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Finite-size scaling and the role of the thermodynamic ensemble in the transition temperature of a dilute Bose gas

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Abstract

We study the Bose–Einstein condensation phase transition in a weakly interacting gas through a perturbative analysis of finite systems. In both the grand canonical and the canonical ensembles, perturbation theory suffers from infrared divergences and cannot directly determine the transition temperature in the thermodynamic limit. However, in conjunction with finite-size scaling, perturbation theory provides a powerful calculation tool. Here we use this combination of perturbation theory and scaling to estimate a shift in the transition temperature in the canonical ensemble consistent with grand canonical calculations.

1. Introduction

Wilkens *et al* [1] derive a surprising and extremely interesting result, namely that as a function of interaction strength the transition temperature of a dilute Bose gas behaves differently in the canonical and grand canonical ensembles. They conclude that in the canonical ensemble, the transition temperature *decreases* with increasing interaction strength, whereas the opposite behaviour has been established in calculations in the grand canonical ensemble [2, 3]. The latter agree with numerical calculations in the canonical ensemble [4, 5] and on the lattice [6, 7].

In this paper we reformulate the ideas of Wilkens *et al* [1] to provide a more explicit comparison with its grand canonical counterparts and with numerical calculations. The calculation is perturbative in nature; we show that such a perturbative scheme fails in the thermodynamic limit due to the presence of infrared divergences. These divergences are common to calculations in both canonical and grand canonical ensembles, and result from long-wavelength fluctuations which dominate all second-order phase transitions. We present a scheme, based upon the finite-size scaling used in numerical calculations of the phase transition [4, 5], which avoids such singularities. In our approach, the phase transition temperature is inferred from the scaling properties of small systems for which perturbation theory converges. Using this novel technique we analytically derive a shift in the transition temperature which agrees with conventional results [2–5].

This paper is structured as follows. First, to lowest order in the interaction strength, we derive, in the spirit of [1], a perturbative expression for the transition temperature. Next, by considering higher-order terms, we show that the perturbation series diverges in the thermodynamic limit. Finally, we use finite-size scaling in conjunction with the perturbation series to correctly derive the shift in the transition temperature.

2. Perturbation theory near T_c

We consider a system of bosons interacting through a short-range potential described by the Hamiltonian

$$H = \sum_q \frac{\hbar^2 q^2}{2m} b_q^\dagger b_q + H_{\mathrm{int}} \tag{1}$$

where

$$H_{\mathrm{int}} = \frac{2\pi\hbar^2 a}{mV} \sum_{pkq} b_p^\dagger b_q^\dagger b_{q-k} b_{p+k} \tag{2}$$

and a is the scattering length, b_q is the annihilation operator for particles with momentum $\boldsymbol{q}$, m is the particle mass and $V \equiv L^3$ is the volume of the system. The free energy to first order in a is

$$F(a) = F_0 + \langle H_{\mathrm{int}} \rangle \tag{3}$$

where the expectation value is in the *free* ensemble, and $F_0 \equiv F(a = 0)$ is the free energy of the non-interacting system. The basic technical difference between the canonical and grand canonical ensembles arises in factoring the four-point expectation value in equation (3); in the grand canonical ensemble

$$\sum_{pqk} \langle b_p^\dagger b_q^\dagger b_{q-k}\, b_{p+k} \rangle_{\mathrm{GC}} = \sum_{pqk} \left(\langle b_p^\dagger b_{q-k} \rangle \langle b_q^\dagger b_{p+k} \rangle + \langle b_p^\dagger b_{p+k} \rangle \langle b_q^\dagger b_{q-k} \rangle \right) \tag{4}$$

$$= 2\langle N \rangle^2 \tag{5}$$

where $\langle N \rangle = \sum_k \langle b_k^\dagger b_k \rangle$ is the mean number of particles. A contribution proportional to N^2 cannot affect the critical temperature, since this term just adds a constant to the free energy, and is compensated by a shift in the chemical potential. In the canonical ensemble, however,

$$\sum_{pqk} \langle b_p^\dagger b_q^\dagger b_{q-k}\, b_{p+k} \rangle_{\mathrm{C}} = 2N^2 - \sum_p \langle N_p (N_p + 1) \rangle \tag{6}$$

where $N_p = b_p^\dagger b_p$. The second tem cannot be compensated by a shift of the chemical potential and does change the transition temperature. The first-order shift in free energy differs in the two ensembles by the term

$$\langle H_{\mathrm{int}} \rangle_{\mathrm{C}} - \langle H_{\mathrm{int}} \rangle_{\mathrm{GC}} = -\frac{2\pi\hbar^2 a}{mV} \sum_p \langle N_p (N_p + 1) \rangle. \tag{7}$$

Although the coefficient of this sum is of order $1/V$, the sum itself diverges as $V^{4/3}$ at the Bose condensation transition. This term of order $V^{1/3}$ is the source of the shift in the critical temperature described in [1]. We now restrict ourselves to the canonical ensemble to determine the role of the term (7). In all subsequent manipulations both the number of particles N and the system size V are held fixed.

2.1. Characterization of condensation

Bose–Einstein condensation occurs when N_0, the number of condensed particles, becomes macroscopic. To explore the transition we study the probability of having N_0 particles in the condensate. This distribution function, $P(N_0)$, is

$$P(N_0) = \frac{1}{Z_N} \operatorname*{Tr}_{N,N_0\,\mathrm{fixed}} \mathrm{e}^{-\beta H} = \frac{1}{Z_N} \mathrm{e}^{-\beta F(N,N_0)} \tag{8}$$

where the trace is taken at fixed N and N_0, and β is the inverse temperature. This equation defines the free energy $F(N, N_0)$; the partition function, $Z_N = \sum_{N_0} \mathrm{e}^{-\beta F(N,N_0)}$, normalizes the probability distribution.

The high-temperature normal phase of the system is characterized by a monotonically decreasing $P(N_0)$, while the low-temperature condensed phase has $P(N_0)$ peaked at $N_0 \neq 0$. The extremes of these regimes are readily quantified. At sufficiently high temperatures, N_0 is Gibbs distributed, $P(N_0) \propto \mathrm{e}^{\beta\mu N_0}$, where $\mu = \partial F/\partial N < 0$ is the chemical potential. At zero temperature in the non-interacting gas all the particles are condensed and $P(N_0) = \delta_{N_0,N}$. At some intermediate temperature the distribution becomes flat at $N_0 = 0$. Wilkens *et al* define T_c by extrapolating this crossover temperature to the thermodynamic limit.

In terms of $F(N, N_0)$, Wilkens *et al*'s criterion for T_c gives an implicit equation for the critical temperature of the interacting system $T_\mathrm{c}^{(a)}$,

$$\left.\frac{\partial F(N, N_0)}{\partial N_0}\right|_{N_0=0,T=T_\mathrm{c}^{(a)}} = 0. \tag{9}$$

As in Fermi liquid theory, $\partial F/\partial N_0$ is the energy of a $k = 0$ quasiparticle measured from the chemical potential [8], and can therefore be expressed as

$$\frac{\partial F}{\partial N_0} = \Sigma(k = 0, \omega = 0) - \mu \tag{10}$$

where $\Sigma(k, \omega)$ is the self-energy at momentum k and energy ω. Thus this criterion for the critical temperature is essentially that used by Baym *et al* [3] in the grand canonical ensemble. An important difference between the two approaches is that in the present calculation only quantities at $N_0 = 0$ are involved. In the canonical ensemble the fluctuations in N_0 are very large at the critical temperature, $\langle N_0^2\rangle - \langle N_0\rangle^2 \sim N^{4/3}$ [9]; as we shall see, the criterion (9) yields a qualitatively different shift in the transition temperature if the derivative is evaluated at the expectation value of N_0 rather than at $N_0 = 0$.

2.2. Perturbative expansion

Following [1], we now attempt to calculate the transition temperature, $T_\mathrm{c}^{(a)}$, by perturbatively expanding (9) in powers of a. Since $\partial F/\partial N_0$ is evaluated at $T = T_\mathrm{c}^{(a)}$, we must consider not only the explicit variation of F with a, but also the implicit contribution due to the dependence of T on a. We use the decomposition $F(a) = F_0 + \Delta F(a)$, where F_0 is the free energy of the non-interacting gas and $\Delta F(a)$ is the correction due to interactions. In the free system, the condensate only contributes to the free energy by reducing the occupation of other modes, i.e.

$$\frac{\partial F_0(N, N_0)}{\partial N_0} = -\frac{\partial F_0(N, N_0)}{\partial N} \equiv -\mu_0 \tag{11}$$

which defines the free chemical potential μ_0, a function of N, N_0 and T. By construction, when $N_0 = 0$ this chemical potential vanishes at the transition temperature of the non-interacting gas, $T_c^{(0)}$, and to first order in the interaction,

$$\left.\frac{\partial F_0}{\partial N_0}\right|_{N_0=0,T=T_c^{(a)}} = -\mu_0(N_0 = 0, T = T_c^{(a)}) \tag{12}$$

$$= -\Delta T_c \left.\frac{\partial \mu_0}{\partial T}\right|_{N_0=0,T=T_c^{(0)}} + \mathcal{O}(a^2). \tag{13}$$

The derivative is taken at fixed N and N_0 and $\Delta T_c = T_c^{(a)} - T_c^{(0)}$ is the shift in the transition temperature for scattering length a. Thus, to first order in a, the left-hand side of equation (9) becomes $\partial(\Delta F)/\partial N_0 - \Delta T_c\, \partial\mu_0/\partial T$, evaluated at $T = T_c^{(0)}$ and $N_0 = 0$. Solving for ΔT_c, we have

$$\Delta T_c = \left.\frac{(\partial(\Delta F)/\partial N_0)}{(\partial\mu_0/\partial T)}\right|_{N_0=0,T=T_c^{(0)}}. \tag{14}$$

Aside from the use of continuous derivatives in place of Wilkens *et al*'s discrete derivatives, this is the result of [1]. Correctly evaluating these functions for a finite-sized system is challenging. We estimate their magnitude by replacing the canonical expectation values in (6) by the grand canonical result $\langle N_k(N_k + 1)\rangle = 2\langle N_k\rangle(\langle N_k\rangle + 1)$, and approximately writing $\langle N_k\rangle \approx (\mathrm{e}^{\beta(\epsilon_k-\mu_0)} - 1)^{-1}$. This assumption provides a simple relationship between $N = N_0 + \sum_k\langle N_k\rangle$ and μ_0. Introducing the number of excited particles $N_{ex} = N - N_0$, we may write

$$\frac{\partial(\Delta F)}{\partial N_0} = -\frac{\partial(\Delta F)}{\partial N_{ex}} = -\left(\frac{\partial(\Delta F)}{\partial\mu_0}\right)\left(\frac{\partial\mu_0}{\partial N_{ex}}\right) \tag{15}$$

$$= \left(\frac{\partial(\Delta F)}{\partial\mu_0}\right)\left(\frac{\partial\mu_0}{\partial T}\right)_{N_{ex}}\left(\frac{\partial T}{\partial N_{ex}}\right)_{\mu_0}. \tag{16}$$

Since all quantities are evaluated in the free ensemble, the derivatives are straightforwardly evaluated, leading to

$$\frac{\Delta T_c}{T_c} \approx -\frac{8\pi\hbar^2 a}{3mNVk_bT}\sum_{k\neq 0}\langle N_k\rangle^3 \tag{17}$$

where $\langle N_k\rangle$ is evaluated at $\mu_0 = 0$. The sum is infrared divergent, scaling as V^2, and yielding a finite-temperature shift proportional to $-an^{1/3}$, where $n = N/V$. The constant of proportionality is of the same order of magnitude as the one calculated in [1] using a sophisticated series of asymptotic expansions; its exact numerical value is unimportant here. The key observation is that contrary to the expected behaviour, the temperature shift predicted by this argument is negative.

This negative temperature shift depends crucially upon the constraint $N_0 = 0$. At finite N_0, the numerator of (14) has an additional contribution due to the derivative of the $p = 0$ term of the sum in (7). This contribution has the opposite sign, and dominates when $N_0 \sim N^{2/3}$, yielding a positive temperature shift. As already emphasized, at the critical temperature, the expectation value of N_0 is of order $N^{2/3}$.

2.3. Breakdown of perturbation theory

We now explore the validity of this perturbation expansion, demonstrating that it breaks down in the thermodynamic limit. Higher-order terms in the expansion of the free energy (3) involve higher powers of the interaction H_{int}. As in first order, the most divergent terms occur when all of the momenta are equal and, at T_c, these terms are of relative size $\langle(\beta H_{\mathrm{int}})^m\rangle/\langle(\beta H_{\mathrm{int}})^{m-1}\rangle \sim aL/\lambda^2$, where $L = V^{1/3}$ is the length of the system, and $\lambda = (2\pi\hbar^2/mk_bT)^{1/2} \sim n^{-1/3}$ is the thermal wavelength, of the order of the interparticle spacing. Thus we see that the perturbation expansion is valid only for sufficiently small $\eta \equiv aL/\lambda^2$.

In any finite system the transition temperature calculated above corresponds to a crossover of finite width δT. One can estimate the width of the crossover from the fluctuations in the number of condensed particles; since the latter scale as [9],

$$\delta T/T \sim \delta N_0/N \sim N^{-1/3}. \tag{18}$$

As long as $\delta T \ll \Delta T_c$, the shift is well defined. Since $\Delta T \propto -an^{1/3}$, the ratio $\Delta T/\delta T$ is of order $aL/\lambda^2 = \eta$, and the shift is only well defined for $\eta \gg 1$. Thus in the limit of small η, where the expansion of the free energy converges, the calculated change in T_c is smaller than the width of the transition and cannot be physically significant. In the other limit $\eta \gg 1$ the expansion of the free energy breaks down. Hence this calculation, as it stands, cannot tell us anything about the transition temperature of a weakly interacting Bose gas.

3. Scaling behaviour

Although perturbation theory breaks down in the thermodynamic limit, it can be used to learn the properties of small systems where $L \ll \lambda^2/a$. We now discuss how finite-size scaling enables one to learn about the $L = \infty$ phase transition by investigating how physical quantities scale with L in these small systems. This technique is commonly used in numerical simulations where it is not feasible to simulate an infinite system. The central assumption of finite-size scaling is that sufficiently close to the critical point all physical quantities scale as functions of the ratio of the correlation length ξ to the system size L. For example, the order parameter scales as

$$\frac{\langle N_0\rangle}{V} \sim L^{-y}\Phi(L/\xi) \tag{19}$$

where $y = \beta/\nu = 1$ is the ratio of the critical exponents for N_0/V and the correlation length, and Φ is a scaling function. As $L/\xi \to \infty$, this function must diverge as $\Phi(L/\xi) \sim (L/\xi)^y$, while as $L/\xi \to 0$, Φ approaches a constant. The latter limit gives a systematic method for finding the critical point ($\xi \to \infty$) by looking solely at the properties of a finite system. In numerical calculations [4,5] one plots $L^y\langle N_0\rangle/V$, or a related quantity such as the superfluid density, as a function of temperature for different system sizes. According to the scaling hypothesis all of these curves should intersect at the critical temperature.

Relations similar to equation (19) also hold for higher moments of the order parameter and imply that at T_c the probability distribution function can be written as

$$P(N_0) = \frac{\lambda^2}{L^2}\psi(N_0\lambda^2/L^2) \tag{20}$$

with some scaling function ψ. We calculate the critical temperature of the interacting system by finding the temperature at which $P(N_0)$ has this scaling form.

3.1. Scaling in the canonical ideal gas

Before using this procedure to calculate ΔT_c, we verify that the scaling relations, (20) and (19), hold in the non-interacting gas. We first derive equation (19) in the grand canonical ensemble

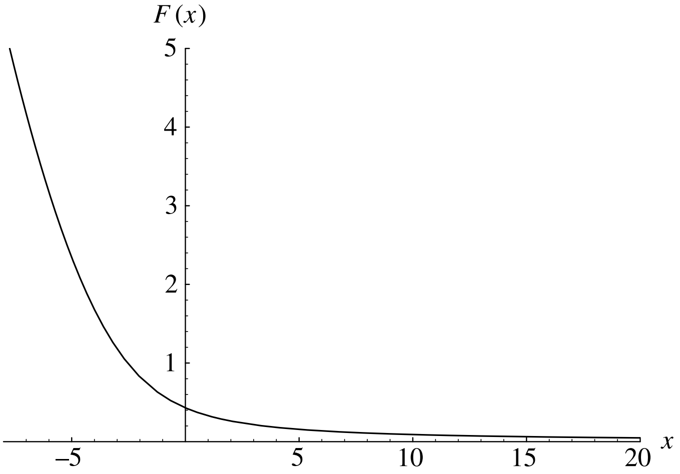

Figure 1. The function $F(x)$, defined as the solution to equation (24), which relates the chemical potential and density of a non-interacting ideal Bose gas via (25).

where the argument is particularly simple. The general strategy is to fix the average density $n = N/V$ and the temperature T, and look at how the order parameter N_0 varies with the system size L. To carry out this approach we need an expression for the chemical potential μ as a function of n, T and L, which requires inverting the relationship,

$$n = \frac{1}{V}\sum_k \frac{1}{e^{\beta(\epsilon_k-\mu)}-1} \tag{21}$$

$$\approx \frac{1}{\lambda^3} g_{3/2}(e^{\beta\mu}) + N_0/V \tag{22}$$

where $g_{3/2}(z) = \sum_j z^j/j^{3/2}$ is a polylogarithm function. The inversion is performed by expanding (22) in powers of $\beta\mu$, noting that $N_0 \approx -1/\beta\mu$. One finds

$$n = \frac{1}{\lambda^3}\left[\zeta\left(\tfrac{3}{2}\right) + \frac{\lambda}{L}\left(-\frac{1}{\beta\mu L^2/\lambda^2} - 2\sqrt{-\pi\beta\mu L^2/\lambda^2}\right) + \cdots\right]. \tag{23}$$

For $\beta\mu \sim \lambda^2/L^2 \sim 1$, the neglected terms are of relative order λ/L. The terms proportional to $1/\beta\mu$ and $\sqrt{-\beta\mu}$ are, respectively, the contributions from the condensed and non-condensed particles. Finding $\beta\mu$ as a function of n, T and L, requires solving a cubic equation. We define the function $F(x)$, plotted in figure 1, as the solution to

$$\frac{1}{F(x)} - 2\sqrt{\pi F(x)} - x = 0 \tag{24}$$

so that the chemical potential can be expressed as

$$\beta\mu = -\frac{\lambda^2}{L^2} F\left(\frac{L}{\lambda}\left(\lambda^3 n - \zeta\left(\tfrac{3}{2}\right)\right)\right). \tag{25}$$

The positive, monotonic $F(x)$ has the properties

$$F(0) = (4\pi)^{-1/3} \tag{26}$$

$$F(x) \underset{x\to-\infty}{\longrightarrow} x^2/4\pi \tag{27}$$

$$F(x) \underset{x\to+\infty}{\longrightarrow} 1/x. \tag{28}$$

Thus, as $L \to \infty$, the order parameter $N_0 \approx -1/\beta\mu$, has three distinct behaviours, corresponding to non-condensed, critical, and condensed regimes, depending on whether n is less than, equal to, or greater than $\zeta\left(\frac{3}{2}\right)/\lambda^3$. In the non-condensed regime, N_0 is microscopic, in the condensed regime, N_0 is extensive, and at the critical point, N_0 scales as (19), with the predicted exponent $y = 1$, i.e.,

$$n < \zeta\left(\tfrac{3}{2}\right)/\lambda^3 \qquad N_0 \sim L^0 \tag{29}$$

$$n = \zeta\left(\tfrac{3}{2}\right)/\lambda^3 \qquad N_0 \sim L^2 \tag{30}$$

$$n > \zeta\left(\tfrac{3}{2}\right)/\lambda^3 \qquad N_0 \sim L^3. \tag{31}$$

The scaling at T_c, equation (30), is consistent with (18), since at the critical point the mean value of N_0 is of the same order as the fluctuations δN_0.

3.2. *Scaling in the canonical ideal gas*

We now perform the equivalent calculation in the canonical ensemble. Starting from the expression $N = N_0 + \sum_k \langle N_k \rangle$, and approximating $\langle N_k \rangle = (\mathrm{e}^{\beta(\epsilon_k - \mu_0(N_0))} - 1)^{-1}$, we solve for μ_0 as a function of N_0. Integrating $\mu_0(N_0)$ with respect to N_0 yields $F(N, N_0)$ and $P(N_0) \propto \mathrm{e}^{-\beta F(N,N_0)}$. As $P(N_0)$ is peaked about the point where $\mu_0 = 0$, we can expand $\sum_k \langle N_k \rangle$ in powers of μ_0. Standard asymptotics [10] yields a series which converges for $|\beta\mu_0| < \pi\lambda^2/L^2$,

$$N_{\mathrm{ex}} = \sum_k \langle N_k \rangle = \left(\frac{L}{\lambda}\right)^3 \zeta\left(\tfrac{3}{2}\right) + \left(\frac{L}{\lambda}\right)^2 f\left(\frac{\beta\mu L^2}{\lambda^2}\right) + \mathcal{O}(L/\lambda) \tag{32}$$

$$f(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!} C_3(k+1) \tag{33}$$

where the coefficients $C_d(k)$ are sums of the form

$$C_d(k) = \frac{\Gamma(k)}{\pi^k} \sum_{n_1, n_2, \ldots, n_d}{}' \frac{1}{\left(n_1^2 + n_2^2 + \cdots + n_d^2\right)^k}. \tag{34}$$

The prime denotes that the term $n_1 = n_2 = \cdots = n_d = 0$ is omitted. These constants are tabulated in table 1. Inversion of the series gives

$$\beta\mu = \frac{\lambda^2}{L^2}\left(-\frac{1}{C_3(2)}M - \frac{C_3(3)}{2(C_3(2))^2}M^2 + \cdots\right) \tag{35}$$

$$M = N_0 \frac{\lambda^2}{L^2} + C_3(1) - \frac{\lambda^2}{L^2}\left(N - \frac{L^3}{\lambda^3}\zeta\left(\tfrac{3}{2}\right)\right) \tag{36}$$

from which the free energy is

$$\beta F_0(N, N_0) = -\int \mathrm{d}N_0\, (\beta\mu_0) \tag{37}$$

$$= \beta\bar{F}_0(N) + \frac{1}{2C_3(2)}M^2 + \frac{C_3(3)}{6(C_3(2))^2}M^3 + \cdots \tag{38}$$

$$\equiv \beta\bar{F}_0(N) + g(M) \tag{39}$$

Table 1. Values of the lattice sum $C_3(k)$, defined in equation (34).

$k = 1$	2	3	4	5	6
−2.8374	1.6752	0.5419	0.4278	0.5039	0.7741

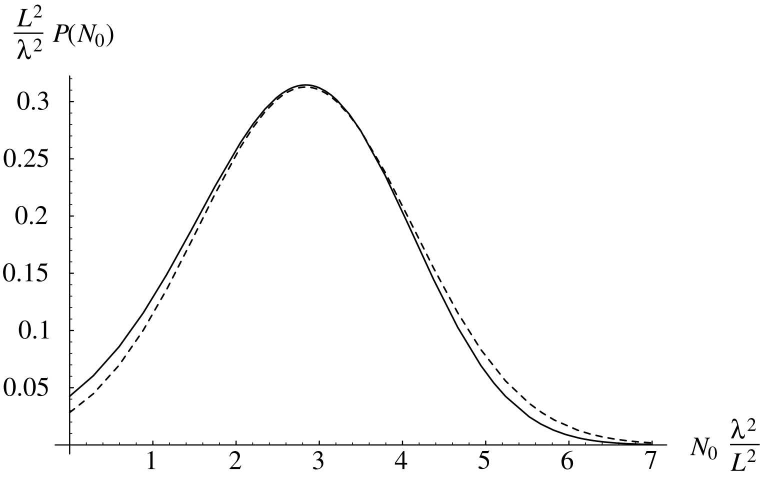

Figure 2. Probability distribution $P(N_0)$ for the number of condensed particles at the critical temperature in a non-interacting Bose gas within the canonical ensemble. The broken curve is a Gaussian approximation. At the critical point, P has the scaling form (20).

where $\bar{F}_0(N)$ is an extensive function which is independent of N_0 and $g(M)$ is defined by equations (38) and (39). If $n = N/V = \zeta\left(\frac{3}{2}\right)/\lambda^3$, then M depends on L only through the variable $N_0\lambda^2/L^2$, implying that $P(N_0)$ is of the form (20). For any other value of the density, M has an additional L dependence, and $P(N_0)$ does not have the desired form, implying that the scaling (20) holds only at T_c. In figure 2 we plot $P(N_0)$ at the critical point. The Gaussian approximation, where only the term proportional to M^2 is kept, is also plotted, and agrees quite well with the full result.

3.3. Calculation of ΔT_c

Having verified the scaling relationships for $P(N_0)$ in the non-interacting gas, we now search for the critical temperature of the interacting gas by perturbatively calculating $P(N_0)$ and finding the temperature at which scaling holds. We continue to use the approximations that $\langle N_k(N_k+1)\rangle = 2\langle N_k\rangle(\langle N_k\rangle+1)$ and $\langle N_k\rangle \approx (\mathrm{e}^{\beta(\epsilon_k-\mu_0)}-1)^{-1}$. To first order in a, at temperature $T = T_c^{(0)} + \Delta T$, the free energy is

$$\beta F[N, N_0] = \beta\bar{F}_0 + g(M_0) - \frac{\Delta T}{T}\frac{\lambda^2}{L^2}N_0 g'(M_0) + \frac{3}{2}\frac{\Delta T}{T}\frac{L}{\lambda}\zeta\left(\tfrac{3}{2}\right)g'(M_0) - \frac{2\pi\hbar^2 a}{mVT}\left(N_0^2 + 2\sum_{k\neq 0} N_k(N_k+1)\right) \tag{40}$$

where the argument $M_0 = N_0(\lambda^2/L^2) + C_3(1)$ is the scaled condensate number measured from the peak of the distribution. The first two terms are the free energy of the non-interacting gas at $T_c^{(0)}$, while the remaining terms give the first-order corrections in ΔT and a. These corrections are only small if $\eta = aL/\lambda^2 \ll 1$. The sum $\sum_{k\neq 0} N_k(N_k+1)$ can be identified with $\partial N_{\mathrm{ex}}/\partial(\beta\mu_0)$, and can be expressed as a series in $\beta\mu_0 L^2/\lambda^2$ via equation (32). Using

(35) to eliminate μ, the corrections are

$$F(T) = F_0(T_c^{(0)}) - \frac{\Delta T}{T}\frac{\lambda^2}{L^2}N_0 g'(M_0) + \frac{L}{\lambda}\left[\frac{3\zeta\left(\frac{3}{2}\right)}{2}\frac{\Delta T}{T}\left(\frac{1}{C_3(2)}M_0 + \frac{C_3(3)}{2C_3(2)^2}M_0^2 + \cdots\right)\right.$$
$$- \frac{2\pi\hbar^2 a}{m\lambda^3 T}\left(C_3(1)^2 + 2C_3(2) - 2\left(C_3(1) + \frac{C_3(3)}{C_3(2)}\right)M_0\right.$$
$$\left.\left. + \left(1 + \frac{C_3(2)C_3(4) - C_3(3)^2}{C_3(2)^3}\right)M_0^2 + \cdots\right)\right]. \tag{41}$$

Comparing with (20), we see that scaling holds if and only if the factor multiplied by L/λ vanishes. Eliminating the coefficient of the first power of M_0 enforces scaling near the peak of $P(N_0)$, in which case

$$\frac{\Delta T}{T} = -\frac{8\pi\hbar^2 a}{3m\lambda^3 T\zeta\left(\frac{3}{2}\right)}\left(C_3(1)C_3(2) + C_3(3)\right) \tag{42}$$

$$\approx 1.6an^{1/3}. \tag{43}$$

The coefficient 1.6 should be compared with the numerical value of 2.3 calculated by Holzmann and Krauth [5]. The discrepancy lies within the accuracy expected of our approximations. The important point to note is that the coefficient is positive and of order unity.

The neglect of terms of higher order in a during the calculation is based on the assumption that they do not change the structure of the scaling function. (We note that recent calculations of ϕ^4 theory on a lattice [6, 7], may indicate that this assumption is not valid.) A more involved study, where these higher-order terms are explicitly calculated, would help verify whether perturbation theory is valid within finite-size scaling.

At this point it would be appealing to repeat the above calculation in the grand canonical ensemble and explicitly verify that the two ensembles yield the same shift in the transition temperature. In the grand canonical ensemble, first-order perturbation theory changes the energy of each momentum state by the same amount. This shift can therefore be absorbed into the chemical potential, leaving the transition temperature unchanged. The first effects start at higher order; exploring how higher-order perturbation theory in conjunction with finite-size scaling can be used to calculate the shift of T_c in the grand canonical ensemble will be discussed in a future publication.

In summary, we demonstrate that infrared divergences prevent the direct application of perturbation theory to calculating the transition temperature of a dilute Bose gas in the canonical ensemble. We use scaling arguments to circumvent this problem and to evaluate ΔT_c within the canonical ensemble, finding results which are consistent with numerical calculations, and with analytic results based on the grand canonical ensemble.

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