Bose-Einstein Condensation Temperature of a Homogeneous Weakly Interacting Bose Gas: PIMC study

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Using a finite-temperature Path Integral Monte Carlo simulation (PIMC) method and finite-size scaling, we have investigated the interaction-induced shift of the phase transition temperature for Bose-Einstein condensation of homogeneous weakly interacting Bose gases in three dimensions, which is given by a proposed analytical expression \( T_c = T_c^0 (1 + c_1 an^{1/3} + c_2' a^2 n^{2/3} + \mathcal{O}(a^3 n)) \), where \( T_c^0 \) is the critical temperature for an ideal gas, \( a \) is the s-wave scattering length, and \( n \) is the number density. We have used smaller number densities and more time slices than in the previous PIMC simulations [Gruter et al., Phys. Rev. Lett. 79, 3549 (1997)] in order to understand the difference in the value of the coefficient \( c_1 \) between their results and the (apparently) other reliable results in the literature. Our results show that \( (T_c - T_c^0) / (an^{1/3}) \) depends strongly on the interaction strength \( an^{1/3} \) while the previous PIMC results are considerably flatter and smaller than our results. We obtain \( c_1 \approx 1.32 \pm 0.14 \), in agreement with results from recent Monte Carlo methods of three-dimensional \( O(2) \) scalar \( \phi^4 \) field theory and variational perturbation theory.

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I. INTRODUCTION

Since the recent achievement of experimental observation of Bose-Einstein Condensation (BEC) in magnetically trapped atomic vapors [1], these inhomogeneous systems have attracted considerable interest from experimental and theoretical sides. In dilute or weakly interacting gases, the Gross-Pitaevskii (GP) theory, a mean-field theory, for the condensate wave function has been enormously successful in describing the extraordinary properties of the condensate. (For a recent review of numerous successful applications of mean field theories in Bose-Einstein condensation in atomic gases see Ref. (2).) However, the determination of the effect of repulsive interactions on the transition temperature of a homogeneous dilute Bose gas at a fixed density has had a long and controversial history [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29].

This non-trivial problem has been treated by different methods with different results. One of the reasons for the multitude of results and methods stems from the fact that the phase transition is second order, and perturbation theory typically breaks down for physical quantities sensitive to the collective long-wavelength modes close to the transition due to infrared (IR) divergences. Moreover, the interaction, no matter how small, changes the universality class of the phase transition from the Gaussian complex-field model to that of the \( XY \)-model.

In the weak interaction (or dilute) limit, the strength of the interatomic interactions can be characterized by the \( s \)-wave scattering length \( a \). The shift \( \Delta T_c = (T_c - T_c^0) \) of the BEC transition temperature of a homogeneous Bose gas away from its ideal-gas value

\[
T_c^0 = \frac{\hbar^2 2\pi}{mk_B} \frac{[n/\zeta(\frac{3}{2})]^{2/3}}
\]

behaves parametrically as

\[
\Delta T_c \rightarrow c_1 an^{1/3},
\]

where \( m \) is the particle mass, \( k_B \) is the Boltzmann constant, \( n \) is the number density, \( \zeta(s) \) is the Riemann zeta function, \( \zeta(\frac{3}{2}) \approx 2.612 \), and \( c_1 \) is a numerical coefficient. Additionally, M. Holzmann et al. [17] have argued that a logarithmic term appears at order-\( a^2 \) in Eq. (2), and they have shown that this term is of the form \( c_2' a^2 n^{2/3} \ln(an^{1/3}) \). They also estimated the value of the numerical coefficient \( c_2' \) using large-\( N_s \) arguments in the three-dimensional \( O(N_s) \) field theory. Later, Arnold et al. [17] were able to show that the transition temperature for a dilute, homogeneous, 3D Bose gas can be expressed to leading order as

\[
\Delta T_c \rightarrow c_1 an^{1/3} + c_2' \ln(an^{1/3}) + c_2'' a^2 n^{2/3} + \mathcal{O}(a^3 n),
\]

where \( c_2' \approx 19.7518 \) can be calculated perturbatively, whereas \( c_1 \) and \( c_2'' \) require non-perturbative techniques. With the help of Monte Carlo data they estimated \( c_2'' \approx 75.7 \); however, a strong debate concerns the values of the other numerical coefficients, especially \( c_1 \) which has been computed using various non-perturbative methods and Monte Carlo techniques. There are numerous estimates for the parameter \( c_1 \) describing the leading deviation of the BEC temperature due to a small repulsive interaction, and the range of variation of different predictions is from 0.34 (Ref. 6) to 4.66 (Ref. 21); these have been summarized for instance in Refs. (10, 16, 30). It appears that the most reliable results so far are obtained by Monte Carlo (MC) simulations of three-dimensional \( O(2) \) scalar \( \phi^4 \) field theory, \( c_1 = 1.29 \pm 0.05 \) determined by Kashurnikov et al. [22] and \( c_1 = 1.32 \pm 0.02 \) determined by Arnold et al. [17], and by variational perturbation theory (VPT), \( c_1 = 1.27 \pm 0.11 \) determined by...
Kastening. In particular, Gruter et al. investigated the dependence of \( \Delta T_c \) numerically using Path Integral Monte Carlo methods. They obtained the value of \( c_1 = 0.34 \pm 0.06 \) after numerical extrapolation of the calculation to the limit \( a \to 0 \). This value is about 4 times smaller than the above results. Holzmann et al. argued that the difference in these results is attributable to a nonanalytic structure, \( a^2 \ln a \), of the transition temperature in \( a \), and that this correction gives rise to a strong dependence on \( a \), even in the very dilute limit. Arnold et al. believed that one likely problem with the PIMC simulation of Gruter et al. is inadequate system size. Kashurnikov et al. stated that the PIMC simulation did not reach the universality region because the minimal value of \( na^3 \) was \( 10^{-5} \).

In this paper, we attempt to understand the difference in the value of the coefficient \( c_1 \) between results from PIMC and the above results. We have used a finite-temperature path-integral Monte Carlo (PIMC) method to study the dependence on interaction strength of the phase transition temperature for Bose-Einstein Condensation of weakly interacting Bose gases in three dimension. Although our PIMC method is the same as that used by Gruter et al., we have used smaller number densities and more time slices than in the previous PIMC simulations, as motivated above.

**II. SIMULATION METHOD AND DEFINITION OF THE PHYSICAL QUANTITIES**

We wish to study the problem of a quantum \( N \)-particle system in order to compute the phase transition temperature \( T_c \) for dilute or weakly interacting Bose gases in three dimensions. We assume that the interparticle interaction can be described by a positive scattering length \( a \) (see, e.g., Refs. [2,3]). The Hamiltonian for this system may be written as

\[
H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j} v(|r_i - r_j|),
\]

where \( v(r) \) is the hard-sphere potential defined by

\[
v(r) = \begin{cases} +\infty & (r < a) \\ 0 & (r > a). \end{cases}
\]

The statistical mechanics of quantum systems is governed by the density matrix. For a system of \( N \) bosons at an inverse temperature \( \beta \), the Bose-symmetrized density matrix is given by

\[
\rho_B(R, R'; \beta) = \frac{1}{N!} \sum_{P} \rho(R, PR'; \beta),
\]

where \( R \) and \( R' \) are two configurations of \( N \) hard spheres. \( P \) denotes a permutation of particle labels among hard spheres, and \( PR \) is one such permutation. Evaluating the density matrix for interacting systems at very low temperatures is complicated by the fact that the kinetic and potential terms in the exponent of the density matrix cannot be separated. We can avoid this problem by inserting \( M - 1 \) intermediate configurations into Eq. (5) to obtain the path-integral formulation of the density matrix:

\[
\rho(R, PR'; \beta) = \int \cdots \int dR_1 dR_2 \cdots dR_{M-1}
\]

\[
\times \rho(R, R_1; \tau) \cdots \rho(R_{M-1}, PR'; \tau),
\]

where \( \beta = 1/k_B T \) and \( \tau = \beta/M \) is the imaginary time step. The problem of evaluating the density matrix at a low temperature \( \beta^{-1} \) has been replaced by the problem of multiple integration of density matrices at a higher temperature \( \tau^{-1} \). The sum over permutations in Eq. (5) combined with the integration in Eq. (6) can be evaluated in path-integral Monte Carlo (PIMC) by a stochastic sampling of the discrete paths \( \{R, R_1, R_2, \cdots R_{M-1}, PR'\} \) using multilevel Monte Carlo sampling, an extension of the standard Metropolis method. The PIMC method is essentially exact, the only necessary input being the interparticle potential or equivalently the scattering length \( a \). In order to use Monte Carlo sampling, we must first provide a pair-product form of the exact two-body density matrices for the high-temperature density matrices that appear in the integrand Eq. (6). We used the high-temperature approximation for the hard-sphere propagator derived by Cao and Berne. In order to choose the value of \( M \), we performed consistency checks by varying \( M \) to see that the results have converged. We used up to fifteen time-slices (\( M = 15 \)). We performed PIMC in the continuum. The particles were confined to a cubic box with volume \( V \) and edge length \( L = V^{1/3} \), to which periodic boundary conditions were applied. We employed the canonical ensemble, i.e. in each simulation we fixed the temperature \( T \), the number of particles \( N \), and the dimensions \( L \) of the simulation cell. 20,000 - 30,000 MC steps are required for equilibration depending on the number density. Statistical averages are collected from 30,000 MC steps after this. In each MC step, we performed 50 - 800 trial moves at each time slice. We performed these calculations partly on IBM SP2 and partly on PC at the University of Georgia. The smallest-density simulations took about 350 CPU hours on IBM SP2.

The scaling functions for the condensate density and the superfluid density are similar and imply that in the (dilute) interacting 3D Bose gas condensation and superfluidity occur at precisely the same temperature. Superfluid density can be calculated using the winding number \( W \) for simulations that have periodic boundary conditions. Nonzero winding numbers occur when particles, through a series of permutations, are permuted with periodic images of themselves. The winding num-
ber is directly related to \( \rho_s \), the superfluid density. The superfluid density is given by \[34\]

\[
\rho_s = \frac{m}{\hbar^2} \frac{\langle W^2 \rangle}{3N},
\]

where the winding number \( W \) is defined by

\[
W = \sum_{i=1}^{N} \int_0^\beta dt \frac{d\phi_i(t)}{dt}.
\]

In order to obtain an estimate of the superfluid transition temperature \( T_c \), we perform a finite-size scaling analysis. Near the critical temperature \( T_c \), the finite-size behavior of the superfluid density obeys the scaled form \[35\]

\[
\rho_s(t, L)/\rho = L^{-\pi/\nu} f(tL^{1/\nu}),
\]

where \( \pi \) is the critical exponent of the bulk superfluid fraction, \( \rho_s(t)/\rho \sim t^\pi \), \( t = (T - T_c)/T_c \), \( \nu \) is the correlation length exponent, \( \xi(t) \sim t^{-\nu} \), and the universal function \( f(tL^{1/\nu}) \) must be analytic for finite argument. It is assumed that \( \pi = \nu \) since this is indicated by experiment \[36\], renormalization-group calculation \[37\], and the Josephson hyperscaling relation \( \pi = (d-2)\nu \). In obtaining an estimate of the critical temperature \( T_c \), we did not use Eq. \[38\] directly because of large statistical errors in our data (see Fig 2(a)). Instead we fit our data for different temperatures \( T \) and several values \( N \) of the total number of particles to a linear form for \( f \)

\[
N^{1/3} \rho_s(t, N)/\rho = f(tN^{1/3\nu}) = f(0) + f_0 N^{1/3\nu} (T - T_c)/T_c,
\]

where the dimensionless \( N^{1/3} \) has replaced the length \( L \). From the fitting, we determined four fitting parameters \( f(0), f_0, \nu, \) and \( T_c \).

**III. SIMULATION RESULTS AND DISCUSSION**

The main goal of this paper is to determine the critical temperature \( T_c \) of a 3D homogeneous system of hard-sphere bosons by path-integral Monte Carlo simulations and finite-size scaling. We have calculated the superfluid fraction \( \rho_s(T, N)/\rho \) for various number densities \( n \) at a fixed hard-sphere diameter \( a \).

In order to check the program carefully, we determined the critical temperature \( T_c^0 \) and the total energy density in the noninteracting case, both of which are known exactly. Fig. 1(a) shows the scaled superfluid fraction \( N^{1/3} \rho_s(t, N)/\rho \), scaled temperature \( tN^{1/3\nu} \), and the resulting linear fit (solid line) to Eq. \[39\] for the noninteracting hard spheres. The best fit parameters are the critical temperature of \( T_c/T_c^0 = 1.000(1) \) and the correlation length exponent of \( \nu = 0.90(6) \), in agreement with the theoretical exact values, namely \( T_c/T_c^0 = 1 \) and \( \nu = 1 \).

From the expression for the specific heat \( c(t, L) \),

\[
c(t, L) = \frac{\partial E(t, L)}{\partial T},
\]

we obtain the energy density \( E(t, L) \), via integration, up to a constant

\[
E(t, L) = c(0, \infty)T + L^{(\alpha-1)/\nu} T_c D(tL^{1/\nu}),
\]
where \( t = (T - T_c)/T_c \). Defining \( dD(x)/dx = g(x) \), we write the specific heat as follows:

\[
c(t, L) = c(0, \infty) + L^{\alpha/\nu} g(tL^{1/\nu}), \tag{13}
\]

where \( g(x) \) is a universal scaling function for the specific heat. For \( t \to 0 \) we obtain

\[
E(0, L) = E_c + E_1 L^{(\alpha-1)/\nu}. \tag{14}
\]

The result of the fit of the energy density data to Eq. (14) is shown in Fig. 1(b). In the fit we used \( \alpha = -1 \) and \( \nu = 1 \) for an ideal Bose gas. If we exclude the data corresponding to the smallest lattice, we obtain an estimate for the energy density in the thermodynamic limit \((N \to \infty)\) which agrees with the exactly known value within an errorbar.

In the interacting case, we have calculated the superfluid fraction and estimated the critical temperatures for various hard-sphere diameters \( a \) at a fixed number density. We can see that the critical temperature approaches \( T_c = T_c^0 \) as the hard-sphere diameter decreases (not shown), as expected.

In order to study the effect of interactions on the transition temperature, we calculated the superfluid fraction \( \rho_s(t, N)/\rho \) and determined the critical temperatures \( T_c(n) \) for various number densities \( 1 \times 10^{-7} \leq n \leq 5 \times 10^{-3} \).

Gruter, Ceperley, and Laloe investigated the dependence of \( \Delta T_c \) numerically using PIMC (to be referred to here as PRL97). In order to compare our estimated critical temperature with PRL97 data, we have calculated the superfluid fraction \( \rho_s(t, N)/\rho \) for \( N = 27, 64, 125, \) and 216 as a function of temperature \( T/T_c^0 \) at a fixed number density \( n = 5 \times 10^{-3} \). Fig. 2 shows our data (Fig. 2(a)) and our result of a linear fit (solid straight line) to the data (Fig. 2(b)) using Eq. (10). Our calculated superfluid fractions \( \rho_s(t, N)/\rho \) are significantly larger than PRL97 data (cf. Fig. 1 of Ref. 6) and our estimated critical temperature is \( T_c/T_c^0 = 1.078(1) \), which is higher than PRL97 data, \( T_c/T_c^0 = 1.057(2) \) (cf. Fig. 2 of Ref. 6). We don’t understand the reason for this large difference. In Fig. 3 we also show the scaled data and the resulting linear fit at the smallest number density \( n = 1 \times 10^{-7} \) we used in this study. Our estimated critical temperature is \( T_c/T_c^0 = 1.0061(14) \).

The resulting dependence of the transition tempera-
FIG. 4: Our calculated dependence of the interaction-induced shift of the transition temperature of a dilute homogeneous Bose gas on the scattering length $an^{1/3}$. (a) $(\Delta T_c/T_c^0)/an^{1/3}$ (b) $T_c/T_c^0$. Whenever not shown, the error bars in our simulation data are smaller than the symbol sizes. We also plotted the PRL97 data (Open circles) and Eq. 3 using Arnold’s results (Solid line). We see that the $(\Delta T_c/T_c^0)/an^{1/3}$ depends on the interaction strength $an^{1/3}$ while the PRL97 data are considerably flatter and smaller than our results (see Fig. 4(a)). Our calculated data approach Arnold’s results. The linear behavior is seen only at small value of $an^{1/3}$ (see Fig. 4(b)). Our calculated data are slightly larger than Eq. 3 using Arnold’s results (Solid line) in the linear region. The dashed straight line is a fit to our data points for the four smallest values of $n$. We found that the slope ($c_1$) is $1.32 \pm 0.14$. This is in agreement with the recent MC values of three-dimensional $O(2)$ scalar $\phi^4$ field theory, $c_1 = 1.29 \pm 0.05$ (Ref. 24) and $c_1 = 1.32 \pm 0.02$ (Ref. 16), and the result by variational perturbation theory (VPT), $c_1 = 1.27 \pm 0.11$ (Ref. 29).

In summary, we have determined the interaction-induced shift of the phase transition temperature for Bose-Einstein condensation of homogeneous weakly interacting Bose gases in three dimensions using PIMC and finite-size scaling. Our results show that $(\Delta T_c/T_c^0)/(an^{1/3})$ depends on the interaction strength $an^{1/3}$ while the previous PIMC results are considerably flatter and smaller than our results. We obtain $c_1 = 1.32 \pm 0.14$, in agreement with results from recent Monte Carlo methods of three-dimensional $O(2)$ scalar $\phi^4$ field theory and variational perturbation theory.

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