Numerical Analysis of Transition Temperature in Bose-Einstein Condensation

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Abstract

We numerically investigate Bose-Einstein condensation (BEC) of finite number atoms in a mean field approximation. For the Bose gas interacting with a weak repulsive potential and trapped in an external parabolic potential, BEC occurs at finite temperature in one- and three-dimensional systems. Comparing free energies between the BEC state and the normal state, we define the transition temperature. The relation between the transition temperature and the repulsive coupling constant shows a simple power law for 1D and 3D systems.

Key words: Bose-Einstein condensation ; transition temperature ; free energy ; order parameter

1. Introduction

In one- and two- dimensional uniform systems, no Bose-Einstein Condensation (BEC) occurs at finite temperature both in free and interacting systems.[1] Recent experiments[2] show that BEC occurs in 1D and 2D interacting bosons under a trapping potential. Although a relation between critical temperature and number of bosons is estimated in free 1D system,[3] BEC transition temperature of interacting bosons is not examined well. In this article, we numerically study BEC of a dilute alkaline atomic gas under a harmonic trapping potential and evaluate BEC transition temperatures for 1D and 3D systems.

2. Formulation and Calculation

The BEC state is identified by the non-vanishing thermal average of a boson field while the thermal average equals zero in a normal state. We decompose the boson field operator Ψ into two parts, an order parameter v ($= \langle\Psi\rangle$) and an operator part ψ, $\Psi = v + \psi$. When $v = 0$, the system is in a normal state (NS) and if $v \neq 0$, the system is in a coherent state (CS).

In the mean field approximation, the equation of motion for $\Psi = v + \psi$ becomes coupled equations,

$$i\hbar\frac{\partial}{\partial t}v = \left(H_0 - \mu + V(v^*v + 2\langle\psi^\dagger\psi\rangle)\right)v \qquad (1)$$

$$i\hbar\frac{\partial}{\partial t}\psi = \left(H_0 - \mu + 2V(v^*v + \langle\psi^\dagger\psi\rangle)\right)\psi + Vvv\psi^\dagger, \qquad (2)$$

where μ is a chemical potential and $V(>0)$ is a repulsive coupling constant of the atom-atom interaction. We neglect a term $\langle\psi\psi\rangle$ in order to consistent with phase invariant symmetry. H_0 includes a trapping harmonic potential and we use a dimensionless form, $H_0 = -\nabla^2 + r^2$, with the unit energy $\hbar\omega_\mathrm{h}$ and the unit length $a_\mathrm{h} = \sqrt{\hbar/m\omega_\mathrm{h}}$. Here m is an atomic mass and ω_h is frequency of the harmonic potential. We also use a temperature scale $T_\mathrm{h} = \hbar\omega_\mathrm{h}/k_\mathrm{B}$ and a coupling constant scale $V_\mathrm{h} = \hbar^2/2ma_\mathrm{h}$.[1]

Considering the equilibrium state, v and μ are evaluated from the self-consistent solution of eq. (1). Expanding ψ with annihilation and creation operators, $a_\ell \mathrm{e}^{-iE_\ell t/\hbar}$ and $a_\ell^\dagger \mathrm{e}^{iE_\ell t/\hbar}$, eq. (2) becomes the eigenequations of the eigen energy E_ℓ. The number of

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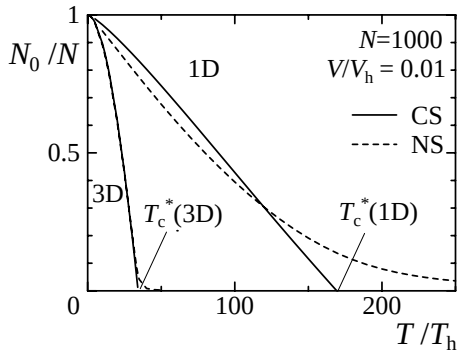

Fig. 1. Fractions of the ordered bosons or the lowest-energy bosons as a function of temperature.

excited bosons N_1 is given by $\int \mathrm{d}\boldsymbol{r}\langle\psi^\dagger\psi\rangle$ and the bose distribution $\langle a_\ell^\dagger a_\ell\rangle = 1/(\mathrm{e}^{E_\ell/k_\mathrm{B}T}-1)$. From the given total number N, the number of ordered bosons N_0 is defined as $N_0 = N - N_1$ which determines the normalization factor of the order parameter $\int \mathrm{d}\boldsymbol{r} v^* v = N_0$. In NS ($v = 0$), the chemical potential μ is determined as satisfying $\int \mathrm{d}\boldsymbol{r}\langle\psi^\dagger\psi\rangle = N$. We perform numerical calculations on real space meshes at intervals of $0.1a_\mathrm{h}$. Boundary conditions of the system are taken as $v = \psi = 0$ for $|r| > 30a_\mathrm{h}$.[4]

3. Results

In Fig. 1, we show the fraction of ordered bosons in CS (solid lines) and the fraction of bosons in the lowest energy state in NS (dashed lines) for 1D and 3D systems. We assume a spherical symmetry in the 3D system, *i.e.* no angular dependence in the distribution of bosons. Solid lines for CS vanish above certain temperature, say T_c^*, while dashed lines for NS exist at higher temperature. The critical temperature T_c^* provides an upper limit of the transition temperature T_c. Since NS can exist even at lower temperature, the transition temperatures of finite number systems will be determined by comparing free energies between CS and NS. We calculate the Helmholtz free energy $F = \Omega + \mu N$, here Ω is the thermodynamical potential.[4] The transition temperature T_c is defined as the crossing point, $F_\mathrm{CS} = F_\mathrm{NS}$.

The transition temperatures are shown in Fig. 2 (solid circles and solid triangles) as a function of the total number of atoms N. As V is decreased, the N-dependence of T_c seems to vanish. There is no variation on V in the N-dependence of T_c^* (open circles and open triangles) for both 1D and 3D systems. Note that the estimation of the critical temperature for non-interacting 1D atoms[3], $N = (T/T_\mathrm{h})\ln(2T/T_\mathrm{h})$ (long dashed line) is in agreement with N-T_c^* relations.

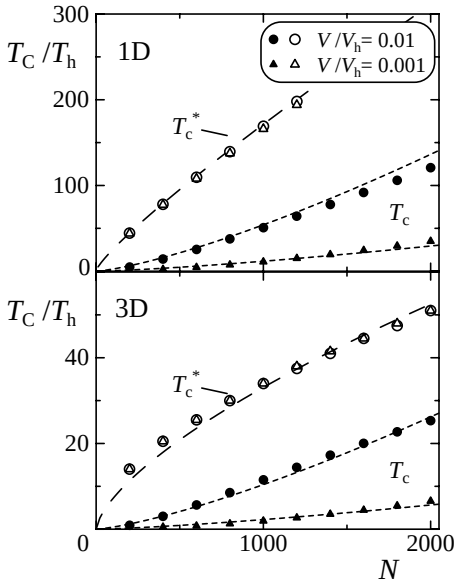

Fig. 2. The transition temperatures T_c as a function of the total number N. The dashed lines are fitted curves (eq.(3)) for each V. The critical temperatures T_c^* are plotted by open circles and open triangles. The long-dashed lines are $N = T\ln(2T)$ (1D) and $T \propto N^{2/3}$ (3D).

From the least mean square fit of the results, we obtain a following relation among T_c, N, and V,

$$T_\mathrm{c}/T_\mathrm{h} = \left(\frac{V/V_\mathrm{h}}{U_\mathrm{d}}\right)^{2/3} N^{4/3}\,, \tag{3}$$

where $U_\mathrm{d} = 4(2\pi)$ for 1D system and $U_\mathrm{d} = \zeta(3)(2\pi)^3$ for 3D system. Dashed lines in Fig. 2 show the relations for each V.

In the mean field approximation, we point out that the transition temperature T_c depends on the coupling constant V while the critical temperature T_c^* is less sensitive to the magnitude of the atom-atom interaction.

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