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Ground state of a homogeneous Bose gas: A diffusion Monte Carlo calculation

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We use a diffusion Monte Carlo method to calculate the lowest-energy state of a uniform gas of bosons interacting through different model potentials, both strictly repulsive and with an attractive well. We explicitly verify that at low density the energy per particle follows a universal behavior fixed by the gas parameter na^3. In the regime of densities typical for experiments in trapped Bose-condensed gases, the corrections to the mean-field energy greatly exceed the differences due to the details of the potential. [S1050-2947(99)04811-8]

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The achievement of Bose-Einstein condensation in magnetically trapped atomic vapors [1] has revived interest in the theoretical study of Bose gases. Mean-field methods provide us with relatively simple predictions both for the equilibrium properties of these systems (energy per particle, density profiles, and condensate fraction) and for the dynamic behavior (frequency of collective excitations and interference effects), which have been found in close agreement with experiments (for a review, see Ref. [2]). In fact, the atomic clouds realized in experiments are very dilute, the average distance between particles being significantly larger than the range of interatomic forces, and mean-field approaches are well suited. However, the investigation of effects beyond mean-field theory is an important task, which would make these systems even more interesting from the point of view of many-body physics. Theoretical studies of these effects have already been proposed, either by analytic inclusion of fluctuations around mean field [3,4] or through numerical calculations based on quantum Monte Carlo methods [5] and, more recently, also on correlated basis function approaches [6]. All of these investigations are based on the idea that, for the values of density relevant in experiments, the details of the interatomic potential can be neglected and one can safely use the hard-sphere model in numerical simulations, and the expansion in powers of the gas parameter na^3, fixed by the number density n and the s-wave scattering length a, in analytic corrections beyond mean field. The main motivation of the present work is to verify the validity of this approach. By using a diffusion Monte Carlo (DMC) method we calculate the ground-state energy of a system of bosons interacting through different two-body model potentials. We explicitly show that for the values of the gas parameter reached in magnetic traps ($na^3 \simeq 10^{-5}$–10^{-4}), the behavior is universal and fixed by na^3 and the corrections to the mean-field energy are much larger than the differences due to the details of the interatomic potential.

The ground state of a homogeneous dilute Bose gas was intensively studied in the 1950s and early 1960s. One of the main results of this investigation is that the ground-state energy can be expanded in powers of $\sqrt{na^3}$. In units of $\hbar^2/2ma^2$ the energy per particle takes the form

$$\frac{E}{N} = 4\pi na^3 \times \left[1 + \frac{128}{15\sqrt{\pi}}\sqrt{na^3} + \frac{8(4\pi - 3\sqrt{3})}{3} na^3 \ln(na^3) + \cdots \right]. \tag{1}$$

The first term corresponds to the mean-field prediction and was already calculated by Bogoliubov [7]. The corrections to mean field have been obtained using perturbation theory; the coefficient of the $(na^3)^{3/2}$ term was first calculated by Lee, Huang, and Yang [8], while the coefficient of the last term was first obtained by Wu [9]. Both of them were originally derived for hard spheres, but it was shown that the same expansion is valid for any repulsive potential with scattering length a [10,11]. Furthermore, Hugenholtz and Pines [11] have shown that the higher-order terms in the expansion (1) depend on the ''shape'' of the interatomic potential. It is worth pointing out that, for the values of na^3 relevant in experiments, the corrections to the mean-field energy are very small ($\simeq 3\%$). In a recent paper, Lieb and Yngvason [12] have also provided a rigorous lower bound for the ground-state energy of a Bose gas holding for non-negative, finite range, spherical, two-body potentials. The lower bound coincides with the Bogoliubov mean-field term: $E/N \geqslant 4\pi(na^3)\hbar^2/2ma^2$. However, what is not well established up to now is the range of validity of the universal law (1).

In realistic systems, the above restrictions for the interatomic potential do not hold because an attractive tail is generally present. In this case the situation for the ground state is different. If the potential does not sustain any many-body bound states and the scattering length is positive, the ground state of the system still behaves like a gas and the expansion (1) should hold. Conversely, in the case of potentials that have two-, three-, or more-body bound states, the ground-state of the system is no longer a homogeneous gas, but a state with clusters of atoms formed. However, if the scattering length is positive, a uniform gas can still exist as a metastable state, which will be long lived at very low densities. Our results for a simple model of interatomic potential with an attractive part show that the energy of the gaslike metastable state still follows the universal law given by Eq. (1).

We consider a system of N spinless bosons with mass m described by the many-body Hamiltonian $\hat{H} = -(\hbar^2/2m)\Sigma_{i=1}^{N}\nabla_i^2 + \Sigma_{i<j}V(|\mathbf{r}_i - \mathbf{r}_j|)$, where $V(r)$ is the two-body, spherical, interatomic potential. The DMC algorithm exactly solves, apart from statistical uncertainty, the N-body Schrödinger equation for the ground-state energy of the system (for further details on the method see for example Ref. [13]). We have used different choices for the potential $V(r)$:

(i) Hard-sphere (HS) potential defined by

$$V(r) = \begin{cases} +\infty & (r<a) \\ 0 & (r>a), \end{cases} \tag{2}$$

where the diameter a of the hard sphere corresponds to the scattering length.

(ii) Soft-sphere (SS) potential defined by

$$V(r) = \begin{cases} V_0 & (r<R) \\ 0 & (r>R), \end{cases} \tag{3}$$

with a scattering length $a = R[1 - \tanh(K_0R)/K_0R]$ with $K_0^2 = V_0 m/\hbar^2$ and $V_0 > 0$. For finite V_0 one has always $R > a$, while for $V_0 \to +\infty$ the SS potential coincides with the HS one with $R = a$. For the SS potential we have considered two choices: $R = 5a$ and $R = 10a$. It is worth noting that the hard sphere and the very soft sphere with $R = 10a$ represent two extreme cases for a repulsive potential. In the HS case, the energy is entirely kinetic, while for the very ''soft'' potential $a \simeq (m/\hbar^2)\int_0^\infty V(r) r^2 dr$, according to the Born approximation, and the energy is almost all potential. This opposite behavior is clearly observed in the curvature of the corresponding two-body distribution function $g(r)$ shown in Fig. 4.

(iii) Hard-core square-well (HCSW) potential defined by

$$V(r) = \begin{cases} +\infty & (r<R_c) \\ -V_0 & (R_c<r<R) \\ 0 & (r>R), \end{cases} \tag{4}$$

for which the s-wave scattering length is given by $a = R_c + (R - R_c)\{1 - \tan[K_0(R - R_c)]/K_0(R - R_c)\}$ with $K_0^2 = V_0 m/\hbar^2$ and $V_0 > 0$. For fixed R_c and R the scattering length coincides with the hard-core radius R_c for $V_0 = 0$ and by increasing V_0 it exhibits resonances each time a two-body bound state appears in the well. In many real potentials (such as in ^{87}Rb and ^{23}Na) the scattering length is much larger than the size of the atom. To reproduce this situation we have chosen $R = 5R_c$ and $a = 10R$ with only one two-body bound state in the well.

In the case of purely repulsive potentials, we directly apply the DMC algorithm to obtain the ground-state energy. For importance sampling we use a Jastrow trial function: $\psi_T(\mathbf{R}) \equiv \psi_T(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \Pi_{i<j} f(r_{ij})$. The Jastrow factor $f(r)$ is chosen as the exact wave function of a pair of particles interacting through $V(r)$ with total energy ϵ for $r \leq \bar{R}$, and for $r > \bar{R}$, a function $f(r) = 1 - Ae^{-r/\alpha}$, which goes rapidly to one. The parameter α is left as a variational parameter, while the coefficient A and the matching point $\bar{R}$ are chosen so that $f(r)$ and its first derivative be continuous at $r = \bar{R}$ and the local energy $(-\hbar^2\nabla^2/2m + V)f(r)/f(r)$ be also continous at $r = \bar{R}$. The energy ϵ is the second variational parameter. Before starting the DMC calculation, we perform a variational Monte Carlo analysis to optimize the parameters of the trial wave function. At low densities, we find that the DMC calculation improves very little on the VMC result. For example, for the HS potential at $na^3 = 10^{-5}$ and in units of $\hbar^2/2ma^2$, $E_{VMC}/N = 1.278(1) \times 10^{-4}$ and $E_{DMC}/N = 1.274(1) \times 10^{-4}$. This means that at low densities $\psi_T(\mathbf{R})$ has a large overlap with the ''true'' ground-state wave function.

The case of the HCSW potential needs a careful treatment. Since the potential has a two-body bound state, the gaslike state is not the ground state. To obtain the energy of the metastable gaslike state it is necessary to project out the bound-state component of the wave function. This can be achieved by using the same trial wave function as for the SS potential (any trial function that is positive in the region where the potential is attractive would be equally appropriate) and then projecting the results for the energy by means of an auxiliary function $\psi_P(\mathbf{R})$ orthogonal to any many-body state with bound pairs. In the Monte Carlo formulation this is realized by the weighted integral $E = \int d\mathbf{R} f(\mathbf{R}, \tau \to \infty) \times [\hat{H}\psi_P(\mathbf{R})]/\psi_T(\mathbf{R}) / \int d\mathbf{R} f(\mathbf{R}, \tau \to \infty)\psi_P(\mathbf{R})/\psi_T(\mathbf{R})$, where $f(\mathbf{R}, \tau \to \infty)$ is the density of walkers generated by the DMC calculation. The projecting function $\psi_P(\mathbf{R})$ is chosen as $\psi_P(\mathbf{R}) = \Pi_{i<j} f_P(r_{ij})$, where $f_P(r)$ coincides with the trial two-body function $f(r)$ for $r > \bar{R}$, while for $r < \bar{R}$ is given by the exact solution for two particles interacting through $V(r)$ with energy $\epsilon > 0$ [we require the same continuity conditions at the matching point $\bar{R}$ as for $f(r)$]. Since the matching point $\bar{R}$ is much larger than the range R of the potential,

TABLE I. Energy per particle for the HS potential.

na^3	E/N (units of $\hbar^2/2ma^2$)	na^3	E/N (units of $\hbar^2/2ma^2$)
10^{-6}	$1.262(1)\times 10^{-5}$	5×10^{-3}	$8.154(6)\times 10^{-2}$
5×10^{-6}	$6.343(1)\times 10^{-5}$	10^{-2}	$1.796(1)\times 10^{-1}$
10^{-5}	$1.274(1)\times 10^{-4}$	5×10^{-2}	1.338(1)
5×10^{-5}	$6.469(3)\times 10^{-4}$	10^{-1}	3.626(7)
10^{-4}	$1.311(1)\times 10^{-3}$	0.166	8.26(2)
5×10^{-4}	$6.880(4)\times 10^{-3}$	0.244	16.7(1)
10^{-3}	$1.424(2)\times 10^{-2}$		

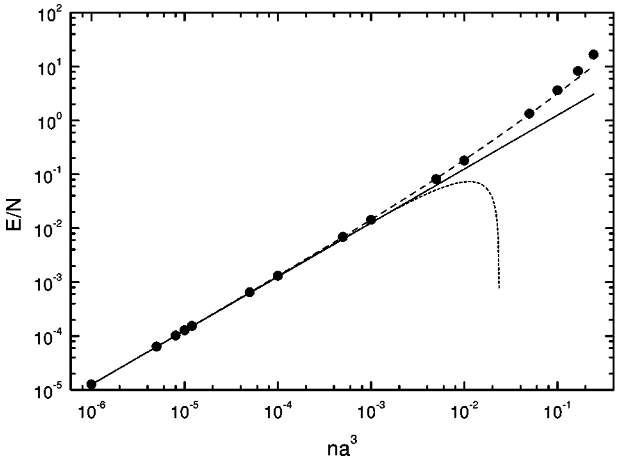

FIG. 1. Equation of state for the HS potential. The solid circles are the DMC energies (error bars are smaller than the size of the symbols); the solid line corresponds to the mean-field prediction [first term in Eq. (1)]; the long-dashed line includes the LHY correction [first two terms in Eq. (1)]; the short-dashed line includes also the logarithmic correction and corresponds to the full expansion (1). The energies are in units of $\hbar^2/2ma^2$.

$f_P(r)$ is orthogonal to the bound-state wave function and $\psi_P(\mathbf{R})$ is orthogonal to any many-body state with one or more bound pairs formed. In this way, we eliminate from the calculation all states with bound pairs. At low densities we expect that bound pairs give the main contribution to the ground state compared to three or more-body bound states. By eliminating these bound pairs we are thus left with the gaslike metastable state with lowest energy.

We are now in a position to discuss our results. In Table I we present the DMC results for the equation of state of the HS potential. In all of the calculations we have used a simulation box containing $N=500$ particles in order to reduce finite size effects well below statistical uncertainty. Previous Monte Carlo calculations of the ground-state energy of the hard-sphere boson system have been performed at densities typical of liquid ^{4}He $(na^3 \simeq 0.1)$ [14,15]. The results for the two highest densities in Table I are compatible with the Green's Function Monte Carlo results of Ref. [15]. In Fig. 1, our results for the HS equation of state are shown together with the various terms of the analytic expansion (1). One can see that the Lee-Huang-Yang (LHY) correction [second term in Eq. (1)] represents a significant improvement on the mean-field prediction and the inclusion of this term allows for a good approximation of the equation of state up to very high densities. On the contrary, the logarithmic correction [third term in Eq. (1)] goes wrong already at intermediate densities $(na^3 \simeq 10^{-3})$.

In Table II, we report the results of the comparison between the various potentials considered in this work (the corresponding results for the HS potential can be read from Table I). At low values of the gas parameter na^3 all potentials give the same results and only at the largest density reported $(na^3 = 10^{-3})$, the results for the SS potential start to deviate from the HS values. The universal behavior is better shown in Fig. 2, where we plot the difference between the calculated energy per particle and the mean-field term and compare it with the LHY correction. It is worth mentioning that this difference is always positive in agreement with the lower bound provided by the mean-field term, as discussed in Ref. [12]. The very low density regime and the relevance of the logarithmic correction is analyzed in the inset of Fig. 2. The HS and SS results show evidence of the presence of this logarithmic correction, however, the effect is tiny and goes rapidly wrong for larger densities. Due to larger error bars no conclusion can be drawn for the HCSW results concerning the logarithmic term.

TABLE II. Energy per particle for the SS and HCSW potential (in units of $\hbar^2/2ma^2$).

	E/N		
na^3	SS $(R=5a)$	SS $(R=10a)$	HCSW
10^{-6}	$1.262(1)\times10^{-5}$	$1.262(1)\times10^{-5}$	$1.262(1)\times10^{-5}$
10^{-5}	$1.274(1)\times10^{-4}$	$1.273(1)\times10^{-4}$	$1.277(2)\times10^{-4}$
10^{-4}	$1.309(1)\times10^{-3}$	$1.303(1)\times10^{-3}$	$1.314(1)\times10^{-3}$
10^{-3}	$1.395(1)\times10^{-2}$	$1.356(1)\times10^{-2}$	$1.430(5)\times10^{-2}$

Another point of interest is the condensate fraction N_0/N, which we calculate from the long-range behavior of the one-body density matrix: $N_0/N=\lim_{r\to\infty}\rho(r)$ (see Ref. [13] for further details). In Fig. 3, we show the results for N_0/N as a function of na^3 for the HS and the two SS potentials. The results are compared with the analytic expansion

$$\frac{N_0}{N}=1-\frac{8}{3\sqrt{\pi}}(na^3)^{1/2}, \tag{5}$$

calculated by Bogoliubov [7]. At low densities this law is universal and agrees very well with the results of the three model potentials. First, deviations from universality start to appear for the $na^3 \simeq 10^{-3}$ result, which coincides with the emergence of deviations in the energy values.

In Fig. 4 we show the two-body distribution function $g(r)$ for hard spheres at various densities. One can clearly see the

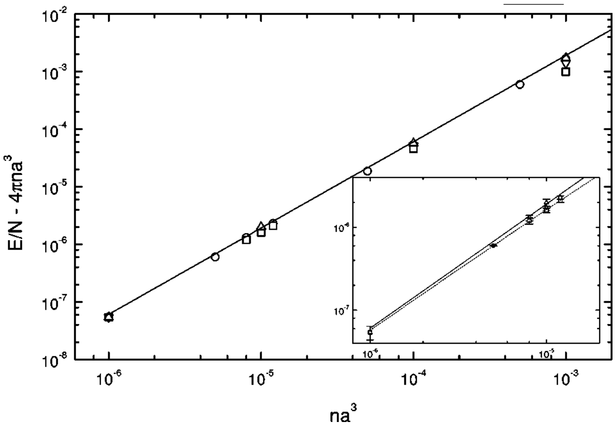

FIG. 2. Corrections to the mean-field energy. Circles, HS potential; down triangles, SS potential $(R=5a)$; squares, SS potential $(R=10a)$; up triangles, HCSW potential; solid line, LHY correction [second term in Eq. (1)]. The error bars are smaller than the size of the symbols. The inset shows the results for the HS, SS $(R=10a)$, and HCSW potentials in the extremely low-density region; the solid line is again the LHY correction, while the dashed line includes the logarithmic correction [second and third term in Eq. (1)]. The energies are in units of $\hbar^2/2ma^2$.

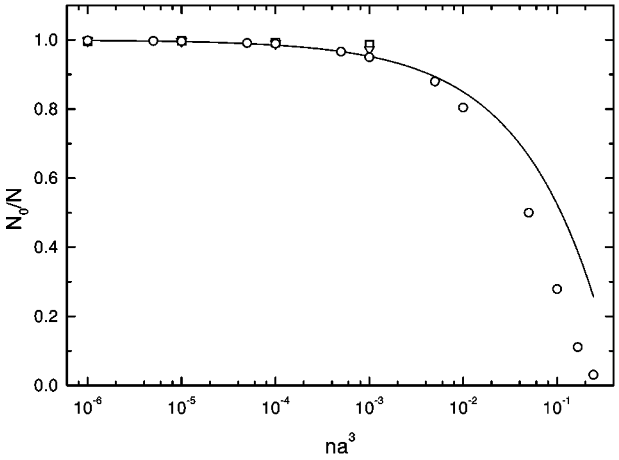

FIG. 3. Condensate fraction as a function of the gas parameter. Circles, HS potential; down triangles, SS potential ($R=5a$); squares, SS potential ($R=10a$). The solid line corresponds to the Bogoliubov expansion (5). The error bars are smaller than the size of the symbols.

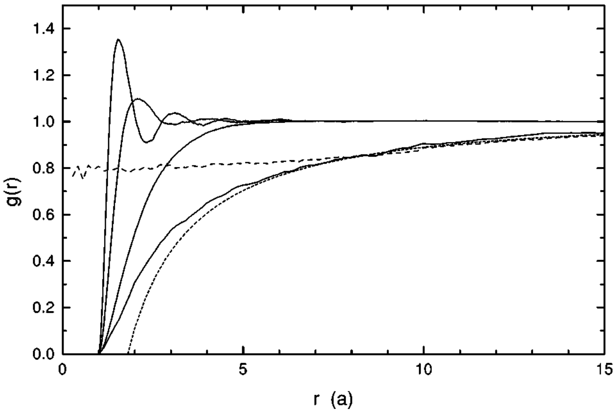

FIG. 4. Two-body distribution function. Solid lines, hard-spheres at densities $na^3=10^{-4}$ (lowermost), 10^{-2}, 0.1, 0.244 (uppermost). Long-dashed line, soft-spheres ($R=10a$) and short-dashed line, Fourier transform of the Bogoliubov static form factor $S(k)$ at the lowest density $na^3=10^{-4}$.

building up of short-range correlations at high densities. The distribution function $g(r)$ can be estimated at low densities using the Bogoliubov result for the static form factor: $S(k)=\hbar^2k^2/2m\epsilon(k)$, where $\epsilon(k)=(\hbar^4k^4/4m^2+gn\hbar^2k^2/m)^{1/2}$ is the usual Bogoliubov dispersion relation with coupling constant $g=4\pi\hbar^2a/m$. The Fourier transform of $S(k)$ gives the distribution function $g(r)$ directly which, for $r\gg a$, exhibits the asymptotic behavior $g(r)\simeq 1-[4\pi^{5/2}(na^3)^{3/2}(r/a)^4]^{-1}$. In Fig. 4 we also compare, at the density $na^3=10^{-4}$, the distribution function obtained from the Bogoliubov $S(k)$ with the $g(r)$ of hard spheres and soft spheres with $R=10a$. The long-range behavior is universal and agrees with the Bogoliubov result, while at short distances the HS and SS potentials give completely different results since in the second case particles can penetrate the repulsive potential. At higher densities the Bogoliubov approximation for $g(r)$ becomes poorer and completely misses the shell structure of the distribution function.

In conclusion, we have shown that, for the values of density realized in magnetic traps, the corrections to mean field are fixed only by the gas parameter na^3 and do not depend on the details of the interatomic potential. These effects, although small, have a simple theoretical description in terms of the parameter na^3 and, possibly, can be singled out in future precision measurements [4].

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