Nonanalytic Dependence of the Transition Temperature of the Homogeneous Dilute Bose Gas on Scattering Length

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(Received 28 March 2001; published 28 August 2001)

We show that the shift in the transition temperature of the dilute homogeneous Bose gas is nonanalytic in the scattering amplitude a. The first correction beyond the positive linear shift in a is negative and of order $a^2 \ln a$. This nonuniversal nonanalytic structure indicates how the discrepancies between numerical calculations at finite a can be reconciled with calculations of the limit $a \to 0$, since the linearity is apparent only for anomalously small a.

DOI: 10.1103/PhysRevLett.87.120403 PACS numbers: 03.75.Fi

The shift of the critical temperature of the dilute homogeneous Bose gas, T_c, with interactions has had a long and controversial history [1–12] (and further references therein). The correction to the ideal gas critical temperature, T_c^0, is now established theoretically [7,8] (see also [6]) to be linear in the scattering length a in leading order

$$\frac{\Delta T_c}{T_c^0} = \frac{T_c - T_c^0}{T_c^0} = c a n^{1/3}, \qquad a n^{1/3} \to 0, \quad (1)$$

where n is the particle density. The variation of T_c is determined primary by large distance, or small momenta, contributions. Because of infrared divergencies around the transition point, pertubation theory is not applicable, and the coefficent c cannot be obtained by simple perturbative techniques. Except in special cases, e.g., a large number of internal degrees of freedom, the constant c must be evaluated numerically.

However, even numerical calculations have not settled this issue. Whereas Ref. [6] provides $c = 2.33 \pm 0.25$ from a direct calculation of the coefficient first taking the limit $a n^{1/3} \to 0$, Ref. [4] predicts $c = 0.34 \pm 0.06$ after numerical extrapolation of the calculation to the limit $a \to 0$. In this paper we show that the difference in these two results is attributable to a nonanalytic structure, $\sim a^2 \ln a$, of the transition temperature in a. This correction, which is negative, does not introduce a new length scale beyond $n^{-1/3}$, but because of its logarithmic character it gives rise to a strong dependence on a even in the very dilute limit, $a n^{1/3} \to 0$. Very recently, Refs. [10,11] obtained $c \simeq 1.3$ from a classical ϕ^4 model on a lattice extrapolated to the continuum, a result qualitatively consistent with the larger value found in Ref. [6]. In these calculations the logarithmic terms enter as corrections to the continuum limit.

Equation (1) is only the beginning of an asymptotic expansion, as one might suspect, since for $a < 0$ the system is unstable. Inclusion of the $a^2 \ln a$ term, when one extrapolates numerical data from finite a values to the limit $a \to 0$, provides a first resolution of the apparent discrepancies between numerical calculations done at finite a [4] and those valid for $a \to 0$ [6,10,11]. To obtain a quantitative estimate, we explicitly calculate the logarithmic correction in a model with N internal degrees of freedom, to leading order in $1/N$. The result suggests that the linear increase of ΔT_c at small but finite a is noticeably suppressed for the physical case of $N = 2$.

We consider a uniform system of bosons of mass m at temperature T, and assume that the two-body interaction can be described by the s-wave scattering length a. Above the critical temperature, the density n is given in terms of a sum over Mastubara frequencies, $z_\nu = 2\pi i \nu T$ ($\nu = \pm 1, \pm 2, \ldots$), of the single particle Green's function $G(k, z)$:

$$n = -T \sum_\nu \int \frac{d^3k}{(2\pi)^3} G(k, z_\nu), \quad (2)$$

where ($\hbar = k_B = 1$)

$$G^{-1}(k, z) = z + \mu - \frac{k^2}{2m} - \Sigma(k, z), \quad (3)$$

and μ is the chemical potential; the condition $\mu = \Sigma(0, 0)$ determines the Bose-Einstein condensation point.

The shift of the critical temperature at fixed density is more conveniently calculated in terms of the shift, $\Delta n_c = n_c(a, T_c) - n_c(0, T_c)$, in the critical density at fixed T; the two shifts are related, to the orders of interest (less than a^2), by $\Delta T_c / T_c = -(2/3) \Delta n_c / n_c$. As shown in [7], the leading linear shift $\Delta T_c^{(1)}$ is given solely by the zero Matsubara frequency term:

$$\frac{\Delta T_c^{(1)}}{T_c^0} = \frac{2 T_c^0}{3n} \int \frac{d^3k}{(2\pi)^3} [G(k, 0) - G_0(k, 0)] \quad (4)$$

$$= \frac{4\lambda}{3\pi\zeta(3/2)} \int_0^\infty dk \frac{U(k)}{k^2 + U(k)}, \quad (5)$$

where $\lambda = (2\pi/mT)^{1/2}$ is the thermal wavelength, $\zeta(3/2) = 2.612\ldots$, G_0 is the Green's function of the ideal Bose gas at T_c^0, and

$$U(k) = 2m[\Sigma(k,0) - \Sigma(0,0)]. \quad (6)$$

At the critical temperature, $U(k)$ can be calculated to order a^2/λ^4 by considering only the $\nu = 0$ sector, which corresponds to a classical field theory. At the transition, $U(k)$ has the scaling structure,

$$U(k) = \frac{a^2}{\lambda^4} \sigma(k\lambda^2/a), \quad (7)$$

from which the linearity of $\Delta T_c^{(1)}$ in a follows [7,8]. If $U(k)$ is calculated by classical field theory, $\Delta T_c^{(1)}$ is strictly linear in a.

The next-to-leading order corrections, $\Delta T_c^{(2)}$, arise in terms with nonzero Matsubara frequencies, both explicitly [Eq. (2)] and in internal loops, in the calculation of $U(k)$. As we show below, the internal loop corrections begin at order a^2 and $a^3 \ln a$; the $a^2 \ln a$ terms may be extracted from

$$\frac{\Delta T_c^{(2)}}{T_c} = \frac{2T_c^0}{3n} \sum_{\nu\neq 0} \int \frac{d^3k}{(2\pi)^3} [G(k,z_\nu) - G_0(k,z_\nu)]. \quad (8)$$

Since the infrared behavior is regular for $\nu \neq 0$, we expand the denominator of G to first order in $\Sigma(k,z_\nu) - \mu$, and write

$$\frac{\Delta T_c^{(2)}}{T_c} \simeq \frac{2T_c^0}{3n} \sum_{\nu\neq 0} \int \frac{d^3k}{(2\pi)^3} \times \frac{\Sigma(k,z_\nu) - \Sigma(k,0) + U(k)/2m}{(z_\nu - k^2/2m)^2}. \quad (9)$$

From pertubation theory we know the functional form of $U(k)$ outside the critical region in k,

$$U(k) \propto \frac{a^2}{\lambda^4} \ln\frac{k\lambda^2}{a}, \qquad k \gg \frac{a}{\lambda^2}; \quad (10)$$

this logarithmic behavior is valid to all orders of pertubation theory, as one can verify by power counting. Since the dominant contribution to the integral in Eq. (9) comes from momenta $k \sim \lambda^{-1}$, the ultraviolet behavior of $U(k)$ generates a logarithmic shift in the critical temperature:

$$\frac{\Delta T_c^{(2)}}{T_c} \propto \frac{a^2}{\lambda^2} \ln\frac{a}{\lambda}. \quad (11)$$

Since $\Sigma(k,z_\nu) - \Sigma(k,0)$ tends to zero for large momenta k, the contribution of this term in Eq. (9) remains of order a^2/λ^2. Thus the next-to-leading order to the critical temperature shift is proportional to $a^2 \ln a$ and is always *negative* for small a.

In order to estimate the shift quantitatively, we calculate it in the large N model. The $\nu = 0$ sector, equivalent to a classical ϕ^4 field theory in three spatial dimensions, is described by the action [13],

$$S\{\phi(r)\} = \int d^3r \left\{ \sum_{i=1}^N \frac{1}{2} [\nabla\phi_i(r)]^2 - m\mu T \sum_i \phi_i^2(r) + \frac{u}{4!} \left[\sum_i \phi_i^2(r) \right]^2 \right\}, \quad (12)$$

with $u = 96\pi^2 a/\lambda^2$. The classical field theory suffers from ultraviolet divergencies, which can be regularized by introducing a large momentum cutoff Λ. As shown in Refs. [7,8], the leading order corrections to the critical density are dominated by long distance properties, and $U(k)$ is independent of the cutoff. Therefore one can derive $U(k)$ with a fixed cutoff Λ in the action, take the limit $\Lambda \to \infty$, and determine the corrections to the critical density from Eqs. (5) and (9).

Instead of this procedure we will obtain the next-to-leading order corrections in an independent way, which has the advantage of making contact with the numerical ϕ^4 lattice calculations. Starting from the finite temperature quantum field action, one can derive the effective action of the classical field theory by integrating pertubatively over the nonzero frequency quantum modes, $\nu \neq 0$, which provides a large momentum cutoff $\Lambda \sim \sqrt{mT} \sim 1/\lambda$ and renormalized effective coefficients of the Euclidean action [13]. Following [8], the corrections to the transition temperature are given in this effective field theory by

$$\frac{\Delta T_c}{T_c} = \frac{4\lambda}{3\pi\zeta(3/2)} \int_0^\Lambda dk \frac{U_\Lambda(k)}{k^2 + U_\Lambda(k)}, \quad (13)$$

where the subscript Λ indicates the explicit dependence on the ultraviolet cutoff which incorporates the leading effects of nonzero Matsubara frequencies.

In the large N limit $U_\Lambda(k)$ is given in terms of the particle-hole bubble, $B(q)$, by

$$U_\Lambda(k) = -\frac{Nu^2}{18} \int_0^\Lambda \frac{d^3q}{(2\pi)^3} \frac{B(q)}{1 + NuB(q)/6} \times \left[\frac{1}{(k-q)^2} - \frac{1}{q^2} \right]; \quad (14)$$

to leading order in $1/N$ in three dimensions [13],

$$B(q) = \frac{1}{8q} - \frac{6}{Ng^*\Lambda} + \mathcal{O}(\Lambda^{-2}), \quad (15)$$

where $g^* = 48\pi^2/N$. Following Ref. [8], we obtain the critical temperature shift

$$\frac{\Delta T_c}{T_c} = \frac{4\lambda}{3\pi\zeta(3/2)} \int_0^\Lambda dk \frac{U_\Lambda(k)}{k^2}. \quad (16)$$

As we see from the Λ dependence of the bubble, Eq. (15), the Λ dependence of $U_\Lambda(k)$ gives rise to higher order corrections in Λ^{-1}. These terms arise effectively from the internal nonzero Matsubara frequencies, and lead to corrections $\sim\Lambda^{-2}\ln\Lambda$ in $\Delta T_c/T_c$, which we can neglect. Thus

$$\frac{\Delta T_c}{T_c} = -\frac{64\lambda}{3\pi\zeta(3/2)}\,\frac{a}{\lambda}\int_0^{\Lambda\tau} dk \int_0^{\Lambda\tau/k} dx\,\frac{1}{k(xk+1)} \times\left[\frac{x}{2}\log\frac{|1+x|}{|1-x|}-1\right], \tag{17}$$

where $\tau = (Nu/48)^{-1}$. To obtain the leading order corrections we differentiate with respect to $\Lambda\tau$, which allows us to isolate the contributions around $\Lambda\tau \to \infty$. Integrating back we find

$$\frac{\Delta T_c}{T_c} = \frac{8\pi}{3\zeta(3/2)}\,\frac{a}{\lambda}\left\{1 + 16N\frac{a}{\lambda^2\Lambda}\ln\frac{Na}{\lambda^2\Lambda} + \mathcal{O}\left(\frac{Na}{\lambda^2\Lambda}\right)\right\}. \tag{18}$$

The integration constant is given by the large N result for the linear shift, Ref. [8]. In contrast to the linear corrections in a, the next-order terms depend on the short length scale properties of the system, modeled by the cutoff Λ, and therefore are not universal.

To estimate the influence of the logarithmic terms we take $N = 2$ and $\Lambda\lambda = (2\pi)^{1/2}$ in Eq. (18). The corrections to the linear behavior of T_c found in this way are precisely those one finds for $N = 2$ by including the particle-hole bubble sum in $U(k)$. The resulting dependence of the transition temperature on a is shown in Fig. 1. For a gas parameter $na^3 \sim 10^{-6}$, corresponding to the experimental region of Bose-Einstein condensation in atomic gases [14] and liquid ^{4}He in Vycor [15], and to the lowest density Monte Carlo data of Ref. [4], the nonlinear corrections depress the linear shift by ~50%; instead of the $a \to 0$ result $c \simeq 2.33$ in Eq. (1), one obtains a coefficient $c \sim 1.2$ for $an^{1/3} \sim 10^{-2}$. Even if the extrapolation from the large N expansion to $N = 2$ is unjustified, this calculation suggests that the logarithmic terms play an important role for present numerical and experimental parameters. The noticeable depression of ΔT_c in this parameter regime is also confirmed by self-consistent numerical model calculations [12].

A qualitatively similar strong dependence on a is found in the renormalization group calculations of Ref. [3], which derives an $a\ln a$ correction [16]. Such a result would follow from Eq. (5) were $U(k)$ to be linear in k up to an ultraviolet cutoff. However, in the regime $a/\lambda^2 \ll \Lambda$, corresponding to the dilute limit, $a/\lambda \ll 1$, $U(k)$ is given by the perturbative result (10) for momenta in the region $a/\lambda^2 \ll k \ll \Lambda$ rather than being linear in k.

The next-to-leading order corrections are important for classical ϕ^4 calculations as well [10,11]; in the universal region where the influence of the ultraviolet cutoff Λ is unimportant ($\Lambda \to \infty$) , classical field theory provides perfect scaling, implying a linear shift of T_c for *all* a. Variations in a of ΔT_c in [10] are due to nonuniversal corrections and are sensitive to the details of the scheme used to regularize the classical ϕ^4 theory [17]. Extrapolation to the universal small coupling region, $a/\lambda^2\Lambda \to 0$, together with finite size scaling to the thermodynamic limit allows one not only to extract the coefficient c of the linear shift in T_c, but should also provide the magnitude of the nonuniversal $a^2\ln a$ corrections for the physical case $N = 2$.

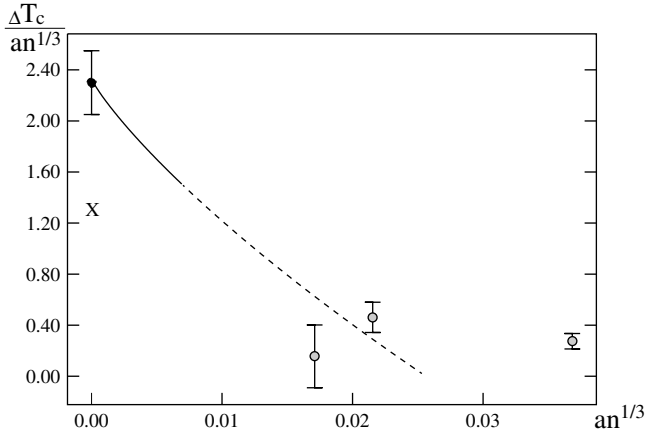

FIG. 1. Dependence of the transition temperature of a dilute homogeneous Bose gas on scattering length, from Eq. (18) for $N = 2$. The falloff of $\Delta T_c/an^{1/3}$ with increasing $an^{1/3}$ arises from the nonuniversal next-to-leading order logarithmic corrections. In the regime where the curve is represented by a dashed line, higher order corrections begin to become important. The dark circle is the calculation of Ref. [6]; the points shown as open circles are the lowest density data from the numerical calculations of Ref. [4]. The data point shown by the cross indicates the numerical results of Refs. [10,11] for a lattice ϕ^4 theory extrapolated to the continuum.

Dominique Vautherin was a source of inspiration to us on this problem. We are grateful to Henk Stoof for stimulating discussions both during his workshop on Bose-Einstein condensation at the Lorentz Center in Leiden, and at the Ecole Normale Supérieure. We also thank Peter Arnold, Nikolay Prokof'ev, and Boris Svistunov for helpful comments on their lattice calculations. Author G. B. would like to thank the ENS for its hospitality in the course of this work. This research was facilitated by the cooperative agreement between the University of Illinois at Urbana-Champaign and the Centre National de la Recherche Scientifique, and supported in part by the NASA Microgravity Research Division, Fundamental Physics Program and by National Science Foundation Grant No. PHY98-00978. Laboratoire Kastler Brossel de l'Ecole Normale Supérieure is *UMR 8552 du CNRS* and *associé à l'Université Pierre et Marie Curie*.

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