Bose-Einstein condensation temperature of a homogeneous weakly interacting Bose gas: Path integral Monte Carlo 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 $T_c = T_c^0 \{ 1 + c_1 a n^{1/3} + [c_2' \ln(an^{1/3}) + c_2''] a^2 n^{2/3} + O(a^3 n) \}$, 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 $\{(T_c - T_c^0)/T_c^0\}/(an^{1/3})$ depends strongly on the interaction strength $an^{1/3}$ while the previous PIMC results are considerably flatter and smaller than our results. We obtain $c_1 = 1.32 \pm 0.14$, in agreement with results from recent Monte Carlo methods of three-dimensional O(2) scalar ϕ^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 [3–29]. This nontrivial 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 $\Delta T_c \equiv (T_c - T_c^0)$ of the BEC transition temperature of a homogeneous Bose gas away from its ideal-gas value

$$T_c^0 = \frac{\hbar^2 2\pi}{m k_B} \left[n/\zeta\left(\frac{3}{2}\right) \right]^{2/3} \qquad (1)$$

behaves parametrically as

$$\frac{\Delta T_c}{T_c^0} \to c_1 a n^{1/3}, \qquad (2)$$

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, Holzmann *et al.* [13] 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, three-dimensional (3D) Bose gas can be expressed to leading order as

$$\frac{\Delta T_c}{T_c^0} = c_1 a n^{1/3} + [c_2' \ln(an^{1/3}) + c_2''] a^2 n^{2/3} + O(a^3 n), \quad (3)$$

where $c_2' \simeq 19.7518$ can be calculated perturbatively, whereas c_1 and c_2'' require nonperturbative 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 nonperturbative 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 ϕ^4 field theory, $c_1 = 1.29 \pm 0.05$ determined by Kashurnikov *et al.* [24] and $c_1 = 1.32 \pm 0.02$ determined by Arnold *et al.* [16], and by variational perturbation theory (VPT), $c_1 = 1.27 \pm 0.11$ determined by Kastening [29]. In particular, Gruter *et al.* [6] investigated the dependence of ΔT_c numerically using path integral Monte Carlo methods. They obtained the value of $c_1 = 0.34 \pm 0.06$ after numerical extrapo-

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lation of the calculation to the limit $a \to 0$. This value is about four times smaller than the above results. Holzmann *et al.* [13] 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.* [16] believed that one likely problem with the PIMC simulation of Gruter *et al.* [6] is inadequate system size. Kashurnikov *et al.* [24] 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 [31] to study the dependence on interaction strength of the phase-transition temperature for Bose-Einstein condensation of weakly interacting Bose gases in three dimensions. 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, equivalent to the interaction of hard spheres of diameter a (see, e.g., Refs. [2,3]). The Hamiltonian for this system may be written as

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j} v(|\mathbf{r}_i - \mathbf{r}_j|), \qquad (4)$$

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

$$v(r) = +\infty \quad (r < a)$$
$$= 0 \quad (r > a).$$

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

$$\rho_B(\mathbf{R}, \mathbf{R}'; \beta) = \frac{1}{N!} \sum_{P} \rho(\mathbf{R}, P\mathbf{R}'; \beta), \qquad (5)$$

where $\mathbf{R}$ and $\mathbf{R}'$ are two configurations of N hard spheres. P denotes a permutation of particle labels among hard spheres, and $P\mathbf{R}$ 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:

$$\rho(\mathbf{R}, P\mathbf{R}'; \beta) = \int \cdots \int d\mathbf{R}_1 d\mathbf{R}_2 \cdots d\mathbf{R}_{M-1}$$
$$\times \rho(\mathbf{R}, \mathbf{R}_1; \tau) \cdots \rho(\mathbf{R}_{M-1}, P\mathbf{R}'; \tau), \qquad (6)$$

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 β^{-1} has been replaced by the problem of multiple integration of density matrices at a higher temperature τ^{-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 $\{\mathbf{R}, \mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_{M-1}, P\mathbf{R}'\}$ using multilevel Monte Carlo sampling [31], an extension of the standard Metropolis method [32]. 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 [33]. 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 15 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 attempted 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 an 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 $\mathbf{W}$ for simulations that have periodic boundary conditions [34]. Nonzero winding numbers occur when particles, through a series of permutations, are permuted with periodic images of themselves. The winding number is directly related to ρ_s, the superfluid density. The superfluid density is given by [34]

$$\frac{\rho_s}{\rho} = \frac{m}{\hbar^2} \frac{\langle \mathbf{W}^2 \rangle}{3\beta N}, \qquad (7)$$

where the winding number $\mathbf{W}$ is defined by

$$\mathbf{W} = \sum_{i=1}^{N} \int_0^{\beta} dt \left(\frac{d\mathbf{r}_i(t)}{dt} \right). \qquad (8)$$

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]
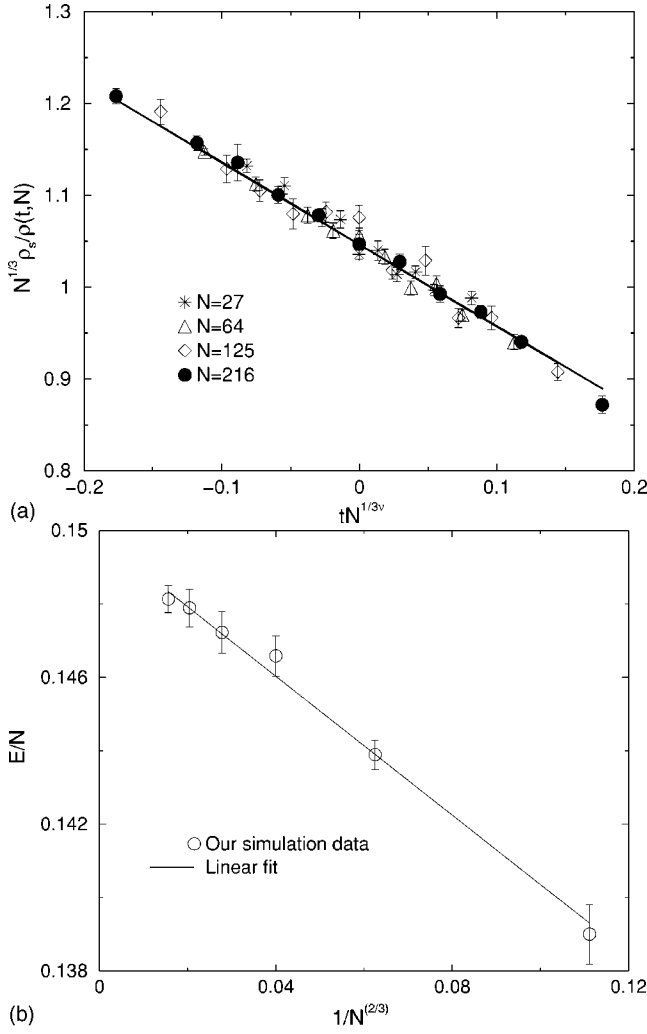
FIG. 1. Results for the noninteracting case at a fixed number density $n = 5 \times 10^{-3}$. (a) The scaled superfluid fraction $N^{1/3}\rho_s(t,N)/\rho$ as a function of scaled temperatures $tN^{1/3\nu}$. The solid line is a linear fit to Eq. (10). The best-fit parameters are the critical temperature of $T_c/T_c^0 = 1.000(1)$ and the correlation length exponent of $\nu = 0.90(6)$. (b) The total energy density as a function of the number of particles with a straight line fit to Eq. (14). From the fit we obtain the energy density in the thermodynamic limit $(N \to \infty)$.

$$\rho_s(t,L)/\rho = L^{-\pi/\nu}f(tL^{1/\nu}), \qquad (9)$$

where π is the critical exponent of the bulk superfluid fraction, $\rho_s(t)/\rho \sim t^{\pi}$, $t = (T-T_c)/T_c$, ν 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. (9) 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,
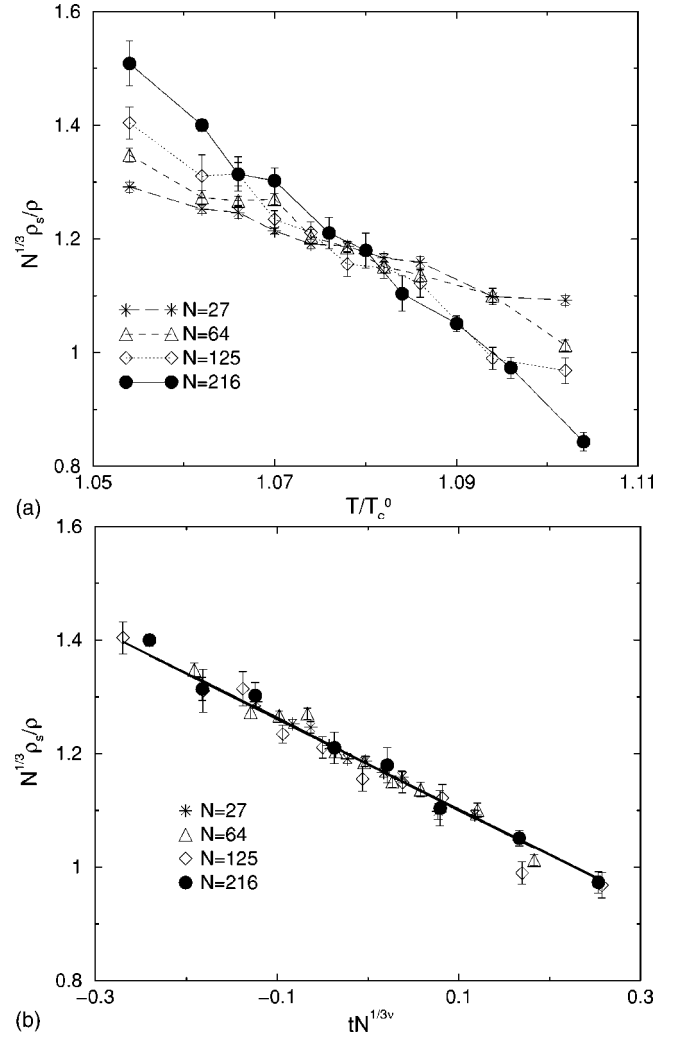

FIG. 2. Determination of the critical temperature T_c at a fixed number density $n = 5 \times 10^{-3}$ for the interacting case. (a) The scaled superfluid fraction $N^{1/3}\rho_s(t,N)/\rho$ as a function of scaled temperatures T/T_c^0. The four lines cross at the critical temperature. (b) Result of our linear fit (solid straight line) to the data from Eq. (10). Our estimated critical temperature is $T_c/T_c^0 = 1.078(1)$.

$$N^{1/3}\rho_s(t,N)/\rho = f(tN^{1/3\nu}) = f(0) + f_0 N^{1/3\nu}(T-T_c)/T_c, \qquad (10)$$

where the dimensionless $N^{1/3}$ has replaced the length L. From the fitting, we determined four fitting parameters $f(0)$, f_0, ν, 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 at a fixed number density $n = 5 \times 10^{-3}$ in the noninteracting case,
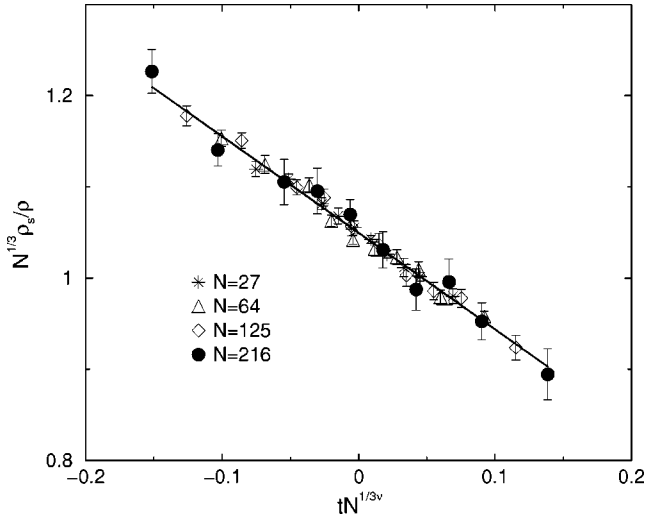
FIG. 3. Scaled superfluid fraction $N^{1/3}\rho_s(t,N)/\rho$ vs $tN^{1/3\nu}$ at the smallest number density $n=1\times10^{-7}$ we used in this study. Our estimated critical temperature is $T_c/T_c^0=1.0061(14)$.

both of which are known exactly. Figure 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. (10) 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 $c(t,L)$,

$$c(t,L) = \frac{\partial E(t,L)}{\partial T}, \tag{11}$$

and a scaling expression for the specific heat [38],

$$c(t,L) = c(0,\infty) + L^{\alpha/\nu}g(tL^{1/\nu}), \tag{12}$$

we obtain the energy density $E(t,L)$ by integrating Eq. (12) up to a constant

$$E(t,L) = c(0,\infty)T + L^{(\alpha-1)/\nu}T_cD(tL^{1/\nu}), \tag{13}$$

where $dD(x)/dx=g(x)$ and $g(x)$ is a universal scaling function for the specific heat. For $t\to0$ we obtain

$$E(0,L) = E_c + E_1L^{(\alpha-1)/\nu}. \tag{14}$$

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 system, we obtain an estimate for the energy density in the thermodynamic limit $(N\to\infty)$ which agrees with the exactly known value within an error bar.

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 temparature, we calculated the superfluid fraction $\rho_s(t,N)/\rho$ and determined the critical temperatures $T_c(n)$ for various number densities $1\times10^{-7}\leq n\leq5\times10^{-3}$.
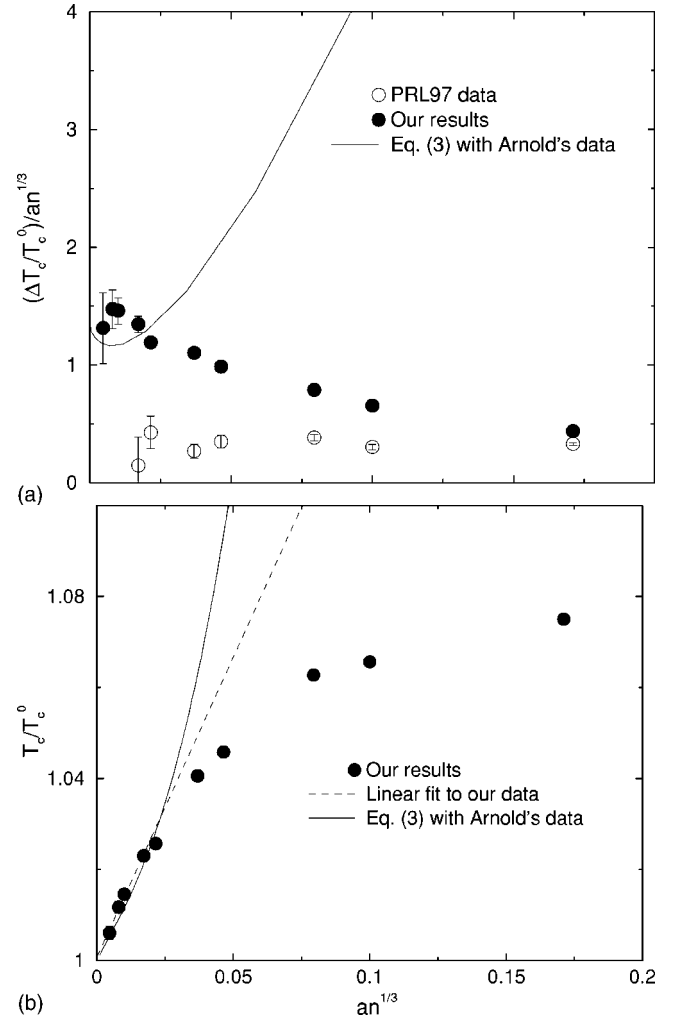

FIG. 4. Our calculated dependence of the interaction-induced shift of the transition temperature of a dilute homogeneous Bose gas on the scattering length $an^{1/3}$: (a) $(\Delta T_c/T_c^0)/an^{1/3}$; (b) T_c/T_c^0. Whenever not shown, the error bars in our simulation data are smaller than the symbol sizes. We also plotted the GCL data (open circles) and Eq. (3) using Arnold's results [16] (solid line). (a) $(\Delta T_c/T_c^0)/an^{1/3}$ depends on the interaction strength $an^{1/3}$ while the GCL data are considerably flatter and smaller than our results. (b) The linear behavior is seen only at small values of $an^{1/3}$. The dashed straight line is a fit to our four smallest data points. We found that the slope (c_1) is 1.32(14).

Gruter, Ceperley, and Laloe [6] investigated the dependence of ΔT_c numerically using PIMC (to be referred to here as GCL). In order to compare our estimated critical temperature with GCL data, we have calculated the superfluid fraction $\rho_s/\rho(T,N)$ for $N=27$, 64, 125, and 216 as a function of temperature T/T_c^0 at a fixed number density $n=5\times10^{-3}$. Figure 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 GCL 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 GCL data, $T_c/T_c^0=1.057(2)$ (cf. Fig. 2 of Ref. [6]). We do not understand the reason for this large difference [39]. 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 temperature (a) $(\Delta T_c/T_c^0)/an^{1/3}$ and (b) T_c/T_c^0 on $an^{1/3}$ is shown in Fig. 4. Whenever not shown, the error bars in our simulation data are smaller than the symbol sizes. We also show comparisons between our results (filled circles), the GCL data (open circles), and Eq. (3) using Arnold's results [16] (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 GCL data are considerably flatter and smaller than our results [see Fig. 4(a)]. Our calculated data approach to 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 [16] (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 ± 0.14. This is in agreement with the recent MC values of three-dimensional O(2) scalar ϕ^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 $\{(T_c - T_c^0)/T_c^0\}/(an^{1/3})$ depends on the interaction strength $an^{1/3}$ while the previous PIMC results [6] 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 ϕ^4 field theory [16,24] and variational perturbation theory [29].

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