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## Transition Temperature of the Homogeneous, Weakly Interacting Bose Gas

Markus Holzmann<sup>1,2,\*</sup> and Werner Krauth<sup>1,†</sup>

<sup>1</sup>CNRS-Laboratoire de Physique Statistique, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France

<sup>2</sup>Laboratoire Kastler-Brossel, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France<sup>‡</sup>

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We present a Monte Carlo calculation for up to  $N \sim 20000$  bosons in 3D to determine the shift of the transition temperature due to small interactions  $a$ . We generate independent configurations of the ideal gas. At finite  $N$ , the superfluid density changes by a certain correlation function in the limit  $a \rightarrow 0$ ; the  $N \rightarrow \infty$  limit is taken afterwards. We argue that our result is independent of the order of limits. Detailed knowledge of the noninteracting system for finite  $N$  allows us to avoid finite-size scaling assumptions.

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Feynman [1] has provided us with a classic formula for the partition function of the canonical noninteracting Bose gas. It represents a “path integral without paths,” as they have been integrated out. What remains is the memory of the cyclic structure of the permutations that were needed to satisfy bosonic statistics,

$$Z_N = \sum_{\{m_k\}} \mathcal{P}(\{m_k\}); \quad \text{with } \mathcal{P}(\{m_k\}) = \prod_{k=1}^N \frac{\rho_k^{m_k}}{m_k! k^{m_k}}. \quad (1)$$

The partitions  $\{m_k\}$  in Eq. (1) decompose permutations of the  $N$  particles into exchange cycles ( $m_i$  cycles of length  $i$  for all  $1 \leq i \leq N$  with  $\sum_k k m_k = N$ ).  $\rho_k$  is a system-dependent weight for cycles of length  $k$ .

In this paper we present an explicit Monte Carlo calculation for up to  $\sim 20000$  bosons in three dimensions, starting from Eq. (1). The calculation allows us to determine unambiguously the shift in the transition temperature  $T_c$  for *weakly interacting* bosons in the thermodynamic limit for an infinitesimal  $s$ -wave scattering length  $a$ . This fundamental question has led to quite a number of different and contradictory theoretical as well as computational answers (cf., e.g., [2–4]).

We will first use Eq. (1) and its generalizations to determine very detailed properties of the finite- $N$  canonical Bose gas in a box with periodic boundary conditions. We then point out that *all* information on the shift of  $T_c$  for weakly interacting gases is already contained in the non-

interacting system. In the linear response regime (infinitesimal interaction), it is a certain correlation function of the noninteracting system which determines the shift in  $T_c$ . This correlation is much too complicated to be calculated directly, but we can *sample* it, even for very large  $N$ . To do so, we generate independent bosonic configurations in the canonical ensemble. We have found a solution [based on Feynman’s formula Eq. (1)] which avoids Markov chain Monte Carlo methods. In our two-step procedure, a partition  $\{m_k\}$  is generated with the correct probability  $\mathcal{P}(\{m_k\})$ . Then, a random boson configuration is constructed for the given partition.

We stress that all our calculations are done very close to  $T_c$ , so that the correlation length  $\xi$  of any macroscopic sample is much larger than the actual system size  $L$  of the simulation. This condition  $L \ll \xi$  allows us to invoke the standard finite-size scaling hypothesis [5], but also to take the  $N \rightarrow \infty$  limit after the limit  $a \rightarrow 0$ .

A key concept in the path integral representation of bosons is that of a *winding number*. Consider first the density matrix  $\rho(r, r', \beta)$  of a single particle [ $r = (x, y, z)$ ] at inverse temperature  $\beta = 1/T$ . In a three-dimensional cubic box of length  $L$  with periodic boundary conditions,  $\rho(r, r', \beta) = \rho(x, x', \beta) \times \rho(y, y', \beta) \times \rho(z, z', \beta)$  with, e.g.,

$$\rho(x, x', \beta) = \sum_{w_x=-\infty}^{\infty} \frac{\exp[(x - (x' + Lw_x))^2/2\beta]}{\sqrt{2\pi\beta}}. \quad (2)$$

In Eq. (2),  $x$  and  $x'$  are to be taken within the periodic box ( $0 < x, x' < L$ ).

It is more convenient to adopt nonperiodic coordinates ( $-\infty < x, x' < \infty$ ), as we will do from here on. In Fig. 1, the path drawn with a thick line can equivalently be tagged by  $(x_1, x'_1)$  or by  $(\tilde{x}_1, \tilde{x}'_1)$ . This notation allows one to keep track of the topology of paths without introducing intermediate time steps  $\tau$ , even for very small systems. With this convention, the winding number of a configuration,  $W = (W_x, W_y, W_z)$ , is defined as

$$W = \sum (r'_i - r_i)/L. \tag{3}$$

The winding number  $W$  in Eq. (3) is the sum of the (integer) winding numbers for each of the statistically uncorrelated cycles which comprise the configuration. The complete statistical weight  $\rho_k$  of a cycle of length  $k$  [cf. Eq. (1)] is given by the sum of the weights  $\rho_{k,w}$  for all winding numbers  $w$ ,

$$\rho_k = \left[ \sum_{w=-\infty}^{\infty} \rho_{k,w} \right]^3; \tag{4}$$

$$\rho_{k,w} = \frac{L}{\sqrt{2\pi k\beta}} \exp\left(-\frac{L^2 w^2}{2k\beta}\right).$$

Pollock and Ceperley [6] have obtained the result

$$\rho_s/\rho = \frac{\langle W^2 \rangle L^2}{3\beta N}, \tag{5}$$

which connects the system's superfluid density  $\rho_s/\rho$  to the winding number in a rigorous fashion.

It is possible to determine the mean square winding number  $\langle W^2 \rangle$  from Eq. (1). We first compute  $\langle w^2 \rangle$  for a given partition  $\{m_k\}$

$$\langle w^2 \rangle_{\{m_k\}} = \sum m_k \langle w^2 \rangle_k. \tag{6}$$

Here,  $\langle w^2 \rangle_k$  is the mean with respect to cycles of length  $k$ ,  $\langle w^2 \rangle_k = 3[\sum_w \rho_{k,w} w^2][\sum_w \rho_{k,w}]^2/\rho_k$ . This yields, by summation over partitions

$$\langle W^2 \rangle = \sum \frac{\rho_k}{k} \langle w^2 \rangle_k Z_{N-k}/Z_N. \tag{7}$$

We have also determined the probability distribution of  $W_x$ .

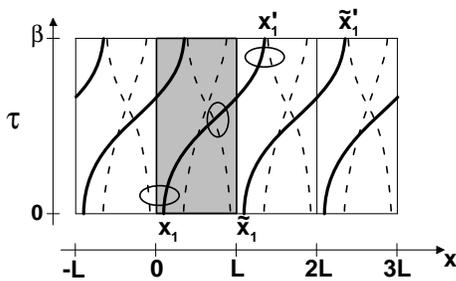


FIG. 1. A one-dimensional periodic simulation box with three bosons. Particles move in imaginary time  $0 < \tau < \beta$  and in periodic space  $0 < x < L$ . We use nonperiodic coordinates.

An analogous calculation formally replaces  $\langle w^2 \rangle_k \rightarrow k$  in Eq. (6), which becomes  $\sum_k k m_k = N$  [cf. Eq. (1)]. Equation (7) is transformed into

$$Z_N = \sum \rho_k Z_{N-k}/N. \tag{8}$$

Equation (8) allows the recursive calculation of the partition function  $Z_N$  if  $Z_1, \dots, Z_{N-1}$  are known [7].

The same relation Eq. (8) allows us to identify

$$k \langle m_k \rangle = \rho_k Z_{N-k}/Z_N \tag{9}$$

as the mean number of particles in a cycle of length  $k$ .

From a different point of view, the quantity  $\sum_k k m_k e^{-\beta k \epsilon_i} / \rho_k$  determines the occupation number of single-particle energy levels  $\epsilon_i$  for a given partition  $\{m_k\}$ . This allows us to compute the average number  $\langle N_i \rangle$  of particles occupying state  $\epsilon_i$  in the bosonic system,

$$\langle N_i \rangle = \sum_{k=1}^N \left\{ e^{-\beta k \epsilon_i} \frac{Z_{N-k}}{Z_N} \right\}. \tag{10}$$

Equation (10) is of crucial importance: We find that  $N_0/N$ , the condensate fraction, is different from the superfluid fraction, as determined from Eqs. (5) and (7) in a finite noninteracting system.

The term  $\{ \}$  in Eq. (10) can be regarded as the probability  $P(n_i \geq k)$  of having at least  $k$  particles in state  $\epsilon_i$ . Taking the sum over all states  $i$ , with the use of Eq. (9), we can connect cycle statistics with the usual occupation number representation,

$$k \langle m_k \rangle = \sum_i P(n_i \geq k). \tag{11}$$

This curious result, which is of practical use in inhomogeneous systems [8], tells us that the discrete derivative of the mean cycle numbers with respect to their length is given by the probability of having  $k$  particles in the same single-particle energy level.

Rescaled superfluid densities  $N_i^{1/3} \rho_s/\rho$  [from Eqs. (5) and (7)] are plotted in Fig. 2a for  $N_1 = 37$ ,  $N_2 = 296$ ,  $N_3 = 2368$ , and  $N_4 = 18944$  as a function of the rescaled temperature  $t = (T - T_c^\infty)/T_c^\infty$ , where  $T_c^\infty$  is the critical temperature for  $N \rightarrow \infty$ .

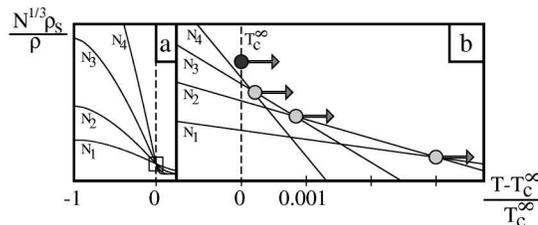


FIG. 2. Rescaled superfluid density of an ideal Bose gas. The curves for different  $N$  with  $N_{i+1} = 8N_i$  intersect approximately at  $T_c^\infty$ , as shown in (a). The close-up view (b) reveals important differences. We determine the shift of the intersection points as a function of the interaction (light arrows). The dark arrow shows schematically the extrapolated shift in the thermodynamic limit.

A finite-size scaling ansatz, which was used in previous Monte Carlo work on the problem [3], assumes that the curves of  $N_i^{1/3} \rho_s/\rho$  for a weakly interacting Bose gas should intersect at the transition temperature, as they do approximately. However, the small-scale Fig. 2b clearly shows the importance of corrections to scaling (cf. [9]) already for the noninteracting gas. By continuity, the corrections to scaling for the weakly interacting Bose gas must be important, especially if the temperature shift due to interactions becomes small.

Our strategy greatly benefits from the solution Eq. (7) for the ideal gas. We compute the intersection point  $(N_i^{1/3} \rho_s/\rho, t)$  for two finite systems with  $N_1$  and  $N_2 = 8N_1$  particles and determine how this point is shifted under the influence of interactions (cf. Fig. 2b). Our arbitrary but fixed ratio  $N_2/N_1 = 8$  facilitates the direct extrapolation in  $N_1$  to  $N_1 \rightarrow \infty$ .

To generate a random partition, we interpret the term  $\rho_k Z_{N-k}/Z_N$  in Eq. (8) as the probability to *split off* a cycle of length  $k$  from a configuration of  $N$  bosons, and to be left with a system of  $N - k$  bosons. We can pick  $k$  with probability  $\sim \rho_k Z_{N-k}$  with a simple “tower of probabilities” strategy [10]. Recursively, we can thus generate an independent random partition  $\{m_k\}$  with great speed. The recursion stops as soon as we have split off a cycle of length  $j$  from a system with  $j$  particles.

To go from a random partition to a random *configuration*, we may treat each cycle separately. For a cycle of length  $k$ , we select a winding number  $w_x$  with probability  $\rho_{k,w_x}$  [cf. Eq. (4)], and analogously for  $w_y$  and  $w_z$ . Towers of probabilities are again used. The cycle starts at a random position  $r = (x, y, z)$  with  $0 < x, y, z < L$ , and ends at  $r' = (x + w_x L, y + w_y L, z + w_z L)$ . Intermediate points are filled in with the appropriate Lévy construction [6]. We have tested our algorithm successfully against the known results (cf. Fig. 2).

We thus generate independent free boson path-integral configurations by a method very different from what is usually done in path-integral (Markov-chain) quantum Monte Carlo calculations, but with an equivalent outcome: Any appropriate operator is sampled with the probability

$$\langle \mathcal{O} \rangle_0 = \frac{\sum_P \int dR [\prod_i \rho(r_i, r'_i)] \mathcal{O}}{\sum_P \int dR [\prod_i \rho(r_i, r'_i)]}. \quad (12)$$

Here,  $\sum_P$  indicates the summation over all permutations  $P$ , and  $r'_i$  is the position of the particle  $P(i)$ . In the presence of interactions, the statistical weight of each configuration is no longer given by the product of the one-particle density matrices  $\pi_0 = [\prod_i \rho(r_i, r'_i)]$ . To lowest order in the interaction, the density matrix is exclusively modified by  $s$ -wave scattering. Likewise, only binary collisions need to be kept. This means that the correct statistical weight is given by

$$\pi_a(r_1, \dots, r_N; r'_1, \dots, r'_N) = \pi_0 \prod_{i < j} g_{ij}(r_i, r_j, r'_i, r'_j). \quad (13)$$

The contribution of collisions is to lowest order in  $a$

$$\prod_{i < j} g_{ij} = 1 - a \sum_{i < j} c_{ij} \quad (14)$$

with

$$c_{ij} = (|r_{ij}|^{-1} + |r'_{ij}|^{-1}) \times \exp[|r_{ij}| |r'_{ij}| (1 + \cos \gamma_{ij}) / 2\beta].$$

Here,  $r_{ij} = r_i - r_j$  and  $\gamma_{ij}$  is the angle between  $r_{ij}$  and  $r'_{ij}$ . Equation (13) corresponds to the popular path-integral Monte Carlo “action” with the following important modifications: (i) no interior time slices are needed, (ii) the interaction may be treated on the  $s$ -wave level, and (iii) the interaction may be expanded in  $a$ . For a consistent evaluation of the interaction with periodic boundary conditions, as schematically represented in Fig. 1, it is best to sum over *all* pairs  $i < j$  shown, with the condition that  $r_i$  be in the original simulation box (shaded in gray). As indicated by the small circles in Fig. 1,  $c_{ij}$  may have important contributions stemming from more than one representative of the path  $(r_j, r'_j)$ , especially for small systems. Of course, a cutoff procedure can be installed.

We now find for the mean-square winding number in the interacting system

$$\langle W^2 \rangle_a = \frac{\langle (1 - aC)W^2 \rangle_0}{\langle (1 - aC) \rangle_0}, \quad (15)$$

where we put  $C = \sum_{i < j} c_{ij}$ . Expanding in  $a$ , this yields

$$\langle W^2 \rangle_a - \langle W^2 \rangle_0 = -a \langle (\Delta W^2) (\Delta C) \rangle_0, \quad (16)$$

where  $\Delta \mathcal{O} = \mathcal{O} - \langle \mathcal{O} \rangle_0$  [11].

For a finite system of  $N$  bosons, the shift in the superfluid density  $\delta \rho_s = \rho_s(a) - \rho_s(0)$  can thus be proven to be linear in  $a$

$$\frac{\delta \rho_s}{\rho} = -\frac{X_N}{\beta N^{1/3}} a \rho^{1/3}, \quad (17)$$

with  $X_N = \langle (\Delta W^2) (\Delta C) \rangle_0 / (3\rho)$ .

To determine quantitatively the shift of the intersection points in Fig. 2, we expand the ideal gas superfluid density around the intersection temperature  $T_s$  of two systems with  $N$  and  $8N$  bosons at the same density,

$$\rho_s/\rho(T)N^{1/3} = \rho_s/\rho(T_s)N^{1/3} + \alpha_N \times [T - T_s]. \quad (18)$$

In this formula, the linear expansion coefficients can be computed. With interactions, only  $\rho_s/\rho(T_s)N^{1/3}$  is modified to linear order in  $a$ .  $\alpha(N)$  remains unchanged, as we restrict the expansion to  $|T - T_s|/T_s \sim a\rho^{1/3}$ . We find the new intersection point of the two systems to be shifted in temperature as

$$\frac{\Delta T_s}{T_s(0)} := \frac{T_s(a) - T_s(0)}{T_s(0)} = \frac{X_{8N} - X_N}{\alpha_{8N} - \alpha_N} a \rho^{1/3}. \quad (19)$$

We have also computed the shift in  $\rho_s/\rho$ , but found

out only that it must be extremely small. We are unaware of any fundamental reason for a vanishing shift in this quantity. In Fig. 3, we plot the shift  $\Delta T_s$  for different system sizes ranging from  $(N_1, N_2) = (37, 296)$  to  $(2368, 18944)$  vs  $N_1^{-1/2}$ . We have not attempted a thorough analysis of the finite-size effects, which already appear negligible for our largest systems.

We conclude that the transition temperature of the weakly interacting Bose gas increases linearly in the scattering length  $a$  by an amount of

$$\frac{\Delta T_C}{T_C} = (2.3 \pm 0.25)a\rho^{1/3}. \quad (20)$$

Our result Eq. (20) is almost an order of magnitude larger than what was found in a previous Monte Carlo calculation [3]. However, this calculation was restricted to very small particle numbers and it used a problematic finite-size scaling ansatz, as pointed out. The agreement of Eq. (20) with the renormalization group calculation [2] seems to be quite good.

It is very interesting to understand whether the result Eq. (20) directly applies to the current Bose-Einstein condensation experiments (cf., e.g., [12,13]). In earlier papers [8,14], we have pointed out the particularities of these finite systems in external potentials (cf. [15] for a general overview). Notwithstanding the differences between the two systems, a relevant parameter is for both cases  $a\rho^{1/3}$ , where the maximum density (at the center of the trap) at the transition point must be taken in the inhomogeneous case. The experimental value is of the order  $a\rho^{1/3} \sim 0.02$ .

Within our method, we can also study finite values of the interaction, even though we no longer compute a correlation function, and also have to introduce interior time slices. Contributions beyond  $s$ -wave scattering need to be monitored, as we have in [14]. For  $N = 125$  bosons we have found agreement with the linear response formula Eq. (16) up to  $a\rho^{1/3} \leq 0.005$ , but a 15% decrease for the full treatment for  $a\rho^{1/3} = 0.023$ . A detailed investigation of this question goes beyond the scope of this paper.

In conclusion, it is worth noting that we have encountered none of the difficulties which usually haunt boson calculations: We work in the canonical ensemble; therefore, the fluctuation anomaly of the grand-canonical Bose gas plays no role. The density remains automati-

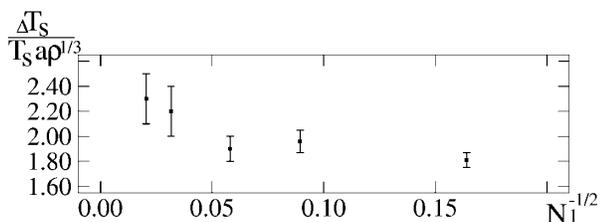


FIG. 3. Shift of the intersection temperature  $\Delta T_s / [T_s(0) a\rho^{1/3}]$  as a function of  $N_1^{-1/2}$  ( $N_2 = 8N_1$ ). The system sizes are  $(N_1, N_2) = (37, 296), (125, 1000), (296, 2368), (1000, 8000),$  and  $(2368, 18944)$ .

cally constant as a function of  $a$  so that an expansion in  $a\rho^{1/3}$  is well defined. At finite  $N$ , we can furthermore prove that the shift in  $\rho_s/\rho$  is linear in the interaction parameter. We have also consistently approached the weakly interacting system from the vantage point of the ideal gas. This allows us to obtain the crucial information on exactly where to do our simulation (cf. Fig. 2). Finally, our extremely powerful direct sampling algorithm has allowed us to partially dispel the curse of Monte Carlo simulations: limitations to small system sizes.

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\*Email address: holzmann@physique.ens.fr

†Email address: krauth@physique.ens.fr  
http://www.lps.ens.fr/~krauth

‡Laboratoire Kastler-Brossel is a unité de recherche de l'Ecole Normale Supérieure et de l'Université Pierre et Marie Curie, associée au CNRS.

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