

## Parametric equation of state of a weakly interacting Bose system

Mingzhe Li,<sup>1</sup> Haixiang Fu,<sup>2</sup> Zhipeng Zhang,<sup>1</sup> and Jincan Chen<sup>1</sup>

<sup>1</sup>*Department of Physics and Institute of Theoretical Physics and Astrophysics, Xiamen University, Xiamen 361005, China*

<sup>2</sup>*Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai 201800, China*

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A uniform dilute Bose system with repulsive interactions is studied in the grand canonical ensemble formalism. We present a parametric equation of state that holds true from high temperatures down to below the transition temperature, thus providing a scheme for exploring the quantum-statistical nature of the Bose-Einstein condensation transition in interacting gases. As an application, the interaction-induced shift of the transition temperature is derived to be  $\Delta T_c/T_c^0 = 2.83n^{1/3}a$ , where  $n$  is the density and  $a$  is the  $S$ -wave scattering length.

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Theoretical study of the weakly interacting Bose gas had a long history (see, e.g., [1,2]) before the realization of Bose-Einstein condensation (BEC). The gas may be described by the parametric equation of state (PES1) [1] as follows:

$$\lambda^3 \frac{P}{k_B T} = g_{5/2}(z) - \frac{2a}{\lambda} [g_{3/2}(z)]^2, \quad (1)$$

$$\lambda^3 n = g_{3/2}(z) - \frac{4a}{\lambda} g_{3/2}(z) g_{1/2}(z), \quad (2)$$

where  $P$  is the pressure,  $T$  is the temperature,  $k_B$  is the Boltzmann constant,  $z$  is the fugacity,  $a$  is the  $S$ -wave scattering length,  $n$  is the particle number density,  $\lambda = \sqrt{2\pi\hbar^2/mk_B T}$  is the thermal wavelength,  $\hbar$  is the Planck constant, and  $g_\alpha(z) = \sum_{j=1}^{\infty} j^{-\alpha} z^j$ . PES1 has broad applications, however, cannot illuminate the effect of atom-atom interactions on the BEC transition temperature, because PES1 fails at extremely low temperatures close to the transition. In the past few years, the effect of interactions on transition temperature has attracted great interest. For a trapped gas, it is predicted [3] and tested [4,5] that repulsive interactions will lower the transition temperature. However, for a homogeneous Bose gas, the effect of interactions on transition temperature  $T_c$  has a controversial history, in the beginning even with regard to the sign of  $\Delta T_c = T_c - T_c^0$  [6–18], where  $T_c^0 = (2\pi\hbar^2/mk_B)[n/\zeta(3/2)]^{2/3}$  [19] is the transition temperature of a uniform noninteracting Bose gas, and  $\zeta[\alpha] = g_\alpha(1)$ . It is now generally recognized that a positive shift of  $T_c$  takes the form  $\Delta T_c/T_c^0 = c_0(na^3)^\gamma$ , but still with dissident estimates of  $c_0$  and/or  $\gamma$  [8–18]. Thus it would be interesting to obtain a new parametric equation of state that can explain this effect.

In the present paper, we study a uniform dilute Bose system with repulsive interactions in the grand canonical ensemble formalism. A treatment on the fugacity is introduced to derive a new parametric equation of state that holds true from high temperatures down to below the transition temperature. As an application of the new parametric equation of state, the interaction-induced shift of the transition temperature is derived to be  $\Delta T_c/T_c^0 = 2.83n^{1/3}a$ .

Let us start from the grand canonical ensemble theory. It has the basic formulas

$$Q_N = \text{Tr} e^{-\beta \hat{H}}, \quad (3)$$

$$Q = \sum_{N=0}^{\infty} z^N Q_N, \quad (4)$$

$$\frac{PV}{k_B T} = \ln Q, \quad (5)$$

$$N = z \frac{\partial}{\partial z} \ln Q, \quad (6)$$

where  $Q_N$  is the partition function of  $N$  particles enclosed in a volume  $V$ ,  $\beta = 1/k_B T$ ,  $\hat{H}$  is the Hamiltonian, and  $Q$  is the grand partition function. The formulas are applicable to systems in gas or BEC phase. Note that they have no precondition whether  $z \leq 1$ , which actually is just a result of an ideal Bose gas but fails for an interacting Bose gas at extremely low temperatures. In fact, PES1 is derived starting from the formulas (3)–(6) with the presumption that  $z \leq 1$  because it expands  $Q$  in powers of  $z$ . This presumption, as shown in the next paragraph, limits the application of PES1 to systems in some regions of the gas phase, and hence furnishes neither information about the condensed phase nor the nature of the condensation [1]. The crucial point is that when a system at lower temperatures with  $z > 1$  is considered, a treatment on the fugacity and the partition function should be done to correctly calculate the grand partition function to arrive at an appropriate equation of state.

For a uniform dilute Bose system with repulsive interactions, the method of pseudopotentials [19] employs the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \frac{4\pi\hbar^2 a}{m} \sum_{i<j} \left[ \delta(\vec{r}_i - \vec{r}_j) \left( \frac{\partial}{\partial r_{ij}} r_{ij} \right) \right], \quad (7)$$

and gives the energy eigenvalues of the system as

$$E = \sum_p N_p \frac{p^2}{2m} + \frac{4\pi\hbar^2 a}{mV} \left( N^2 - \frac{1}{2}N - \frac{1}{2} \sum_p N_p^2 \right), \quad (8)$$

where  $N_p$  is the number of particles with momentum  $p$ . The validity of the foregoing expression requires that

$$a/\lambda \ll 1 \quad \text{and} \quad n^{1/3}a \ll 1. \quad (9)$$

These conditions limit the validity of Eq. (8) to systems at low densities with weak interactions. The chemical potential  $\mu$  is the energy to add a particle to the system with the entropy and volume being held constant as follows:

$$\mu = \left( \frac{\partial E}{\partial N} \right)_{S,V}. \quad (10)$$

Notice that a particle added to the system will go to the zero-momentum state at temperatures  $T \leq T_c$ , and the entropy associated with the zero-momentum state is zero. Hence from Eqs. (8) and (10), the chemical potential can be expressed as  $\mu = 4\pi\hbar^2 a(2N - N_0)/mV$  [20], where  $N_0$  is the number of condensed particles. Thus the chemical potential varies with temperature no matter when the system is in gas phase or condensed phase. The chemical potential at the transition point is

$$\mu_c = 8\pi\hbar^2 an/m, \quad (11)$$

and half this value at zero temperature, with fugacities  $z > 1$ . Thus, when the partition function and the grand partition function are calculated, an effective fugacity  $z'$  should be introduced by

$$z = z' \exp(8\pi\hbar^2 an/mk_B T) = z' \exp[4(\lambda^3 n)(a/\lambda)]. \quad (12)$$

In Eq. (12) the fugacity  $z$  has two factors, the factor  $\exp(8\pi\hbar^2 an/mk_B T)$  concerns the effect of atom-atom interactions, and the other factor  $z'$  is the dissociative fugacity apart from the interaction effect. Clearly, the definition of this effective fugacity only causes a difference in normalization, but will not change the probability that the system be in an energy level state, which is a foundation of the ensemble theory.

Correspondingly, Eqs. (3) and (4) are rewritten as

$$\begin{aligned} Q'_N &= \text{Tr} e^{-\beta(\hat{H} - \varepsilon_0)}, \\ Q &= \sum_{N=0}^{\infty} (z')^N Q'_N, \end{aligned} \quad (13)$$

where  $\varepsilon_0 = 8\pi\hbar^2 an/m$ . Expanding  $Q'_N$  and  $Q$  in ascending powers of  $a$ ,

$$\begin{aligned} Q'_N &= Q'_N{}^{(0)} + Q'_N{}^{(1)} + Q'_N{}^{(2)} + \dots, \\ Q &= Q^{(0)} + Q^{(1)} + Q^{(2)} + \dots, \end{aligned} \quad (14)$$

one has

$$\begin{aligned} Q'_N{}^{(0)} &= \text{Tr} e^{-\beta\hat{H}_0}, \\ Q'_N{}^{(1)} &= -\beta \text{Tr}[e^{-\beta\hat{H}_0}(\hat{H}_1 - \varepsilon_0)], \end{aligned}$$

$$Q^{(n)} = \sum_{N=0}^{\infty} (z')^N Q'_N{}^{(n)}, \quad (15)$$

and

$$\begin{aligned} \ln Q &= \ln \left[ Q^{(0)} \left( 1 + \frac{Q^{(1)}}{Q^{(0)}} + \frac{Q^{(2)}}{Q^{(0)}} + \dots \right) \right] \\ &= \ln Q^{(0)} + \frac{Q^{(1)}}{Q^{(0)}} + \left[ \frac{Q^{(2)}}{Q^{(0)}} - \frac{1}{2} \left( \frac{Q^{(1)}}{Q^{(0)}} \right)^2 \right] + \dots. \end{aligned} \quad (16)$$

With the help of Eqs. (15) and (16), Eq. (5) may be expressed, retaining to order  $a/\lambda$ , as

$$\begin{aligned} \frac{P}{k_B T} &= \frac{1}{V} \ln \frac{1}{1-z'} + \frac{1}{\lambda^3} g_{5/2}(z') + 2a\lambda^2 \frac{N^2 + \frac{1}{2}N + \frac{1}{2} \sum_p N_p^2}{V^2} \\ &\approx \frac{1}{\lambda^3} g_{5/2}(z') + \frac{2a}{\lambda^4} [g_{3/2}(z')]^2. \end{aligned} \quad (17)$$

Equation (17) is obtained by ignoring the term  $V^{-1} \ln(1-z')^{-1}$  which is at most  $O(2a\lambda^2 n_0^2/N_0)$ , and neglecting  $\sum_p N_p^2$  in comparison with  $N^2$  which is valid for temperatures as low as around  $T_c$ , and approximating  $\lambda^3 n$  to  $g_{3/2}(z')$ . The last approximation is based on  $Q^{(1)} \ll Q^{(0)}$  and is appropriate in the limit of weak atom-atom interactions. Finally, substituting Eqs. (5) and (17) into Eq. (6), and making use of

$$z \frac{\partial g_\alpha(z)}{\partial z} = g_{\alpha-1}(z), \quad (18)$$

results in

$$n = \frac{1}{V} \frac{z'}{1-z'} + \frac{1}{\lambda^3} g_{3/2}(z') + \frac{4a}{\lambda^4} g_{3/2}(z') g_{1/2}(z'). \quad (19)$$

Expressions (17) and (19) constitute our new parametric equation of state (PES2). PES2 is significant in that it holds true from high temperatures down to below the transition temperature where the fugacity exceeds 1. The feature that it holds true across  $T_c$  provides a scheme for exploring the quantum-statistical nature of the BEC transition.

PES2 reduces to describe the ideal Bose gas as long as we let  $a=0$ . In this specific case, PES2 may also be formulated in terms of polylogarithms. It is interesting that any ideal gas, whether Fermi, Bose, or classical, can be given a unified picture with polylogarithms and many analytic properties follow explicitly [21].

PES2 includes PES1 in describing the gas phase because Eq. (17) reduces to Eq. (1) readily. A scaling operator  $\hat{S}$  defined as

$$\hat{S} = e^{\eta z \partial/\partial z} = \sum_{l=0}^{\infty} \frac{1}{l!} \left( \eta z \frac{\partial}{\partial z} \right)^l, \quad (20)$$

transforms a function by

$$\hat{S}[f(z)] = f(e^{\eta z}). \quad (21)$$

Applying this operator with parameter  $\eta = -4(\lambda^3 n)/(a/\lambda)$  on Bose functions and retaining to order  $a/\lambda$  yields

$$\begin{aligned} g_\alpha(z') &= g_\alpha \{ z \exp[-4(\lambda^3 n)/(a/\lambda)] \} \\ &= g_\alpha(z) - 4(a/\lambda)(\lambda^3 n)g_{\alpha-1}(z), \end{aligned} \quad (22)$$

where Eq. (18) has also been used. To order  $a/\lambda$ , Eq. (17) reduces to Eq. (1) with the help of Eq. (22). Thus all performance of gas given by PES1 in literature may also be obtained with PES2.

Moreover, PES1 fails in a small gas region with temperature right above  $T_c$  where  $z > 1$ , thus gases in this regime should be described with PES2 instead of PES1.

Let us look into Eqs. (17) and (19) to find out the interaction effects on  $T_c$  and  $P$ . The right-hand sides of Eqs. (17) and (19) rise with  $z'$ , until as  $z' \rightarrow 1$ , the former approaches a finite value while the latter diverges. This shows an increase in  $n$  but with no contribution to  $P$ , and manifests the congregation of particles in the ground state. Thus BEC occurs at  $z' = 1$ . The corresponding fugacity and chemical potential are, respectively,

$$z_c = 1 + 4\zeta(3/2)\frac{a}{\lambda_c}, \quad (23)$$

and

$$\mu_c = 4\zeta(3/2)k_B T_c \frac{a}{\lambda_c}, \quad (24)$$

which are in accordance with the conclusions in Ref. [2], and consistent with our base of defining  $z'$ . At the phase transition, Eq. (17) gives

$$\left( \lambda^3 \frac{P}{k_B T} \right)_c = \zeta(5/2) + 2[\zeta(3/2)]^2 \frac{a}{\lambda_c}, \quad (25)$$

which is exactly what was obtained in Ref. [2] by comparing the thermodynamic functions for the gaseous phase and the degenerate phase.

The manner  $g_{1/2}(z')$  diverges as  $z' \rightarrow 1$  is interesting [22],

$$\begin{aligned} g_{1/2}(z') &= \sqrt{\pi}(1-z')^{-1/2} + \zeta(1/2) + 0.208(1-z') \\ &\quad - 0.0128(1-z')^2 + \dots, \end{aligned} \quad (26)$$

i.e., the divergence comes from the term  $\sqrt{\pi}(1-z')^{-1/2}$ , while

the rest of the terms converge to  $\zeta(1/2) = -1.46$ . The Bose distribution has a form of  $1/[\exp(\varepsilon - \mu)/k_B T - 1]$ , so the particle number in the ground state, which contributes to the divergence in Eq. (19), has the fate of taking a form  $b\delta^{-1} + d$  with  $d$  definitely equal to 0, and  $\delta$  as an infinitesimal. Consequently, in separating  $n$  into a diverging  $n_0$  and a converging  $n_e$ ,  $n_0$  should take exactly the effect of the first term in Eq. (26) as follows:

$$n_0 = \frac{1}{V} \frac{z'}{1-z'} + \frac{4a}{\lambda^4} g_{3/2}(z') \sqrt{\pi}(1-z')^{-1/2}, \quad (27)$$

$$n_e = \frac{1}{\lambda^3} g_{3/2}(z') + \frac{4a}{\lambda^4} g_{3/2}(z') \zeta(1/2), \quad (28)$$

with  $z' \rightarrow 1$ . Equation (28) gives

$$\left( \frac{T_c}{T_c^0} \right)^{-3/2} = 1 + \frac{4a}{\lambda_c} \zeta(1/2), \quad (29)$$

which leads to

$$\frac{\Delta T_c}{T_c^0} = \frac{-8\zeta(1/2)}{3[\zeta(3/2)]^{1/3}} n^{1/3} a = 2.83 n^{1/3} a. \quad (30)$$

On the interaction-induced shift of the transition temperature, we have  $\gamma = 1/3$  in agreement with Refs. [9–18], while our analytic expression for  $c_0$  takes a value of 2.83 closest to the result given in Ref. [11]. The shift of critical temperature stems from the last term in Eq. (17), which accounts for quantum fluctuation and reflects the energy level shifts induced by the interactions, but not due to the introduction of the effective fugacity.

It is perceptible that repulsive mutual interactions shift  $T_c$  in opposite directions in the homogeneous and inhomogeneous Bose gases. BEC in the inhomogeneous case is a condensation in both momentum and real space; repulsive mutual interactions will counteract the congregating of particles around the potential center to form BEC and hence lower the critical temperature. But in the homogeneous case, BEC is a condensation in momentum space and not in real space; repulsive interactions will favor the homogeneity and thus increase the critical temperature.

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