Bose-Einstein condensation in a trap: the case of a dense condensate

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We consider the Bose-Einstein condensation of atoms in a trap where the density of particles is so high that the low-density approach of Gross [J. Math. Phys. (N.Y.) **4**, 195 (1963)] and Pitaevskii (V. L. Ginsburg and L. P. Pitaevskii, Zh. Éksp. Teor. Fiz. **34**, 1240 (1958) [Sov. Phys. JETP **7**, 1858 (1958)]) will not be applicable. For this purpose we use the slave boson representation which is valid for hard-core bosons at any density. This description leads to the same results as the Gross-Pitaevskii approach in the low-density limit, but for higher densities, it predicts the depletion of the condensate in the regions where the density of the atomic cloud is high. [S1050-2947(97)07408-8]

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I. INTRODUCTION

Atoms in a magnetic trap present an interesting system for the analysis of highly degenerate gases. The trap plays the role of a three-dimensional confining potential well and by using advanced experimental techniques, such as laser and evaporative cooling, it is possible to study the gas over a wide range of parameters, such as temperature or density of particles. One of the most spectacular achievements of such techniques was the observation of the Bose-Einstein (BE) condensation in gases composed of alkali-metal atoms [1]. BE condensation, originally studied in terms of the ideal (noninteracting) Bose gas, requires a minimal density of bosons $\rho_0 = g_{3/2}(1)/\lambda^3$, where $\lambda = (2\pi\hbar^2/mk_BT)^{1/2}$ is the de Broglie wave length and $g_{3/2}(1) \approx 2.612$. On the other hand, it is known that the density of the condensate in an interacting Bose gas at high density is depleted if the total density exceeds a certain value. For instance, the condensate in the bulk of ^{4}He is only about 10% at zero temperature. On the surface, however, the condensate can reach almost 100% because of the reduced total density. This phenomenon was observed in numerical simulations of an interacting Bose gas [2] and in analytic calculations including an attractive interaction [3] or in a slave boson approach to a hard-core Bose gas [4]. The effect can be understood as a reduction of long-range correlations, necessary for the formation of a condensate, which is caused by increasing fluctuations due to an increasing density of interacting particles. There is an approach to the dilute interacting Bose gas due to Ginzburg and Pitaevskii [5] and Gross [6], analogous to the Ginzburg-Landau approach for second-order phase transitions. As in the general Ginzburg-Landau approach, the Gross-Pitaevskii (GP) approach is an expansion in powers of the order parameter field up to fourth order. It works very well close to the critical point, however, away from it, where the order parameter is not small anymore, it may significantly deviate from the correct result. This is not a problem in a homogeneous system with a uniform order parameter, since we can restrict the theory to a regime where the order parameter is small. In an inhomogeneous system, e.g., in a trap, the order parameter varies in the system. Therefore, it is not sufficient, unless the system is very dilute, to assume that the order parameter is small in some spatial region because it can be large in another region of the system. The interparticle interactions in the GP approach are approximated by a hard-core two-body potential with contributions only from the s-wave scattering length. This approximation is quite satisfactory for the extremely dilute gases satisfying the condition $na^3 \ll 1$, where n is a density of particles and a is the scattering length. The physical implication of this condition is that it is highly improbable for three or more particles to interact with each other simultaneously. Therefore, it is clear that as the density of particles in the condensate increases, the likelihood of the three-body and higher-order interactions will also increase, making it necessary to go beyond the GP approach. Even though the recent experiments on the BE in magnetic traps were based on dilute systems of bosons with $na^3 \approx 10^{-6}$, it is foreseeable that experiments can be performed where the Bose gas is dense. This is already indicated by the history of these experiments: the number of particles in the condensate has increased by three orders of magnitude [7], as compared to the early results. In this context it is interesting to study the condensate including higher-order interaction effects, expected in systems at higher density. The purpose of this article is to apply a method, which goes beyond the GP approach, to analyze an interacting Bose gas in a trap at arbitrary densities.

The rest of the paper consists of two parts: in the first (Sec. II) part we discuss the case of a dilute Bose gas using the GP approach. This includes a mean-field theory based on the nonlinear Schrödinger equation and the Thomas-Fermi approximation. In the second part (Sec. III) the Bose gas with hard-core interaction is defined as a functional integral in a slave boson representation. From the latter we derive an effective functional integral for the order-parameter field which describes the BE condensate. The new effective functional integral, which also constitutes the main result of this work, is valid for an arbitrary condensate density, and takes account of the three-body and higher-order effects in the interparticle interactions, at a finite temperature. We apply this approach to the problem of BE condensation in a trap in Sec. III A, and study the behavior of the condensate wave function as a function of chemical potential (which controls the particle density) by means of a mean-field theory based on the Thomas-Fermi approximation again. However, like the GP approach, the limitation of the present work is its inabil-

ity to account for the effects of the atoms outside of the condensate on the condensate itself. Such an extension will be the subject of a future publication.

II. DILUTE BOSE GAS

The Bose gas, defined as a grand canonical ensemble of bosons, can be described in second quantization, for instance, using a functional integral representation [8]. The fluctuations with respect to time (i.e., quantum fluctuations) have a gap $k_B T$ at nonzero temperature T due to the Matsubara frequencies $\omega_n = n k_B T$ ($n = 0, 1, \ldots$). The condensation of bosons is characterized by a spontaneous breaking of a $U(1)$ symmetry (the phase degree of freedom of the complex boson field). This implies a Goldstone mode which describes gapless fluctuations in space. Thus the latter fluctuations are relevant for the condensation, whereas the fluctuations with $\omega_n \neq 0$ can be neglected because of the gap $k_B T$. Thus it is sufficient to consider the ω_0 component of the quantum field $\Phi(x, \omega_0) \equiv \Phi_x$, since we are only interested in static properties of the condensate near the phase transition. This approximation has been used in the discussion of the condensation of a Bose gas in translational invariant systems [5,6] as well as in a harmonic trap [9–12].

As an introduction, we present the GP approach of a grand canonical Bose gas. The latter is defined by the partition function [8]

$$ Z = \int e^{-S_{GP}} \prod_x d\Phi_x d\Phi_x^* . \tag{1} $$

The bosons in the condensate are described by the complex field Φ, which is controlled by the GP action of a dilute hard-core Bose gas [5,6]

$$ S_{GP} = \sum_{x,x'} \Phi_x t_{x,x'} \Phi_{x'}^* - \sum_x \left(\mu |\Phi_x|^2 - \frac{u}{2} |\Phi_x|^4 \right). \tag{2} $$

Since this model is based on a Bose gas with hard-core interaction [13], only three independent parameters enter: the chemical potential μ, the scattering length of the hard-core interaction a, and the mass of the bosons. The coupling constant u is proportional to the scattering length [13], whereas the mass enters into the hopping rate $\tau = \Sigma_x t_{x,x'} < 0$, which has the same energy scale as μ. Formally, the action (2) is defined on a lattice with lattice constant a. This is a good approximation of the hard-core gas with scattering length a if one is only interested in length scales large compared to a. This is the case in the experiments because the typical size of the condensate is 5×10^{-4} cm, whereas $a \approx 5 \times 10^{-7}$ cm [10]. Usually the hopping term $\Sigma_{x,x'} \Phi_x t_{x,x'} \Phi_{x'}^*$ is replaced by the continuum approximation $\Phi_x \tau [1 + (1/6a^2) \nabla^2] \Phi_x^*$ and the sum by a formal integral, for simplicity.

The magnetic trap can be modeled by introducing a confining potential V_x, for instance, a harmonic potential. It is convenient to use a dimensionless expression for the action in Eq. (2) as given in Refs. [9,10]. The parameters of a gas with about 5000 ^{87}Rb atoms, studied in the experiment by Anderson et al. [1], has been estimated in Ref. [10]: The shape of the trap is anisotropic with the potential

$V_x = x_1^2 + x_2^2 + 8x_3^2 - \mu_0$. The coupling constant of the interaction of the ^{87}Rb atoms is $u \approx 813$ and the effective chemical potential $\mu_0 - \tau \approx 16.3$.

Mean-field theory

The properties of the condensate (e.g., the density) can be evaluated using the saddle-point approximation of the action S_{GP}. This is equivalent to the approximation which neglects fluctuations of Φ_x (classical field approximation). The classical field Φ_x is a solution of the nonlinear Schrödinger equation

$$ [(\tau/6a^2) \nabla^2 + \tau + V_x + u|\Phi_x|^2] \Phi_x = 0. \tag{3} $$

This nonlinear differential equation is complicated and generally one has to resort to numerical methods to obtain its exact solutions. However, in order to understand its behavior in the high-density limit one can neglect the kinetic-energy term because, in that case, the nonlinear term of the equation is dominant. This is known as the Thomas-Fermi approximation. In a translational invariant system (i.e., $V_x = -\mu_0$) the Thomas-Fermi approximation gives a linear behavior for the condensate density as a function of μ_0

$$ \rho_c \propto |\Phi_x|^2 = (1/u)(\mu_0 - \tau) \Theta(\mu_0 - \tau), \tag{4} $$

where Θ is the Heaviside step function. The condensate density increases ad infinitum upon increasing μ_0. This behavior is in disagreement with the depletion of the condensate expected at higher total densities. It also contradicts the fact that the hard-core potential limits the density of the Bose gas. The reason behind this behavior is that in the GP approach the hard-core condition is implemented by a two-body δ function potential. However, in the high-density limit when a large number of particles are close to each other, this potential does not provide a strong enough repulsion needed for the strict imposition of the hard-core condition. In other word, corrections due to three-body and higher-order effects will become equally important. This reflects that the GP approach is realistic only for a dilute Bose system: The linear behavior is correct near the critical point, where $|\Phi|^2 \sim 0$ but the slope of the density of the condensate is less than linear as one goes away from the critical point. And finally it decreases, indicating the depletion of the condensate at higher total densities. By the same argument one can also obtain the inhomogeneous condensate density for the case of a high-density Bose gas composed of alkali-metal atoms in a trap confined by a potential V_x [9]

$$ \rho_x \propto |\Phi_x|^2 = -(1/u)(V_x + \tau) \Theta(-V_x - \tau). \tag{5} $$

One may try to correct the high-density behavior of the GP approach by including terms such as $|\Phi_x|^6, |\Phi_x|^8, \ldots$ in the GP action [Eq. (2)] to account for the three-body and higher-order interactions terms. But our feeling is that one will need to go to very high orders in this expansion to obtain the correct limiting behavior. However, in this work we propose an alternative approach which restores the correct high-density behavior of an inhomogeneous Bose gas by imposing a strict hard-core condition by adopting a slave boson representation. This approach is an extension of a similar approach formulated earlier by one of us [4], for the

case of a homogeneous Bose gas. In the following section we will develop and apply the aforementioned slave boson based approach to study the hard-core Bose gas in a harmonic trap.

III. SLAVE BOSON APPROACH

The slave boson representation was originally developed for fermion systems (e.g., the Hubbard model) [14]. The advantage of using a slave boson representation in the case of strongly interacting electrons is that one can account for many effects of strong correlations at the mean-field level of this representation [14]. For the Bose gas, in contrast to the Hubbard model of the fermion gas, the dilute limit describes already interesting physics, such as BE condensation. The dilute limit of a Bose gas can be described quite adequately by traditional approaches, such as the GP approach, which takes into account only the two-particle interactions. However, it is intuitively obvious that as the density of particles in the BE condensate increases, the nature of interparticle interactions will become more and more complex, and one will need to take even three-body and higher effects into account. It was demonstrated by one of us that the slave boson representation allows one to describe the dynamics of a Bose gas at arbitrary densities [4], which is what we review next. For the case of bosons, the slave boson representation is even easier to formulate because there are only two states per site in a hard-core system: a site is either empty (represented by a complex field e_x) or occupied by a single boson (represented by a complex field b_x). A hopping process of a boson appears as an exchange of an empty site with a singly occupied site. Following the standard arguments [14], this picture can be translated into a slave boson action $S_{\rm sb}$ of the form

$$\sum_x \left[\sum_{x'} b_x^* e_x t_{x,x'} b_{x'} e_{x'}^* + V_x b_x^* b_x + i\lambda_x (e_x^* e_x + b_x^* b_x - 1) \right].$$
(6)

Here again we have neglected fluctuations with respect to time because they have a gap $k_B T$ at a nonzero temperature T, as discussed in Sec. II. The field λ_x enforces the constraint $e_x^* e_x + b_x^* b_x = 1$ which guarantees that a site is either empty or singly occupied. This becomes clear if we consider the partition function where we integrate over all fields

$$Z = \int e^{-S_{\rm sb}} \prod_x d\lambda_x db_x db_x^* de_x de_x^*.$$
(7)

The λ field creates a Dirac δ function for the constraint. The slave boson fields e_x and b_x can be combined to a collective field $b_x^* e_x \to \Phi_x$. Then the constraint field λ and the slave boson fields can be integrated out which finally leads to the action for the collective field Φ. This was demonstrated in detail in Ref. [4]. Here we only present the results: The new partition function reads

$$Z = \int e^{-S_b - S_1} \prod_x d\Phi_x d\Phi_x^*,$$
(8)

with the hopping (''kinetic'') term

$$S_b = \sum_{x,x'} \Phi_x (1-t)_{x,x'}^{-1} \Phi_{x'}^*,$$

$$\approx \sum_x (1-\tau)^{-1} |\Phi_x|^2 + \frac{\tau}{6a^2(1-\tau)^2} \Phi_x (\nabla^2 \Phi^*)_x,$$
(9)

and the potential term

$$S_1 = -\sum_x \ln\left(e^{-V_x/2 - 1/4} \int d\varphi_x e^{-\varphi_x^2} \right.$$

$$\left. \times \frac{\sinh(\sqrt{(\varphi_x - V_x/2)^2 + |\Phi_x|^2})}{\sqrt{(\varphi_x - V_x/2)^2 + |\Phi_x|^2}} \right).$$
(10)

$S_b + S_1$ is a generalization of the GP action to systems with arbitrary density. It agrees with Eq. (2) in the dilute regime after expanding S_1 in powers of $|\Phi_x|^2$ up to second order: $S_1 = a_1 |\Phi_x|^2 + a_2 |\Phi_x|^4 + o(|\Phi|^5)$ can be compared with the potential of the dimensionless GP energy. For instance, we find for $V_x = 0$ the coefficients $a_1 = -1/6$ and $a_2 = 1/180$. In general, both coefficients of the expansion depend on V_x. That means the composite field Φ of the slave boson approach must be rescaled by $(813/2a_2)^{1/4}$ in order to get the equivalent of the field Φ of the GP approach. Furthermore, there is a renormalized chemical potential $(1-\tau)^{-1} - 1/6$ instead of τ in Eq. (2). τ can be fixed by comparing the slave boson result and the GP result in the vicinity of a vanishing condensate. We found with the above-mentioned parameters $\tau \approx -5.5$. Going beyond the dilute regime the effective potential of the slave boson representation deviates significantly from the GP potential: it grows only linearly for large $|\Phi_x|$ in contrast to the $|\Phi_x|^4$ behavior of the GP case. Therefore, the ''confinement'' of the condensate is much weaker and allows a destruction of the latter by fluctuations. The strong potential in the GP case makes the condensate very robust against fluctuations with sufficiently large $|\Phi_x|$.

An interesting quantity for the characterization of the condensate is the momentum distribution of condensate atoms [9]. For the case of a inhomogeneous condensate, the condensate wave function obviously is not an eigenfunction of the momentum. However, we do expect the momentum distribution to be sharply peaked around zero momentum and its shape to be determined both by the trap parameters and the interparticle interactions [1]. In the continuum limit that we are considering here, the momentum distribution can be evaluated from the field Φ as [9]

$$\langle \Phi_k \Phi_{-k}^* \rangle = \sum_{x,x'} e^{ik(x-x')} \langle \Phi_x \Phi_{x'}^* \rangle,$$
(11)

where the average is taken with respect to the effective action $\langle \cdots \rangle = Z^{-1} \int \cdots e^{-S_b - S_1} \prod_x d\Phi_x d\Phi_x^*$. In order to calculate this quantity we use a saddle-point approximation for the functional integral described in Sec. III A.

A. Mean-field theory

The total density and the density of the condensate in the trap can be calculated again from the saddle-point approximation. For the present case we feel that it is sufficient be-
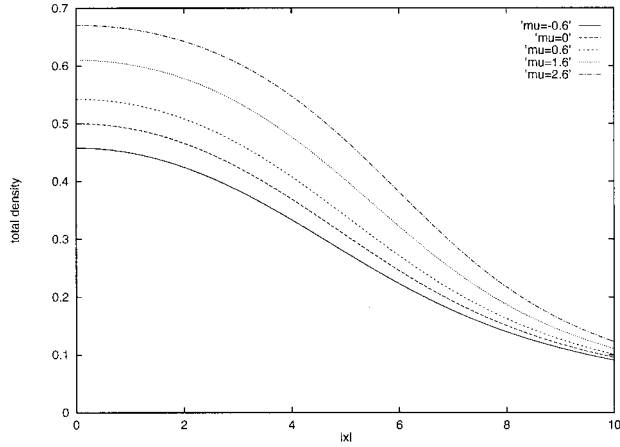
FIG. 1. Total density of bosons in a harmonic trap as a function of the distance $|x|$ from the center of the trap for the chemical potential $\mu_0 = -0.6, 0, 0.6, 1.6, 2.6$. The total density at a given distance $|x|$ increases as the chemical potential increases. This result assumes the equilibrium of the grand canonical ensemble of bosons, a condition which may be violated in the experiment.

cause thermal fluctuations will not be important at the small temperatures at which the BE condensation occurs in these systems. However, if one needed to account for thermal fluctuations, one could do so by studying the deviations around the saddle point in the functional integral of Eq. (8) [8]. That means we have to look for a solution Φ_x which minimizes $S_b + S_1$. This problem is analogous to the minimization of the GP energy, discussed above. Instead of the nonlinear Schrödinger equation (3), we have a generalization of this equation for the slave boson approach

$$[(\tau/6a^2)\nabla^2 + (1-\tau)]\Phi_x + (1-\tau)^2 \frac{\partial S_1}{\partial \Phi_x^*} = 0. \quad (12)$$

This nonlinear differential equation is even more complicated than the nonlinear Schrödinger equation. Therefore, we again apply the Thomas-Fermi approximation

$$\Phi_x + (1-\tau)\frac{\partial S_1}{\partial \Phi_x^*} = 0. \quad (13)$$

$\partial S_1/\partial \Phi_x^*$ contains higher-order terms (three-body interactions, etc.) which are important for the dense regime. However, inclusion of the kinetic-energy term will only be necessary if more complicated structures (e.g., vortex states [10]) are considered. Since the accuracy of the Thomas-Fermi approximation increases with increasing density, it is particularly suitable for our case where we are interested in the high-density regime.

The total density of bosons can be evaluated from $\partial \ln Z/\partial \mu_0$. This quantity is measured with respect to a lattice Bose gas with lattice spacing a. The maximal density is $n=1$, where we have one boson per site (i.e., one boson in a volume element a^3). In the trap the maximum is at the center and it decreases monotonically with $|x|$ (cf. Fig. 1). Solutions for an isotropic trap are presented for different values of μ_0. In reality, of course, the number of bosons N is measured and μ_0 must be determined self-consistently for N while solving Eq. (12). However, in this case, we have used
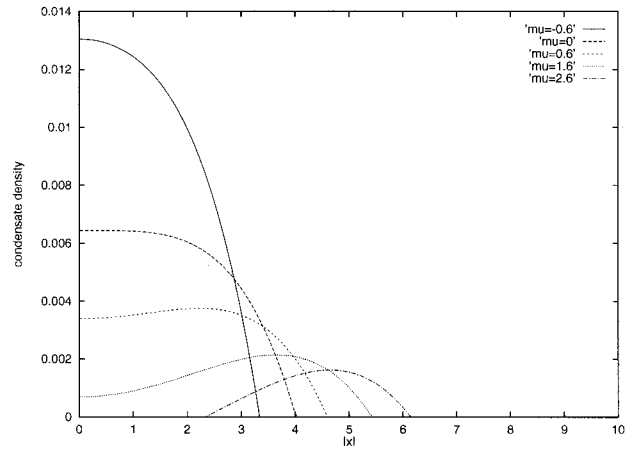

FIG. 2. Density of the condensate in the trap, normalized by the volume, for the μ_0 values of Fig. 1. The surface of the condensate grows with increasing μ_0, and the condensate for the lowest density already has the parabolic shape found in the GP approach.

μ_0 as a parameter which controls the number N, and hence, the density of atoms in the trap, and assigned it different values so as to solve Eq. (13) for different values of the particle density. Solutions of Eq. (13) for the density of the condensate are given in Fig. 2. The maximum of the condensate appears always at positions in the trap where the total density is 0.5. This reflects the duality of bosons and holes in the hard-core Bose gas on the lattice. If the total density is less than 0.5 everywhere in the trap, the density of the condensate decays monotonically with $|x|$. This result demonstrates that the condensate is depleted at the center of the trap if the total density of bosons is larger than 0.5. Consequently, it is difficult to create an extended condensate in a potential where the bosons are concentrated at the center with high density. However, known experiments on a Bose gases are far away from such high densities.

The correlation function of the order-parameter field $\Phi_x = |\Phi_x| e^{i\varphi_x}$ can be approximated by neglecting the fluctuations of $|\Phi_x|$ as

$$\langle \Phi_x \Phi_{x'}^* \rangle \approx \overline{\Phi_x} \, \overline{\Phi_{x'}^*} \langle e^{i\varphi_x - i\varphi_{x'}} \rangle, \quad (14)$$

where $\overline{\Phi_x}$ is a solution of Eq. (13). [The global phase of $\overline{\Phi_x}$, of course, is not determined by Eqs. (12) or (13) due to symmetry.] The phase coherence of the fluctuating phase φ_x may be larger than the size of the condensate because of the off-diagonal long-range order in a three-dimensional Bose gas [15]. Therefore, the momentum distribution, defined by Eq. (11) and the continuum limit can be approximated by [9]

$$f(k) = \left| \int d^3x \, e^{ikx} \overline{\Phi_x} \right|^2. \quad (15)$$

The momentum distribution of the condensate atoms obtained using Eq. (15), based on the solution of Eq. (13) is plotted in Fig. 3 for several values of the chemical potential μ_0. Upon inspecting Fig. 3, one immediately observes that the momentum distribution becomes even sharper due to
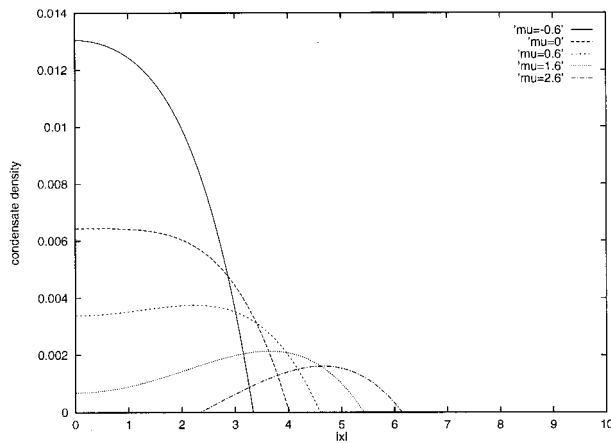
FIG. 3. Momentum distribution of condensate particles in the trap for the μ_0 values of Fig. 1. The sharpness of the distribution increases with increasing μ_0.

depletion. This is a consequence of the spreading of the condensate due to depletion, which supports small momenta.

IV. CONCLUSIONS

In conclusion, we have studied the condensation of a three-dimensional high-density Bose gas in a harmonic trap. We demonstrated the unphysical nature of the solutions that one obtains if one applies the traditional approach of Gross and Pitaevskii to study such a system. We identified that the reason behind this behavior was that the GP action ignores the three-body and the higher-order interactions which become important at high densities. In this work we proposed an alternative approach based on the slave boson representation, which accounts for these complex interactions at high densities by satisfying the hard-core condition strictly. Our approach leads to solutions which are well behaved at high densities and predicts depletion of the condensate in the regions of high densities (mainly the center of the trap) which one would expect on intuitive grounds. We also study the momentum distribution of the atoms in the trap and observe a narrowing of the momentum distribution in the high-density limit. This approach is expected to be of little application for the low-density condensates which are presently being created in experiments, but we hope that it can be tested in the future when experimentalists may be able to realize a dense Bose gas in a trap. We also plan to apply this approach to study the structure of vortices in a high-density inhomogeneous Bose gas, results of which will be presented in a future publication.

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