

Equation of state of Bose gases beyond the universal regime

Martí Planasdemunt-Hospital¹, Jordi Pera^{1,*}, and Jordi Boronat^{1,†}*Departament de Física, Universitat Politècnica de Catalunya, Campus Nord B4-B5, 08034 Barcelona, Spain*

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The equation of state of dilute Bose gases, in which the energy only depends on the s -wave scattering length, is rather unknown beyond the universal limit. We have carried out a set of diffusion Monte Carlo calculations up to gas parameters of 10^{-2} to explore how the departure from the universality emerges. Using different model potentials, we calculate the energies of the gas in an exact way, within some statistical noise, and report the results as a function of the three relevant scattering parameters: the s -wave scattering length a_0 , the s -wave effective range r_0 , and the p -wave scattering length a_1 . If the effective range is not large, we observe universality in terms of a_0 and r_0 up to gas parameters of 10^{-2} . If r_0 grows, the regime of universality in these two parameters is reduced and effects of a_1 start to be observed. In the (a_0, r_0) universal regime we propose an analytical law that reproduces fairly well the exact energies.

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The experimental realization of the Bose-Einstein condensed state (BEC) [1,2] has allowed for the study of a dilute Bose gas whose main properties were predicted theoretically many years ago. The high tunability of the interaction strength in these systems offers a unique platform to gain accurate insight on their properties. However, this intriguing feature cannot be carried out as far as theory would like due to the metastability of dilute BEC gases in the laboratories [3]. Three-body losses frequently hinder the achievement of large densities n and universality in terms of the gas parameter $x = na_0^3$, with a_0 the s -wave scattering length, is what is normally observed. Nevertheless, we already know of experimental results that go beyond universality: the Fermi polaron in two dimensions [4,5], dilute Bose-Bose liquid drops [6,7], and dipolar gases [8,9].

The first terms of the equation of state of Bose gases were calculated a long time ago and proved to be dependent only on the gas parameter x ,

$$\frac{E_u}{N} = c_{\text{MF}} x + c_{\text{LHY}} x^{3/2} + c_{\text{WU}} x^2 \ln x, \quad (1)$$

with the energy in units of $\hbar^2/(2ma_0^2)$. The universal constants in Eq. (1) are

$$c_{\text{MF}} = 4\pi, \quad (2)$$

$$c_{\text{LHY}} = \frac{512\sqrt{\pi}}{15}, \quad (3)$$

$$c_{\text{WU}} = \frac{32\pi(4\pi - 3\sqrt{3})}{3}. \quad (4)$$

*Contact author: jordi.pera@upc.edu†Contact author: jordi.boronat@upc.edu

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The first term in Eq. (1) is the mean-field or Hartree-Fock term [10]. The second one was first calculated by Lee, Huang, and Yang (LHY) [11] and incorporates quantum fluctuations at the lowest order, and finally the last one was obtained by Wu [12]. The LHY and Wu terms were first derived by a hard-sphere interaction and, later on, it was proved that they are also valid for repulsive potentials with the same s -wave scattering length a_0 [13–16]. Beyond E_u/N (1), the energy of the Bose gas is no longer a universal expression depending only on the s -wave scattering length of the potential. Hugenholtz and Pines [17] proposed a continuation of the series (1) in the form

$$\frac{E}{N} = \frac{E_u}{N} + d_1 x^2 + d_2 x^{5/2} \ln x + \dots, \quad (5)$$

with new coefficients d_i which must depend on the shape of the interatomic potential. These parameters are expected to be related to scattering parameters corresponding to a larger momentum transfer, essentially the s -wave effective range r_0 and the p -wave scattering length a_1 , and also to three-body s -wave contributions [18–21]. This perturbative series for a dilute Fermi gas is well settled up to third order of the gas parameter, the terms beyond the universal regime being known, some of them with analytic expressions and the rest with integrals that are numerically estimated [22,23]. In the expansion for fermions, which is not within the scope of this Letter but provides context in the field and allows for comparison, the analytic terms depend explicitly on r_0 and a_1 . Contrarily, the knowledge of the nonuniversal terms for the equation of state of a Bose gas is very reduced up to now due to difficulties in the calculation of the required Feynman diagrams. The most recent attempt to continue the perturbative series was carried out by Braaten [18,19]. In this Letter, an expression beyond the LHY term is proposed with terms that correspond to three-body contributions and another one that depends on r_0 . The weight of the three-body term was determined by a fitting procedure to diffusion Monte Carlo (DMC) results available at that time [24]. As these data were focused to low densities, this parameter was determined with a large uncertainty.

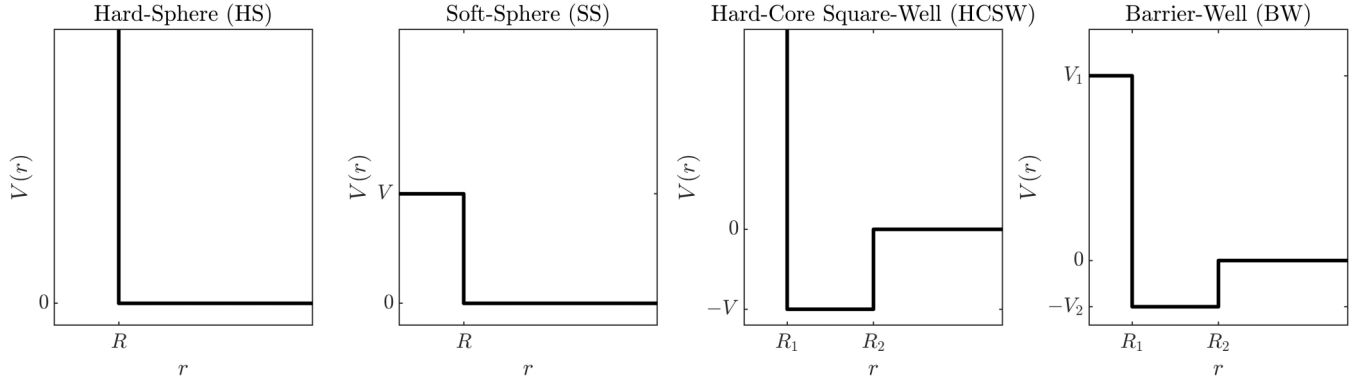


FIG. 1. Model potentials used in the DMC calculations.

In this Letter, we study the equation of state of Bose gases beyond the universal limit using the DMC method [25]. Using different model potentials (Fig. 1), from which we know the low-energy scattering parameters, we explore an extended universality, but now in terms of a_0 , r_0 , and a_1 . Our results show that this hypothesis is approximately correct within a certain domain of r_0 values and maximum density and that results with different interactions, sharing common scattering values, are always closer. We discuss the limitations of the Braaten series [18] to reproduce the DMC results, mainly when the density grows. We propose an empirical form that fits well all the DMC data for a limited set of $|r_0| \lesssim 2$ values and gas parameters up to 1×10^{-2} .

The DMC method solves stochastically the imaginary-time Schrödinger equation providing exact results for the ground-state energy and other properties of the system, within some statistical noise [25]. To reduce the variance one introduces a trial wave function that acts as importance sampling, leading the sampling to regions where the exact wave function is expected to be large and, importantly, eliminating divergences when the potential becomes singular. The model that we use is a standard Jastrow wave function $\Psi_J(\mathbf{R}) = \prod_{i < j}^N f(r_{ij})$, with $f(r)$ a two-body correlation function. We build $f(r)$ as the two-body solution, properly symmetrized to account well with the periodic boundary conditions [see specific details in the Supplemental Material (SM) [26]]. The time step and the average number of configurations (*walkers*) is adjusted to eliminate any systematic bias in the results. It is worth noting that our Green's function is accurate to second order in the time step $\Delta\tau$, reducing in this way the time-step dependence and allowing for the use of larger $\Delta\tau$ values, which reduce the correlation length. The model potentials used in our simulations are shown in Fig. 1 and their characteristic values are chosen to produce the desired scattering parameters.

Our simulations work with finite numbers of particles N , confined in a cubic box of size L^3 , to get the expected bulk density $n = N/L^3$, and thus it is important to study any finite-size effect. This is particularly important in our case because we need to work with the largest possible accuracy. For a fixed density and interaction, we carry on a set of simulations with an increasing number of particles, typically in the range $N = 50$ –700. Then, we get the energy in the thermodynamic limit E_0/N using the linear law $E/N = E_0/N + \alpha 1/N$ [26], with α a constant obtained from the fit to the DMC data. The time step and asymptotic population of walkers are chosen to

eliminate any significant bias coming from these two technical parameters.

Scattering theory at low energy, and up to momentum transfer k^2 , can be developed using three scattering parameters: the a_0 and a_1 scattering lengths [27,28],

$$a_l^{2l+1} = \frac{1}{2l+1} \int_0^\infty V(r) r^{l+1} u_l^{(0)}(r) dr, \quad (6)$$

corresponding to $l = 0$ and $l = 1$, respectively, and the s -wave effective range

$$r_0 = \frac{2}{a_0^2} \int_0^\infty [(r - a_0)^2 - u_0^{(0)2}(r)] dr. \quad (7)$$

In Eqs. (6) and (7), $V(r)$ is the interaction potential, l is the angular momentum quantum number, and $u_l^{(0)}$ is the reduced radial wave function, the solution of the radial two-body Schrödinger equation for that potential, with zero energy and angular momentum l . For the model potentials used in our work, these three parameters are analytically known as a function of the parameters defining the interaction [27]. The inverse problem, that is, to know the potential parameters for a given set of scattering parameters, is not trivial due to the complex character of the equations to solve. To this end, we implemented a stochastic search that proved to be very efficient (see SM [26]).

In Fig. 2 (left panel), we show the departure from the universal regime plotting the DMC energies using the universal energy (1), with $c_{\text{Wu}} = 0$, as a reference. From here on, we do not include the logarithmic Wu contribution because it presents a pathological behavior when x grows, even below the universal limit [24]. We have studied densities from $na_0^3 = 10^{-4}$ up to 10^{-2} and the potentials shown in Fig. 1. Below 10^{-3} , the differences between the different calculations are tiny and not visible at the scale of the plot. This result agrees with previous estimations obtained using also DMC [24], but now the accuracy is improved by using modern CPUs that allow for a more accurate determination of finite-size effects. By increasing the density, one can appreciate that as the energies spread and, at the larger value analyzed in our work (10^{-2}), the effect of finite-range effects is clear. A first significant finding of our study is that energies appear ordered from low to high values of r_0 . To better analyze a possible universality in the (a_0, r_0) plane, we show in Fig. 2 (right panel) a zoom-in at a regime of r_0 values around one. Organized in different colors, we show the energies obtained using different

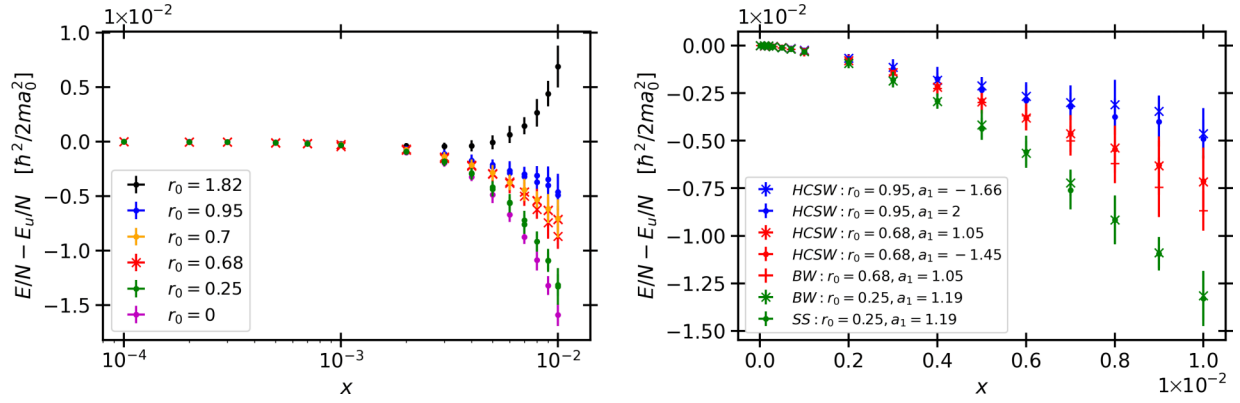


FIG. 2. Left: DMC energies using different model potentials with a common value of the s -wave effective range r_0 and s -wave scattering length a_0 . The scattering length is used as the unit length everywhere. To show the departure from the universal regime, we subtract the universal term (1) from the energy per particle. Right: DMC energies using different potentials for values of $|r_0| < 2$. The same colors stand for common r_0 values.

potentials that share a common r_0 value. As one can see, at least in this window of r_0 values, the universality in terms of the two s -wave scattering parameters is clearly observed up to the largest density explored here. However, as we will discuss later on, the range of two-parameter universality is significantly reduced when r_0 becomes larger. The role of the p -wave scattering length in the cases reported in Fig. 2 (right panel) is quantitatively below our error bars, since in the figure we plot energies with the same r_0 but distinct a_1 .

Braaten [18] proposed a continuation of the perturbative series beyond the universal regime (1) in the form

$$\frac{E}{N} - \frac{E_u}{N} = 4\pi x \left[\left(c_0 + \frac{4\pi - 3\sqrt{3}}{6\pi} \ln \bar{x} \right) \bar{x} + \left(\frac{8(4\pi - 3\sqrt{3})}{3\pi^2} \ln \bar{x} + c_1 - \frac{16}{15\pi} r_0 \right) \bar{x}^{3/2} \right], \quad (8)$$

with $\bar{x} = 16\pi x$. The parameter c_0 , termed c_E in Ref. [18], is the three-body contact parameter [29–32]. Braaten *et al.* obtained the value of c_0 by fitting Eq. (8) to DMC energies of Ref. [24], but the scarce data available and their relatively large statistical errors made its estimation difficult. The results found were dependent on the specific interaction, for instance for a hard-sphere potential they obtained $c_0 = -0.9 \pm 0.5$ and for a soft-sphere one $c_0 = -1.8 \pm 0.8$. It is worth noticing that our results for c_0 are compatible with the estimations in Ref. [18], within the statistical errors.

With the new data obtained in the present letter we have repeated the Braaten analysis. We selected energies for effective ranges $|r_0| < 2$ and used both the original model (8) and the one in Eq. (8) but without the logarithmic terms. In both cases, we get statistically compatible fits ($\chi^2/\nu \lesssim 1$) only for gas parameters $x \leq 4 \times 10^{-3}$. With the complete Braaten model (8), we obtained $c_0 = 2.20 \pm 0.06$ and $c_1 = 0.57 \pm 0.16$, whereas, without the logarithmic terms, $c_0 = -0.73 \pm 0.06$ and $c_1 = 1.33 \pm 0.15$, the latter showing a slightly better χ^2/ν . The three-body contact parameter c_0 in Eq. (8) keeps a rather constant value $c_0 = 1.2 \pm 0.1$ for

energies corresponding to gas parameters $x \leq 7 \times 10^{-4}$. Its absolute value is close to the original Braaten estimation but the sign that we obtain is changed. In Fig. 3, we show the better Braaten equation (8), restricted to the density regime where it is compatible with our results, and the set of DMC points used for the fit (see the table of all the DMC energies in SM [26]).

We extended our DMC calculations up to gas parameters $x = 10^{-2}$, a value which clearly goes beyond the validity of Eq. (8). Inspired by the series expansion proposed by Hugenholtz and Pines [17] (5) we found an empirical equation of state in the form

$$\frac{E}{N} - \frac{E_u}{N} = 4\pi x \left[c_0 \bar{x} + \left(c_1 - \frac{16}{15\pi} r_0 \right) \bar{x}^{3/2} + (c_2 + c_4 r_0) \bar{x}^2 + (c_3 + c_5 r_0) \bar{x}^{5/2} \right], \quad (9)$$

which reproduces well our results. Compared with Eq. (8), we notice that we have suppressed the logarithmic terms and increased the order of the expansion up to powers $x^{7/2}$. We verified that we need to go with this power in the series if energies up to $x = 1 \times 10^{-2}$ are going to be reproduced. Regarding the logarithmic terms, we did not observe any improvement in the law (9) with their inclusion and thus we finally removed them. The best set of parameters are reported in Table I, with a value $\chi^2/\nu < 1$. The equations of state for different r_0 values in the range $|r_0| < 2$ are shown, together with the DMC energies, in Fig. 3. As one can appreciate, Eq. (9) is able to reproduce quite accurately the exact energies. For dilute Fermi gases, it is well known that series beyond the

TABLE I. Set of optimal parameters of Eq. (9).

c_0	-1.29 ± 0.07
c_1	5.4 ± 0.4
c_2	-9.9 ± 0.9
c_3	6.2 ± 0.6
c_4	2.5 ± 0.08
c_5	-2.33 ± 0.12

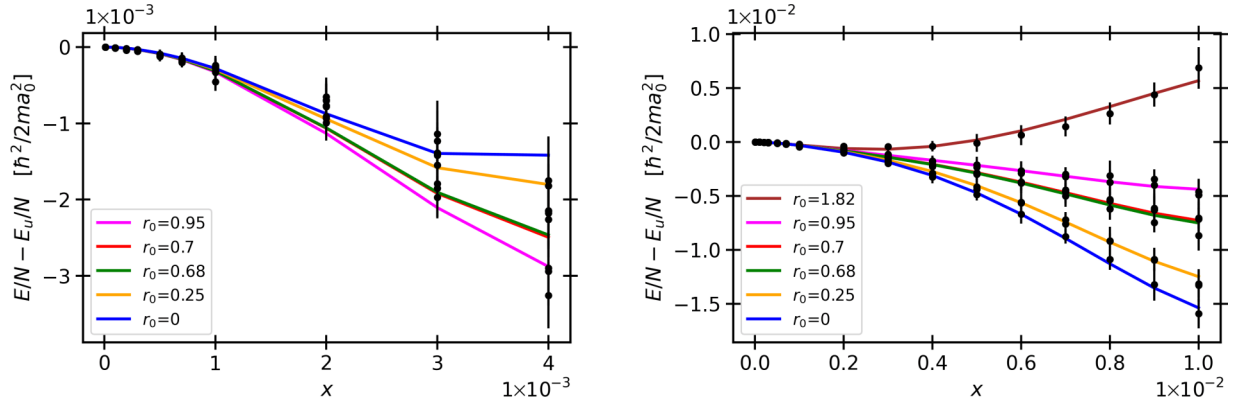


FIG. 3. Left: Braaten equation of state (8) (lines) and the set of DMC energies used for the fit (points with error bars). Right: Our proposal for the equation of state (9) (lines) and the DMC energies included in the fit (points with error bars). The best parameters are reported in Table I.

universal terms include both the s -wave effective range and the p -wave scattering length a_1 [22,23]. In the range of r_0 values used for the fit of Eq. (9), we tried to include also in the equation of state of a Bose gas the respective values of a_1 that we also know (see SM [26]). We used different models to include the a_1 values in the equation of state. However, we were not able to discern any effect by introducing these values in the fit. This can also be understood by looking at our results plotted in Fig. 3. There, we show results that have in common r_0 but not a_1 and any meaningful difference is not appreciated.

We carried out more DMC calculations covering larger values of the effective range. However, we were not able to get a reliable equation of state, as Eq. (9), including this extended regime. In Fig. 4, we report the energies obtained for these additional cases, with $r_0 = 19.7$ and $r_0 = -4.96$. For the positive r_0 case, we use two different potentials, hard-core square-well and barrier-well, and the negative case corresponds to a SS model. The first observation on these results is the breaking of universality, in terms of the pair (a_0, r_0) , for the case of large r_0 at gas parameters $x \gtrsim 3 \times 10^{-3}$. Therefore, the two-parameter universal range depends on the $|r_0|$ value, becoming smaller when it grows. The case of the large r_0 is particularly interesting. In the figure, we show three different calculations with a common r_0 value, two of them

sharing the same p -wave scattering length. Although it is not perfect, we can see that the energies are closer when the triplet (a_0, r_0, a_1) is the same. This indicates that the role of a_1 , which was negligible for small $|r_0|$, becomes significant when the effective range is larger.

We have analyzed if the equation of state (9), fitted to a regime of small effective ranges, is able to reproduce cases out of this domain, even in an approximate form. In Fig. 4, we show with solid lines the predictions of Eq. (9) with the parameters contained in Table I for the two new cases with $r_0 = 19.7$ and $r_0 = -4.96$. The nonuniversal corrections in both cases are significantly larger than the cases analyzed before (see the different energy scales in Figs. 2 and 4) but still the predictions are rather close to the exact results. Of course, Eq. (9) cannot reproduce the dependence on a_1 observed for $r_0 = 19.7$ because this scattering parameter is not included in the model. For the Bose equation of state, a perturbative model which includes a_1 is lacking, to the best of our knowledge. Noticeably, in the case of fermions, a_1 appears explicitly in the expansion, combined linearly with the effective range. As a first and rather crude attempt, we summed a_1^3 to r_0 in the term $\bar{x}^{3/2}$ of Eq. (9) without any refitting procedure. In a second model, we assumed $r_0 + \beta a_1^3$ with β an adjusting parameter, but the behavior of the energy with a_1 was worse than with a fixed $\beta = 1$ value. Notice that we add a_1^3 because the phase shift of p -wave scattering is proportional to $k^3 A_1$, A_1 being a volume that is usually written as a_1^3 [27]. The results obtained are shown in Fig. 4 with dashed lines. For the two small $|a_1|$ values, the introduction of a_1 into the equation of state does not improve the results. However, for the largest $|a_1|$ the result is surprisingly accurate. It is also remarkable that the introduction of this scattering parameter reproduces well the ordering of the DMC energies when a_1 changes.

Summarizing, we have explored the equation of state of dilute Bose gases by a large set of DMC calculations of energies, covering a large range of scattering parameters and using different model potentials. The goal of this intensive work was to provide a valuable set of results in order to explore the behavior of the equation of state when universality in terms of the s -wave scattering length ceases. In this regard, this is a continuation of work initiated some years ago in Ref. [24] that allowed to determine the approximated limit of the universality. We have carried out our calculations up to gas parameters

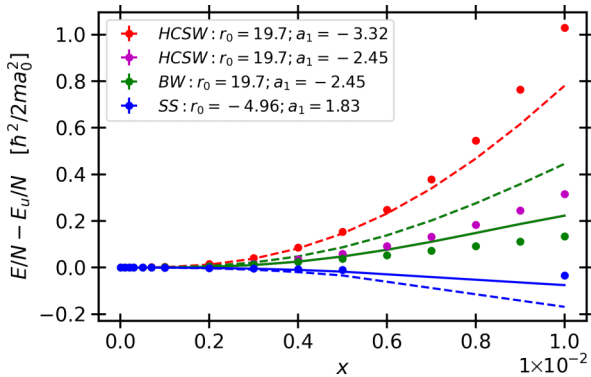


FIG. 4. DMC energies for large $|r_0|$ not included in the fit of Eq. (9). The error bars are smaller than the size of the symbols. The solid lines stand for the application of Eq. (9) and the dashed lines incorporate the value of a_1 in the equation of state, as commented in the text.

$x = 10^{-2}$, quite far from the limit of universality $x < 10^{-3}$. Our results show sizable deviations of the universal terms, with both positive and negative departures. In the regime $|r_0| < 2$, we clearly observe universality in terms of (a_0, r_0) , since energies calculated with different model potentials, but sharing these two scattering parameters, are statistically compatible up to $x \simeq 10^{-2}$. In this regime, the equation of state of Bose gases proposed by Braaten [18] reproduces our results but in a smaller density domain, $x < 4 \times 10^{-3}$. We proposed a new equation of state, with terms up to $x^{7/3}$, that reproduces quite accurately the DMC energies up to $x = 10^{-2}$. We used additional energies corresponding to larger values of r_0 to check the validity of our law out of the regime used for the fitting. Contrarily to the energies for small effective range, we observed a sizable effect of the p -wave scattering length. By fixing the set of three parameters (a_0, r_0, a_1) , we recovered universality, although for not so large values of x .

By introducing in the equation of state the a_1 length, we improve our model, mainly for larger values of a_1 . We hope that our DMC calculations [26] can serve to stimulate further theoretical work to improve the equation of state of Bose gases beyond the universal limit. Also, from the experimental side, the estimation of r_0 can serve to effectively improve the study of Bose gases in regimes where the interactions are stronger. Finally, the introduction of the new equation of state in the extended Gross-Pitaevskii formalism [3] can enlarge significantly its domain of applicability.

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