

Monte Carlo simulations of the unitary Bose gas

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We investigate the zero-temperature properties of a diluted homogeneous Bose gas made of N particles interacting via a two-body square-well potential by performing Monte Carlo simulations. We tune the interaction strength to achieve arbitrary positive values of the scattering length and compute by Monte Carlo quadrature the energy per particle E/N and the condensate fraction N_0/N of this system by using a Jastrow ansatz for the many-body wave function, which avoids the formation of the self-bound ground state and describes instead a (metastable) gaseous state with uniform density. In the unitarity limit, where the scattering length diverges while the range of the interatomic potential is much smaller than the average distance between atoms, we find a finite energy per particle [$E/N = 0.70 \hbar^2(6\pi^2n)^{2/3}/2m$, with n the number density] and a quite large condensate fraction ($N_0/N = 0.83$).

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One of the most intriguing topics in modern quantum physics is the characterization of the universal properties of an ultracold and dilute atomic gas in the so-called unitary regime [1], i.e., when the two-body scattering length a is tuned to very large values by using the Feshbach resonance technique [2] and the range R of the interatomic potential is much smaller than the average distance r_0 between atoms [3]. It is now understood that the unitary regime is characterized by remarkably simple universal laws, arising from scale invariance, and has connections with fields as diverse as nuclear physics and string theory [4]. In recent years the unitary Fermi gas has been largely investigated both experimentally and theoretically [5], while its bosonic counterpart has been only marginally addressed theoretically [6–11] because it is generally considered to be experimentally inaccessible [12].

Contrary to the case of Fermi gases, a Bose gas with attractive interactions is mechanically unstable at low T and thus most of the studies have been focused only on repulsive Bose gases. However, in the strongly repulsive regime there is a huge increase of the three-body recombination rates close to a Feshbach resonance [9,13], which makes it very difficult to reach an equilibrium state. Very recent experimental observations [14–17], however, provided a foundation for future investigations even for the degenerate Bose gas, showing that the three-body dynamics that spoils the unitary regime is slow enough with respect to the two-body one so that the degenerate Bose gas evolves dynamically on time scales fast compared to losses, thus allowing a unitary Bose gas to be experimentally created and probed dynamically. In spite of these promising results, however, the behavior of a Bose gas in this metastable regime is still not well understood and in the recent literature on the subject quite different predictions on its bulk properties have been reported [6,8–11].

The bosonic unitary regime is a formidable challenge for many-body theories. Due to the strong interaction, the standard mean-field theories are inadequate and the metastability of the system also rules out all those (*ab initio* or not) microscopic theories that are explicitly devised to search for the ground state. In particular, no attempt has been made yet to derive the equation of state of bosons at unitarity using microscopic quantum Monte Carlo approaches as done for fermion gases

[18,19]. The reason is that a positive scattering length a is associated with the presence of two-body bound states of energy $e_b = -\hbar^2/2ma^2$ in the interaction potential. This makes the gaslike state unstable and drives the system towards a self-bound ground state (cluster formation).

In this Rapid Communication we address the problem of the metastable unitary Bose gas by using quantum Monte Carlo method where the many-body wave function is based on a Jastrow ansatz that explicitly avoids the formation of the self-bound ground state. We compute the energy per particle E/N and the condensate fraction N_0/N of the metastable Bose gas by numerically simulating a large number of bosons interacting via a square-well two-body potential of radius R in a periodically repeated cubic cell. We study the metastable state by tuning the value of the s -wave scattering length a via the two-body potential parameters, keeping the system in the dilute regime $R/r_0 \ll 1$ [where $r_0 = (3/4\pi n)^{1/3}$ is the average distance among particles and n the number density]. In the weak-coupling regime ($a/r_0 \ll 1$) we recover the familiar results for the weakly interacting Bose gas [20]. In the strong-coupling regime ($a/r_0 \gg 1$) we reach the unitarity limit, finding a finite and positive energy per particle $E/N = 0.70\varepsilon_B$ [$\varepsilon_B = \frac{\hbar^2}{2m}(6\pi^2n)^{2/3}$ is the characteristic energy emerging at unitarity for a Bose gas] and a large condensate fraction $N_0/N = 0.83$.

Before giving the details of our calculations, we briefly review the approximate theoretical methods used so far to approach the problem of a Bose unitary gas and quote their main results for the energy and condensate fraction. One of the simplest methods that provides better insight than the mean-field approach without suffering the limitation of full microscopic techniques is the lowest-order constrained variational (LOCV) method [21]. The LOCV recipe is based on a Jastrow wave function where the pair function $f(r)$ for small distances is the exact solution $f_2(r)$ of the two-body Schrödinger equation, while it is set to 1 beyond a certain healing length. In the unitarity limit, the LOCV method predicts, for a condensed Bose gas, a finite value for the energy per particle $E/N = \xi\varepsilon_B$ [6], with $\xi = 1.75$. Other viable strategies that have been used to study this system are renormalization-group (RG) [9,11] and hypernetted-chain

(HNC) approximations [10], both of which have a long history in the study of strongly correlated systems. The RG approach provides the values $\xi = 0.39$ [9] and $\xi = 0.85$ [11], while an extrapolation from intermediate to very large scattering lengths of results from an HNC approach gives $\xi \simeq 0.67$ [10]. The value $\xi = 0.48$ has also been proposed, based on a variational approach on the momentum distribution [8]. The results for the condensate fraction N_0/N are even more scattered: The LOCV method gives a null condensate fraction [6] and variational and RG arguments lead to $N_0/N \simeq 0.5$ [8,11], while the HNC approach provides the value $N_0/N = 0.75$ [10]. The fact that the theoretical predictions are so scattered is a signature of the absence of a standard procedure to deal with the metastable nature of the Bose gas at unitarity.

In our Monte Carlo calculations we treat $N = 500$ atomic bosons in a cubic simulation box with periodic boundary conditions. The system is governed by the Hamiltonian

$$\hat{H} = \sum_{i=1}^N -\frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i<j=1}^N v(|\vec{r}_i - \vec{r}_j|), \quad (1)$$

with the two-body potential $v(|\vec{r}_i - \vec{r}_j|)$ given by

$$v(r) = \begin{cases} -U_0 & \text{for } 0 < r < R \\ 0 & \text{for } r > R, \end{cases} \quad (2)$$

where R is the range of the potential and $-U_0 = -\hbar^2 k_0^2/m$ is the well depth. The corresponding scattering length reads $a = R[1 - \tan(k_0 R)/k_0 R]$ and the effective range is $r_e = R(1 - R^2/3a^2 - 1/k_0^2 a R)$ [22]. We have chosen k_0 in such a way that there is a single bound state in the potential well and the scattering length is positive. When computing the properties of the system in the unitary limit, which is the main goal of the present work, the inequality $r_e \ll r_0 \ll a$ must be satisfied. In order to verify it we have considered R/r_0 values smaller than 0.01 and a/r_0 as large as 10 000. Notice that as a diverges r_e becomes equal to R .

To construct the many-body wave function we rely on a standard Jastrow-Feenberg ansatz, keeping explicit only the two body-correlations:

$$\psi_J(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \prod_{i<j} f(|\vec{r}_i - \vec{r}_j|). \quad (3)$$

Since the temperature is zero in our simulations and the Bose gas is dilute, its physical properties are governed by two-body interactions (at least in the metastable unitary regime) and the low-energy scattering of two particles can be safely approximated with the solution of the two-body problem [6,10]. We thus construct the pair function $f(r)$ in Eq. (3) starting from the exact solution of the two-body Schrödinger equation

$$\left[-\frac{\hbar^2}{m} \frac{d^2}{dr^2} + v(r) \right] r f_2(r) = \varepsilon r f_2(r), \quad (4)$$

where $\varepsilon = \hbar^2 k^2/m$ is the smallest positive energy compatible with the imposed periodic boundary conditions. For the potential (2), the solution of (4) reads

$$r f_2(r) = \begin{cases} A \sin(\kappa r) & \text{for } 0 < r < R \\ B \sin(\kappa r + \delta) & \text{for } r > R, \end{cases} \quad (5)$$

where $\kappa^2 = k^2 + k_0^2$ and the parameters A , B , and δ are fixed by the matching conditions at $r = R$ and by normalization [23].

In the limit where the range R of the two-body potential goes to zero the interparticle interaction in Eq. (4) can be replaced by the Bethe-Peierls boundary conditions [6,24] on the pair function

$$\lim_{r \rightarrow 0} \frac{[r f_2(r)]'}{r f_2(r)} = -\frac{1}{a}. \quad (6)$$

In this case $f_2(r)$ is given by

$$r f_2(r) = A \sin(\kappa r + \delta), \quad (7)$$

where the parameter δ is now fixed by Eq. (6) and A by the normalization [25].

In order to account for many-body effects, which typically become relevant when r is of the same order of r_0 , $f(r)$ is smoothly joined with a constant at a certain distance R_m [6]. This is required also in order to account for the periodic boundary conditions imposed on the simulation box. With such a wave function, however, when the scattering length diverges, the equilibrium configuration is not a uniform gas, as desired, but rather it is a compact cluster of atoms in equilibrium with the vacuum, whose radius is about 10 times the effective range of the potential and 0.001 times the average distance r_0 in the uniform system. This is due to a maximum in the probability density provided by $r^2 f_2^2(r)$ at short distances (order of R), which favors configurations where the atoms are close to one another (dimers, trimers, etc.). In order to keep the system in a uniform phase (metastable state) we should correct $f(r)$ at small distances to prevent particles from dwelling into this regions. The underlying idea originates from Feynman's comments on the construction of the ground-state wave function for liquid ^4He [26].

There are different ways to implement such a correction, ranging from imposing the three-body repulsive condition in quantum Monte Carlo methods [27] to enforcing the equivalent hard-sphere condition in the hyperradius formalism [28]. These methods need an explicit way to include higher-order correlations, which are not known, thus requiring extra approximations. In our approach we simply set to zero the value of the pair function up to the outermost node R_n of $f_2(r)$. This is indeed reasonable because, due to the extreme diluteness of the gas, in the metastable unitary regime the particle pairs should experience only the tails of the wave function. Our choice also has the advantage of keeping all the formalism in the two-body sector.

The pair function then reads

$$f(r) = \begin{cases} 0 & \text{for } 0 < r < R_n \\ f_2(r) & \text{for } R_n < r < R_m \\ 1 & \text{for } r > R_m. \end{cases} \quad (8)$$

The continuity and boundary conditions on $f(r)$, plus the requirement that $f'(R_m) = 0$, fix all the free parameters in $f(r)$ except for R_m . As already pointed out in Ref. [6], one cannot simply treat R_m as a variational parameter since this procedure would lead to the undesired minimizing value $R_m = 0$. We thus choose to fix R_m through a normalization condition $4\pi n \int_0^{R_m} r^2 f_2(r) dr = 1$ as in the LOCV approach [6].

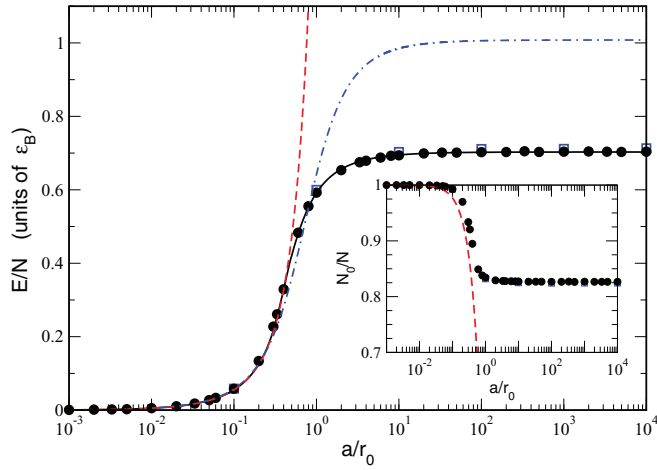


FIG. 1. (Color online) Energy per particle E/N (in units of ε_B) and condensate fraction N_0/N (inset) as a function of the scaled scattering length a/r_0 for two values of the two-body potential range R/r_0 : 0.01 (open squares) and 0 (closed circles). The dashed line is the mean-field prediction of Bogoliubov with the LHY correction [29] and the dot-dashed line is the fit of Ref. [30] to quantum Monte Carlo results for the unitary Fermi gas [18]. The solid line is the fit of our Monte Carlo data as described in the text.

There are other possible choices for R_m , such as $R_m = L/2$ as used in quantum Monte Carlo (MC) studies of unitary Fermi gases [18,19], but such a choice could lead in the present case to the unwanted condition $r_0 < R_n$ for large values of a .

Summarizing, we proposed a many-body wave function of the Jastrow-Feenberg form (3) with the two-body correlation function obeying three basic requirements, i.e., (i) it provides long-range correlations as dictated by an attractive short-range potential with the actual scattering length a , (ii) it keeps the density uniform by preventing the formation of clusters, and (iii) it is normalized while keeping the position of the last node of the actual two-body scattering wave function.

In Fig. 1 we report the calculated energy per particle

$$\varepsilon = \frac{E}{N} = \frac{1}{N} \frac{\langle \psi_J | \hat{H} | \psi_J \rangle}{\langle \psi_J | \psi_J \rangle} \quad (9)$$

as a function of the scaled scattering length a/r_0 for two different values of the scaled two-body potential range R/r_0 . The MC simulations used to compute ε never count less than 2×10^6 sampled configurations and both the sparse and the block averaging techniques [31] have been adopted to prevent correlations among the sampled configurations.

The open squares are the results obtained at $R/r_0 = 0.01$ with $f_2(r)$ given by Eq. (5), while the closed circles are obtained with $R/r_0 = 0$, i.e., with $f_2(r)$ given by Eq. (7). The two sets of data are very close, showing that with $R/r_0 = 0.01$ the system is indeed dilute and displays (universal) properties that depend only on the s -wave scattering length a [3,5].

We have also considered an alternative form for $f(r)$, which instead of being strictly zero in the range $0 < r < R_n$ is smoothly connected to a third-order polynomial in $r = R_n$ and fulfills the condition $f(0) = 0$. This leaves a free parameter that can be variationally optimized. We found, however, that the resulting energy is always larger than the one obtained with

(8). In particular, the variational optimization returns a wave function as flat (and as small) as possible within the range $0 < r < R_n$, thus confirming the quality of our ansatz (8).

In the weakly interacting regime ($a/r_0 \ll 1$) our results, as shown in Fig. 1, agree with the well known universal Bogoliubov prediction [32] with the Lee-Huang-Yang (LHY) correction [29]:

$$\varepsilon_{\text{LHY}}(x) = \varepsilon_B \left(\frac{4}{3\pi^2} \right)^{1/3} x \left[1 + \frac{128}{15\sqrt{\pi}} \sqrt{\frac{3}{4\pi}} x^{3/2} \right]$$

where $x = a/r_0$. In the strong-coupling regime ($a/r_0 \gg 1$) our data reach a plateau in a way that is qualitatively similar to the behavior found for a unitary Fermi gas on the Bose-Einstein condensation (BEC) side of BCS-BEC crossover (also shown for comparison in Fig. 1), but the convergence is to a lower value, namely, $\varepsilon/\varepsilon_B = 0.70$. This value is well below the LOCV prediction of 1.75 based on the LOCV method [6] and is slightly larger than the average value of RG approaches [9,11], the HNC result [10], and the variational estimate of [8].

The obtained MC data are well interpolated by the function

$$\varepsilon(x)/\varepsilon_B = \begin{cases} \varepsilon_{\text{LHY}}(x)/\varepsilon_B + ax^3 & \text{for } x < 0.3 \\ c_3x^3 + c_2x^2 + c_1x + c_0 & \text{for } 0.3 < x < 0.5 \\ b_0 + b_1 \tanh(b_2/x - 1) & \text{for } x > 0.5 \end{cases} \quad (10)$$

and a fit procedure provides the values $a = 0.21$, $b_0 = 0.45$, $b_1 = -0.33$, and $b_2 = 0.54$, while the parameters $c_3 = -6.64$, $c_2 = 7.16$, $c_1 = -1.46$, and $c_0 = 0.19$ are fixed by smoothness and continuity constraints in $r = 0.3$ and 0.5 . The function $\varepsilon(x)$ is shown with a solid line in Fig. 1.

The parametrization (10) of the equation of state allows us to obtain other useful quantities via standard thermodynamical relations, for example, the chemical potential $\mu = \partial_n(n\varepsilon)$, the pressure $P = n^2 \partial_n \varepsilon$, the sound velocity, $c_s^2 = n/m \partial_n \mu$, and also Tan's two-body contact density [33] $C_2 = (8\pi n m a^2 / \hbar^2) d\varepsilon/da$, which describes the $1/k^4$ tail of the momentum distribution $\rho(k)$ at large momenta. Our results are shown in Fig. 2. Note that at unitarity $C_2 = \alpha n^{4/3}$, with $\alpha = 9.02$. This value compares acceptably well with previous theoretical estimates $\alpha = 10.3$ [10], 32 [11], and 12 [34] and is a factor of 2 smaller than the value extrapolated from experimental results on a trapped gas in the local-density approximation $\alpha = 22$ [33].

The many-body wave function (3) gives direct access also to the one-body density matrix $\rho_1(\vec{r} - \vec{r}')$ whose limiting value at large distances provides the condensate fraction N_0/N [22]. In the inset of Fig. 1 we plot the behavior of N_0/N as a function of a/r_0 for two values of R/r_0 . Our data follow the Bogoliubov prediction $\frac{N_0}{N} = 1 - \frac{8}{3\sqrt{\pi}} \left(\frac{3}{4\pi} x^3 \right)^{1/2}$ (dashed line in Fig. 1) up to about $a/r_0 = 0.01$, while in the unitary limit our data converge to a constant value $N_0/N = 0.83$. The LOCV method predicts in the same limit $N_0/N = 0$ [6], while the HNC value $N_0/N = 0.78$ [10] is compatible with our result. For completeness, we recall that the RG method developed in Ref. [11] and the variational approach in Ref. [8] suggest instead $N_0/N \sim 0.5$.

In conclusion, we have studied the zero-temperature unitary Bose gas via a Jastrow ansatz on the many-body wave function that avoids the formation of the self-bound ground state and

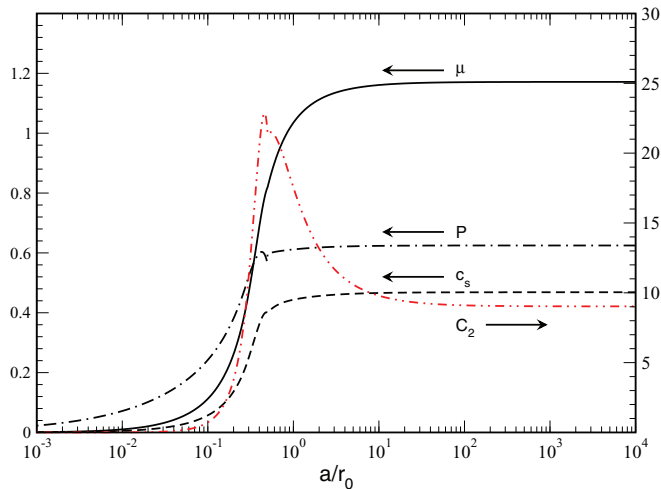


FIG. 2. (Color online) Chemical potential μ (in units of ε_B), pressure P (in units of $n\varepsilon_B$), sound velocity c_s (in units of $v_B = \sqrt{2\varepsilon_B/m}$), and two-body contact density C_2 (in units of $n^{4/3}$) as a function of the scaled scattering length a/r_0 as obtained from the parametrization (10) of the equation of state. Arrows indicate the axis with the corresponding scale.

then computed the energy per particle and the condensate fraction by Monte Carlo quadrature. In the unitary limit we have found a finite value both for the energy per particle and for the condensate fraction. This is a clear signature of a universal behavior in which the properties of the system depend only on the average distance between the particles encoded in their density. The fact that the universal value of the energy per particle for the unitary gas is lower for bosons than for fermions is not completely unexpected since the antisymmetry of the fermionic wave function results in an effective excluded-volume effect that increases the energy [35]. From the Monte Carlo data of the energy per particle we have also derived the chemical potential, the pressure, the sound velocity, and the contact density as a function of the s -wave scattering length. We believe our predictions can be tested with the ongoing experiments [15–17] on ultracold vapors of bosonic alkali-metal atoms.

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