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Critical Temperature Shift in Weakly Interacting Bose Gas

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With a high-performance Monte Carlo algorithm we study the interaction-induced shift of the critical point in weakly interacting three-dimensional $|\psi|^4$ -theory (which includes quantum Bose gas). In terms of critical density, n_c , mass, m , interaction, U , and temperature, T , this shift is universal: $\Delta n_c(T) = -Cm^3T^2U$, the constant C found to be equal to 0.0140 ± 0.0005 . For quantum Bose gas with the scattering length a this implies $\Delta T_c/T_c = C_0an^{1/3}$, with $C_0 = 1.29 \pm 0.05$.

The problem of interaction-induced shift of the critical temperature in a weakly interacting Bose gas has been attracting a lot of theoretical effort during recent years [1–5]. Apart from an apparent fundamental interest, the study of this problem has been strongly stimulated by the experimental achievement of Bose-Einstein condensation in ultra-cold gases [6] and, correspondingly, the perspective of experimental verification of theoretical predictions. The first experimental study of the critical temperature of interacting Bose gas was reported recently for the ⁴He-Vycor system [7].

Despite a considerable number of papers dealing with the issue, the answer for the critical temperature shift still remains a matter of controversy. As it follows from simple analysis of dimensions, the result should have the form

$$\frac{\Delta T_c}{T_c} = C_0an^{1/3}, \quad (1)$$

where C_0 is a dimensionless constant. There are reasonable physical arguments for C_0 to be positive [2], and most studies predict that $C_0 > 0$. However, there is a profound discrepancy between different approaches in the value of C_0 . The range of variation of different predictions is an order-of-magnitude large: 0.34 [2], 0.7 [3], 2.3 [5], 2.9 [4], 4.66 [1]. As far as the experiment of Ref. [7] is concerned, where the law (1) was clearly observed, it should be realized that the only quantity that was really measured was the product C_0a . Therefore, until the accurate value of the scattering length a is available, it is impossible to make a reliable conclusion about C_0 [8].

Though Eq. (1) formally looks like a perturbative correction in terms of the gas parameter $an^{1/3}$, physically it is clear that this is not the case (cf., however, [5]), because in the thermodynamic limit any finite interaction, no matter how small, changes the universality class of the phase transition: while the ideal Bose gas belongs to the universality class of the Gaussian complex-field model, the interacting system pertains to the XY-model universality class. Due to this fact the first-principle analytic description of the interacting Bose gas at the critical point is rather difficult. To the best of our knowledge, up to now there was done only one *ab initio* Monte Carlo

simulation of the interacting gas in the context of ΔT_c (Grüter, Ceperley, and Laloë, Ref. [2]). An alternative Monte Carlo approach by Holzmann and Krauth [5] was based on a *hypothesis* that Eq. (1) can be obtained in a (rather sophisticated) perturbative way, by simulating an ideal gas.

The goal of this Letter is to develop a numeric scheme for describing weakly interacting Bose gas in the fluctuation region, which, in particular, could produce an accurate result for C_0 . The crucial point that renders this aim attainable is the universality of the long-wave behavior of weakly interacting $|\psi|^4$ -theories in the fluctuation region at transition point: All these theories, no matter quantum or classical, continuous or discrete, lead to a generic long-wave Hamiltonian (cf., e.g., [4])

$$H = \int \left\{ \frac{1}{2m} |\nabla \psi|^2 + \frac{U}{2} |\psi|^4 \right\} d\mathbf{r}. \quad (2)$$

From this universality it follows that in *any* such system the shift of the critical density (which is not sensitive to the ultra-violet cutoff of the theory) is given by the formula (from now on $\hbar = 1$)

$$\Delta n_c(T) = -Cm^3T^2U, \quad (3)$$

where C is a universal constant. Then, the critical temperature shift (which is not universal, being sensitive to the short-wave physics) can be obtained for each particular system from the obvious relation

$$\frac{\Delta T_c}{\Delta n_c} = -\frac{dT_c^{(0)}(n)}{dn}, \quad (4)$$

where $T_c^{(0)}$ is the critical temperature of the corresponding ideal system. From Eq. (4) one readily obtains for the quantum Bose gas

$$C_0 \approx 91.8C. \quad (5)$$

The universality of the density shift (3) suggests that it can actually be calculated not in a continuous quantum system, where simulations are computationally expensive, but in a discrete classical model

$$H = - \sum_{\langle ij \rangle} [\psi_i^* \psi_j + \text{c.c.}] + \frac{U}{2} \sum_i |\psi_i|^4, \quad (6)$$

where i and j stand for the sites of 3D cubic lattice, $\langle ij \rangle$ denotes nearest-neighbor sites, and ψ_i is a complex variable. The long-wave behavior of the discrete system (6) is described by the Hamiltonian (2) with $m = 1/2$. The advantage of utilizing model (6) for numeric analysis is associated with the existence of a very powerful Worm algorithm for simulating discrete classical systems of this type [10].

Analysis of dimensions. We start with rendering general considerations leading to Eq. (3). Consider the grand canonical counterpart of the Hamiltonian (2)

$$H' = \int \left\{ -\frac{1}{2m} |\nabla \psi|^2 + \frac{U}{2} |\psi|^4 - \tilde{\mu} |\psi|^2 \right\} d\mathbf{r}. \quad (7)$$

Here $\tilde{\mu}$ is an effective chemical potential [which, generally speaking, does not coincide with the bare chemical potential of the original system for which H' plays the role of the effective Hamiltonian]. As the field ψ describes only the long-wave modes of the original system, it is supposed to have some ultra-violet cutoff:

$$\psi(\mathbf{r}) = \sum_{k < k_0} a_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}}. \quad (8)$$

The choice of k_0 is arbitrary as long as k_0 is larger than the momentum k_c which characterizes the momentum region where harmonics are strongly coupled to each other ($k \gg k_c$ harmonics are almost free). If $k_0 \sim k_c$, then all three terms in Eq. (7) are of the same order, and we have the following relations

$$k_c^2/m \sim |\tilde{\mu}| \sim \tilde{n}U, \quad (9)$$

$$\tilde{n} \sim \langle |\psi|^2 \rangle \sim \sum_{k < k_c} n_k, \quad (10)$$

where $n_k = \langle |a_{\mathbf{k}}|^2 \rangle$ and $\langle \dots \rangle$ means statistical averaging.

According to Eq. (10), $\tilde{n} \sim k_c^3 n_{k_c}$. Since k_c is a momentum separating strongly coupled long-wave harmonics from ideal short-wave ones, the order-of-magnitude estimate for n_{k_c} may be obtained from the ideal gas formula :

$$n_{k_c} \sim \frac{T}{k_c^2/2m - \tilde{\mu}} \sim \frac{T}{\tilde{\mu}}. \quad (11)$$

Substituting this back to Eqs. (9)-(10) we see that

$$k_c \sim m^2 T U, \quad \tilde{n} \sim m^3 T^2 U. \quad (12)$$

Consider now the shift of the critical density

$$\Delta n_c(T) = \sum_{\mathbf{k}} [n_{\mathbf{k}}^{(\text{crit})} - n_{\mathbf{k}}^{(\text{crit},0)}], \quad (13)$$

where $n_{\mathbf{k}}^{(\text{crit})}$ and $n_{\mathbf{k}}^{(\text{crit},0)}$ are the occupation numbers at the critical density (corresponding to a given temperature T) for interacting and non-interacting system, respectively. The main contribution to the sum in Eq. (13) comes from $k \sim k_c$, since at $k \gg k_c$ the terms $n_{\mathbf{k}}^{(\text{crit})}$ and $n_{\mathbf{k}}^{(\text{crit},0)}$ are almost equal and compensate each other. At $k \sim k_c$ one can use the estimate (11), which means that $\Delta n_c \sim \tilde{n}$, and we arrive at Eq. (3).

Numeric procedure and results. Our Monte Carlo scheme is based on the Worm-algorithm simulation of the high-temperature expansions for the two-point correlator $\langle \psi_i^* \psi_j \rangle$ in the grand canonical ensemble. (The description of this approach and performance tests see in Ref. [10]).

To proceed, we need a formal definition of the critical point for finite system with linear dimension L , which, on one hand, is consistent with the thermodynamic limit $L \rightarrow \infty$, and, on the other hand, is convenient from the computational viewpoint. We adopt the following definition. By critical we understand the point where the condensate density equals to

$$n_0^{(\text{crit})}(L) = T/(3.75L). \quad (14)$$

This definition is optimized for the ideal gas (minimal finite-size corrections for the total density). Nevertheless, it proved to be quite satisfactory for the interacting system as well, including the limit of strong interaction.

The classical model (6) possesses an obvious similarity property: The transformation $\psi \rightarrow \sqrt{T}\psi$, $U \rightarrow U/T$ reduces the problem to the corresponding $T = 1$ case. Hence, without loss of generality, we set $T = 1$.

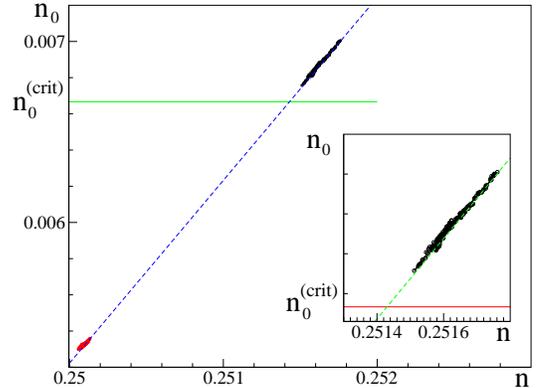


FIG. 1. Co-variance of n_0 and n for $U = 1$, $L = 40$, and two different values of μ . Data points correspond to successive Monte Carlo outputs (n, n_0) . The crucial observation here is that fluctuations of n_0 and n are strongly correlated, and follow the line: $\delta n_0 / \delta n \approx d\tilde{n}_0 / d\tilde{n}$, where bars above the symbols denote statistic limits. With changing chemical potential the whole linear-shape pattern just shifts along its axis. We thus obtain $n_c(U = 1, L = 40) = 0.25143(3)$ from this plot.

The procedure of determining the critical density is as follows. We iteratively tune the chemical potential μ until (14) is satisfied with a required accuracy, and then calculate the corresponding density. For small U , where a high precision is required to resolve a small effect [11], we radically improve the efficiency of the pinpointing procedure by utilizing the covariance (see Ref. [12]) in the statistical fluctuations of Monte Carlo data for n_0 and n . The existence of strong covariance between fluctuations of n_0 and n (Fig. 1) allows one to extract the dependence $n_0(n)$ with significantly higher accuracy than the accuracy of separate calculations of $n_0(\mu)$ and $n(\mu)$.

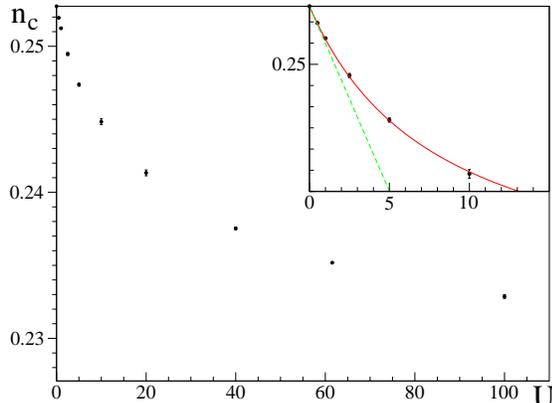


FIG. 2. Critical ratio $(n/T)_c$ for the model (6), as a function of interaction U . The upper bound of the box corresponds to $(n/T)_c = 0.25274$ of the ideal system, and the lower bound corresponds to the $U \rightarrow \infty$ limit, which is the XY-model with $(n/T)_c \approx 0.22708$. Insert: The critical density at small U . The dashed line corresponds to Eq. (3) with $C = 0.0140$. The solid line corresponds to more accurate approximation Eq. (17) at $L \rightarrow \infty$: $\Delta n_c = -Cm^3T^2U/(1+b_0U)$ with $b_0 = 0.123$.

Prior to inspecting the region of small U , it is instructive to consider the behavior of the critical density for the model (6) at finite interactions, in view of a remarkable contrast to the quantum case. In a quantum gas with the parameter $an^{1/3}$ of order unity, the shift of the critical temperature is determined by a competition of two effects [2]: (i) the suppression of the long-wave fluctuations of density (which stimulates condensation), and (ii) the depletion of the long-wave components of the field (which effectively reduces density, and thus drives the system away from the phase transition). The first circumstance dominates at small interaction, while for larger $an^{1/3}$ the second effect takes over. Following this competition, the shift of the critical temperature goes through a maximum around $an^{1/3} \lesssim 1$, and then goes down finally becoming negative [2,7]. While the first effect is of classical-field nature and thus is relevant to (6), the second effect is of quantum nature, and does not have any classical analog. That is why in the classical system we expect that the (negative) shift of the critical density

will be a monotonous function of U . This is precisely what is revealed by our simulation (Fig. 2). The critical density is monotonously decreasing with interaction, saturating at $U \rightarrow \infty$ to the known value $(n/T)_c \approx 0.22708$ corresponding to the XY-model (see, e.g., Ref. [13]). [As an illustration of the fact that the criterion (14) works reasonably well for the strongly interacting system, we reproduced the above-mentioned critical point of the XY-model with the accuracy of 5 significant digits by the brut-force simulation of large systems with $L = 160$, and checked that finite-size systematic errors are almost irrelevant already for $L = 40$.]

Now we turn to the region of small U . As the accuracy of calculations can be significantly improved by a proper finite-size analysis of the data, we begin with generalizing relation (3) to the finite-size case. We note that in the limit $U \rightarrow 0$ the only relevant lengthscale is the mode-coupling radius

$$r_c = \frac{2\pi}{k_c} \sim \frac{1}{m^2TU}, \quad (15)$$

Hence, r_c defines the characteristic size of the system that can be considered as macroscopic with respect to (small) interaction: The system is in the proper thermodynamic limit if, and only if $L \gg r_c$. In the limit $L \ll r_c$ interactions can be treated perturbatively, and thus are essentially irrelevant. From this consideration we arrive at the following generalization of Eq. (3):

$$\frac{\Delta n_c(T, L)}{m^3T^2U} = -f(r_c/L) + \mathcal{O}(U), \quad (16)$$

where the particular form of the dimensionless function f depends on the definition of $n_c(L)$, apart from universal limits $f(0) = C$ and $f(\infty) = 0$. On the basis of Eq. (16), we employ the following scaling function which should adequately describe the limit $U \rightarrow 0, L \rightarrow \infty$

$$-\frac{\Delta n_c(T, L)}{m^3T^2U} = \frac{C}{1 + b_0U + (a_1 + b_1U)x^\eta}, \quad (17)$$

where $x = 1/(Lm^2TU)$ and $\eta = 1.038$ [13] in accordance with expected asymptotic behavior of the finite-size corrections for XY-type models. Fitting parameters C, b_0, a_1 , and b_1 were obtained by stochastic optimization ($C = 0.0140, a_1 = 1.29, b_0 = 0.123, b_1 = 0.744$). As is seen from Fig. 3, the scaling function (17) works extremely well. With errorbars defined from the uncertainty of the fitting procedure, for the constant C we have

$$C = 0.0140 \pm 0.0005, \quad (18)$$

which, according to Eq. (5), means

$$C_0 = 1.29 \pm 0.05. \quad (19)$$

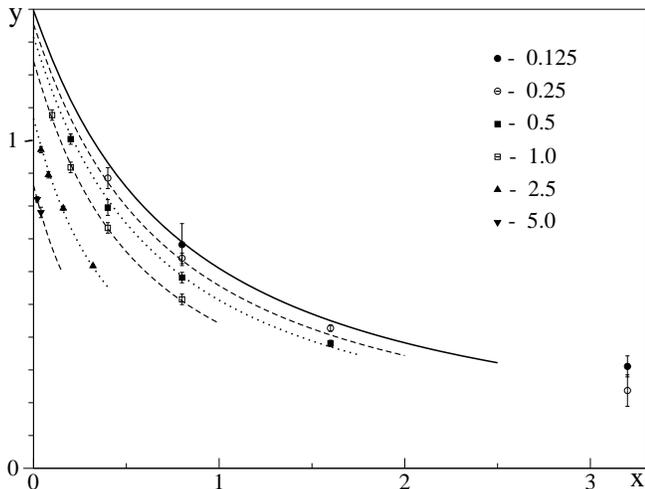


FIG. 3. Scaling plot of $y = 10^2 \Delta n_c / (m^3 T^2 U)$ vs $x = 1 / (L m^2 T U)$ at small U . The upper curve is given by the scaling function at $U = 0$. Note that while this function is not supposed to fit the data at $x \geq 1$, actually it is rather accurate up to $x \sim 3$.

While the particular form of $f(x)$ in the region $0 < x < \infty$ is sensitive to the definition of $n_c(L)$, the typical scale $x \sim x_c$ of significant variation of $f(x)$ from its limiting value $f(0)$ depends only on the mode-coupling radius: $x_c \sim 1 / (r_c m^2 T U)$. From Fig. 3 we deduce

$$r_c \approx 1 / (m^2 T U). \quad (20)$$

Using Eq. (20), one can readily estimate how small should be the interaction for a particular weakly interacting system to demonstrate the universal long-wave behavior. The generic requirement is that r_c be much larger than other microscopic lengthscales at which the behavior of the system becomes non-universal (due to the discreteness of the system, or/and quantization of occupation numbers). The most severe requirement for the quantum Bose gas is $r_c \gg \lambda_T$, where $\lambda_T \approx n^{-1/3}$ is the thermal de Broglie wavelength at the Bose condensation point. In terms of the gas parameter this means $an^{1/3} \ll 0.025$, and we immediately realize that neither Monte Carlo simulation of Ref. [2], nor the experiment of Ref. [7] have reached the universality region: In both cases the minimal value of na^3 was $\sim 10^{-5}$, while our estimate shows that one may expect universality only at $na^3 \lesssim 10^{-7}$.

In conclusion, we have developed a Monte Carlo approach for the study of weakly interacting $|\psi|^4$ -theories in the fluctuation region. With this technique we obtained an accurate result for the critical temperature of weakly interacting three-dimensional Bose gas, and established a criterion of its applicability. We note that the method can be also applied to weakly interacting Bose gas in two dimensions. The CPU time required for collecting high-precision data reported above is equivalent to two years on PIII-733 processor.

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