Bogoliubov inequality and Bose-Einstein condensates with repulsive and attractive interactions

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The Hohenberg theorem on the absence of Bose-Einstein condensation (BEC) in homogeneous systems of space dimensions $D \leqslant 2$ is based on a well-known Bogoliubov inequality. Applied to an assembly trapped in a harmonic potential we show that the Bogoliubov inequality rules out BEC in all dimensions at finite temperatures. However, this conflicting result with both theory and experiment disappears when the effect of the order parameter is properly taken into account in the boson-field commutation relations. For a hard-sphere Bose gas the theory is consistent with the expansion of the condensate when a positive scattering length is increased, as well as the collapse of the condensate when the sign of the scattering length is reversed and it reaches a minimum critical value.

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I. INTRODUCTION

The observation of Bose-Einstein condensation (BEC) in magnetically trapped atomic gases [1–3] has caused renewed theoretical investigations into this unique phenomenon [4]. Questions of a more general nature concern the space dimensionality, the confining potential, the repulsive or attractive character of the atomic forces, the finite particle assembly as it relates to the thermodynamic limit, and the continuous spectrum approximation. A rigorous analysis of BEC dependence upon the space dimension was first carried out by Hohenberg [5]. This work applies to both noninteracting and interacting uniform systems enclosed in a D-dimensional box with periodic boundary conditions. The Hohenberg theorem states that in the thermodynamic limit BEC can occur only in three dimensions (3D). It is based on an exact Bogoliubov inequality [6]. If, given the existence of BEC's order parameter, the inequality is violated, then BEC is ruled out. In other words, the Bogoliubov inequality provides a sufficient condition for the absence of BEC and a necessary condition for its presence.

In the present work we apply the Bogoliubov inequality to an assembly of bosons confined in a harmonic trap (HAT). The Bose-Einstein phase transition strictly takes place in the thermodynamic limit. Since the experiments are performed with finite assemblies of *N* particles, we shall refer to BEC as the macroscopic occupation of the lowest state such that the condensate fraction remains finite in the limit of large *N*. We show that if the boson field satisfies the canonical commutation relations the Bogoliubov inequality rules out BEC in every dimension at finite temperatures. However, this conflicting result with experiment and theory disappears if the order parameter is properly taken into account in the commutation relation. In this fashion, the results found for the ideal Bose gas (IBG) are consistent with current predictions, whether *N* is finite or infinite. The formalism explicitly reveals the role of the interparticle interaction in BEC. In particular, it will be shown that the results are consistent with a recent experiment by Cornish *et al.* on condensates with widely tunable interactions [7]. The outline of the paper is as follows. The basic formalism is presented in Sec. II. In Sec. III we work out the IBG. Section IV deals with interacting systems. Finally, in Sec. V alternative symmetry-breaking methods, other than the Bogoliubov prescription, are discussed in regard to the Bogoliubov inequality.

II. BASIC FORMALISM

We consider an assembly of *N* bosons at temperature *T* below the BEC transition temperature T_c. The number of particles in the ground state, N_0, is then a finite fraction of *N*. The system occupies a *D*-dimensional volume *V*. In space-dependent confining potentials the condensation also takes place in coordinate space. For potentials whose domains are infinite we assume that this condensation allows the definition of an effective *V* such that N/V is kept constant in the thermodynamic limit. In the next section this volume is specifically defined for the case of an isotropic HAT.

The BEC order parameter stems from the observation first made by Dirac that the macroscopic occupation of the lowest state allows one to interpret the zero-mode annihilation and creation operators as *c* numbers whenever $N_0+1\sim N_0$ [8]. In fact, the Dirac ansatz was shown to be asymptotically exact in the thermodynamic limit [9]. Bogoliubov made use of the Dirac ansatz in his pioneering work on the microscopic theory of superfluidity [10]. This procedure became known as the Bogoliubov prescription and has since underlain most of the field-theoretic treatments of BEC. The Bogoliubov prescription breaks the gauge symmetry and leads to the order parameter that characterizes the long-range order of the BEC transition.

Now, according to the Bogoliubov prescription the annihilation and creation operators in momentum space satisfy the commutation relations

$$[b_0,b_0^\dagger]=0, \tag{2.1}$$

$$[b_p,b_q^\dagger]=\delta_{p,q} \quad (p\neq 0), \tag{2.2}$$

$$[b_p,b_q]=[b_p^\dagger,b_q^\dagger]=0. \tag{2.3}$$

Underlying Eq. (2.1) is the Dirac ansatz,

$$b_0=b_0^\dagger=N_0^{1/2}, \tag{2.4}$$

The boson field ψ can be expanded in a complete orthonormal set of single-particle wave functions φ_p that satisfy the boundary conditions on the surface of V,

$$\psi(x)=\sum_p b_p\varphi_p(x), \quad \psi^\dagger(x)=\sum_p b_p^\dagger\varphi_p^*(x). \tag{2.5}$$

From Eqs. (2.1)–(2.3) there follow the commutation relations

$$[\psi(x),\psi^\dagger(y)]=\delta(x-y)-\eta(x,y), \quad \eta(x,y)\equiv\varphi_0(x)\varphi_0^*(y), \tag{2.6}$$

$$[\psi(x),\psi(y)]=[\psi^\dagger(x),\psi^\dagger(y)]=0, \tag{2.7}$$

where φ_0 denotes the single-particle ground-state wave function. Equation (2.6) has been used previously in connection with the homogeneous superfluid ^{4}He [11].

The total particle number operator

$$\hat{N}=\int d^Dx\,\psi^\dagger\psi=\sum_p b_p^\dagger b_p \tag{2.8}$$

satisfies the commutation relations

$$[\hat{N},\psi]=-\psi+\psi_0=-\psi', \quad [\hat{N},\psi^\dagger]=\psi^\dagger-\psi_0^\dagger=\psi'^\dagger, \tag{2.9}$$

where we have split the field operator as

$$\psi=\psi_0+\psi', \quad \psi_0=b_0\varphi_0, \quad \psi'=\sum_{p\neq 0} b_p\varphi_p. \tag{2.10}$$

The counterpart of Eq. (2.4) is the condensate wave function defined by the anomalous average

$$\langle\psi(x)\rangle=\langle\psi_0(x)\rangle=N_0^{1/2}\varphi_0(x). \tag{2.11}$$

The broken gauge symmetry is exhibited by the transformation

$$e^{i\alpha\hat{N}}\psi e^{-i\alpha\hat{N}}=\psi_0+\psi' e^{-i\alpha}, \tag{2.12}$$

where α is an arbitrary real parameter. Since Eq. (2.12) is a consequence of Eq. (2.6), $\eta(x,y)$ plays the role of a symmetry-breaking function.

We next consider the Bogoliubov inequality. It relates ensemble averages at temperature T as follows:

$$\langle\{A^\dagger,A\}\rangle\langle[B^\dagger,[\hat{H},B]]\rangle\geqslant 2k_BT|\langle[A^\dagger,B]\rangle|^2, \tag{2.13}$$

where the curly brackets represent the anticommutator, $\hat{H}$ is the system's Hamiltonian, and the operators A and B are arbitrary provided the ensemble averages exist. This rigorous inequality stems from the Schwarz inequality and the fluctuation-dissipation theorem [5,12]. Hence, it has a general character, the thermal averages applying to both canonical and grand canonical ensembles of either boson or fermion systems. It has been used to prove the absence of long-range order in 1D and 2D superfluids and superconductors [5] as well as in various kinds of magnetic and crystalline ordering [13,14].

Following Chester, Fisher, and Mermin [15] in their reformulation of Hohenberg's work, we choose for A and B the respective Fourier transforms

$$a_k=V^{-1/2}\int d^Dx\,e^{-ikx}\psi(x), \tag{2.14}$$

$$\rho_k=\int d^Dx\,e^{-ikx}\psi^\dagger(x)\psi(x). \tag{2.15}$$

As pointed out by these authors, the wave vector $k(\neq 0)$ may be thought of as an auxiliary mathematical variable that need not label physical momentum states. Hence, it is not restricted by the boundary conditions imposed by the confining potential. The boundary conditions must be satisfied by the single-particle wave functions $\varphi_p(x)$. From Eqs. (2.13)–(2.15) one obtains the usual expression for the Bogoliubov inequality, i.e.,

$$(\langle a_k^\dagger a_k\rangle+\tfrac{1}{2})\langle[\rho_k^\dagger,[\hat{H},\rho_k]]\rangle\geqslant|\langle[a_k^\dagger,\rho_k]\rangle|^2k_BT. \tag{2.16}$$

Now, from Eqs. (2.5) and (2.14) one has

$$\langle a_k^\dagger a_k\rangle=\frac{1}{V}\sum_{p,q}\langle b_p^\dagger b_q\rangle\int\int d^Dx\,d^Dy\,e^{ik(x-y)}\varphi_p^*(x)\varphi_q(y), \tag{2.17}$$

and from the completeness relation of $\varphi_p(x)$ it follows immediately that

$$\int\frac{d^Dk}{(2\pi)^D}\langle a_k^\dagger a_k\rangle=\frac{1}{V}\sum_p\langle b_p^\dagger b_p\rangle=\frac{N}{V}\equiv n, \tag{2.18}$$

where $N=\langle\hat{N}\rangle$. This is a subtle result because the (continuum) k integration is related to the possibly discrete summation over p states. Indeed, as stressed in [15], the wave vector k can assume a continuum of values even when the confining potential is finite. Combining Eqs. (2.16) and (2.18) we arrive at the inequality

$$n\geqslant\int\frac{d^Dk}{(2\pi)^D}\left(\frac{|\langle[a_k^\dagger,\rho_k]\rangle|^2k_BT}{\langle[\rho_k^\dagger,[\hat{H},\rho_k]]\rangle}-\frac{1}{2}\right). \tag{2.19}$$

From the above remarks it is important to realize that Eq. (2.19) implies neither the thermodynamic limit nor the continuous spectrum approximation of the actual physical system. Hence, it can be applied to finite-(N,V) systems. The Bogoliubov inequality is then satisfied if the following integral is finite:

$$I_D\equiv\frac{k_BT}{(2\pi)^D}\int d^Dk\,\frac{|\langle[a_k^\dagger,\rho_k]\rangle|^2}{\langle[\rho_k^\dagger,[\hat{H},\rho_k]]\rangle}<\infty. \tag{2.20}$$

The denominator of the integrand depends on the system's Hamiltonian. On the other hand, the numerator has a general expression in terms of the single-particle ground-state wave function. From Eqs. (2.5)–(2.7) and (2.11) we readily obtain

$$|\langle[a_k^\dagger,\rho_k]\rangle|^2=\frac{N_0}{V}\left(\int d^Dx\,\varphi_0^*(x)-\int\int d^Dx\,d^Dy\,e^{ik(x-y)}\varphi_0^*(x)|\varphi_0^*(y)|^2\right)^2, \tag{2.21}$$

where the double integral comes from $\eta(x,y)$ in Eq. (2.6). Thus, the numerator in Eq. (2.20) depends linearly on N_0. If the integral (2.20) diverges one must then assume that $N_0=0$, which means that BEC is ruled out.

It is clear from Eq. (2.16) that

$$\langle[\rho_k^\dagger,[\hat{H},\rho_k]]\rangle\geqslant 0. \tag{2.22}$$

This thermal average plays a key role because it underlies the convergence or divergence of Eq. (2.20). In homogeneous systems Eq. (2.22) is, in general, identical to the *f*-sum rule. It will be shown that the inequality (2.22), by itself, furnishes additional information on BEC of inhomogeneous systems in a HAT.

III. IDEAL BOSE GAS

We consider an assembly of N bosons of mass m confined in a D-dimensional isotropic HAT with angular frequency ω at temperature $T<T_c$. The Hamiltonian then equals

$$\hat{H}_0=\hat{N}\hbar\omega. \tag{3.1}$$

The zero-point energy is irrelevant because $\hat{H}_0$ enters the calculations only through commutators. The single-particle ground-state wave function is given by

$$\varphi_0(x)=(\pi l^2)^{-D/4}e^{-x^2/2l^2}, \tag{3.2}$$

where the average width of the Gaussian is

$$l=\left(\frac{\hbar}{m\omega}\right)^{1/2}. \tag{3.3}$$

The symmetry-breaking function in Eq. (2.6) is now real, i.e., $\eta(x,y)=\varphi_0(x)\varphi_0(y)=\eta(y,x)$, and the fundamental commutation relation of the condensed system becomes

$$[\psi(x),\psi^\dagger(y)]=\delta(x-y)-\left(\frac{m\omega}{\pi\hbar}\right)^{D/2}e^{-m\omega(x^2+y^2)/2\hbar}. \tag{3.4}$$

Given the Bogoliubov prescription this result is exact. In a homogeneous system confined in a box of volume L^{-D}, with periodic boundary conditions, the symmetry-breaking function equals $\eta=L^{-D}$. The periodic boundary conditions allow an arbitrarily large box so that L^{-D} is usually neglected, as in the case of the Hohenberg work. In Eq. (3.4), however, η cannot be neglected. In fact, η will be necessary in obtaining results in agreement with current predictions.

As advanced in the beginning of Sec. II, a finite volume V can be defined by virtue of the condensation in coordinate space. For the isotropic HAT the condensate is symmetrically distributed within a D-dimensional sphere centered at the origin. The noncondensate behaves as a saturated vapor surrounding the condensate [16,17]. Hence, one can define a spherical volume V that contains an average of N_0 condensed particles and $N-N_0$ excited ones. This can be accomplished by introducing a range parameter R associated with the harmonic potential in the form [18]

$$V(x)=\frac{1}{2}m\omega^2x^2=\frac{1}{2}V_0\left(\frac{x}{R}\right)^2. \tag{3.5}$$

The energy V_0 is constant and R equals

$$R=\frac{1}{\omega}\left(\frac{V_0}{m}\right)^{1/2}. \tag{3.6}$$

For $D\geqslant 2$ the thermodynamic limit is achieved when $N\to\infty$ and $\omega\to 0$ such that $N\omega^D$ is kept constant [19]. In this case N/R^D can be interpreted as an average density that remains fixed in the thermodynamic limit. Accordingly, we take for V the D-dimensional spherical volume with radius R,

$$V=\frac{2\pi^{D/2}}{D\Gamma(D/2)}R^D, \tag{3.7}$$

where Γ is the gamma function. The probability of finding a particle in the exterior of V must be negligible. Since I_D will depend only on $\varphi_0(x)$, it is thus required that $|\varphi_0(x)|^2\sim 0$, $x\geqslant R$. The ratio between Eqs. (3.3) and (3.6) is

$$\frac{l}{R}=\left(\frac{\hbar\omega}{V_0}\right)^{1/2}\propto N^{-1/(2D)}. \tag{3.8}$$

The proportionality sign stems from constant $N\omega^D$. For large N then $R\gg l$. As an illustration we take $R=5l$ (e.g., $N\sim 10^6$ and $l/R\sim 2N^{-1/6}$ in 3D), so that $|\varphi_0(5l)/\varphi_0(0)|^2=e^{-25}\sim 10^{-11}$. Therefore the probability of finding a particle on the surface of V is 10^{-11} smaller than that at its center [20].

Hereafter we assume that φ_0 is vanishingly small on the surface of V. In this fashion the integration of the Gaussian functions can be performed over their entire range. Accordingly, substitution of Eq. (3.2) in Eq. (2.21) leads to the Fourier transform of Gaussian functions. For convenience to the reader we quote the specific transform:

$$\int d^Dx\,e^{ikx}\varphi_0^n(x)=[2n^{-1}(\pi l^2)^{1-(n/2)}]^{D/2}e^{-l^2k^2/2n}. \tag{3.9}$$

The integrals in Eq. (2.21) then yield

$$|\langle[a_k,\rho_k]\rangle|^2=2^{D-1}\Gamma(D/2)N_0\left(\frac{\hbar\omega}{V_0}\right)^{D/2}(1-e^{-3l^2k^2/4})^2. \tag{3.10}$$

In the evaluation of $\langle[\rho_k^\dagger,[\hat{N},\rho_k]]\rangle$ it is convenient to consider the general commutation relation (2.6) instead of Eq. (3.4). From Eqs. (2.6), (2.8), and (2.15), we have

$$[\hat{N},\rho_k]=\int\int d^Dx\, d^Dy\, e^{-iky}[\eta^*(x,y)\psi^\dagger(y)\psi(x)-\text{H.c.}], \tag{3.11}$$

where H.c. denotes Hermitian conjugation. By making use of the orthonormal property of $\varphi_p(x)$, the x integration yields

$$[\hat{N},\rho_k]=\sqrt{N_0}\int d^Dy\, e^{-iky}(\varphi_0\psi^\dagger-\varphi_0^*\psi). \tag{3.12}$$

Equation (3.11) is crucial: if $\eta(x,y)$ were absent from Eq. (2.6), the commutator $[\hat{N},\rho_k]$ would vanish identically. Hence, Eq. (2.16) would be only satisfied at $T=0$, namely, BEC could occur only at absolute zero. This shows that the last term in Eq. (3.4) plays a key role.

Now, the second commutator is readily obtained from Eqs. (2.15) and (3.12), i.e.,

$$[\rho_k^\dagger,[\hat{N},\rho_k]]=2N_0-\sqrt{N_0}\int\int d^Dx\, d^Dy\, e^{ik(x-y)}\times[\eta(x,y)\varphi_0(y)\psi^\dagger(x)+\text{H.c.}]. \tag{3.13}$$

By taking the ensemble average only the zero-mode amplitudes do not vanish and we obtain

$$\langle[\rho_k^\dagger,[\hat{N},\rho_k]]\rangle=2N_0\left(1-\int\int d^Dx\, d^Dy\, e^{ik(x-y)}|\eta(x,y)|^2\right), \tag{3.14}$$

and from Eqs. (3.1) and (3.14) there follows the general expression

$$\langle[\rho_k^\dagger,[\hat{H}_0,\rho_k]]\rangle=2N_0\hbar\omega\left(1-\left|\int d^Dx\, e^{ikx}|\varphi_0(x)|^2\right|^2\right). \tag{3.15}$$

Now, making use of the specific function (3.2) one has, from Eq. (3.9),

$$\langle[\rho_k^\dagger,[\hat{H}_0,\rho_k]]\rangle=2N_0\hbar\omega(1-e^{-l^2k^2/2}). \tag{3.16}$$

Finally, combining Eqs. (3.10) and (3.16), and performing the angle-variable integration, Eq. (2.20) yields

$$I_D=\frac{Dk_BT(\hbar\omega)^{(D/2)-1}}{2\pi^{D/2}V_0^{D/2}}\int_0^\Lambda dk\, k^{D-1}\frac{(1-e^{3l^2k^2/4})^2}{1-e^{-l^2k^2/2}}, \tag{3.17}$$

where Λ is the ultraviolet cutoff. This cutoff is justified by the following argument. Ultraviolet divergences do not occur in condensed matter physics due to the intrinsic upper cutoff, which is the inverse of a typical interparticle distance. Hence, an ultraviolet cutoff can be introduced in the p summation of the physical p states in Eq. (2.18). Since the k integration of the auxiliary wave vector is connected to the p summation by Eq. (2.18), it is then natural to extend the cutoff to the k integral. In fact, the k integral first introduced by Chester, Fisher, and Mermin displays such an upper cutoff [15].

The integral in Eq. (3.17) is discussed in the Appendix. It does not exhibit any infrared divergence and is independent of N. The behavior of I_D is then dictated by $\omega^{(D/2)-1}$. For a constant potential I_D is convergent whether N is finite or infinite. Thus the Bogoliubov inequality is satisfied in all dimensions. Only the standard thermodynamic limit ($N\to\infty$, $\omega\to 0$, and $N\omega^D$ constant) rules out BEC in 1D. But this criterion applies only in 2D and 3D, whereby T_c remains constant in this limit. These results are consistent with the work of Ketterle and van Druten [21].

IV. INTERACTING BOSE GAS

In this section the Bose gas in the isotropic HAT is endowed with a two-particle interaction $U(|x-y|)$. It is straightforward to verify that the general expression for the associated second quantized operator $\hat{U}$ contributes to Eq. (2.22) only if $\eta\neq 0$. Thus η makes the Bogoliubov inequality interaction dependent. We shall assume a contact interaction defined by the pseudopotential $U(x,y)=U_0\delta(x-y)$. In 3D this corresponds to the first order of a hard-sphere Bose gas (HSBG) in the limit of low densities and temperatures [22]. In 2D and 1D the respective hard-disk and hard-rod interactions are more complex and may not be physically realistic. By contrast, the HSBG model is simple and yet useful in the analysis of most experimental data. Nevertheless, we shall work out the general formalism in D dimensions but applications will be performed in 3D only. Accordingly, the pseudopotential leads to the interaction operator

$$\hat{U}=\tfrac{1}{2}U_0\int d^Dx\, \psi^\dagger\psi^\dagger\psi\psi. \tag{4.1}$$

In 3D the interaction constant equals

$$U_0=\frac{4\pi a\hbar^2}{m}, \tag{4.2}$$

where the hard-sphere diameter equals the s-wave scattering length a. If $a>0$ ($a<0$) the interaction corresponds to an effective repulsion (attraction).

We next determine the contribution of Eq. (4.1) to Eq. (2.22). In the evaluation of $[\hat{U},\rho_k]$ the δ-function contribution of Eq. (2.6) vanishes identically, as expected in the normal phase. Using the notation

$$\int d^Dx\equiv\int_x, \tag{4.3}$$

the η function in Eq. (2.6) yields

$$[\hat{U},\rho_k]=U_0\int_x\int_y e^{-iky}[\psi^\dagger(y)\eta(y,x)|\psi(x)|^2\psi(x)-\text{H.c.}]. \tag{4.4}$$

After lengthy but straightforward algebra Eq. (2.22) becomes

$$\langle[\rho_k^\dagger,[\hat{U},\rho_k]]\rangle = U_0\int_x\int_y\langle\psi^\dagger(x)|\psi(x)|^2\eta(x,y)\psi(y)+\text{H.c.}\rangle \tag{4.5a}$$

$$-U_0\int_x\int_y e^{ik(x-y)} \times\langle\psi^\dagger(x)|\psi(x)|^2\eta(x,y)\psi(y)+\text{H.c.}\rangle \tag{4.5b}$$

$$+2U_0\int_x\int_y\int_z e^{ik(z-y)}\langle\psi^\dagger(y)\eta(y,x) \times|\psi(x)(x)|^2\eta(x,z)\psi(z)+\text{H.c.}\rangle \tag{4.5c}$$

$$-U_0\int_x\int_y\int_z e^{ik(z-y)} \times\langle\psi^\dagger(x)\psi^\dagger(x)\eta(x,y)\psi(y)\eta(x,z)\psi(z) +\text{H.c.}\rangle \tag{4.5d}$$

$$-U_0\int_x\int_y\int_z e^{ik(z-y)} \times\langle\psi^\dagger(x)|\psi^\dagger(x)|^2\eta(x,y)\eta(y,z)\psi(z) +\text{H.c.}\rangle. \tag{4.5e}$$

The Hermitian conjugate terms simply have the effect of multiplying the thermal averages of the integrals in Eq. (4.5) by a factor of 2. Substituting the field operators by the expansion (2.5) and denoting the (4.5a)–(4.5e) terms, respectively, by

$$\langle[\rho_k^\dagger,[\hat{U},\rho_k]]\rangle = Q_a+Q_b+Q_c+Q_d+Q_e, \tag{4.6}$$

we finally obtain

$$Q_a=2U_0\sum_{pqr}\langle b_p^\dagger b_q^\dagger b_r b_0\rangle\int_x\varphi_p^*\varphi_q^*\varphi_r\varphi_0, \tag{4.7a}$$

$$Q_b=-2U_0\sum_{pqrs}\langle b_p^\dagger b_q^\dagger b_r b_s\rangle\int_x e^{ikx}\varphi_p^*\varphi_q^*\varphi_r\varphi_0\int_y e^{-iky}\varphi_0^*\varphi_s, \tag{4.7b}$$

$$Q_c=4U_0\sum_{pqrs}\langle b_p^\dagger b_q^\dagger b_r b_s\rangle\int_x|\varphi_0|^2\varphi_q^*\varphi_r \times\int_y e^{-iky}\varphi_p^*\varphi_0\int_z e^{ikz}\varphi_0^*\varphi_s, \tag{4.7c}$$

$$Q_d=-2U_0\sum_{pqrs}\langle b_p^\dagger b_q^\dagger b_r b_s\rangle\int_x\varphi_p^*\varphi_q^*\varphi_0^2 \times\int_y e^{-iky}\varphi_0^*\varphi_r\int_z e^{ikz}\varphi_0^*\varphi_s, \tag{4.7d}$$

$$Q_e=-2U_0\sum_{pqrs}\langle b_p^\dagger b_q^\dagger b_r b_s\rangle\int_x\varphi_p^*\varphi_q^*\varphi_r\varphi_0 \times\int_y e^{-iky}|\varphi_0|^2\int_z e^{ikz}\varphi_0^*\varphi_s. \tag{4.7e}$$

These equations allow one to separate Eq. (4.6) into powers of N_0 in the form

$$\langle[\rho_k^\dagger,[\hat{U},\rho_k]]\rangle = U_0 l^{-D}(N_0^2W_0+N_0W_1+W_2), \tag{4.8}$$

where W_i $(i=0,1,2)$ are dimensionless quantities independent of N_0. The $N_0^2W_0$ term corresponds to the ground-state contribution. In this case Eq. (4.7) shows that $Q_c+Q_d+Q_d$ vanishes identically and Q_a+Q_b gives

$$W_0=2l^D\left(\int_x|\varphi_0|^4-\int_x e^{ikx}|\varphi_0|^4\int_y e^{-iky}|\varphi_0|^2\right). \tag{4.9}$$

N_0W_1 results from the interaction between the condensed and uncondensed particles. After some algebra it follows from Eq. (4.7) that

$$W_1=4l^D\sum_{p\neq 0}\langle b_p^\dagger b_p\rangle\left(\int_x|\varphi_0|^2|\varphi_p|^2 - \int_x e^{ikx}|\varphi_0|^2|\varphi_p|^2\int_y e^{-iky}|\varphi_0|^2 - \int_x e^{ikx}\varphi_p^*|\varphi_0|^2\varphi_0\int_y e^{-iky}\varphi_0^*\varphi_p + \int_x|\varphi_0|^4|\int_y e^{iky}\varphi_0^*\varphi_p|^2 - \int_x\varphi_p^*|\varphi_0|^2\varphi_0\int_y e^{-iky}|\varphi_0|^2\int_z e^{ikz}\varphi_0^*\varphi_p\right). \tag{4.10}$$

The W_2 contribution comes from interactions among excited particles, where none of the summation indices in Eq. (4.7) represents the lowest state.

The ground state is nondegenerate and φ_0 is presumably an even and positive function. On the other hand, excited states are degenerate where φ_p corresponds to a set of quantum numbers $p=\{p_1,\cdots,p_D\}$. Hence, φ_p can be represented by a linear combination of even and odd functions, $\varphi_p=\varphi_p^{(+)}+\varphi_p^{(-)}$. By expanding the exponential functions in Eq. (4.10) the imaginary part vanishes and the only contribution comes from the real part that corresponds to the cosine expansion. Due to the orthonormal property of φ_p the k-independent term cancels out and the leading term W_1' becomes

$$W_1' = 4l^D \frac{k^2}{2!} \sum_{p\neq 0} \langle b_p^\dagger b_p \rangle \bigg(\int_x x^2 |\varphi_0|^2 |\varphi_p|^2 + \int_x |\varphi_0|^2 |\varphi_p|^2 \int_y y^2 |\varphi_0|^2 + \int_x |\varphi_0|^2 \bigg| \int_y y \varphi_0^* \varphi_p^{(-)} \bigg|^2 + \int_x \varphi_p^{(+)*} |\varphi_0|^2 \varphi_0 \int_y y^2 \varphi_0^* \varphi_p^{(+)} - \int_x x \varphi_p^{(-)*} |\varphi_0|^2 \varphi_0 \int_y y \varphi_0^* \varphi_p^{(-)} \bigg). \tag{4.11}$$

Now, since φ_p is normalized, the y integral in Eq. (4.9) cannot be greater than unity. In addition, the second x integral in Eq. (4.9) cannot be greater than the first x integral. Therefore, $W_0 > 0$. Clearly, $W_1' > 0$, and one might expect that $W_1 > 0$, too. In any event, $N_0^2 W_0 > N_0 W_1 + W_2$, so that the sign of Eq. (4.8) is dictated by U_0. This is ensured by the following argument. Previous results show that the density distribution of the condensate appears as a sharp peak superimposed on the broad distribution of the thermal cloud. As T decreases the height of the condensate peak increases while the tails of the thermal component diminish and eventually disappear at very low temperatures [4,23]. Therefore, $N - N_0 \ll N_0$ in the region occupied by the condensate.

We next apply the above results to the 3D case. The numerator of the I_3 integral is given by Eq. (2.21) and the denominator by Eqs. (3.15) and (4.8). The last then reads

$$\hbar\omega K + \frac{4\pi a \hbar^2}{ml^3}(N_0 W_0 + W_1 + N_0^{-1} W_2) \geqslant 0, \tag{4.12}$$

where the inequality comes from Eq. (2.22) and K denotes twice the expression within the parentheses in Eq. (3.15). Taking into account Eq. (3.3) and neglecting $N_0^{-1} W_2$ we rewrite Eq. (4.12) as

$$\chi \equiv \frac{4\pi a}{lK}(N_0 W_0 + W_1) \geqslant -1. \tag{4.13}$$

This parameter is proportional to the ratio between the interaction and kinetic-energy averages. It is then a useful quantity in modeling the experiments. For instance, if $\chi \gg 1$ the Thomas-Fermi approximation greatly simplifies the mean-field predictions [24–26].

For $a > 0$, the condition (4.13) is obviously satisfied. Repulsive interactions decrease I_3 and hence favor the occurrence of BEC.

For attractive interactions ($a < 0$) Eq. (4.13) leads to a maximum number of condensed particles determined by $\chi = -1$. Beyond this critical number the condensate becomes unstable against collapse. Thus, for $a < 0$, Eq. (4.13) gives

$$\frac{N_0 |a|}{l} \leqslant \frac{K}{4\pi W_0} - \frac{|a| W_1}{l W_0}. \tag{4.14}$$

We now carry out an estimate of the Eq. (4.14) upper bound. Since $|a| \ll l$, we neglect the second term in the right side of Eq. (4.14). The first term depends only on the single-particle ground-state wave function. We take for the latter the noninteracting function (3.2). Accordingly, K is obtained from Eq. (3.16) while the integrals in Eq. (4.9) are of the form (3.9). The result is

$$\frac{K}{W_0} = (2\pi)^{3/2} \frac{1 - e^{-l^2 k^2/2}}{1 - e^{-3l^2 k^2/8}}. \tag{4.15}$$

The fraction lies in the interval $[1, \frac{4}{3}]$ and N_c must correspond to the lower limit. Thus, to lowest order, one has

$$\frac{N_c |a|}{l} = \sqrt{\pi/2} = 1.25. \tag{4.16}$$

This is about twice the values obtained by the numerical solution of the Gross-Pitaevskii equation [27,28], as well as by variational estimates [4,25,29–31] and the use of an effective potential [32]. Considering the approximations involved, especially the neglect of W_1 / W_0, which is expected to decrease N_c, the (4.16) estimate is not unreasonable. The N_c barrier is by now well established. For ^{7}Li atoms ($a = -1.46$ nm and $l = 3\ \mu$m [2]) one has $N_c \sim 1300$ [33–35]. Although this represents few particles in comparison with the $a > 0$ condensates, the Bogoliubov prescription still holds because the condition $N_0 + 1 \sim N_0$ is valid even in this case.

We finally conclude this section by showing that the Bogoliubov inequality is consistent with previous theoretical and experimental results.

To first order in scattering length the HSBG leads to the mean-field theory described by the Gross-Pitaevskii equation. Numerical solution of this equation for repulsive interactions ($a > 0$) reveals a broadening of the condensate peak with a consequent reduction of the density as a increases. For attractive interactions ($a < 0$) the behavior is the opposite: the peak narrows and the density increases [4]. For $a > 0$ excellent agreement has been found between the numerical solution and the experimental results [36]. Such a density variation is consistent with the lower bound of n given by the Bogoliubov inequality, Eq. (2.19). For $a > 0 (a < 0)$ the denominator (4.12) decreases (increases) I_3, thereby decreasing (increasing) the lower bound of Eq. (2.19).

In a recent experiment Cornish *et al.* were able to reverse the sign of the scattering length in condensed ^{85}Rb [7]. When a was switched from repulsive to attractive there was a critical point where the condensate first collapsed and subsequently emitted a burst of high-energy atoms, leaving a smaller condensate at the core. On again reversing a up to the repulsive regime the core reexpanded with increasing a. Now, let N_0 be fixed in a 3D isotropic HAT. As a decreases so does $\chi \propto a N_0$ and I_3 increases. The collapse of the condensate takes place at a critical scattering length $a_c < 0$, such that $a_c N_0$ reaches its minimum value determined by $\chi = -1$. At this point I_3 diverges and thereby Eq. (2.19) implies an infinite density (the collapse). The stability condition ($\chi > -1, I_3 < \infty$) can be restored by a sudden decrease of the condensed particles (the burst). A subsequent increase of a

allows an increase of the condensate (core). When the scattering length becomes positive the number of condensed particles is no longer limited by Eq. (4.13). As a increases further toward the Feshbach resonance the density lower bound diminishes with decreasing I_3. Hence, the condensate can expand by an increase of N_0 and/or by a decrease in density.

V. DISCUSSION

The foregoing theory is based on the Bogoliubov prescription and its effect on the field commutation relation. Given the Bogliubov prescription the general formalism in Sec. II is exact. The function η in Eq. (2.6) plays a key role. If $\eta=0$, the Bogoliubov inequality rules out BEC in noninteracting and interacting systems at finite temperatures in all HAT dimensions. An important and unique consequence of $\eta\neq 0$ consists in the dependence of the Bogoliubov inequality on the interparticle interaction. In particular, it reveals the drastically distinct behavior when the sign of the s-wave scattering length is reversed.

In addition to the Bogoliubov prescription there are two alternative methods that also break the gauge symmetry of Bose assemblies. One may then inquire into the effect of these procedures upon the Bogoliubov inequality.

One such method is the shift transformation [37]. Denoting by $c_k, c_k^\dagger$ the standard Bose amplitudes the transformation acts on the zero mode $c_0\to b_0+\sqrt{N_0}$, such that $\langle c_0\rangle=0$ and $\langle b_0\rangle=\sqrt{N_0}$. Since this transformation preserves the canonical commutation relations the Bogoliubov inequality implies the absence of BEC in HATs for $T>0$.

The other method consists in removing the gauge group by adding to the Hamiltonian a small perturbation of the form [38]

$$\hat{H}_{\rm SB}=-\int d^D x(\zeta\psi^\dagger+\zeta^*\psi), \tag{5.1}$$

where ζ is a fictitious field. The total Hamiltonian then reads $\hat{H}=\hat{H}_0+\hat{U}+\hat{H}_{\rm SB}$, where $\hat{H}_{\rm SB}$ stabilizes the anomalous averages (2.11). In analogy with magnetic systems, the symmetry-breaking field ζ is allowed to vanish at the end of the calculations. As in the shift transformation, neither $\hat{H}_0$ nor $\hat{U}$ contributes to Eq. (2.22) on account of the canonical commutation relations. On the other hand, one can readily show that $\hat{H}_{\rm SB}$ leads to

$$\langle[\rho_k^\dagger,[\hat{H},\rho_k]]\rangle=\int d^D x(\zeta\langle\psi^\dagger\rangle+\zeta^*\langle\psi\rangle). \tag{5.2}$$

Therefore, the denominator in Eq. (2.20) becomes k independent as well as the numerator, for the double integral in Eq. (2.21) is absent when $\eta=0$. The integral in Eq. (2.20) then equals a D-dimensional spherical volume whose radius is the ultraviolet cutoff. Clearly, I_D diverges with $\zeta\to 0$, and the Bogoliubov inequality rules out BEC for $T>0$.

We are thus led to conclude that only through the Bogoliubov prescription, and when it is properly accounted for by the field commutation relation (2.6), does the Bogoliubov inequality become consistent with current theoretical and experimental results. On one hand, this conclusion singles out the Bogoliubov prescription among other symmetry-breaking procedures. On the other hand, it strengthens the commutation relation (2.6) that underlies the present work.

APPENDIX: THE INTEGRAL IN EQ. (3.17)

In this Appendix we find a close estimate for the integral in Eq. (3.17), i.e.,

$$J_D\equiv\int_0^\Lambda dk\, k^{D-1}\frac{(1-e^{-3l^2k^2/4})^z}{1-e^{-l^2k^2/2}}. \tag{A1}$$

In terms of the variable

$$u\equiv e^{-l^2k^2/4}, \tag{A2}$$

the fraction in Eq. (A1) becomes

$$\begin{aligned}\frac{(1-u^3)^2}{1-u^2}&=-u^4-u^2+2u+1+\frac{2}{1+u}\\&=1-u^2-u^4+2u^2(1-u+u^2-u^3+\cdots).\end{aligned} \tag{A3}$$

We see from Eq. (A3) that the cutoff is only needed for the integration of the u-independent term. In regard to the terms $k^{D-1}u^n$ we let $\Lambda\to\infty$, so that

$$\int_0^\infty dk\, k^{D-1}u^n=\frac{2^{D-1}\Gamma(D/2)}{l^D n^{D/2}}. \tag{A4}$$

From Eqs. (A1)–(A4) and after a slight rearrangement we finally obtain

$$J_D=\frac{\Lambda^D}{D}+\frac{2^D\Gamma(D/2)}{l^D}\left(1-\frac{1}{2^{(D/2)+1}}-\frac{1}{2^{D+1}}-S_D\right), \tag{A5}$$

where S_D stands for the convergent series

$$S_D=1-\frac{1}{2^{D/2}}+\frac{1}{3^{D/2}}-\frac{1}{4^{D/2}}+\cdots. \tag{A6}$$

The values in each dimension are

$$S_1=(1-2^{1/2})\zeta(1/2)=0.605, \tag{A7}$$

$$S_2=\ln 2=0.693, \tag{A8}$$

$$S_3=(1-2^{-1/2})\zeta(3/2)=0.765, \tag{A9}$$

where ζ is the Riemann zeta function.

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