\omega_j}{\partial\Delta_0}\left(\frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}-1\right) + \hbar\omega_j\frac{\partial^2\hbar\omega_j}{\partial\Delta_0\partial\hbar\Sigma}\right\}.\end{aligned} \tag{A11}$$

As in the previous calculation, the first and second derivatives of $\hbar\omega_j$ with respect to Δ_0 and $\hbar\Sigma$ can be calculated by perturbing the Hamiltonian according to $H=H_0+\delta H$, with

$$\delta H = \begin{pmatrix}\delta\hbar\Sigma & \delta\Delta_0\\ -\delta\Delta_0 & -\delta\hbar\Sigma\end{pmatrix}.$$

The energy levels then shift to second order according to

$$\begin{aligned}\delta\hbar\omega_j &= \frac{\partial\hbar\omega_j}{\partial\hbar\Sigma}\,\delta\hbar\Sigma + \frac{\partial\hbar\omega_j}{\partial\Delta_0}\,\delta\Delta_0 + \frac{1}{2}\left(\frac{\partial^2\hbar\omega_j}{\partial\hbar\Sigma^2}\,\delta\hbar\Sigma^2\right.\\ &\quad\left. + 2\frac{\partial^2\hbar\omega_j}{\partial\hbar\Sigma\,\partial\Delta_0}\,\delta\hbar\Sigma\,\delta\Delta_0 + \frac{\partial^2\hbar\omega_j}{\partial\Delta_0^2}\,\delta\Delta_0^2\right).\end{aligned} \tag{A12}$$

Comparing this again with the perturbative expression for the energy shift Eq. (A8), we find that

$$\frac{\partial\hbar\omega_j}{\partial\Delta_0} = \frac{(j|\delta H|j)}{\delta\Delta_0} = \left(j\left|\frac{\partial H}{\partial\Delta_0}\right|j\right) = 2\int d\vec{r}\,u_j(\vec{r})v_j(\vec{r}). \tag{A13}$$

Moreover, the second order derivative in Eq. (A11) can be written as

$$\begin{aligned}&\frac{\partial^2\hbar\omega_j}{\partial\Delta_0\partial\hbar\Sigma}\\ &\quad= \sum_{i\neq j}\frac{\left(j\left|\frac{\partial H}{\partial\Delta_0}\right|i\right)\left(i\left|\frac{\partial H}{\partial\hbar\Sigma}\right|j\right) + \left(j\left|\frac{\partial H}{\partial\hbar\Sigma}\right|i\right)\left(i\left|\frac{\partial H}{\partial\Delta_0}\right|j\right)}{\hbar\omega_j-\hbar\omega_i}.\end{aligned} \tag{A14}$$

Therefore Eq. (A11) becomes

$$\begin{aligned}\frac{\partial E_g}{\partial \Delta_0} = \sum_j & \Bigg\{ \int d\vec{r}\, u_j(\vec{r}) v_j(\vec{r}) - \frac{1}{2}\left(j\left|\frac{\partial H}{\partial \Delta_0}\right|j\right)\left(j\left|\frac{\partial H}{\partial \hbar\Sigma}\right|j\right) \\ & - \frac{1}{2}\sum_{i\neq j} \frac{\hbar\omega_j}{\hbar\omega_j - \hbar\omega_i} \times \Bigg[\left(j\left|\frac{\partial H}{\partial \Delta_0}\right|i\right)\left(i\left|\frac{\partial H}{\partial \hbar\Sigma}\right|j\right) \\ & + \left(j\left|\frac{\partial H}{\partial \hbar\Sigma}\right|i\right)\left(i\left|\frac{\partial H}{\partial \Delta_0}\right|j\right)\Bigg]\Bigg\} \\ = \sum_j & \int d\vec{r}\, u_j(\vec{r}) v_j(\vec{r}) - \frac{1}{4}\sum_j \Bigg[\left(j\left|\frac{\partial H}{\partial \Delta_0}\frac{\partial H}{\partial \hbar\Sigma}\right|j\right) \\ & + \left(j\left|\frac{\partial H}{\partial \hbar\Sigma}\frac{\partial H}{\partial \Delta_0}\right|j\right)\Bigg] \\ = \sum_j & \int d\vec{r}\, u_j(\vec{r}) v_j(\vec{r}), \end{aligned} \tag{A15}$$

since

$$\frac{\partial H}{\partial \Delta_0} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad \frac{\partial H}{\partial \hbar\Sigma} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Combining all results, Eq. (A10) becomes

$$\begin{aligned}\frac{\partial E_g}{\partial \Delta_0} &+ \sum_j N(\hbar\omega_j)\frac{\partial \hbar\omega_j}{\partial \Delta_0} - \frac{1}{2}\langle \psi\psi\rangle_t - \frac{1}{2}\langle \psi^\dagger\psi^\dagger\rangle_t \\ &= \sum_j \int d\vec{r}\, u_j(\vec{r}) v_j(\vec{r})[1+2N(\hbar\omega_j)] - \frac{1}{2}\langle\psi\psi\rangle_t \\ &\quad - \frac{1}{2}\langle \psi^\dagger\psi^\dagger\rangle_t = 0, \end{aligned} \tag{A16}$$

which completes the proof.

To gain even more confidence in our expression for Ω, it is useful to see whether

$$N = \int d\vec{r}\, n(\vec{r}) = \int d\vec{r} \langle \psi^\dagger(\vec{r})\psi(\vec{r})\rangle_t = -\left.\frac{\partial \Omega}{\partial \mu}\right|_{\hbar\Sigma,\Delta_0^\dagger,\Delta_0} \tag{A17}$$

is satisfied. To prove this, we first notice that $n^2(\vec{r}) = (\hbar\Sigma(\vec{r})/2T^{2B})^2$ and that according to the matrix form of the Hamiltonian [cf. Eq. (9)]

$$\frac{\partial \hbar\omega_j}{\partial \mu} = -\frac{\partial \hbar\omega_j}{\partial \hbar\Sigma}. \tag{A18}$$

Therefore, we can make use of our previous results in Eqs. (A5) and (A7) to obtain

$$\begin{aligned}\left.\frac{\partial \Omega}{\partial \mu}\right|_{\hbar\Sigma,\Delta_0^\dagger,\Delta_0} &= \frac{\partial E_g}{\partial \mu} + N(\hbar\omega_j)\frac{\partial \hbar\omega_j}{\partial \mu} \\ &= -\left\{\frac{\partial E_g}{\partial \hbar\Sigma} + N(\hbar\omega_j)\frac{\partial \hbar\omega_j}{\partial \hbar\Sigma}\right\} \\ &= -\sum_j \int d\vec{r}\{[|u_j(\vec{r})|^2 + |v_j(\vec{r})|^2] \\ &\quad \times N(\hbar\omega_j) + |v_j(\vec{r})|^2\} \\ &= -\int d\vec{r}\, n(\vec{r}), \end{aligned}$$

as desired.

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