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The Transition Temperature of the Dilute Interacting Bose Gas

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We show that the critical temperature of a uniform dilute Bose gas increases linearly with the s-wave scattering length describing the repulsion between the particles. Because of infrared divergences, the magnitude of the shift cannot be obtained from perturbation theory, even in the weak coupling regime; rather, it is proportional to the size of the critical region in momentum space. By means of a self-consistent calculation of the quasiparticle spectrum at low momenta at the transition, we find an estimate of the effect in reasonable agreement with numerical simulations.

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Determination of the effect of repulsive interactions on the transition temperature of a homogeneous dilute Bose gas at fixed density has had a long and controversial history [1–5]. While [1] predicted that the first change in the transition temperature, T_c, is of order the scattering length a for the interaction between the particles, neither the sign of the effect nor its dependence on a has been obvious. Recent renormalization group studies [4] predict an increase of the critical temperature. Numerical calculations by Grüter, Ceperley, and Laloë [6], and more recently by Holzmann and Krauth [7], of the effect of interactions on the Bose-Einstein condensation transition in a uniform gas of hard sphere bosons, and approximate analytic calculations by Holzmann, Grüter, and Laloë of the dilute limit [8], have shown that the transition temperature, T_c, initially *rises linearly* with a. The effect arises physically from the change in the energy of low momentum particles near T_c [8]. Here we analyze the leading order behavior of diagrammatic perturbation theory, and argue that T_c increases linearly with a. We then construct an approximate self-consistent solution of the single particle spectrum at T_c which demonstrates the change in the low momentum spectrum, and which enables us to calculate the change in T_c quantitatively.

We consider a uniform system of identical bosons of mass m, at temperature T close to T_c and use finite temperature quantum many-body perturbation theory. We assume that the range of the two-body potential is small compared to the interparticle distance $n^{-1/3}$, so that the potential can be taken to act locally and be characterized entirely by the s-wave scattering length a. Thus we work in the limit $a \ll \lambda$, where $\lambda = (2\pi\hbar^2/mk_BT)^{1/2}$ is the thermal wavelength. (We generally use units $\hbar = k_B = 1$.)

To compute the effects of the interactions on T_c, we write the density n as a sum over Matsubara frequencies $\omega_\nu = 2\pi i\nu T$ ($\nu = 0, \pm1, \pm2, \ldots$) of the single particle Green's function, $G(k,z)$:

$$n = -T\sum_\nu \int \frac{d^3k}{(2\pi)^3} G(k,\omega_\nu), \qquad (1)$$

where

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

with μ the chemical potential. The Bose-Einstein condensation transition is determined by the point where $G^{-1}(0,0) = 0$, i.e., where $\Sigma(0,0) = \mu$.

The first effect of interactions on Σ is a mean field term $\Sigma_{\rm mf} = 2gn$, where $g = 4\pi\hbar^2 a/m$; the factor of 2 comes from including the exchange term. Such a contribution, independent of k and z, has no effect on the transition temperature, as it can be simply absorbed in a redefinition of the chemical potential. To avoid carrying along such trivial contributions we define:

$$\frac{\hbar^2}{2m\zeta^2} = -(\mu - 2gn). \qquad (3)$$

The quantity ζ may be interpreted as the mean field correlation length. In the mean field approximation, ζ becomes infinite at T_c; however, in general, it remains finite, and functions here as an infrared cutoff.

Because the effects of interactions are weak, one could imagine calculating the change in T_c in perturbation theory. However, such calculations are plagued by infrared divergences. Power counting arguments reveal that the leading contribution to the self-energy, $\Sigma(k \ll \zeta^{-1}, 0)$, of a diagram of order a^n has the form:

$$\Sigma_n \sim T\left(\frac{a}{\lambda}\right)^2\left(\frac{a\zeta}{\lambda^2}\right)^{n-2}. \qquad (4)$$

In perturbation theory about the mean field, with the mean field criterion for the phase transition, $\zeta \to \infty$ at T_c, all Σ_n diverge, starting with a logarithmic divergence at $n = 2$. More generally, the approach of ζ towards λ^2/a in magnitude signals, according to the Ginsburg criterion, the onset of the critical region. Beyond, perturbation theory breaks down, since all Σ_n in Eq. (4) are of the same order of magnitude.

Even though the theory is infrared divergent, we can isolate the leading correction to the change in T_c, which, as we show, is of order a. Since the infrared divergences occur only in terms with zero Matsubara frequencies we separate, in Eq. (1), the contribution of the $\nu = 0$ terms, writing

$$n(a,T) = -T\int \frac{d^3k}{(2\pi)^3}[G_{\nu=0}(k) + G_{\nu\neq 0}(k)], \qquad (5)$$

where $G_{\nu\neq 0}(k)$ is the sum of terms with $\nu \neq 0$. Similarly, the density of a noninteracting system with condensation temperature T is given by

$$n^0(T) = -T\int \frac{d^3k}{(2\pi)^3}[G^0_{\nu=0}(k) + G^0_{\nu\neq 0}(k)]$$
$$= \int \frac{d^3k}{(2\pi)^3}\frac{1}{e^{k^2/2mT} - 1} = \frac{\zeta(3/2)}{\lambda^3}, \qquad (6)$$

where $\zeta(3/2) = 2.612$. Since the nonzero Matsubara frequencies regularize the infrared behavior of the momentum integrals, the dependence of the $\nu \neq 0$ terms in Eq. (5) on a is nonsingular at T_c. These terms, of order a^2 at least, can be neglected. Thus to order a,

$$n(a,T_c) - n^0(T_c) = -T_c\int \frac{d^3k}{(2\pi)^3}[G_0(k) - G_0^0(k)]. \qquad (7)$$

To calculate the change in T_c at fixed density we equate $n(a,T_c)$ at T_c with $n^0(T_c^0)$ at the free particle transition temperature T_c^0 and observe that $n^0(T_c) = (T_c/T_c^0)^{3/2} n^0(T_c^0)$; thus in lowest order the change in transition temperature $\Delta T_c = T_c - T_c^0$ is given by

$$\frac{3}{2}\frac{\Delta T_c}{T_c} n^0(T_c^0) = T_c\int \frac{d^3k}{(2\pi)^3}[G_{\nu=0}(k) - G^0_{\nu=0}(k)], \qquad (8)$$

where $\Delta T_c = T_c - T_c^0$. Thus

$$\frac{\Delta T_c}{T_c} = \frac{4\lambda}{3\pi\zeta(3/2)}\int_0^\infty dk\, \frac{U(k)}{k^2 + U(k)}, \qquad (9)$$

where $U(k) \equiv 2m[\Sigma_{\nu=0}(k) - \mu]$.

Equation (9) for the leading correction to the critical temperature is crucial. The criterion for spatially uniform condensation is that $U(0) = 0$; above the transition, $U(0) > 0$. At the transition, $k^2 + U(k) > 0$ for $k > 0$. At large wave numbers, $U \to 1/\zeta^2 > 0$, and in the critical region, as we discuss below, U is also positive. Although we have not proved it rigorously, numerical simulations indicate that U is generally positive for $k > 0$, which implies that the integral in Eq. (9) and hence ΔT_c is positive.

In the critical region, $k < k_c$, where k_c defines the scale of the critical region in momentum space, $G_{\nu=0}$ has the scaling form [9] $G^{-1}_{\nu=0}(k) = -k^{2-\eta}k_c^{\eta}F(k\xi)$; ξ is the coherence length which diverges at T_c as $|T - T_c|^{-\nu}$, and F is a dimensionless function, with $F(\infty) \sim 1$. The critical index, η, is given to leading order in the $\epsilon = 4 - d$ expansion by $\epsilon^2/54$ [10]. At T_c, $G^{-1}_{\nu=0}(k) \sim -k^{2-\eta}k_c^{\eta}$, and thus $U \sim +k^{2-\eta}$. Both terms in Eq. (8) give a contribution of order k_c, so that $\Delta T_c/T_c \sim k_c$. As we shall see, $k_c \sim a/\lambda^2$, and hence $\Delta T_c/T_c \sim a/\lambda$.

To study the leading behavior in a quantitatively, we need concentrate only on the $\nu = 0$ sector where the full finite temperature theory reduces to a classical field theory [10] defined by the action:

$$S\{\phi(r)\} = \frac{1}{2mT}\int d^3r\Big[\nabla\phi^*(r)\cdot\nabla\phi(r) + \frac{1}{\zeta^2}|\phi(r)|^2$$
$$+ 4\pi a(|\phi(r)|^2 - \langle|\phi(r)|^2\rangle)^2\Big]; \qquad (10)$$

the probability of a given field configuration entering the computation of expectation values is proportional to $e^{-S\{\phi(r)\}}$.

The classical theory is ultraviolet divergent, but superrenormalizable. The divergences appear only in the two-loop self-energy, $\Sigma^{(2)}_{\nu=0}$—effectively the second order self-energy written in terms of the full $G_{\nu=0}$ rather than the zeroth order Green's functions—and can be removed by simple renormalization of the mean field coherence length, ζ. Since, henceforth, we calculate only in the classical theory, we drop the subscript $\nu = 0$. The second order self-energy is

$$\Sigma(k) = -2g^2\int \frac{d^3q}{(2\pi)^3}B(q)\frac{T}{\epsilon_{\mathbf{k}-\mathbf{q}}}, \qquad (11)$$

where $\epsilon_k = (k^2 + \zeta^{-2})/2m$, and the ($\nu = 0$) particle-hole bubble,

$$B(q) = \int \frac{d^3p}{(2\pi)^3} \frac{T}{\epsilon_p \epsilon_{\mathbf{p+q}}}, \tag{12}$$

is given by

$$B(q) = \frac{2\pi^2\zeta}{T\lambda^4} b(\zeta q); \tag{13}$$

$b(x) \rightarrow 1/x$ for $x \gg 1$ and $b(0) = 1/\pi$.

The integral in Eq. (11) is logarithmically divergent in the ultraviolet. But in the full theory the momentum integrals are cut off by distribution functions, $f = (e^{k^2/2mT} - 1)^{-1}$, and the ultraviolet behavior is regular. To control this divergence we introduce an ultraviolet momentum cutoff, Λ, in the classical theory, recognizing that it is in fact effectively determined in the full theory. Then

$$2m\Sigma(k) = -32\pi^2 \frac{a^2}{\lambda^4} \int_0^{\Lambda\zeta} dx\, x b(x) L(k\zeta, x), \tag{14}$$

where

$$L(k\zeta, x) = \frac{1}{k\zeta} \ln\left[\frac{(x + k\zeta)^2 + 1}{(x - k\zeta)^2 + 1}\right]. \tag{15}$$

The divergent part of the integral comes from the large x tail of $b(x)$, and contributes $-128(a/\lambda^2)^2 \ln(\Lambda\zeta)$ to $2m\Sigma$.

More generally we carry out a diagrammatic expansion of Σ in terms of the *self-consistent* $\nu = 0$ Green's function, defined by $2mG^{-1}(k) = -k^2 + \zeta^{-2} + 2m\Sigma(k, a, G, \Lambda)$. Note that the dependence of Σ on ζ enters only through the dependence of Σ on G. We define a *renormalized* mean field coherence length by

$$\frac{1}{\zeta_R^2} = \frac{1}{\zeta^2} - 128\left(\frac{a}{\lambda^2}\right)^2 \ln(\Lambda\zeta_R). \tag{16}$$

Then $G^{-1}(k)$ is given by

$$-2mG^{-1}(k) = k^2 + \zeta_R^{-2} + 2m\Sigma_F(k, a, G), \tag{17}$$

where

$$\Sigma_F(k, a, G) = \Sigma(k, a, G, \Lambda) + 128\left(\frac{a}{\lambda^2}\right)^2 \ln(\Lambda\zeta_R) \tag{18}$$

is independent of Λ. As a function of ζ_R, the Green's function is independent of the cutoff.

In fact, a simple power counting argument shows that the finite part of the self-energy has the form

$$\Sigma_F(k, a, G) = \frac{1}{2m\zeta_R^2} \sigma(k\zeta_R, J), \tag{19}$$

where

$$J = a\zeta_R/\lambda^2. \tag{20}$$

To see this structure we note that a term in the self-energy of order a^n is the product of a dimensionless function of $k\zeta_R$ times the Σ_n of Eq. (4), with ζ replaced by ζ_R [11].

The criterion for condensation, $\zeta_R^{-2} + 2m\Sigma_F(0, a, G) = 0$, implies that

$$1 + \sigma(0, J) = 0. \tag{21}$$

Since $\sigma(0)$ is a well-behaved function of only the parameter J, Eq. (21) determines the critical value of $J = J^*$ for condensation, a dimensionless number independent of the parameters of the original problem. At condensation, the renormalized mean field coherence length ζ_R tends to infinity as $a \rightarrow 0$, with the product $a\zeta_R$ fixed, thus preventing a perturbative expansion in a.

At condensation $U(k) = [\sigma(k\zeta_R, J^*) + 1]/\zeta_R^2$, and Eq. (9) implies the change in T_c

$$\frac{\Delta T_c}{T_c} = \frac{a}{\lambda}\left[\frac{4}{3\pi\zeta(3/2)} \frac{1}{J^*} \int_0^\infty dx \frac{\sigma(x, J^*) + 1}{x^2 + \sigma(x, J^*) + 1}\right]. \tag{22}$$

Since J^* is determined by the condition (21), the result for $\Delta T_c/T_c$ is linear and expected to be positive in a/λ.

We turn now to calculating ΔT_c explicitly within a simple self-consistent model based on taking only the zero frequency component of the leading two-loop approximation self-energy, given by Eq. (11). We construct the ϵ_p as self-consistent quasiparticle energies at the transition, i.e., solutions of the equation:

$$G^{-1}(k, \epsilon_k) = 0 = \epsilon_k - \frac{k^2}{2m} - [\Sigma(k) - \Sigma(0)]. \tag{23}$$

The low momentum behavior of ϵ_k is determined by a familiar argument [12]. In order that the integral (11) converge in the infrared limit, ϵ_k must behave, modulo possible logarithmic corrections, as $\sim k^\alpha$, where $\alpha < 2$. In this case, the term $k^2/2m$ in (23) can be neglected at small k. We then expand $\Sigma(k)$ about $k = 0$. For $1 \le \alpha < 4/3$ the self-energy is sufficiently convergent that $\Sigma(k) - \Sigma(0) \sim k^2$ at small k, and thus cannot be the correct self-consistent solution. For α with $4/3 < \alpha < 2$ one has $\Sigma(k) - \Sigma(0) \sim +k^{6-3\alpha}$, so we find self-consistency, $\Sigma(k) - \Sigma(0) \sim k^\alpha$, for $\alpha = 3/2$. We write the small k part of the spectrum as

$$\epsilon_k = k_c^{1/2} k^{3/2}/2m. \tag{24}$$

Here k_c is the wave vector around which the $k^{3/2}$ at low k crosses over to the $k^2/2m$ free-particle behavior.

To extract the low momentum structure, below the scale k_c, we evaluate the most divergent terms of

$$\Sigma(k) - \Sigma(0) = -2g^2 T \int \frac{d^3q}{(2\pi)^3} B(q)\left(\frac{1}{\epsilon_{\vec{k}-\vec{q}}} - \frac{1}{\epsilon_q}\right); \tag{25}$$

at small k. Since the $k^{3/2}$ structure arises from the small q behavior of the integral; we evaluate the bubble $B(q)$, Eq. (12), at small q with the spectrum (24) for $k < k_c$ and $k^2/2m$ for $k > k_c$. Then

$$B(q) = \frac{4m}{\pi\lambda^2 k_c}[\ln(k_c/q) + c], \tag{26}$$

with $c \approx 2 + 2\ln 2 - \pi/2 = 1.816$. Thus,

$$\Sigma(k) - \Sigma(0) = \frac{1024\pi}{15m}\left(\frac{a}{\lambda^2}\right)^2\left(\frac{k}{k_c}\right)^{3/2}. \qquad (27)$$

Identifying the right side of Eq. (27) with $k_c^{1/2}k^{3/2}/2m$, we derive

$$k_c = 32\left(\frac{2\pi}{15}\right)^{1/2}\frac{a}{\lambda^2} \approx 20.7\,\frac{a}{\lambda^2}. \qquad (28)$$

As expected, the scale of the unusual low momentum structure is a/λ^2.

Let us, for a first quantitative estimate, assume a spectrum at T_c of the form $\epsilon_k = k_c^{1/2}k^{3/2}/2m$ for $k \ll k_c$, and $(k^2 + k_c^2)/2m$ for $k \gg k_c$. We smoothly interpolate between these limits, writing $U(k) = k_c^{1/2}k^{3/2}/[1 + (k/k_c)^{3/2}]$. Thus $\int dk\, U/(k^2 + U) \simeq 1.2k_c$, so that with Eq. (28),

$$\frac{\Delta T_c}{T_c} \simeq 2.9an^{1/3}. \qquad (29)$$

By comparison, Grüter, Ceperley, and Laloë [6] find $\Delta T_c/T_c \approx 0.34an^{1/3}$, while the more recent calculation of Holzmann and Krauth yields $\Delta T_c/T_c \approx (2.2 \pm 0.2)an^{1/3}$. The agreement of the numerical coefficient, given the simplicity of the approximations in evaluating the effect of interactions on the transition temperature, is satisfying. As will be reported in a fuller paper [14], this estimate agrees with that derived from the numerical self-consistent solution of Eq. (23).

The lowest two-loop calculation does not account fully for the modification of the transition temperature; indeed, at the critical point, all diagrams become comparable [13,14]. Consider, for example, summing the bubbles describing the repeated scattering of the particle-hole pair in B [15], thus replacing B in Eq. (11) by

$$B_{\text{eff}}(q) = \frac{B(q)}{1 + 2gB(q)}, \qquad (30)$$

where the two accounts for the exchange terms. The denominator at small q, from Eq. (26), is given by

$$1 + 2gB(q) = 1 + \frac{32a}{\lambda^2 k_c}[\ln(k_c/q) + c]. \qquad (31)$$

Since $k_c \sim a/\lambda^2$, the correction is of order unity, and serves to modify the spectrum, recalculated from Eq. (25) with (31), from $k^{3/2}$ to $k^{2-\eta}$, with [14] $\eta \simeq (1/2) - 1/(2c + k_c\lambda^2/16a) \simeq 0.36$.

To estimate J^*, we calculate $\Sigma(0)$ from Eq. (11) with the 3/2 spectrum and the leading log in $B(q)$, Eq. (26), and neglect the contribution for $q > k_c$. Then $\Sigma(0) \simeq -\kappa^2a^2/2m\lambda^4$, and $\sigma(0, J) \simeq -\kappa^2J^2$, so that at T_c, $J^* \simeq 1/\kappa = 3/(32\sqrt{2} + 3c)$. The self-consistent solution of Eq. (23) yields [14] $J^* \simeq 0.07$.

The modification at T_c of the spectrum of particles at low momenta should have direct experimental consequences in trapped Bose condensates. While a $k^2/2m$ particle spectrum yields a flat distribution v^2dn/dv of velocities, a more rapidly rising spectrum, e.g., the $k^{3/2}$ discussed here, depletes the number of low momentum particles. These effects become more pronounced with a larger number of particles and flatter traps, as the level spacing ceases to control the low-energy behavior.

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