Effect of Interactions on the Critical Temperature of a Dilute Bose Gas

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Abstract

Due to the observation of Bose-Einstein condensation in dilute atomic $^{87}\text{Rb}$ and $^{23}\text{Na}$ vapors last year, there is currently a great interest in the properties of a degenerate Bose gas. One aspect that is not yet understood is the effect of the interatomic interactions on the critical temperature of the phase transition. We present here a renormalization group study of the weakly-interacting Bose gas and predict the critical temperature at which Bose-Einstein condensation occurs as a function of the (positive) scattering length $a$ of the interatomic potential.

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After a long history of trying to master stabilization and cooling, the correct road towards Bose-Einstein condensation in a dilute gas has now finally been found. Indeed, last year a Bose condensate was observed in the magnetically trapped and evaporatively cooled alkali gases $^{87}$Rb and $^{23}$Na [1,2]. Initiated by this breakthrough, extensive experimental and theoretical studies will surely follow in the near future to fathom the physics of Bose-Einstein condensation in inhomogeneous gases. Superfluidity [3], the Josephson effect and vortex dynamics are just a few examples of phenomena that are very interesting, but in first instance also very difficult to experimentally measure or create. Aspects that appear to be more easily accessible and will be subject of scrutiny first, are e.g. collective excitations [4] and the critical temperature of the phase transition. With respect to this latter point, the recent experiments claim to observe a critical temperature that is shifted upward compared to the ideal gas value, as the measured degeneracy parameter $n_c \Lambda_{th}^3$ at the transition is smaller than $\zeta(3/2) \simeq 2.612$. The exact magnitude of the shift however, is still uncertain. Here $n$ is the density and $\Lambda_{th} = (2\pi\hbar^2/mk_B T)^{1/2}$ the thermal de Broglie wavelength of the atoms in the gas.

A shift in the critical temperature can be expected because the gas contains a finite number of particles. However, this effect is negligible for the large number of atoms used in the experiments [3], and would shift the critical temperature downwards. In addition, a shift can arise because the atoms are interacting via an (effectively) repulsive potential. Concerning this latter aspect, it is important to note that existing approaches to the weakly-interacting Bose gas using the Bogoliubov (or Popov) theory actually do not predict a shift in the critical temperature [3]. Since these theories are of mean-field type, one might naively expect that critical fluctuations will depress the critical temperature, which would again contradict the experimental data. To settle this issue, and also give a quantative prediction for the shift of the critical temperature, we report here on a renormalization group (RG) calculation for the homogeneous Bose gas.

In most applications, the RG method is used to obtain information about universal properties of the system considered, such as critical exponents. Nonuniversal properties depend
on the (usually unknown) ultraviolet cutoff $\Lambda$ of the theory. However, in our case we can eliminate this cutoff dependence because we have sufficient information on the microscopic details of the dilute Bose system. Therefore, we are also able to determine nonuniversal properties of the system as we will see shortly.

In principle, we treat here only the homogeneous Bose gas with effectively repulsive interactions, which implies that the interatomic potential has a positive scattering length $a$.

However, as the number of particles $N \gg 1$, the critical temperature $T_c$ is much larger than the energy splitting $\hbar \omega$ between the levels in the harmonic oscillator traps used experimentally. As the width of the region in which finite-size effects are important is of $O(T_c(\bar{\hbar} \omega/k_B T_c))$, one can practically for all temperatures use a local density approximation to describe the gas in the center of the trap. As a result, the critical conditions we find here for the homogeneous gas are essentially also valid for the central density of a trapped Bose gas, and in particular pertain also to the $^{87}$Rb and $^{23}$Na experiments.

In the functional formulation of the grand canonical partition function, the action for the dilute Bose system in momentum and frequency space is written as

$$S[a^*, a] = \sum_{k,n} (-i\hbar \omega_n + \epsilon_k - \mu)a_{k,n}^* a_{k,n}$$

$$+ \frac{1}{2\hbar \beta V} \sum_{k,k',q} V_q a_{k+q,n+m}^* a_{k'-q,n'-m} a_{k',n'} a_{k,n} , \quad (1)$$

where $\omega_n = 2\pi n/\hbar \beta \equiv 2\pi nk_B T/\hbar$ are the bosonic Matsubara frequencies, $\epsilon_k = \hbar^2 k^2 / 2m$, $\mu$ is the chemical potential, $V$ is the volume of the system, $V_q = \int d\mathbf{x} V(\mathbf{x}) e^{-i\mathbf{q} \cdot \mathbf{x}}$ is the Fourier transform of the interaction potential, and $a_{k,n}^*$ and $a_{k,n}$ are the Fourier components of the fields $\psi^*(\mathbf{x}, \tau)$ and $\psi(\mathbf{x}, \tau)$, creating respectively annihilating a particle at position $\mathbf{x}$ and (imaginary) time $\tau$. The specific form of the potential $V(\mathbf{x})$ or its corresponding scattering length is in first instance immaterial to the derivation of the RG equations.

The renormalization of the various terms in the effective action is obtained by successively integrating out high momentum shells $d\Lambda$ of infinitesimal width [7]. In the operator language this is equivalent to performing the trace in the grand canonical partition function...
over the most rapidly oscillating one-particle states, and then constructing a new effective Hamiltonian for the less rapidly oscillating states. Technically, this first step of Wilson’s RG transformation boils down to calculating the Feynman diagrams renormalizing the vertices of interest, where the integration over the internal momenta is restricted to the afore-mentioned momentum shell. The type of diagrams contributing to the renormalization when the thickness of the momentum shell $d\Lambda$ is infinitesimal, are the so-called one-loop diagrams only. This follows from the fact that each extra loop introduces an extra factor of $d\Lambda$ \[8\]. The second step in Wilson’s RG transformation consists of a rescaling of the momenta, frequencies and fields such that the original cutoff is restored and the coefficient of $(-i\hbar \omega_n + \epsilon_k) a_{k,n}^* a_{k,n}$ is kept equal to one. If one neglects the renormalizations from the first step, this procedure yields the so-called trivial scaling of the vertices and reveals the relevance of the vertices considered.

In principle, the action in Eq. (1) does not possess a real sharp ultraviolet cutoff $\Lambda$. However, the typical behavior of the Fourier transform of the two-body interaction potential is such that there is an effective ultraviolet cutoff around the momentum scale set by the scattering length $a$ of this potential. Below this value, the Fourier transform is practically momentum independent and equal to $V_0$. As in the Bose systems considered here we always have that $h/a \gg h/\Lambda_{th}$, the momentum range in which the particles in the gas reside falls well below this cutoff. Thus, we represent the interaction potential by the momentum independent value $V_0$ for $q$ less than a cutoff $\Lambda$ of $O(1/a)$ and zero for $q > \Lambda$.

Modelling the potential as described, implies that the nonuniversal properties we find from an RG calculation will in first instance be sensitive to the specific value of the cutoff $\Lambda$ taken in the calculations. However, at this point our knowledge about the microscopic details of the Bose gas comes in to resolve this problem because we know that the two-body interaction potential $V_q$ has to renormalize to the two-body $T$-matrix $T^{2B}((k - k')/2 + q, (k - k')/2; \hbar^2 (k - k')^2/m)$ when we include all possible two-body scattering processes in the vacuum. The two-body $T$-matrix has roughly the same momentum dependence as $V_q$, and is in particular constant and equal to $4\pi a \hbar^2/m$ in the range of thermal momenta and
energies. Thus, given an ultraviolet cutoff $\Lambda$, we can fix the RG equations by demanding that for the two-body problem $V_0$ indeed correctly renormalizes to $4\pi a\hbar^2/m$. Since this value is, due to the inequality $a/\Lambda \ll 1$, already attained before we enter into the thermal regime as we integrate out more and more momentum shells, this indeed leads to a correct description of the properties of the Bose gas which is independent of the ultraviolet cutoff $\Lambda$. Having eliminated the cutoff dependence in this manner, we are then in a position to determine also the nonuniversal properties of the dilute Bose gas such as most notably the critical temperature. Furthermore, we can perform the calculation for any (positive) value of the scattering length, thus being able to describe any atomic species with effectively repulsive $s$–wave scattering. The results we find are therefore relevant to the experiments using $^{87}$Rb, $^{23}$Na, but for instance also for future experiments with $^1$H and other atoms having a positive scattering length.

When deriving the equations governing the renormalization of the various terms in the action, one has to proceed differently, depending on the sign of the chemical potential. For negative chemical potential the derivation of the RG equations is most straightforward as one can start directly from Eq. (1) to obtain the Feynman diagrams. For positive chemical potential the derivation is much more involved since in this case the space and time independent part of the effective action, i.e. $-\mu |a_{0,0}|^2 + V_0 |a_{0,0}|^4 / 2\hbar \beta V$, has a Mexican hat shape and one first has to expand the action around the correct extremum by performing the shift $a_{0,0} \to a_{0,0} + \sqrt{n_0 \hbar \beta V}$ introducing the condensate density $n_0$. Only after that can one find the Feynman diagrams contributing to the renormalization.

We will first focus on the situation of negative chemical potential, and restrict ourselves to operators which are relevant or marginal at the critical temperature. The chemical potential $\mu$ and the two-body interaction term $V_0$ are both relevant there. The vertex $U_0$ from the three-body interaction term, schematically written as $U_0 |\psi(x, \tau)|^6 / 6$ and in principle also present in the Hamiltonian of the system, is marginal, and would thus have to be included in the set of RG equations describing the change or ‘flow’ of the vertices during the process of integrating out momentum shells. However, since we are studying the dilute Bose gas it it
expected that three-body interactions will in general have only an extremely small influence on the properties to be calculated. Only near the critical temperature can there be some effect as at that point all fluctuations become important. This we have checked explicitly by numerically solving the coupled set of RG equations including and excluding the three-body interaction. Indeed, the above argument is corroborated by our findings, which show that the influence of \( U_0 \) on e.g. the density, even in the critical region, is typically smaller than 1% in the regime where \( na^3 \ll 1 \). In the following we will, therefore, neglect the three-body interaction and focus on the renormalization of \( \mu \) and \( V_0 \) only. For negative chemical potential, the RG equations are then given by

\[
\frac{d\mu}{dl} = 2\mu - \frac{\Lambda^3}{\pi^2} V_0 N(\epsilon_\Lambda - \mu) 
\]

\[
\frac{dV_0}{dl} = -V_0 - \frac{\Lambda^3}{2\pi^2} \frac{V_0^2}{\beta N(\epsilon_\Lambda - \mu)} 
\]

\[
- \frac{2\Lambda^3}{\pi^2} V_0^2 \beta N(\epsilon_\Lambda - \mu)[N(\epsilon_\Lambda - \mu) + 1].
\]

At a particular value of \( l \), the region in momentum space that has been integrated out is the shell running from \( |k| = \Lambda e^{-l} \) to \( |k| = \Lambda \). Here, \( N(\epsilon_\Lambda - \mu) = 1/(e^{\beta(\epsilon_\Lambda - \mu)} - 1) \) is the Bose-Einstein distribution function containing \( \epsilon_\Lambda = h^2 \Lambda^2 / 2m \) in its argument since after each step we have rescaled the momenta to retain the cutoff at \( \Lambda \). Furthermore, as a result of this rescaling we have that the temperature scales as \( T(l) = T e^{2l} \). The nontrivial term in Eq. (2a) originates from the sum of the Hartree and Fock diagrams, whereas the nontrivial terms in Eq. (2b) stem from the ladder diagram and the bubble diagram respectively.

Next we consider the case of positive chemical potential. Introducing the condensate density through the shift mentioned above, we generate, next to a linear term proportional to \( (a_{0,0} + a_{0}^*) \), normal and anomalous selfenergies \( \sum_{k,n} (h \Sigma_{11} a_{k,n}^* a_{k,n} + h \Sigma_{12} (a_{k,n}^* a_{-k,-n}^* + a_{k,n} a_{-k,-n})) / 2 \) and the term \( \sum_{k,n} \sum_{q,m} \Gamma_3 (a_{q,m}^* a_{k-q,n-m}^* a_{k,n} + a_{k+q,n+m}^* a_{q,m} a_{k,n}) / \sqrt{n_0 V} \) into the action [4]. In first instance we have, due to the neglect of the three-body interactions, that \( h \Sigma_{11} = 2n_0 V_0 \), \( h \Sigma_{12} = n_0 V_0 \), and \( \Gamma_3 = \sqrt{n_0 V} \). Moreover, the magnitude of the condensate is found by eliminating the linear term in the action, which gives \( n_0 = \mu / V_0 \).
Performing a Bogoliubov transformation to diagonalize the quadratic part of the action facilitates the calculation of the one-loop diagrams contributing to the renormalization of the vertices of interest. One of these corresponds to the linear term in the action. After every step of the RG transformation we have to eliminate this term by performing a shift in $a_{0,0}$ in order to remain in the minimum of the action. Clearly this gives the equation describing the change of the condensate density. Proceeding with the selfenergies, we find that they obey the Hugenholtz-Pines relation $\mu(l) = \hbar \Sigma_{11}(l) - \hbar \Sigma_{12}(l)$ implicite from the $U(1)$ symmetry of the problem \cite{[9]}. As a result, we only have to consider the diagrams contributing to $\hbar \Sigma_{12}$ to obtain the renormalization of the quadratic part of the action. Finally, due to the neglect of the three-body interactions, we have again from $U(1)$ symmetry that $\Gamma_3(l) = \sqrt{n_0(l)V_0(l)}$ and $V_0(l) = \hbar \Sigma_{12}(l)/n_0(l)$. These relations allow the action to be recast into the explicitly $U(1)$ symmetric form of Eq. (1) at any point during renormalization. Consequently, from the RG equations for $\hbar \Sigma_{12}$ and $n_0$, we can deduce the equations describing the flow of the chemical potential $\mu$ and the two-body interaction $V_0$. This leads to

$$\frac{d\mu}{dl} = 2\mu - \frac{\Lambda^3}{2\pi^2} V_0 \left[ \frac{2\epsilon^3_{\Lambda} + 6\mu \epsilon^3_{\Lambda} + \mu^3}{2\hbar^3 \omega^3_{\Lambda}} (2N(\hbar \omega_{\Lambda}) + 1) - 1 \right]$$

$$\frac{dV_0}{dl} = -V_0 - \frac{\Lambda^3}{2\pi^2} V_0^2 \left[ \frac{(\epsilon_{\Lambda} - \mu)^2}{2\hbar^3 \omega^3_{\Lambda}} (2N(\hbar \omega_{\Lambda}) + 1) \right] + \frac{(2\epsilon_{\Lambda} + \mu)^2}{\hbar^2 \omega^2_{\Lambda}} \beta N(\hbar \omega_{\Lambda}) [N(\hbar \omega_{\Lambda}) + 1] \right] \right] ,$$

where the Bose-Einstein distribution function now contains the Bogoliubov dispersion $\hbar \omega_{\Lambda} = \sqrt{\epsilon^2_{\Lambda} + 2\mu \epsilon_{\Lambda}}$. Eqs. (2) and (3) constitute the flow equations in the case of negative and positive chemical potential respectively, and completely describe the system in the dilute gas approximation. Note that both sets coincide when $\mu$ is taken equal to zero, implying that the flow is continuously differentiable, also at $\mu = 0$.

Finally, we have to fix the RG equations as explained above. From Eq. (2b) we recognize that in a vacuum, i.e. $N(\epsilon_{\Lambda} - \mu) = 0$, the renormalization of the interaction between two particles is governed by
\[
\frac{dV_0}{dl} = -V_0 - \frac{\Lambda^3}{2\pi^2} V_0^2 \frac{1}{2(\epsilon_\Lambda - \mu)}.
\]  

(4)

As expected, this is just the differential form of the Lippmann-Schwinger equation for the two-body \(T\)-matrix at energy \(2\mu\), \(T^{2B}(0,0;2\mu)\). As the two-body \(T\)-matrix is energy independent for low energies, we can neglect \(\mu\) and use \(T^{2B}(0,0;2\mu) = 4\pi a \hbar^2 /m\). The requirement is now that, given an ultraviolet cutoff \(\Lambda\), \(V_0\) flows to the value \(4\pi a \hbar^2 /m\). This can be ascertained by choosing the right initial condition for \(V_0\). More precisely, we find from Eq. (4) that \(V_0(l = 0) = 4\pi a \hbar^2 / (m(1 - 2a\Lambda/\pi))\) leads to the correct result. Clearly, we can describe different atomic species by only changing the value of the scattering length \(a\) used in this equation. Note again that this boundary value also assures the correct renormalization of the full RG equations (2)-(3), because the other terms in the right-hand side of these equations are insensitive to the cutoff. Put differently, these terms only start to contribute to the flow in the range of thermal momenta, but at that point \(V_0\) has already correctly renormalized to \(4\pi a \hbar^2 /m\).

Having found the correct boundary conditions, \(\mu(l = 0)\) being the bare chemical potential in Eq. (1), we can now numerically integrate the RG equations. In Fig. 1 we depict the trajectories resulting from these calculations. The temperature is fixed and the bare chemical potential is raised going from a lower curve to a higher curve. We can determine the corresponding density by noting that \(n = n_0 + \sum_{k,n} \langle a^\dagger_{k,n} a_{k,n} \rangle\), which we can also cast into a differential equation yielding the building up of the density as we integrate out more and more momentum shells. The trajectory flowing into the fixed point \((\mu^*,V_0^*)\) corresponds after removal of the trivial scaling to a chemical potential renormalizing exactly to zero, and therefore to a condensate density renormalizing exactly to zero. For values higher than this (positive) bare critical chemical potential we find \(n_0 > 0\), and we are in the condensed phase.

Thus, the critical density of the dilute Bose system is determined by the set Eq. (3). Moreover, we can find the usual critical exponent \(\nu\) pertaining to the divergence of the correlation length as we approach the critical temperature, i.e. \(\xi\) behaves as \(\xi_0 \propto (T - \)
$T_c/T_c \sim \nu$, by linearizing the flow equations around the fixed point and calculating the largest eigenvalue. This gives $\nu = 0.685$, which is to be compared with the value $\nu = 0.67$ found from an $\epsilon$–expansion of the $O(2)$ model [11] and also measured in $^{4}$He experiments. The agreement is surprisingly good, indicating that we are indeed accurately describing the Bose gas with the derived RG equations, also in the critical region.

We now turn to the ultimate goal of this study, namely the effect of interactions on the critical temperature of Bose-Einstein condensation. At fixed temperatures we vary the (bare) chemical potential to find the trajectories flowing into the fixed point. As mentioned above, this yields the critical densities for these specific temperatures and gives us the $n_c-T$ relation. We repeat this for different values of the scattering length to obtain the dependence of the critical temperature on the strength of the interaction. All curves fall on one single curve if we plot the degeneracy parameter $n_c\Lambda_\text{th}^3$ at which Bose-Einstein condensation occurs versus $a/\Lambda_\text{th}$. This curve is depicted in Fig. 2, where we normalized $n_c\Lambda_\text{th}^3$ to the ideal gas value $\zeta(3/2)$. As seen from Fig. 2 we always have that $n_c\Lambda_\text{th}^3 < \zeta(3/2)$, which leads to the conclusion that the critical temperature of the weakly-interacting Bose gas is raised with respect to the ideal gas value, in qualitative agreement with the recent experiments. The main reason for the lower value of $n_c\Lambda_\text{th}^3$ is that at the critical point, the effective chemical potential renormalizes from a positive initial value exactly to zero. Due to the Bogoliubov dispersion, this behavior depresses the occupation of the non-zero momentum states relative to the ideal gas case.

In summary, we have derived renormalization group equations for the dilute Bose gas. Using our knowledge of the two-body scattering problem, we have effectively eliminated the ultraviolet cutoff from our theory, and obtained also information on nonuniversal properties. As such, we have determined the effect of repulsive interactions on the critical temperature of Bose-Einstein condensation, and found that it is raised with respect to the ideal gas value. Preliminary Quantum Monte Carlo calculations seem to confirm this result [11]. From our calculations we predict that for the $^{87}$Rb and $^{23}$Na experiments the critical temperature can be raised with as much as 10 %. This appears to be a very promising result because one
might expect that an effect of this magnitude can very well be measured in future, more accurate, experiments.

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FIGURES

FIG. 1. Flow diagram resulting from the RG equations. The fixed point is indicated with an asterix and its eigenvectors by the dotted lines.

FIG. 2. The normalized critical degeneracy parameter versus $a/\Lambda_{th}$. 
Figure 1.
Figure 2.