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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 $0.0140 \pm 0.0005$. For quantum Bose gas with the scattering length $a$ this implies $\Delta T_c/T_c = C_0 a n^{1/3}$, 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 \cite{1, 2, 3, 4, 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 \cite{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 $^4$He-Vycor system \cite{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

$$\frac{\Delta T_c}{T_c} = C_0 a n^{1/3},$$  \hspace{1cm} (1)

where $C_0$ is a dimensionless constant. There are reasonable physical arguments for $C_0$ to be positive \cite{6}, 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 \cite{2, 3}, 0.7 \cite{3}, 2.3 \cite{4}, 2.9 \cite{5}, 4.66 \cite{6}. As far as the experiment of Ref. \cite{7} is concerned, where the law \cite{6} was clearly observed, it should be realized that the only quantity that was really measured was the product $C_0 a$. Therefore, until the accurate value of the scattering length $a$ is available, it is impossible to make a reliable conclusion about $C_0$. \cite{6}

Though Eq. (1) formally looks like a perturbative correction in terms of the gas parameter $a n^{1/3}$, physically it is clear that this is not the case (cf., however, \cite{6}), 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 \textit{ab initio} Monte Carlo simulation of the interacting gas in the context of $\Delta T_c$ (Grüter, Ceperley, and Laloë, Ref. \cite{2}). An alternative Monte Carlo approach by Holzmann and Krauth \cite{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., \cite{6})

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

From this universality it follows that in \textit{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 $h = 1$)

$$\Delta n_c(T) = -Cm^3T^2U, \hspace{1cm} (3)$$

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

$$\frac{\Delta T_c}{\Delta n_c} = -\frac{dT_c^{(0)}(n)}{dn}, \hspace{1cm} (4)$$

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

$$C_0 \approx 91.8C. \hspace{1cm} (5)$$

The universality of the density shift \cite{6} suggests that it can actually be calculated not in a continuous quantum system, where simulations are computationally expensive, but in a discrete classical model

\begin{center}

\begin{tabular}{c}
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\end{center}
\[
H = - \sum_{<ij>} [\psi_i^* \psi_j + \text{c.c.}] + \frac{U}{2} \sum_i |\psi_i|^4 ,
\]

where \(i\) and \(j\) stand for the sites of 3D cubic lattice, \(<ij>\) denotes nearest-neighbor sites, and \(\psi_i\) is a complex variable. The long-wave behavior of the discrete system (6) is described by the Hamiltonian (6) 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 [14].

Analysis of dimensions. We start with rendering general considerations leading to Eq. (6). Consider the grand canonical counterpart of the Hamiltonian (6)

\[
H' = \int \left\{ -\frac{1}{2m} |\nabla \psi|^2 + \frac{U}{2} |\psi|^4 - \tilde{\mu} |\psi|^2 \right\} d\mathbf{r} .
\]

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 \(\psi\) describes only the long-wave modes of the original system, it is supposed to have some ultra-violet cutoff:

\[
\psi(\mathbf{r}) = \sum_{k<k_0} a_k e^{i\mathbf{k}\cdot\mathbf{r}} .
\]

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. (6) are of the same order, and we have the following relations

\[
k_c^2/m \sim |\tilde{\mu}| \sim \tilde{n}U ,
\]

\[
\tilde{n} \sim \langle |\psi|^2 \rangle \sim \sum_{k<k_c} n_k ,
\]

where \(n_k = \langle |a_k|^2 \rangle\) and \(\langle \ldots \rangle\) means statistical averaging.

According to Eq. (11), \(\tilde{n} \sim k_c^3 n_{k_c}\). 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:

\[
n_{k_c} \sim \frac{T}{k_c^2/2m - \tilde{\mu}} \sim \frac{T}{\tilde{\mu}} .
\]

Substituting this back to Eqs. (6)-(11) we see that

\[
k_c \sim m^2 TU , \quad \tilde{n} \sim m^3 T^2 U .
\]

Consider now the shift of the critical density

\[
\Delta n_c(T) = \sum_k [n_k^{(\text{crit})} - n_k^{(\text{crit},0)}] ,
\]

where \(n_k^{(\text{crit})}\) and \(n_k^{(\text{crit},0)}\) 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 \(n_k^{(\text{crit})}\) and \(n_k^{(\text{crit},0)}\) are almost equal and compensate each other. At \(k \sim k_c\) one can use the estimate (14), which means that \(\Delta n_c \sim \tilde{n}\) and we arrive at Eq. (6).

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. [14].)

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

\[
n_0^{(\text{crit})}(L) = T/(3.75L) .
\]

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 \(\mu\). 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: \(\delta n_0/\delta n \approx d\delta n/d\delta n\), 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.](image-url)
The existence of strong covariance between fluctuations

\[ b_L \text{approximation Eq. (17) at larger circumstance dominates at small interaction, while for the system away from the phase transition). The first field (which effectively reduces density, and thus drives } \]

\[ (n/T)_c \approx 0.22708 \] corresponding to the \( XY \)-model (see, e.g., Ref. [13]). As an illustration of the fact that the criterion \( b \) 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 \( b \) to the finite-size case. We note that in the limit \( U \to 0 \) the only relevant lengthscale is the mode-coupling radius

\[ r_c = \frac{2\pi}{k_c} \sim \frac{1}{m^2 TU} \] (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. \( b \):

\[ \frac{\Delta n_c(T, L)}{m^3 T^2 U} = -f(r_c/L) + O(U) \] (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. \( b \), we employ the following scaling function which should adequately describe the limit \( U \to 0 \), \( L \to \infty \)

\[ - \frac{\Delta n_c(T, L)}{m^3 T^2 U} = \frac{C}{1 + b_0 U + (a_1 + b_1 U) e^\eta} \] (17)

where \( x = 1/(L m^2 TU) \) and \( \eta = 1.038 \) 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 \( b \) works extremely well. With errorbars defined from the uncertainty of the fitting procedure, for the constant \( C \) we have

\[ C = 0.0140 \pm 0.0005 \] (18)

which, according to Eq. \( b \), means

\[ C_0 = 1.29 \pm 0.05 \] (19)
mal value of reached the universality region: In both cases the mini-

culation of Ref. [2], nor the experiment of Ref. [7] have

and we immediately realize that neither Monte Carlo sim-

Bose gas is numbers). The most severe requirement for the quantum

ness of the system, or/and quantization of occupation

lar scale

Using Eq. (20), one can readily estimate how small should

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

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cal scale x \sim x_c of significant variation of f(x) from its

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In conclusion, we have developed a Monte Carlo ap-

proach 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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