Transition Temperature of a Uniform Imperfect Bose Gas

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We calculate the transition temperature of a uniform dilute Bose gas with repulsive interactions, using a known virial expansion of the equation of state. We find that the transition temperature is higher than that of an ideal gas, with a fractional increase $K_0(na^3)^{1/6}$, where n is the density, a is the S-wave scattering length, and K_0 is a constant given in the paper. This disagrees with all existing results, analytical or numerical.

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The weakly interacting Bose gas is an old subject that has found new life since the experimental discovery of Bose-Einstein condensation in ultracold trapped atoms. Although there is a vast literature on the subject, the transition temperature of the interacting gas remains a controversial subject, even in the uniform case. In this note, we present a calculation that is simple and transparent, in the hope that it will settle the controversy.

In the gas phase, the equation of state of a general system is given in the virial expansion in the parametric form [1]

$$\begin{aligned} \lambda^3 \beta P &= \sum_{\ell=1}^{\infty} b_\ell z^\ell, \\ \lambda^3 n &= z \frac{\partial}{\partial z} (\lambda^3 \beta P) = \sum_{\ell=1}^{\infty} \ell b_\ell z^\ell, \end{aligned} \tag{1}$$

where P is the pressure, n is the particle density, z is the fugacity, $\beta = (k_B T)^{-1}$, and $\lambda = \sqrt{2\pi\beta\hbar^2/m}$ is the thermal wavelength. The "cluster integral" b_ℓ expresses the property of an ℓ-particle system in infinite volume. For the ideal Bose gas, we have

$$\begin{aligned} \lambda^3 \beta P &= g_{5/2}(z), \\ \lambda^3 n &= g_{3/2}(z), \end{aligned} \tag{2}$$

where

$$g_\alpha(z) \equiv \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell^\alpha}. \tag{3}$$

No single-particle state has a macroscopic occupation in this phase. However, the function $g_{3/2}(z)$ is monotonic, and bounded by $g_{3/2}(1) = \zeta(3/2) = 2.612$. Thus, particles must go into the zero-momentum state when $\lambda^3 n > \zeta(3/2)$, making this state macroscopically occupied. Thus, the thermal wavelength at transition is $\lambda_0 = [\zeta(3/2)]^{-1/3} n^{-1/3}$, and this gives the transition temperature of the ideal Bose gas at a fixed density n:

$$T_0 = \frac{2\pi\hbar^2}{mk_B} [\zeta(3/2)]^{-2/3} n^{2/3}. \tag{4}$$

Now consider a uniform imperfect Bose gas with repulsive interactions with equivalent hard-sphere diameter a (S-wave scattering length). We denote the transition temperature by T_c, and its fractional shift by

$$\frac{\Delta T}{T_0} \equiv \frac{T_c - T_0}{T_0}. \tag{5}$$

In an early statement on the subject [2], it was argued that $\Delta T > 0$, since a spatial repulsion leads to momentum-space attraction [3], and this would make the imperfect gas more ready to condense. However, a Hartree-Fock calculation by Fetter and Walecka [4], and one by Girardeau [5] based on a mean-field method, yield the opposite sign $\Delta T < 0$. A calculation of the grand partition function to one-loop order by Toyoda [6] also yields a negative sign. Specifically, Toyoda obtains

$$\left(\frac{\Delta T}{T_0}\right)_{\text{Toyoda}} = -K_0 (na^3)^{1/6}, \tag{6}$$

where

$$K_0 = \frac{8\sqrt{2\pi}}{3[\zeta(3/2)]^{2/3}} = 3.527. \tag{7}$$

Barring calculational errors, this must be considered reliable, since it is the lowest-order result of a systematic expansion. All subsequent calculations, alas, yield answers different from this and from one another. Stoof [7] gives $\Delta T = [16\pi/3\zeta(3/2)](a/\lambda_0)$, while Bijlsma and Stoof [8] discuss renormalization-group equations that give a result consistent with $\Delta T \sim a$. A numerical calculation based on Monte Carlo simulation by Grüter *et al.* [9] gives $\Delta T/T_0 = c_0(na^3)^\gamma$, where $c_0 = 0.34 \pm 0.06$, and $\gamma = 0.34 \pm 0.03$. A recent calculation involving some mean-field assumptions [10] gives $\Delta T/T_0 = 0.7(na^3)^{1/3}$. Thus, there is no consensus on how ΔT should depend on the scattering length, nor even the sign.

We shall calculate T_c using the parametric equation of state obtained some time ago [11] via a calculation of all cluster integrals to order a^2:

$$\begin{aligned} \lambda^3 \beta P &= g_{5/2}(z) - \frac{2a}{\lambda}[g_{3/2}(z)]^2 \\ &\quad + 8\left(\frac{a}{\lambda}\right)^2 h(z) + O\left(\frac{a}{\lambda}\right)^3, \\ \lambda^3 n &= z\frac{\partial}{\partial z}(\lambda^3 \beta P) = g_{3/2}(z) - \frac{4a}{\lambda} g_{3/2}(z) g_{1/2}(z) \\ &\quad + 8\left(\frac{a}{\lambda}\right)^2 z\frac{dh(z)}{dz} + O\left(\frac{a}{\lambda}\right)^3, \end{aligned} \tag{8}$$

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where P is the pressure, and

$$h(z) = [g_{3/2}(z)]^2 g_{1/2}(z) + \sum_1^\infty \sum_1^\infty \sum_1^\infty \frac{z^{\ell+m+n}}{\sqrt{\ell mn}\,(\ell + m)(\ell + n)}. \quad (9)$$

We shall work only to lowest order in a, and take from the second equation of (8)

$$\lambda^3 n = g_{3/2}(z)\left[1 - \frac{4a}{\lambda}\, g_{1/2}(z)\right] + O(a)^2. \quad (10)$$

As a function of z, the right side rises through a maximum at some value $z = z_c$, and then approaches $-\infty$ as $z \to 1$. We must require $z \to 0$, as $n \to 0$. As n increases at fixed temperature, z increases monotonically until it reaches z_c, beyond which there is no solution. The assumption of no macroscopic occupation breaks down at this point, which marks the transition point of the Bose-Einstein condensation.

Since the treatment is valid only when $a/\lambda \ll 1$, we put

$$z_c = 1 - \delta \qquad (\delta \ll 1). \quad (11)$$

The maximum can be located with the help of the expansions [12]

$$g_{3/2}(z_c) \approx \zeta(3/2) - 2\sqrt{\pi}\,\delta^{1/2}, \qquad g_{1/2}(z_c) \approx \sqrt{\pi}\,\delta^{-1/2}. \quad (12)$$

We then find

$$\delta = \frac{2a}{\lambda}\,\zeta(3/2). \quad (13)$$

The critical temperature T_c can be found by substituting this value into (10), with the result

$$\frac{\Delta T}{T_0} = K_0(na^3)^{1/6}, \quad (14)$$

where K_0 is given in (7). Thus, we agree exactly with Toyoda except for the sign.

We close with some comments:

(1) Our result $\Delta T \sim \sqrt{a}$ indicates that it cannot be continued to $a < 0$. This is a reflection of the fact that a gas with attractive interactions will collapse, rendering the scattering-length description invalid.

(2) In a mean-field approximation, the density is given by (2), except that z is replaced by $z\exp(-8\pi\hbar^2 an/mk_BT)$. It is clear that this leads to $\Delta T = 0$. On the other hand, the mean-field result yields (8) to lowest order in a, and raises the question whether $\Delta T = 0$ in our calculations, if we were capable of summing the virial series to all orders. Barring an usual conspiracy, the answer is no, because the virial expansion differs from mean-field theory in $O(a^2)$, and is therefore not the same as mean-field theory.

(3) We have obtained ΔT by approaching the transition point from the high-temperature side, and that is why the virial expansion is useful. It appears to be more difficult to obtain it from the low-temperature side, because, in the usual technique involving the Bogoliubov transformation, the quasiparticles reduce to noninteracting particles at the transition point. An adequate treatment of the region $z_c < z < 1$ must go beyond the usual Bogoliubov approach. Only then can we determine the order of the phase transition.

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