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Limits of validity for a semiclassical mean-field two-fluid model for Bose–Einstein condensation thermodynamics

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Abstract

We reinvestigate the Bose–Einstein condensation (BEC) thermodynamics of a weakly interacting dilute Bose gas under the action of a trap using a semi-classical two-fluid mean-field model in order to find the domain of applicability of the model. Such a model is expected to break down once the condition of diluteness and weak interaction is violated. We find that this breakdown happens for values of coupling and density near the present experimental scenario of BEC. With the increase of the interaction coupling and density the model may lead to unphysical results for thermodynamic observables. © 2000 Published by Elsevier Science B.V. All rights reserved.

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1. Introduction

The recent experimental observation of Bose–Einstein condensation (BEC) in a weakly interacting dilute gas of ^{87}Rb [1,2], ^{23}Na [3], ^{7}Li [4,5], and ^{1}H [6] employing magnetic traps at ultra-low temperatures calls for a theoretical investigation on various aspects of the condensate. The condensate consists of few thousands to few millions of atoms confined by the trap potential. As the temperature is lowered below the critical temperature T_0 of BEC, the condensate starts to form and finally at 0 K all the available atoms will be condensed. In the absence of a microscopic equation, the condensate

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is usually described by the mean-field Gross–Pitaevskii (GP) equation [7,8]. One of the primary interest on the process is to study the thermodynamic observables of the system, such as, the condensate fraction, internal energy, and specific heat.

There have been several comprehensive studies on temperature dependencies of thermodynamic observables of the condensate using semiclassical mean-field two-fluid models [9–15]. The physical ingredients of these models are quite similar. One such model using the GP wave function provides satisfactory description of the temperature dependencies of the thermodynamic observables in two [13], and three [12,16] dimensions. These studies employed an iterative solution of the system of equations involved. For the condensation of a system composed of 40 000 trapped ^{87}Rb atoms with repulsive interatomic interaction, the iterative scheme converged rapidly and provided a satisfactory account of the condensate fraction, internal energy, and specific heat [12]. Similar conclusion was also reached in the study of condensation of ^{7}Li atoms [16]. In the case of ^{7}Li, the attractive interatomic interaction is responsible for collapse if the number of atoms is larger than approximately 1400 [17–19].

Here we reinvestigate critically the BEC of a weakly interacting dilute gas in two and three dimensions using the two-fluid mean-field model mentioned above in order to define the domain of its applicability. We have included the two-dimensional BEC in this study because of considerable recent interest in this topic [13,20–25]. We employ the usual iterative solution of the nonlinear two-fluid mean-field model and study the convergence of the iterative scheme. Although, the convergence is rapid for a weakly interacting dilute system, with an increase of the strength of interaction and/or density, the model breaks down and leads to physically unacceptable results for the thermodynamic observables. Specifically, below the critical temperature, the model may yield negative specific heat.

However, it is well-known that the mean-field description of the condensate via the GP equation as used in the semiclassical models above should hold under the condition of diluteness of a weakly interacting Bose gas and is expected to break down once the conditions of diluteness and weak interaction are violated (see, for example Ref. [15, p. 474]). The breakdown should happen for a large number of condensed particles reflecting a large density as well as for a large modulus of the scattering length denoting a strong interatomic interaction. These two conditions correspond to a large nonlinearity of the system and may lead to a breakdown of the mean-field two-fluid thermodynamic model [9,15]. In addition, the finite size of the system may necessitate corrections in the thermodynamic model as we are away from the real thermodynamic limit $N \to \infty$, $V \to \infty$, where N is the number of particles and V the volume of the system.[1] Nevertheless, exact numerical conditions for the breakdown of the mean-field thermodynamical model have never been investigated. In this work by performing numerical calculations we identify such conditions. We find that the semiclassical model may break down under possible present experimental conditions of BEC of a trapped Bose gas.

[1] These limitations of the thermodynamic model are discussed in Section 5 of Ref. [15].

We present the semiclassical model in Section 2, numerical results in Section 3, and conclusions in Section 4.

2. Mean-field model

We consider a system of N bosons with repulsive interaction at temperature T under the influence of a trap potential. The condensate is described by the following GP wave function in the Thomas–Fermi approximation [12,13]:

$$|\Psi(r)|^2 = \frac{\mu - V_{\rm ext} - 2gn_1(r)}{g}\theta(\mu - V_{\rm ext} - 2gn_1(r))\,, \tag{1}$$

where $\theta(x)$ is the step function, $\theta(x) = 0$ if $x < 0$ and 1 otherwise. Here, $V_{\rm ext}(r) \equiv m\omega^2 r^2/2$ is the trap potential, g the strength of the repulsive interaction between the atoms, m the mass of a single bosonic atom, ω the angular frequency, μ the chemical potential, and $n_1(r)$ represents the distribution function of the noncondensed bosons. As we are interested in studying the limits of validity of the semiclassical mean-field model and not in simulating a particular experimental situation, we consider a spherically symmetric trap both in two and three dimensions. The noncondensed particles are treated as non-interacting bosons in an effective potential [26]

$$V_{\rm eff}(r) = V_{\rm ext}(r) + 2gn_1(r) + 2g|\Psi(r)|^2\,. \tag{2}$$

Thermal averages are calculated with a standard Bose distribution of the noncondensed particles in chemical equilibrium with the condensate governed by the same chemical potential μ. In particular the density $n_1(r)$ is given by [12,13,26]

$$n_1(r) = \frac{1}{(2\pi\hbar)^{\mathscr{D}}}\int \frac{{\rm d}^{\mathscr{D}} p}{\exp[\{p^2/2m + V_{\rm eff}(r) - \mu\}/k_{\rm B}T] - 1}\,, \tag{3}$$

where $k_{\rm B}$ is the Boltzmann constant, and $\mathscr{D}(\equiv 2, 3)$ is the dimension of space. Eqs. (1)–(3) above are the principal equations of the present model. The total number of particles N of the system is given by the number equation

$$N = N_0 + \int \frac{\rho(E)\,{\rm d}E}{\exp[(E-\mu)/k_{\rm B}T] - 1}\,, \tag{4}$$

where $N_0 \equiv \int |\Psi(r)|^2 {\rm d}^{\mathscr{D}} r$ is the total number of particles in the condensate. The critical temperature T_0 is obtained as the solution of Eq. (4) with N_0 and μ set equal to 0. The semiclassical density of states $\rho(E)$ of noncondensed particles is given by [12,13]

$$\rho(E) = \frac{2\pi m^{\mathscr{D}/2}}{(2\pi\hbar)^{\mathscr{D}}}\int_{V_{\rm eff}(r)<E} [8(E - V_{\rm eff}(r))]^{(\mathscr{D}-2)/2}\,{\rm d}^{\mathscr{D}} r\,. \tag{5}$$

The average single-particle energy of the noncondensed particles is given by [12]

$$\langle E\rangle_{\rm nc} = \int \frac{E\rho(E)\,{\rm d}E}{\exp[(E-\mu)/k_{\rm B}T] - 1}\,. \tag{6}$$

The kinetic energy of the condensate is assumed to be negligible and its interaction energy per particle is given by $\langle E\rangle_{\rm c} = (g/2)\int |\Psi(r)|^4\,{\rm d}^{\mathscr{D}} r$. The quantity of experimental

interest is the average energy $\langle E\rangle = [\langle E\rangle_{\rm nc}(N-N_0)/2 + \langle E\rangle_{\rm c}]/N$, which we calculate in the following. The specific heat is defined by $C = {\rm d}\langle E\rangle/{\rm d}T$ [12].

Eqs. (1)–(5) are to be solved iteratively. The iteration is started at a fixed temperature with a trial chemical potential μ using $n_1(r) = 0$. Then $\Psi(r)$ and $V_{\rm eff}(r)$ are calculated using Eqs. (1) and (2). With these results $n_1(r), \Psi(r)$, and $V_{\rm eff}(r)$ are recalculated. This procedure is repeated until desired precision is obtained. The results for the lowest order of iteration with $n_1(r) = 0$ will be denoted by $I = 1$, and successive orders by $I = 2, 3, \ldots$. With the solutions $\Psi(r)$ and $V_{\rm eff}(r)$ so obtained, the density of states $\rho(E)$ of Eq. (5) is calculated. Then it is seen if they satisfy the number equation (4). If Eq. (4) is satisfied the desired solution is obtained. If not, the initial trial μ is varied until the number equation is satisfied. In each order of iteration we calculate the condensate fraction N_0/N and energy $\langle E\rangle$.

3. Numerical study

First, we consider the three-dimensional case. In this case, the coupling g is given by $g = 4\pi\hbar^2 a/m$, where a is the scattering length. Usually, a dimensionless coupling is introduced via $\eta \equiv (mg/\pi\hbar^2)/a_{\rm ho} = 4a/a_{\rm ho}$, where $a_{\rm ho} = \sqrt{\hbar/m\omega}$. The semiclassical model under consideration should break down as either η or N is increased. This will violate the condition of weak interaction and diluteness. In the case of experiment on BEC of ^{87}Rb, $\eta = 0.025$ and $N = 40\,000$ [1,2,12]. To test our calculational scheme, first we solve the present model for $\eta = 0.025$ and $N = 40\,000$. Our results are very similar to those of Ref. [12]. The small difference between these two calculations is due to the use of an isotropic harmonic oscillator potential in this work and an anisotropic potential in Ref. [12]. In this case, specific heat is positive at all temperatures. Next, we increase η and N. We find that as η and N are increased, the energy develops a maximum at a temperature below T_0. Consequently, the specific heat becomes negative for an interval of temperature above this maximum. To show this violation in a pronounced way here we show the results for the following three cases: (a) $\eta = 0.1$, $N = 10^6$, (b) $\eta = 0.1$, $N = 10^7$, and (c) $\eta = 0.5$, $N = 10^6$. In the case of ^{23}Na, the experimental N was as high as 10^7 [3]. As the interaction is repulsive in both ^{87}Rb and ^{23}Na, it should be possible to have 10^7 atoms in a BEC of ^{87}Rb under favorable experimental conditions. Hence, these values of the parameters are within the present experimental scenario. In Fig. 1(a), (b) and (c) we plot $\langle E\rangle/Nk_{\rm B}T_0$ and N_0/N versus T/T_0 for different iterations for the above three cases. We find that the energies are acceptable under conditions of diluteness and very weak interactions, but as η and N increases the average energy of the system may have a maximum leading to a negative specific heat above the maximum. From Fig. 1(a)–(c) we find that this violation happens in the case (c) which has the largest η and N. We verified that for sufficiently large values of η and N the lowest-order energy also leads to negative specific heat.

Next, we consider the two-dimensional case. In this case, in analogy with the three-dimensional case, a dimensionless coupling is introduced by $\eta \equiv (mg/\pi\hbar^2)$.

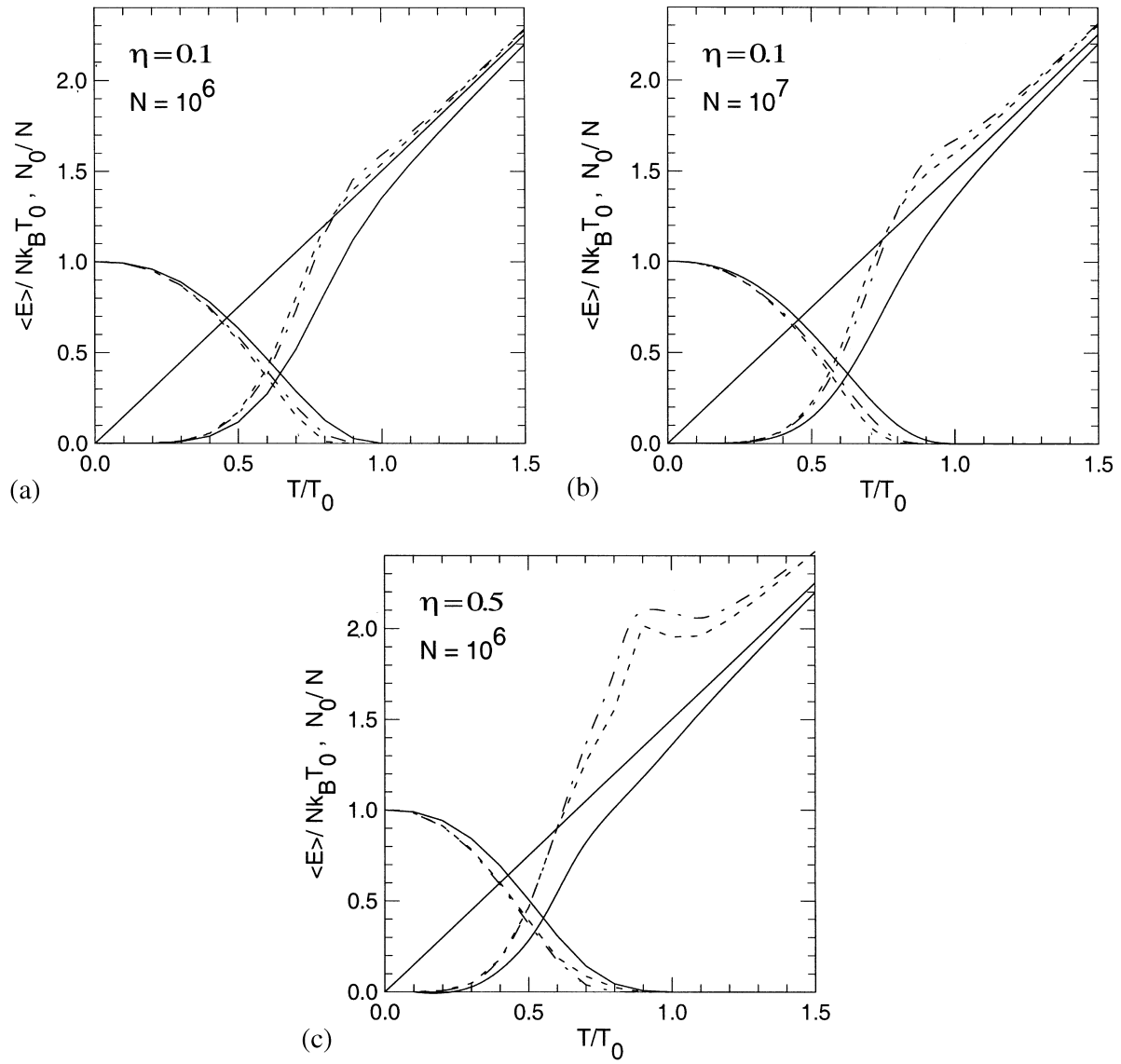

Fig. 1. Condensate fraction N_0/N and energy $\langle E\rangle/Nk_BT_0$ in three dimensions as a function of T/T_0 for (a) $\eta=0.1$ and $N=10^6$, (b) $\eta=0.1$ and $N=10^7$, and (c) $\eta=0.5$ and $N=10^6$ for iterations $I=1$ (full line), 2 (dashed-dotted line), and 4 (dotted line). The straight line represents the classical Maxwell–Boltzman result of energy.

This coupling is already dimensionless, whereas we needed to divide it by a_{ho} in three dimensions to make it dimensionless. First, we repeat the calculations reported in Ref. [13] and our results are in agreement with that study. In addition, in agreement with our finding in three dimensions, we find that for small values of η and N the equations of the model converge well and lead to acceptable values for condensate fraction N_0/N and energy $\langle E\rangle/Nk_BT_0$. For larger values of η and/or N, the condensate fraction N_0/N is quite acceptable with a temperature dependence similar to that in three dimensions. However, the energy produces a maximum as N and η increase. Hence, we shall be limited to a consideration of energy only.

As there is no experimental guideline for probable values of N and η in two dimensions, as in Ref. [13], we consider $N=10^5$ and $\eta=0.1$, 1, and 10. In Fig. 2 we plot

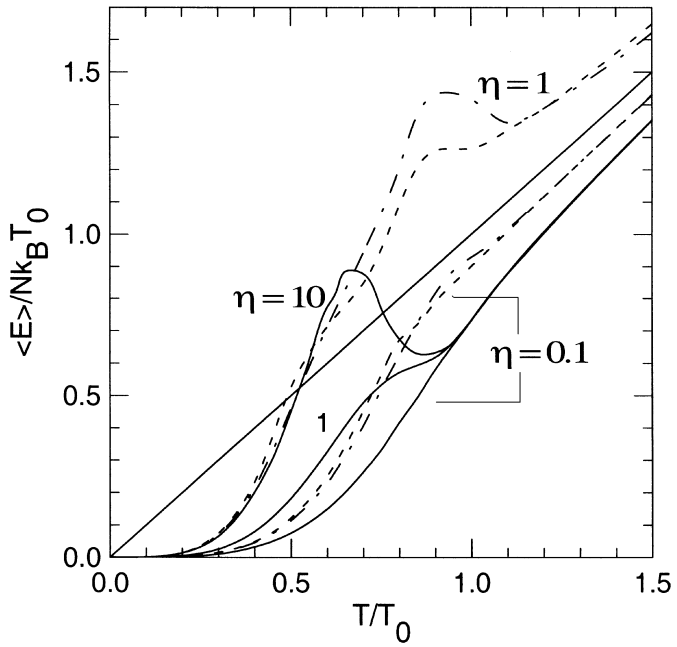

Fig. 2. Energy $\langle E\rangle/Nk_{\mathrm{B}}T_0$ in two dimensions as a function of T/T_0 for $N = 10^5$ and $\eta = 0.1$, 1, and 10 for iterations $I = 1, 2$ and 4. Notations are the same as in Fig. 1. The curves are labeled by the values of η.

the temperature dependence of average energy $\langle E\rangle/Nk_{\mathrm{B}}T_0$ for different iterations. The lowest-order results for $\eta = 0.1$ and 1 are in agreement with those of Ref. [13]. The classical Maxwell–Boltzmann result for a noninteracting gas is also shown in Fig. 2. For a weakly interacting gas with $\eta = 0.1$, the energies for all orders of iteration are acceptable. For a stronger interaction with $\eta = 1$, the lowest-order energy is acceptable. However, in this case the energies for all orders of iteration produce maxima leading to negative specific heat. For $\eta = 10$, the lowest-order result already leads to a negative specific heat.

In addition to the trouble discussed above, the mean-field model may exhibit another unacceptable behavior. We see in Figs. 1 and 2, that the energy of the system could be larger than the corresponding classical Maxwell–Boltzmann result for a noninteracting ideal gas. We recall that for BEC to materialize, the energy of the condensate should be smaller than the corresponding energy of the noncondensed system. However, one should consider the correction to the classical result above due to the presence of the trap and the interatomic interaction. In all our calculations we have noted that $k_{\mathrm{B}}T_0 \gg \hbar\omega$, so that for temperatures close to T_0 considered above the correction to the classical energy due to the presence of the trap can be neglected. The same is also true for the interatomic interaction at temperatures close to T_0, for the values of η considered in this study. Consequently, the energy of the condensate of the mean-field model could be larger than the classical result signaling a breakdown of the model.

It is well known that the semiclassical model requires $k_{\mathrm{B}}T_0 \gg \hbar\omega$ and the Thomas–Fermi approximation does not hold for very small number of atoms in the condensate. For the cases studied here $k_{\mathrm{B}}T_0$ is typically 50–100 times larger than $\hbar\omega$ and Thomas–Fermi approximation apparently seems to be valid for the condensates. The diluteness

condition for the validity of the GP equation $na^3 \ll 1$ is also valid in three dimensions, where n is the density. For the case considered in Fig. 1(a), $N = 10^6$, $a = 50$ nm, for a condensate of typical dimension 100 μm, $na^3 \sim 10^{-3} \ll 1$. The values of na^3 are larger for Figs. 1(b) and (c). Nevertheless, we find that these values of diluteness and coupling set a limit to the applicability of the semiclassical mean-field two-fluid models for studying BEC thermodynamics.

4. Conclusion

In conclusion, we reexamined the problem of BEC under the action of a trap potential using a two-fluid mean-field model [12,13] in both two and three dimensions. We employed an iterative solution scheme of the system of equations. Although the system leads to rapid convergence for a weakly interacting dilute system, with the increase of coupling and particle number the iterative scheme leads to physically unacceptable results for thermodynamic observables. Specifically, this may lead to a maximum in energy responsible for a negative specific heat. In three dimensions the breakdown of the mean-field model happens for values of coupling and particle number, which are not so remote from present experimental scenario for repulsive interatomic interaction. In addition, the energy of the condensate could be larger than the corresponding classical energy of the system, which is another independent unacceptable result of the model. The larger values of the coupling η and N considered in this work possibly sets a limit to the applicability of the mean-field equations for BEC. Summarizing, the most important finding of this study is that the iterative solution of the mean-field model of Refs. [12,13] for a condensate may lead to unphysical thermodynamical properties for medium to large coupling and number of particles.

Despite the above deficiency of the mean-field two-fluid thermodynamical models, they continue to be very useful in many cases. The virtue of these models is the simplicity and ability to yield results in agreement with experiment for weak interactions and dilute systems. As a theoretically sound description of the BEC thermodynamics seems to be unmanagably complicated, these simple mean-field two-fluid models remain as attractive simple alternatives to study thermodynamical properties provided that proper attention is paid to remain inside the domain of their validity.

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