Large-\(N\) properties of a non-ideal Bose gas

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Abstract

We rigorously discuss the large-\(N\) thermodynamics of a Bose gas with a short-range two-body potential. Considering the system as a mixture of \(N\) identical components with a symmetric interaction we calculate numerically the temperature dependence of the leading-order corrections to the depletion of the Bose–Einstein condensate and to the isothermal compressibility.

Keywords: \(1/N\) expansion, Bose–Einstein condensation, critical behavior

1. Introduction

The \(1/N\) expansion is known to be a powerful tool in field theory [1] and in condensed matter physics, where it has allowed us to describe the properties of frustrated quantum antiferromagnets [2], strongly coupled low-density quantum gases [3], unitary Fermi superfluids [4], fermions possessing the finite-temperature Stoner instability [5], graphene [6, 7], impurity states in the dilute critical Bose condensate [8], etc. It has also been proven to be a valuable method for the approximate calculations of critical exponents [9]. In the large-\(N\) limit, some field-theoretical [10] and statistic-mechanical [11] models can be solved exactly, and every time the behavior of these systems is non-trivial [12].

Large-\(N\) expansion in the context of Bose system theory was previously used in different variations including summation of diagrams in a particle–hole channel for the Galilean-invariant [13, 14], relativistic [15], and two-component [16] many-boson systems as well as ladder summation of particle–particle diagrams for the normal state Bose gases [17], but a full numerical analysis of the problem at finite temperatures in the Bose condensed phase is lacking. The application of this method to two-dimensional (2D) Bose systems [18] revealed a very interesting phenomenon, namely, the appearance of the thermally stimulated roton minimum in the spectrum of collective excitations. The role of thermal and quantum fluctuations in the formation of thermodynamics of an imperfect Bose gas with various boundary conditions was studied in [19]. Recently, we have demonstrated [20] that the application of this technique to the problem of critical temperature calculation for a Bose gas a with point-like repulsive interaction leads to a result which coincides semi-quantitatively well with that...
of the Monte Carlo simulations [21, 22] in a wide range of the interaction parameter values. The latter observation inspires confidence to use the large-$N$-based theories for studying the finite-temperature thermodynamic properties of a Bose gas not only in the dilute limit.

In the present article, using the large-$N$ expansion method, we calculate the full temperature dependence of the leading-order corrections to the condensate density and isothermal compressibility for a Bose gas with a short-ranged two-body repulsion in the superfluid phase.

2. Model and method

We consider a Bose mixture consisting of $N$ identical components with symmetric zero-range interparticle interaction $\Phi(r) = (g/N)\delta(r) \frac{\partial}{\partial r}$, where the coupling constant is related to the $s$-wave scattering length $a$ and mass of particles $m$ in the following way: $g = 4\pi\hbar^2a/m$. This model, after introducing auxiliary real field $\varphi(x)$ and making use of the Hubbard–Stratonovich transformation, is described by the following imaginary time action [20]:

$$S = \int dx \psi^*_\sigma(x) \{ \partial_\tau - \xi - i\varphi(x) \} \psi_\sigma(x) - \frac{N}{2g} \int dx \varphi^2(x), \quad (1)$$

where $x \equiv (\tau, r)$, $\xi = -\hbar^2\nabla^2/2m - \mu$, $\int dx = \int_{0}^{T} d\tau \int d^3 r$, periodic complex fields $\psi_\sigma(x)$ describe $N$ sorts of Bose particle whose number is controlled by chemical potential $\mu$, and the summation over repeating index $\sigma = 1, 2, \ldots, N$ is implied. As usual, in the symmetry broken phase one singles out the condensates of two fields $\psi_\sigma(x) = \psi_0^0 + \tilde{\psi}_\sigma(x)$, $\varphi(x) = \varphi_0 + \tilde{\varphi}(x)$ with constraints $\int d^3 r \tilde{\psi}_\sigma(x) = \int d^3 r \tilde{\varphi}(x) = 0$ imposed on the fluctuational terms. The steepest-descent method for the grand canonical potential $(\partial\Omega/\partial\varphi_0)\varphi_0 = 0$, $(\partial\Omega/\partial\tilde{\varphi}^\ast_0)\varphi_0 = 0$ fixes the value of $i\tilde{\varphi}_0 = ng\langle n \rangle$ (here $\langle n \rangle$ is the density of each sort of particles) and generates the ‘gap’ equation

$$\mu\psi_0 - ng\psi_0 - i\frac{T}{V} \int dx \langle \tilde{\varphi}(x) \tilde{\psi}_\sigma(x) \rangle = 0, \quad (2)$$

where $T$ is the temperature and $\langle \ldots \rangle$ denotes statistical averaging. The above equation possesses at least two physically distinct solutions. The trivial one $\psi_0 = 0$ describes properties of the system in the high-temperature region, while the second solution determines the chemical potential in the Bose condensed phase.

Action (1) after the shift of fields $\varphi(x), \psi_\sigma(x)$ in the four-momentum space reads

$$S = \sum_p \left\{ \omega_p - \tilde{\xi}_p \right\} \psi^\ast_{\sigma,p} \psi_{\sigma,p} - \frac{N}{2g} \sum_Q |\varphi_Q|^2$$

$$- i \sum_{Q, \sigma} \varphi_Q \left\{ \psi^\ast_0 \psi_{\sigma,-Q} + \psi^\ast_{\sigma,0} \psi^\ast_0 \right\} - i \sqrt{\frac{T}{V}} \sum_{Q, p} \varphi_Q \psi^\ast_{\sigma,p} \psi_{\sigma,p,-Q}, \quad (3)$$

where capital letters denote four-momenta $P \equiv (\omega_p, p \neq 0), Q \equiv (\omega_q, q \neq 0)$ (here $\omega_q, \omega_p$ are bosonic Matsubara frequencies) and $\tilde{\xi}_p \equiv \varepsilon_p - \tilde{\mu}$ with $\varepsilon_p = \hbar^2p^2/2m$ being the free-particle dispersion. We also used notation for the shifted chemical potential $\tilde{\mu} = \mu - ng$.

Action (3) without the last term is a quadratic form over fields $\psi_{\sigma,p}, \varphi_Q$, and the problem of calculation of the appropriate averages $\langle \psi^\ast_{\sigma,p} \psi_{\sigma,p} \rangle, \langle \varphi_Q \psi_{\sigma,-Q} \rangle, \langle \psi^\ast_{\sigma,p} \varphi_Q \rangle$, etc., reduces to the diagonalization of a square matrix of size $2N + 1$. It is important to note that these calculations can be exactly performed in the general case for an arbitrary $N$ with the result
\[
\langle \psi_{\sigma,p}^* \psi_{\sigma',p} \rangle = \frac{\delta_{\sigma,\sigma'}}{\xi_p - i\omega_p} - \frac{1}{N} \frac{\xi_p + i\omega_p}{\xi_p^2 - \omega_p^2 + E_p^2} |\psi_0|^2 g,
\]
\[
\langle \psi_{\sigma,p} \psi_{\sigma',-p} \rangle = -\frac{1}{N} \frac{\psi_0^2 g}{\omega_p^2 + E_p^2},
\]
\[
\langle \psi_{\sigma,p}^* \phi_{-p} \rangle = -i\psi_0 g \frac{\xi_p - i\omega_p}{N} \frac{\xi_p}{\omega_p^2 + E_p^2},
\]
\[
\langle \phi_{-p} \phi_{Q-q} \rangle = g \frac{\omega_p^2 + \xi_p^2}{N} \frac{1}{\omega_q^2 + E_q^2},
\]
where \(\delta_{\sigma,\sigma'}\) is the Kronecker delta. At this stage the formulated approximation is nothing but the celebrated Bogoliubov theory for an \(N\)-component Bose system with symmetric inter- and intra-species interactions and characteristic quasiparticle spectrum \(E_q^2 = \xi_q^2 + 2\xi_q n_0 g\) (where \(n_0 = |\psi_0|^2\)). Furthermore, by setting \(N = 1\) in equations (4) and (5) we recover (up to a sign, of course) the well-known expressions (see, for instance [23]) for the normal and anomalous Green’s functions in the simplest approximation. Inclusion of the last term in the action breaks the exact integrability of the partition function, but in the leading order over the expansion parameter \(1/N\) the result is easily obtained. To do this, one has to replace in the above formulas the bare interaction parameter \(g\) with the density-fluctuation-induced effective potential \(g(Q) \equiv g/[1 + g\Pi(Q)]\), where the polarization operator reads
\[
\Pi(Q) = \frac{T}{V} \sum_p \frac{1}{\xi_p - i\omega_p} \frac{1}{\xi_{[p+q]} - i\omega_{p+q}}.
\]
Additionally, we have to shift \(\xi_p \rightarrow \xi_p + \Sigma^{(1)}(P)/N\) in the denominator of the first term of equation (4) by the \(1/N\) correction to the diagonal element of self-energy (see figure 2) \(\Sigma^{(1)}(P)\), which in our approximation is given by
\[
\Sigma^{(1)}(P) = \frac{T}{V} \sum_Q \frac{g(Q)(\xi_q^2 + \omega_q^2)}{E_q^2(Q) + \omega_q^2} \frac{1}{\xi_{[p+q]} - i\omega_{p+q}}.
\]
where \(E(Q) = E_{Qk \rightarrow \xi(Q)}\). A very important feature of our approximation is that it preserves the Nepomnyashchy–Nepomnyashchy identity [24] for the self-energy of the normal Green’s function. Indeed, taking the limit \(P \rightarrow 0\) in the above self-energy and substituting equation (6) (with the replacement \(g \rightarrow g(Q)\) in the ‘gap’ equation (2) one readily obtains that \(\tilde{\mu} = \Sigma^{(1)}(0)/N\). This guarantees that the one-particle spectrum (which coincides with the spectrum of collective modes in this approximation), in accordance with the Hugengoltz–Pines relation [25], will be gapless in the Bose condensate phase. At high temperatures the quantity \(\Sigma^{(1)}(0)/N - \tilde{\mu}\) is always positive definite and up to the leading order in the expansion over \(1/N\) plays a role of an effective chemical potential that signals the occurrence of the Bose–Einstein condensation (BEC) transition. A very similar parameter appears in extension of the Beliaev techniques [26] on the finite-temperature region. Finally, it should be emphasized that the formulated approach has much in common with the so-called dielectric formalism [27–29] applied to Bose condensed systems, where the analogue of our leading-order \(1/N\) treatment is the celebrated random phase approximation (RPA). However, despite dielectric formalism the large-\(N\) technique allows us to perform controllable approximate calculations.
in terms of a formal dimensionless expansion parameter \(1/N\), which leads to the disparity in results of these two approaches even in the simplest approximation. In particular, a very important self-energy correction (9), which is of order \(1/N\) and renormalizes the one-particle spectrum as well as shifting the critical temperature of an interacting Bose system, is not taken into account in the original RPA. A possible resolution of this problem can be found in various generalizations of the RPA, which were comprehensively studied in [30].

3. Results and discussion

Having calculated correlator (4) up to \(1/N\)-terms we are in a position to obtain the thermodynamic functions and the Bose condensate depletion. The main differences between the large-\(N\) expansion and Bogoliubov’s theory are expected at finite temperatures, especially in the narrow region of the critical point, where developed thermal fluctuations have a profound effect on the behavior of Bose systems.

Both the temperature and interaction-induced depletion of the BEC density of each sort can be calculated in a standard manner:

\[
n_0 = n - \lim_{\tau \to +0} \frac{T}{V} \sum_p e^{i\tau \omega_p} \langle \psi^*_\sigma p \psi_{\sigma, p} \rangle,
\]

where in the adopted approximation we have to substitute \(\langle \psi^*_\sigma p \psi_{\sigma, p} \rangle = (4) - \frac{1}{\pi} \Sigma^{(1)}(p)/(\tilde{\xi}_p - i\omega_p)^2\) (recall \(g \to g(Q)\)) and to replace \(\tilde{\mu} \to 0\) in all the \(1/N\)-terms. Now the condensate disappears at the \(1/N\)-corrected critical temperature

\[
\frac{T_c}{T_0} = 1 + \frac{1}{N} f^{(1)}(an^{1/3}) + \ldots,
\]
where $T_0$ is the BEC transition temperature of the ideal Bose gas and function $f(1)(an^{1/3})$ is calculated in [20]. The numerical computations of the temperature dependence of $n_0$ (see figure 3) in dimensionless units $t = T/T_c$ (here $T_c$ already takes into account shift (11)) were performed at $N = 1$ and for three values of the gas parameter, namely $an^{1/3} = 0.01, 0.125,$ and $0.345$. The last two correspond to the maximum of the critical temperature shift and to the value where it becomes zero again [20], respectively. Note that in the case of a dilute Bose gas when $an^{1/3} = 0.01$ we found a satisfactory agreement (see inset) with the results of the essentially exact Monte Carlo simulations [26]. From the obtained graphical dependences of the condensate density the general tendency is clearly viewed: the increase of the two-body interaction lifts the condensate curve rescaled on the ground-state (Bogoliubov’s in our case) value above the ideal gas result. This conclusion of the large-$N$ approach should be compared with various finite-temperature self-consistent beyond-Bogoliubov treatments [31–35] and numerical approaches [36]. Moreover, a recent experimental test of the Bogoliubov ground-state depletion [37] gives us hope for forthcoming verification of our finite-temperature results. The distinct feature of the $1/N$ expansion is that it possesses non-trivial critical behavior. In particular, it is easy to show by analyzing the zero Matsuraba frequency term in equation (10) that the condensate depletion demonstrates a logarithmic non-analyticity in the close vicinity of the BEC transition temperature $T_c$

$$n_0/n \propto \delta t - \frac{4}{N\pi^2} \delta t \ln \delta t + \ldots$$

(12)

(here $\delta t = \frac{T - T_c}{T_c}$), where the universal power-law behavior of the order parameter $\psi_0 \sim (\delta t)^\beta$ is clearly visible. Of course, the exponent $\beta = 1/2 - 2/(N\pi^2) \rightarrow 0.2973 \ldots$ calculated here reproduces the large-$N$ result of [38], but is far from the values of $0.3485(2)$ [39] and $0.3486(1)$ [40] obtained for a single-component Bose system’s universality class in the Monte Carlo simulations. These findings, however, together with the value of the Fisher exponent $\eta = 4/(3N\pi^2)$ [8, 41] obtained with the same accuracy, determine the critical behavior of the three-dimensional Bose system in the large-$N$ limit.
In the present article we also focus on the derivation of the $1/N$ correction to inverse susceptibility $(\partial \mu^{(1)}/\partial n)_T$ of the Bose gas in the condensed phase rescaled on the zero-temperature (Lee–Huang–Yang) result $16g\sqrt{na^3/\pi}$. Dotted and dashed lines correspond to the values of the gas parameter $an^{1/3} = 0.125$ and $an^{1/3} = 0.345$, respectively. The inset shows the result for the dilute limit $an^{1/3} = 0.01$.

In the present article we also focus on the derivation of the $1/N$ correction to inverse susceptibility $(\partial \mu^{(1)}/\partial n)_T$. This quantity determines the first sound velocity $c_2 = n/m(\partial \mu/\partial n)_T$ in the Bose condensate and can be measured in the appropriate experiments. The simplest way to deal with the problem of its calculation in the Bose-condensed phase is to obtain the beyond-mean-field correction to the chemical potential with the use of equation (2) (or equivalently equation (9)),

$$\mu = ng + \mu^{(1)}/N,$$

where the $1/N$ shift is given by

$$\mu^{(1)} = \frac{T}{V} \sum_Q \left( \frac{g(Q)e_q}{E^2(Q) + \omega^2_q} - \frac{g\epsilon_q}{E^2_q + \omega^2_q} \right) + \frac{1}{2V} \sum_{q\neq0} g \left( \frac{\epsilon_q}{E_q} - 1 \right) + \frac{1}{V} \sum_{q\neq0} g\epsilon_q n(E_q/T)$$

(here $n(x) = 1/(e^x - 1)$ is the Bose distribution and we singled out standard Bogoliubov corrections (last two terms) explicitly), and then to evaluate straightforwardly the derivative with respect to $n$.

The results of numerical calculations for function $\kappa^{(1)}(t) (t = T/T_c)$ determining the temperature dependence of the compressibility $(\partial \mu/\partial n)_T = g \left[ 1 + \frac{16}{N} \sqrt{\frac{na^3}{\pi}} \kappa^{(1)}(t) \right]$ are presented in figure 4. In order to compare regimes of various coupling strengths we have chosen the same values of the gas parameter as previously used for the condensate calculations. From general arguments it becomes clear that the temperature effects should be more visible in the behavior of the sound velocity of a dilute Bose gas, while in the case of intermediate interaction strength the compressibility is less sensitive to the temperature changes due to the increasing role of phonon excitations. These intuitive conclusions are confirmed by direct numerical
computations, and the general tendency of the obtained curves is in qualitative agreement with
the observed temperature behavior of the first sound velocity in liquid $^4$He [42]. As is seen
from figure 4 the calculated isothermal compressibility is finite at $T_c$, but one can easily show
that, like the condensate depletion (12), its leading-order temperature dependence is log-linear
in the vicinity of the critical point. Obviously this is a hint of a universal power-law behavior
of the inverse susceptibility close to the BEC transition temperature.

4. Conclusions

In summary, by means of the $1/N$ expansion we studied the thermodynamic properties of a
Bose gas in the condensed phase. At absolute zero this approach in the simplest approximation
recovers the well-known results for thermodynamics of a weakly interacting Bose gas, but
the presence of a formal small parameter, namely the inverse number of components, allows
us to perform controllable calculations not only in the dilute limit. The main differences of
our consideration in comparison with the conventional Bogoliubov theory were found in the
finite-temperature region, where the large-$N$ expansion provided the qualitatively correct shift
of the Bose–Einstein condensation critical temperature, changed the order of the phase trans-
ition, and generally impacted crucially on the thermodynamics of the system. In particular,
working in the first order over the expansion parameter we determined the full temperature
dependence of the condensate density for a Bose system with point-like repulsion. By varying
interparticle interaction we were able to cover both the dilute limit and the case of interme-
diate couplings. The temperature behavior of the Bose condensate calculated in the present
article is in qualitative agreement with the dependence of the condensate fraction in superfluid
helium observed in the Monte Carlo simulations (see, for instance [43]). The evaluation of
the inverse susceptibility revealed a natural tendency for the sound velocity to become less
sensitive to the thermal effects with increasing strength of the repulsive two-body potential.
The proposed approach, after some modifications, can be used to describe a recent experiment
[44], which has made available measurements of the finite-temperature behavior of sound
velocity in a uniform 2D Bose gas. Finally, it was also shown that the large-$N$ expansion was
able to capture the correct temperature dependence of basic thermodynamic functions of Bose
condensates both in the low-temperature limit and in the narrow region of the critical point.

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