

Thermal field theory of bosonic gases with finite-range effective interaction

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We study a dilute and ultracold Bose gas of interacting atoms by using an effective field theory which takes into account the finite-range effects of the interatomic potential. Within the formalism of functional integration from the grand canonical partition function, we derive beyond-mean-field analytical results which depend on both the scattering length and the effective range of the interaction. In particular, we calculate the equation of state of the bosonic system as a function of these interaction parameters both at zero and finite temperature including one-loop Gaussian fluctuation. In the case of zero-range effective interaction, we explicitly show that, due to quantum fluctuations, the bosonic system is thermodynamically stable only for very small values of the gas parameter. We find that a positive effective range above a critical threshold is necessary to remove the thermodynamical instability of the uniform configuration. Remarkably, also for relatively large values of the gas parameter, our finite-range results are in quite good agreement with recent zero-temperature Monte Carlo calculations obtained with hard-sphere bosons.

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I. INTRODUCTION

The experimental achievement of Bose-Einstein condensation with dilute and ultracold alkali-metal atoms [1–3] has triggered many theoretical investigations of weakly interacting Bose gases. The key theoretical tool for the description of these bosonic systems at zero temperature is the Gross-Pitaevskii equation [4], where the nonlocal interatomic interaction is approximated by a local contact interaction characterized by only one physical parameter, the s -wave scattering length a_s . Also, quantum and thermal fluctuations have been analyzed within this contact approximation of the interatomic potential (see, for instance, Refs. [5–10]), which can be interpreted as a zero-range effective field theory (EFT) of the dilute Bose gas [8,11,12]. In the last years the EFT approach to the Bose gas has been extended including finite-range effects due to the effective range r_s of the interaction potential. It has been shown that this approach gives a modified Gross-Pitaevskii equation [13–19] for the condensate and nonuniversal effects for quantum fluctuations at zero temperature [8,11,12,15].

In this paper, by using finite-temperature functional integration [9,20], we show that with a zero-range repulsive interaction, the uniform configuration of the Bose gas becomes thermodynamically unstable at large values of the gas parameter due to Gaussian quantum fluctuations. This puzzling problem is solved by including the effects of the effective range r_s of the interaction potential. In particular, we derive the beyond-mean-field (one-loop, Gaussian) equation of state of the bosonic system at zero temperature. This equation of state (see also Refs. [8,11]) depends on both the scattering length a_s and the effective range r_s of the interaction. We prove that a positive effective range r_s above a critical threshold ($r_s/a_s > 0.25$) is necessary to remove the thermodynamical instability of the uniform configuration for large values of the gas parameter. In the case of a hard-core interaction potential, where $r_s/a_s = 2/3$, our EFT results for the ground-state energy are in quite good agreement with zero-temperature Monte Carlo calculations [21]. Finally,

we include thermal fluctuations and obtain analytically a finite-temperature equation of state which is reliable at low temperatures.

II. PARTITION FUNCTION OF THE SYSTEM

In the study of the interacting Bose gas, we adopt the path integral formalism, where bosonic atoms are described by a complex field $\psi(\mathbf{r}, \tau)$. Within this framework, all the relevant thermodynamical properties of the system can be computed starting from the grand canonical partition function \mathcal{Z} at finite temperature [20]

$$\mathcal{Z} = \int \mathcal{D}[\psi, \psi^*] \exp\left(-\frac{S[\psi, \psi^*]}{\hbar}\right), \quad (1)$$

where

$$S[\psi, \psi^*] = \int_0^{\hbar\beta} d\tau \int d^3\mathbf{r} \mathcal{L}(\psi, \psi^*) \quad (2)$$

is the Euclidean action and $\beta \equiv 1/(k_B T)$ with k_B being the Boltzmann's constant. The grand potential Ω , as a function of the chemical potential μ and the temperature T , can be obtained by [20]

$$\Omega = -\frac{1}{\beta} \ln \mathcal{Z}. \quad (3)$$

By working in the grand canonical ensemble, the nonlocal Lagrangian density of interacting identical bosons is given by

$$\begin{aligned} \mathcal{L} = & \psi^*(\mathbf{r}, \tau) \left[\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} - \mu \right] \psi(\mathbf{r}, \tau) \\ & + \frac{1}{2} \int d^3\mathbf{r}' |\psi(\mathbf{r}', \tau)|^2 V(|\mathbf{r} - \mathbf{r}'|) |\psi(\mathbf{r}, \tau)|^2, \end{aligned} \quad (4)$$

where $V(|\mathbf{r} - \mathbf{r}'|)$ is the spherically-symmetric two-body interaction potential between bosons.

III. ZERO-RANGE EFFECTIVE POTENTIAL

In order to get analytical results, several authors showed that it is worthwhile to replace the interatomic potential with a pseudopotential which must reproduce low-energy scattering properties and energy shifts of the original one [12]. Dealing with ultracold and dilute atoms, the usual, and most simple, scheme consists in replacing $V(r)$ with the zero-range Fermi pseudopotential $V_{p,0}(r) = g_0 \delta^{(3)}(r)$, where $\delta^{(3)}(r)$ is the Dirac delta function. Clearly, the Fourier transform $\tilde{V}_{p,0}(q)$ of $V_{p,0}(r)$ reads

$$\tilde{V}_{p,0}(q) = g_0, \quad (5)$$

where g_0 is given, from scattering theory, by $g_0 = 4\pi\hbar^2 a_s/m$ with a_s the s -wave scattering length [6,8]. Consequently, the Lagrangian density becomes

$$\mathcal{L} = \psi^*(\mathbf{r}, \tau) \left[\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} - \mu \right] \psi(\mathbf{r}, \tau) + \frac{1}{2} g_0 |\psi(\mathbf{r}, \tau)|^4, \quad (6)$$

$$\mathbf{M}(Q) = \beta \begin{pmatrix} -i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + 2g_0\psi_0^2 & g_0\psi_0^2 \\ g_0\psi_0^2 & i\hbar\omega_n + \frac{\hbar^2 q^2}{2m} - \mu + 2g_0\psi_0^2 \end{pmatrix}. \quad (9)$$

Integrating over the bosonic fields $\tilde{\eta}(Q)$ and $\tilde{\eta}^*(Q)$, we obtain the Gaussian grand potential

$$\begin{aligned} \Omega_g &= \frac{1}{2\beta} \sum_Q \ln \text{Det}[\mathbf{M}(Q)] \\ &= \frac{1}{2\beta} \sum_{\mathbf{q}} \sum_{n=-\infty}^{+\infty} \ln [\beta^2 (\hbar^2 \omega_n^2 + E_{\mathbf{q}}^2)], \end{aligned} \quad (10)$$

where $E_{\mathbf{q}}$ is the dispersion relation:

$$E_{\mathbf{q}}(\mu, \psi_0) = \sqrt{\left(\frac{\hbar^2 q^2}{2m} - \mu + 2g_0\psi_0^2 \right)^2 - g_0^2 \psi_0^4}. \quad (11)$$

The sum over bosonic Matsubara frequencies gives [8]

$$\frac{1}{2\beta} \sum_{n=-\infty}^{+\infty} \ln [\beta^2 (\hbar^2 \omega_n^2 + E_{\mathbf{q}}^2)] = \frac{E_{\mathbf{q}}}{2} + \frac{1}{\beta} \ln (1 - e^{-\beta E_{\mathbf{q}}}), \quad (12)$$

and, in this way, taking into account Eq. (6) one finds the grand potential [8–10]

$$\Omega(\mu, \psi_0) = \Omega_0(\mu, \psi_0) + \Omega_g(\mu, \psi_0) + \Omega_g^{(T)}(\mu, \psi_0), \quad (13)$$

where

$$\Omega_0(\mu, \psi_0) = \left(-\mu \psi_0^2 + \frac{1}{2} g_0 \psi_0^4 \right) L^3 \quad (14)$$

is the mean-field contribution (assuming a real ψ_0) with L^3 the volume of the system,

$$\Omega_g^{(0)}(\mu, \psi_0) = \frac{1}{2} \sum_{\mathbf{q}} E_{\mathbf{q}}(\mu, \psi_0) \quad (15)$$

The mean-field (saddle-point) plus Gaussian (one-loop) approximation is obtained setting

$$\psi(\mathbf{r}, \tau) = \psi_0 + \eta(\mathbf{r}, \tau) \quad (7)$$

and expanding the action $S[\psi, \psi^*]$ of Eq. (2) around the uniform and constant ψ_0 up to quadratic (Gaussian) order in $\eta(\mathbf{r}, \tau)$ and $\eta^*(\mathbf{r}, \tau)$. We find that in the momentum space, the Gaussian contribution of quantum fluctuation is described by

$$S_g[\tilde{\eta}, \tilde{\eta}^*] = \frac{1}{2} \sum_Q (\tilde{\eta}^*(Q), \tilde{\eta}(-Q)) \mathbf{M}(Q) \begin{pmatrix} \tilde{\eta}(Q) \\ \tilde{\eta}^*(-Q) \end{pmatrix}, \quad (8)$$

where $Q = (\mathbf{q}, i\omega_n)$ is the $3 + 1$ vector denoting the momenta \mathbf{q} and bosonic Matsubara frequencies $\omega_n = 2\pi n/(\beta\hbar)$. The matrix $\mathbf{M}(Q)$ is the inverse fluctuation propagator, given by the following:

is the zero-point energy of bosonic excitations, i.e., the zero-temperature contribution of quantum Gaussian fluctuations, while

$$\Omega_g^{(T)}(\mu, \psi_0) = \frac{1}{\beta} \sum_{\mathbf{q}} \ln (1 - e^{-\beta E_{\mathbf{q}}(\mu, \psi_0)}) \quad (16)$$

takes into account thermal Gaussian fluctuations.

Imposing the crucial condition

$$\frac{\partial \Omega_0(\mu, \psi_0)}{\partial \psi_0} = 0, \quad (17)$$

one gets

$$\psi_0(\mu) = \sqrt{\frac{\mu}{g_0}} \quad (18)$$

and the well-known Bogoliubov spectrum of collective excitations

$$E_{\mathbf{q}}(\mu) = \sqrt{\frac{\hbar^2 q^2}{2m} \left(\frac{\hbar^2 q^2}{2m} + 2\mu \right)}. \quad (19)$$

Remarkably, the spectrum is now gapless as required by the Goldstone theorem. Now, one can replace ψ_0 with its classical value given by Eq. (18) and, after removing the ultraviolet divergence (for a detailed review see Ref. [10]) in $\Omega_g^{(0)}(\mu) = \Omega_g^{(0)}(\mu, \psi_0(\mu))$, the zero temperature grand potential becomes

$$\Omega_g^{(0)}(\mu) = \frac{8}{15\pi^2} \left(\frac{m}{\hbar^2} \right)^{3/2} \mu^{5/2}. \quad (20)$$

The pressure $P(\mu)$ of the system is simply related to the grand potential $\Omega(\mu)$ by the formula

$$P(\mu) = -\frac{\Omega(\mu)}{L^3}. \quad (21)$$

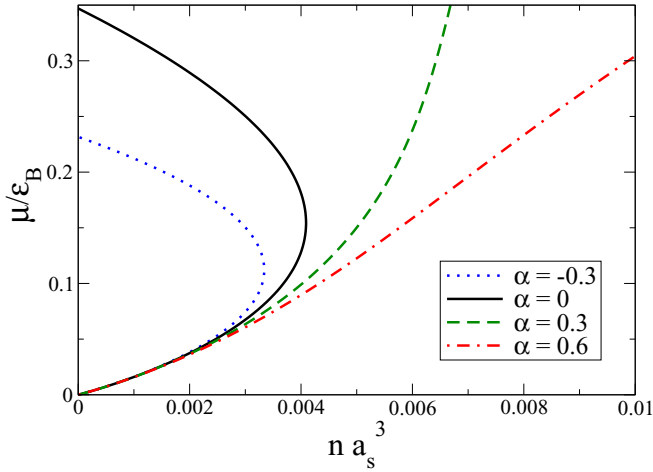


FIG. 1. Chemical potential μ vs gas parameter na_s^3 obtained with beyond-mean-field (Gaussian) EFT, Eq. (42), for different values of the adimensional ratio $\alpha = 2r_s/a_s$. Here, $\epsilon_B = \hbar^2/(ma_s^2)$ is the characteristic energy of the interacting Bose gas, a_s is the s -wave scattering length, r_s is the effective range, and n is the number density.

At zero temperature, the beyond-mean-field pressure $P(\mu)$ as a function of the chemical potential μ is then given by

$$P(\mu) = \frac{\mu^2}{2g_0} - \frac{8}{15\pi^2} \left(\frac{m}{\hbar^2}\right)^{3/2} \mu^{5/2}, \quad (22)$$

and it agrees with the result derived in 1960 by Lee and Yang [22] within the framework of quantum statistical mechanics. Equation (22) has been also obtained in Ref. [23] by using a functional approach. It is important to stress that the pressure P given by Eq. (22) becomes negative, i.e., unphysical, for a large value of the chemical potential μ . Actually, the uniform configuration is thermodynamically stable if and only if

$$\frac{\partial^2 P(\mu)}{\partial \mu^2} > 0. \quad (23)$$

Equation (22) implies thermodynamical instability for $\mu > \mu_c = \pi(\hbar^2/(2m))^{3/4}/\sqrt{2g_0}$.

The zero-temperature number density n can be derived from the grand potential by using this thermodynamic formula

$$n(\mu) = -\frac{\partial \Omega(\mu)}{\partial \mu}, \quad (24)$$

which gives

$$n(\mu) = \frac{\mu}{g_0} - \frac{4}{3\pi^2} \left(\frac{m}{\hbar^2}\right)^{3/2} \mu^{3/2}. \quad (25)$$

From this equation one can easily numerically determine μ as a function of na_s^3 . The result is the solid line of Fig. 1. The plot clearly shows that in the absence of finite-range corrections the chemical potential has two branches and there are no solutions above a critical value of the gas parameter na_s^3 . This result, which is full consistent with the discussion of Eq. (23), means that for $na_s^3 > 0.004$ the uniform configuration does not exist anymore.

We observe that a simple analytical result is obtained from Eq. (25) by using a perturbative expansion where $g_0 n \ll \mu$. In

this way, one gets

$$\mu(n) = g_0 n + \frac{4g_0}{3\pi^2} \left(\frac{m}{\hbar^2}\right)^{3/2} (g_0 n)^{3/2}. \quad (26)$$

The first term of this chemical potential was derived by Bogoliubov [24], while the second term is the one deduced by Lee, Huang, and Yang [25]. However, it is extremely important to remind that Eq. (26) is obtained assuming a very small gas parameter na_s^3 (perturbative scheme above mean-field plus Gaussian results) and it cannot be used when the system is thermodynamically unstable according to the general equation Eq. (25). Close to the instability, the contribution of Gaussian fluctuations to the grand potential, given by Eq. (20), becomes of the same order of the mean-field term; this signals that quantum fluctuations are strong enough to destabilize the uniform configuration. The critical value $(na_s^3)_c \simeq 0.004$ specifies the upper threshold of applicability of the zero-range Gaussian theory and, consequently, of Eq. (26). We shall now show that the inclusion of an effective-range interaction in the thermodynamics can remove the instability by assuring a positive sign of the second derivative of the pressure.

IV. FINITE-RANGE EFFECTIVE POTENTIAL

An improvement of the contact (zero-range) approximation can be achieved by replacing the interaction potential $\tilde{V}(\mathbf{q})$ with the finite-range pseudopotential

$$\tilde{V}_{p,2}(q) = g_0 + g_2 q^2. \quad (27)$$

The relation with the true interatomic potential appearing in Eq. (4) is given by the following relations:

$$g_0 = \tilde{V}(0) = \int d^3\mathbf{r} V(r) \quad (28)$$

and

$$g_2 = \frac{1}{2} \tilde{V}''(0) = -\frac{1}{6} \int d^3\mathbf{r} r^2 V(r), \quad (29)$$

where $\tilde{V}(\mathbf{q}) = \int d^3\mathbf{r} \exp(i\mathbf{q} \cdot \mathbf{r}) V(r)$. It has been shown [12,15] that, in real space, the pseudopotential in (27) is given by

$$V_p(r) = g_0 \delta(r) - \frac{g_2}{2} [\overleftarrow{\nabla}^2 \delta(r) + \delta(r) \overrightarrow{\nabla}^2]. \quad (30)$$

The connection with experimental quantities such as the s -wave scattering length a_s and the s -wave effective range r_s can be established by requiring the matching between the expansion parameters of Eq. (27) and the ones obtained by a more general pseudopotential $V_p(q)$. Several authors [8,11,12] adopt

$$\tilde{V}_p(q) = \frac{4\pi\hbar^2 \tan[\delta_0(q)]}{m q}, \quad (31)$$

which depends on the s -wave phase shift $\delta_0(q)$. Notice that $\delta_0(q)$ is related to the scattering length a_s and the effective range r_s by the equation

$$\delta_0(q) = \arctan\left(\frac{1}{-\frac{1}{a_s} + \frac{1}{2}r_s q^2 + O(q^4)}\right). \quad (32)$$

One can expand $\tilde{V}_p(q)$ and $\delta_0(q)$, respectively, Eq. (31) and Eq. (32), up to the second order for small q . In this way, one finds that the coupling constants g_0 and g_2 are related to the physical parameters a_s and r_s according to

$$g_0 = \frac{4\pi\hbar^2}{m}a_s, \quad (33)$$

which is a well-known relation, and

$$g_2 = \frac{2\pi\hbar^2}{m}a_s^2r_s. \quad (34)$$

By using the pseudopotential in Eq. (27) the nonlocal Lagrangian density given by Eq. (4) becomes

$$\begin{aligned} \mathcal{L} = & \psi^*(\mathbf{r}, \tau) \left[\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} - \mu \right] \psi(\mathbf{r}, \tau) \\ & + \frac{g_0}{2} |\psi(\mathbf{r}, \tau)|^4 - \frac{g_2}{2} |\psi(\mathbf{r}, \tau)|^2 \nabla^2 |\psi(\mathbf{r}, \tau)|^2. \end{aligned} \quad (35)$$

This is the finite-range effective field theory (EFT) we shall use in the remaining part of the paper. Gaussian (one-loop) results of Eq. (35) have been obtained in Refs. [8,11,12], but mainly in the perturbative regime within one-loop calculations and at zero temperature. Here we explicitly prove that, working in regions where the gas parameter is small, the inclusion of the effective-range term can remove the instability of the zero-range theory. Moreover, we compare our EFT calculations with Monte Carlo data and analyze also finite-temperature effects.

By using the Lagrangian density derived in Eq. (35) in the Eq. (2), the stationary Gross-Pitaevskii equation for the space-dependent field $\psi_0(\mathbf{r})$ can be derived by means of the saddle-point approximation

$$\delta S[\psi_0^*(\mathbf{r}), \psi_0(\mathbf{r})] = 0, \quad (36)$$

which leads to

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + g_0 |\psi_0(\mathbf{r})| - g_2 \nabla^2 |\psi_0(\mathbf{r})|^2 \right] \psi_0(\mathbf{r}) = \mu \psi_0(\mathbf{r}). \quad (37)$$

Equation (37) was derived for the first time in Ref. [15] for a Bose gas under external confinement. In this case, simulations based on Eq. (37) leads to a better agreement with Quantum Monte Carlo data concerning, for example, the ground-state energy [15]. Moreover, by using Eq. (37) it is possible to study, also in the absence of an external confining potential, how space dependent topological solutions, such as vortex and solitons, are affected by this effective-range expansion [19].

As in the previous section, in the remaining part of the paper we adopt the shift of Eq. (7) and expand the action $S[\psi, \psi^*]$ of Eq. (2) around a uniform and stationary ψ_0 up to quadratic (Gaussian) order in $\eta(\mathbf{r}, \tau)$ and $\eta^*(\mathbf{r}, \tau)$, but now using (35) instead of (6). Formally, we find again Eqs. (13)–(16) for the grand potential Ω but now the dispersion relation reads

$$\begin{aligned} E_q(\mu, \psi_0) = & \left\{ \left[\frac{\hbar^2 q^2}{2m} - \mu + \psi_0^2 (g_0 + \tilde{V}_{p,2}(q)) \right]^2 \right. \\ & \left. - \psi_0^4 \tilde{V}_{p,2}(q)^2 \right\}^{1/2}. \end{aligned} \quad (38)$$

By using Eqs. (17) and (18) to remove the dependence on ψ_0 in E_q , we obtain

$$E_q(\mu) = \sqrt{\frac{\hbar^2 q^2}{2m} \left((1 + \chi\mu) \frac{\hbar^2 q^2}{2m} + 2\mu \right)}, \quad (39)$$

where

$$\chi = \frac{4m}{\hbar^2} \frac{g_2}{g_0} \quad (40)$$

takes into account finite-range effects of the interatomic potential.

A. Zero-temperature results

The zero-temperature Gaussian grand potential $\Omega_g^{(0)}(\mu)$, given by Eq. (15), is ultraviolet divergent with $E_q(\mu)$ given by Eq. (39). However, this divergence can be regularized with dimensional regularization [26]. For a recent review of this and other regularization methods applied to the dilute and ultracold atomic systems, one can see Ref. [10]. In this way, we find

$$\frac{\Omega_g^{(0)}}{L^3} = \frac{8}{15\pi^2} \left(\frac{m}{\hbar^2} \right)^{3/2} \frac{\mu^{5/2}}{(1 + \chi\mu)^2}. \quad (41)$$

The zero-temperature number density n is obtained by using the number equation (24) with Ω given by Eq. (13) with Eqs. (14), (15), and (41). We obtain

$$\begin{aligned} n(\mu) = & \frac{\mu}{g_0} - \frac{4}{3\pi^2} \left(\frac{m}{\hbar^2} \right)^{3/2} \frac{\mu^{3/2}}{(1 + \chi\mu)^2} \\ & + \frac{64}{15\pi^2} \left(\frac{m}{\hbar^2} \right)^{5/2} \frac{g_2}{g_0} \frac{\mu^{5/2}}{(1 + \chi\mu)^3}. \end{aligned} \quad (42)$$

From this equation, we determine μ as a function of na_s^3 for different values of χ at fixed density n . The results are shown in Fig. 1, where α is proportional to the ratio g_2/g_0 in adimensional units, namely,

$$\alpha = \frac{\hbar^2}{ma_s^2} \chi = 4 \frac{g_2}{g_0 a_s^2} = 2 \frac{r_s}{a_s}. \quad (43)$$

As previously discussed, Fig. (1) clearly shows that in the absence of finite-range corrections ($\alpha = 0$) the chemical potential μ versus n has no solutions above the critical value 0.004 of the gas parameter na_s^3 . This problem is indeed solved by using a positive value of α larger than about 0.25, while for $\alpha < 0$ the problem gets worse. The different behavior of numerical solutions of Eq. (42) for $\alpha \neq 0$ compared to Eq. (25) (equivalent to $\alpha = 0$ case) can be understood thanks to modified dependence from μ of Eq. (41): for $\alpha \gtrsim 0.25$, the finite-range Gaussian correction never becomes of the same order, or bigger, of the mean-field term. Differently from the zero-range case, the finite-range correction manages to control the growth of fluctuations and it stabilizes the system, as highlighted by the dashed and dashed-dotted lines in Fig. 1; for these values of α , there is no critical value of the gas parameter.

It is interesting to compare it with quantum Monte Carlo (QMC) data obtained for a Bose gas of hard spheres by using the path-integral ground-state method [21], as done in Fig. 2. In the case of hard spheres, the s -wave scattering length a_s and effective range r_s are related by $r_s/a_s = 2/3$ (see, for

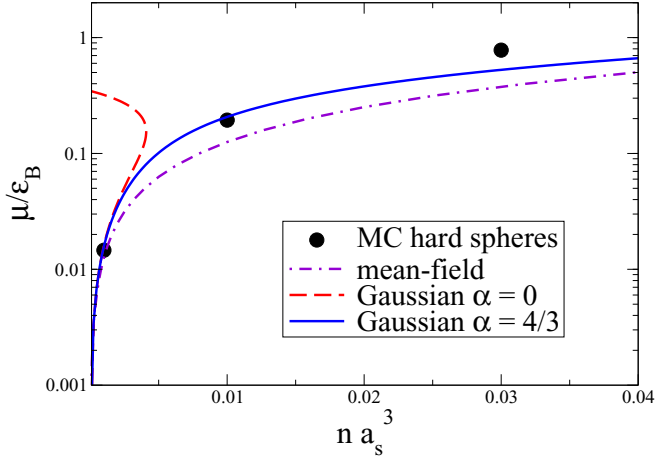


FIG. 2. Monte Carlo (MC) data (filled circles) of the chemical potential μ vs gas parameter na_s^3 for a Bose gas of hard spheres [21]. Dot-dashed line is the mean-field theory, $\mu = 4\pi\hbar^2 a_s n/m$. Solid and dashed lines are the results of our zero-temperature Gaussian EFT, Eq. (42), for two different values of the effective-range adimensional parameter $\alpha = 2r_s/a_s$. The case $\alpha = 0$ corresponds to usual scheme with a zero-range interaction while $\alpha = 4/3$ correspond to the case of a hard-core interaction potential. Also here $\epsilon_B = \hbar^2/(ma_s^2)$ is the characteristic energy of the interacting Bose gas, a_s is the s -wave scattering length, r_s is the effective range, and n is the number density.

instance, Refs. [15,16,19]). The adimensional parameter α , Eq. (43), of our theory must be $\alpha = 4/3$ in order to model the hard-sphere Bose gas. The figure shows that the Monte Carlo data (filled circles) are reproduced reasonably well by our EFT with $\alpha = 4/3$ (solid line) also for quite large values of the gas parameter na_s^3 . So, by including the finite-range Gaussian corrections in Eq. (42), we are able to recover the zero-range results, which is reliable at very low values na_s^3 and surely not above $na_s^3 \simeq 0.004$, but we can reproduce the QMC data for a more dense system. The range of applicability of our finite-range theory is of the order shown in the horizontal axis of Fig. 2.

QMC simulations are performed with a hard-core potential, which has a finite range. Our theory, at a Gaussian level, introduces an effective range r_s whose relation with the scattering length a_s of the hard-core potential is $r_s = (2/3)a_s$. In the case of the hard-core potential, at fixed scattering length a_s (and consequently at fixed effective range r_s), by increasing the gas parameter na_s^3 one increases the density n and, at the same time, the average distance $d \simeq n^{-1/3}$ between atoms reduces. In this way, d becomes comparable with the effective range r_s and finite-range effects of the interatomic potential are then sizable.

We stress that, at two-loop level (next-to-Gaussian), the correction to energy density proportional to na_s^3 is characterized by an unknown coefficient which cannot be specified in the zero-range framework [27]. This coefficient can be expressed in terms of the s -wave scattering length and a three-body coupling not easy to determine experimentally. It is remarkable that, at least for alkali atoms, second-order quantum corrections are proportional to the logarithm of an additional length scale fixed by the van der Waals interaction.

B. Finite-temperature results

The finite-temperature one-loop contribution to the equation of state is obtained from $\Omega_g^{(T)}(\mu)$, which can be written as

$$\frac{\Omega_g^{(T)}(\mu)}{L^3} = -\frac{1}{6\pi} \int_0^\infty dq q^3 \frac{dE_q}{dq} \frac{1}{e^{\beta E_q(\mu)} - 1}. \quad (44)$$

Introducing the variable $x = \beta E_q(\mu)$, we get

$$\frac{\Omega_g^{(T)}(\mu)}{L^3} = -\frac{1}{6\pi^2\beta} \int_0^\infty dx q(x,\mu)^3 \frac{1}{e^x - 1}, \quad (45)$$

where $q(x,\mu)$ is given by

$$q(x,\mu) = \sqrt{\frac{2m\mu}{\hbar^2(1+\chi\mu)}} \sqrt{-1 + \sqrt{1 + \frac{(1+\chi\mu)x^2}{\mu^2\beta^2}}}. \quad (46)$$

Expanding this expression at low temperature T , we find

$$\frac{\Omega_g^{(T)}(\mu)}{L^3} = -\frac{\pi^2}{90} \left(\frac{m}{\hbar^2}\right)^{3/2} \frac{(k_B T)^4}{\mu^{3/2}} \left(1 - \frac{5\pi^2}{7} (k_B T)^2 \frac{1+\chi\mu}{\mu^2}\right), \quad (47)$$

and the finite-temperature contribution $n_g^{(g)}$ to the total number density n reads

$$n_g^{(T)}(\mu) = -\frac{\pi^2}{60} \left(\frac{m}{\hbar^2}\right)^{3/2} \frac{(k_B T)^4}{\mu^{5/2}} \left(1 - \frac{5\pi^2}{21} (k_B T)^2 \frac{7+5\chi\mu}{\mu^2}\right). \quad (48)$$

Thus, within the perturbative expansion approach ($|\mu - g_n| \ll 1$) previously discussed, the finite-temperature equation of state reads

$$\mu(n) = \mu_0(n) + \mu_g^{(0)}(n) + \mu_g^{(T)}(n), \quad (49)$$

where $\mu_0(n) + \mu_g^{(0)}(n)$ is given by Eq. (26) and

$$\begin{aligned} \mu_g^{(T)}(n) = & -\frac{\pi^2}{60} g_0 \left(\frac{m}{\hbar^2}\right)^{3/2} \frac{(k_B T)^4}{(g_0 n)^{5/2}} \\ & \times \left[1 - \frac{5\pi^2}{21} (k_B T)^2 \frac{7+5\chi(g_0 n)}{(g_0 n)^2} \right]. \end{aligned} \quad (50)$$

Notice that Eq. (49), with Eqs. (26) and (50), generalizes the old familiar result obtained in 1958 by Lee and Yang [28].

V. CONCLUSIONS

We have used a finite-temperature Gaussian (one-loop) functional integration to obtain the equation of state for a dilute and ultracold gas of bosons with uniform number density n , taking into account both the scattering length a_s and the effective range r_s of the interatomic interaction. The divergent zero-point energy of the system has been regularized by performing dimensional regularization. Our analytical results at zero and finite temperature, which are non trivial generalizations of old but familiar formulas [22,24,25,28] depending only on the scattering length a_s , are in quite good agreement with recent Monte Carlo calculations [21] also for relatively large values of the gas parameter na_s^3 . As discussed by Braaten, Hammer, and Hermans [11], the Gaussian grand

potential can be improved taking into account also two-loop corrections but, in this case, a three-body interaction is needed to regularize the divergent two-loop grand potential [11,27]. On this respect, a self-consistent derivation of an effective field theory with a three-body term starting from a nonlocal two-body interaction potential is still missing and it surely deserves a deep investigation.

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- [1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. Wieman, and E. A. Cornell, *Science* **269**, 198 (1995).
- [2] C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, *Phys. Rev. Lett.* **75**, 1687 (1995).
- [3] K. B. Davis, M. O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Phys. Rev. Lett.* **75**, 3969 (1995).
- [4] E. P. Gross, *Nuovo Cimento* **20**, 454 (1961); L. P. Pitaevskii, *Sov. Phys. JETP* **13**, 451 (1961).
- [5] H. Shi and A. Griffin, *Phys. Rep.* **304**, 1 (1998).
- [6] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, *Rev. Mod. Phys.* **71**, 463 (1999).
- [7] A. J. Leggett, *Rev. Mod. Phys.* **73**, 307 (2001).
- [8] J. O. Andersen, *Rev. Mod. Phys.* **76**, 599 (2004).
- [9] A. M. J. Schakel, *Boulevard of Broken Symmetries* (World Scientific, Singapore, 2008).
- [10] L. Salasnich and F. Toigo, *Phys. Rep.* **640**, 1 (2016).
- [11] E. Braaten, H.-W. Hammer, and S. Hermans, *Phys. Rev. A* **63**, 063609 (2001).
- [12] R. Roth and H. Feldmeier, *Phys. Rev. A* **64**, 043603 (2001).
- [13] A. Parola, L. Salasnich, and L. Reatto, *Phys. Rev. A* **57**, R3180(R) (1998).
- [14] J. J. Garcia-Ripoll, V. V. Konotop, B. A. Malomed, and V. M. Perez-Garcia, *Math. Comput. Simul.* **62**, 21 (2003).
- [15] H. Fu, Y. Wang, and B. Gao, *Phys. Rev. A* **67**, 053612 (2003).
- [16] A. Collin, P. Massignan, and C. J. Pethick, *Phys. Rev. A* **75**, 013615 (2007).
- [17] H. Veksler, S. Fishman, and W. Ketterle, *Phys. Rev. A* **90**, 023620 (2014).
- [18] N. T. Zinner and M. Thogersen, *Phys. Rev. A* **80**, 023607 (2009); M. Thogersen, N. T. Zinner, and A. S. Jensen, *ibid.* **80**, 043625 (2009).
- [19] F. Sgarlata, G. Mazzarella, and L. Salasnich, *J. Phys. B* **48**, 115301 (2015).
- [20] A. Atland and B. Simons, *Condensed Matter Field Theory* (Cambridge University Press, Cambridge, 2006).
- [21] M. Rossi and L. Salasnich, *Phys. Rev. A* **88**, 053617 (2013).
- [22] T. D. Lee and C. N. Yang, *Phys. Rev.* **117**, 12 (1960).
- [23] T. Haugset, H. Haugerud, and F. Ravndal, *Ann. Phys.* **266**, 27 (1998).
- [24] N. N. Bogoliubov, *Izv. Akad. Nauk Ser. Fiz.* **11**, 77 (1947) [*J. Phys. (USSR)* **11**, 23 (1947)].
- [25] T. D. Lee, K. Hang, and C. N. Yang, *Phys. Rev.* **106**, 1135 (1957).
- [26] G. 't Hooft and M. Veltman, *Nucl. Phys. B* **44**, 189 (1972).
- [27] E. Braaten and A. Nieto, *Phys. Rev. B* **55**, 8090 (1997); *Eur. Phys. J. B* **11**, 143 (1999).
- [28] T. D. Lee and C. N. Yang, *Phys. Rev.* **112**, 1419 (1958).