Bose atoms in a trap: A variational Monte Carlo formulation for the universal behavior at the van der Waals length scale

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We present a variational Monte Carlo formulation for the universal equations of state at the van der Waals length scale [B. Gao, J. Phys. B **37**, L227 (2004)] for N Bose atoms in a trap. The theory illustrates both how such equations of state can be computed exactly, and the existence and the importance of long-range atom-atom correlation under strong confinement. Explicit numerical results are presented for $N=3$ and 5, and used to provide a quantitative understanding of the shape-dependent confinement correction that is important for few atoms under strong confinement.

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I. INTRODUCTION

Few atoms in a trap, which can in principle be realized, e.g., through a Mott transition from a degenerate quantum gas in a optical lattice [1,2], is a fundamental system for studying atomic interactions and correlations. It has many features of a many-atom system, yet still sufficiently simple to be amenable to a number of different theoretical approaches that can check against and learn from each other. These methods include, for example, the Monte Carlo methods (see, e.g., Refs. [3–7]), and the hyperspherical methods [8–14].

Unlike the problem of two identical atoms in a symmetric harmonic trap, which can be reduced to a one-dimensional (1D) problem and be solved exactly [15–19], the problem of N atoms in a trap ($N>2$) is much more complex. Partly due to this complexity, and partly due to our previously limited understanding of atomic interaction based on the effect-range theory [20,21], existing studies of N atoms in a trap, with virtually no exception, have relied on potential models that do not reflect the true nature of atomic interaction except for the scattering length. In other words, they provide understanding only at the level of shape-independent approximation. This approximation clearly breaks down for dense systems with $\rho\beta_6^3 \sim 1$ or greater [22,23]. Here $\rho=N/V$ is the atomic number density, and $\beta_6=(mC_6/\hbar^2)^{1/4}$ is the length scale associated with the van der Waals interaction, $-C_6/r^6$, between atoms. For an inhomogeneous system of atoms in a trap, the shape-independent approximation may also break down, even for fairly small values of $\rho\beta_6^3$, due to strong confinement [16–19,24], as characterized by $a_0/a_{ho} \sim 1$, where a_0 is the s wave scattering length, and $a_{ho}=(\hbar/m\omega)^{1/2}$ is the length scale associated with the trapping potential. This effect, which we call the shape-dependent confinement correction [24], can be understood qualitatively as due to the energy dependence of the scattering amplitude, which is always shape dependent [16–19,24].

Going beyond the shape-independent approximation requires understandings of atomic interaction and correlations at shorter length scales. Fortunately, universal properties persist because atoms have the same *types* of long-range interactions, such as $-C_6/r^6$ for atoms in ground state. The development of the angular-momentum-insensitive quantum defect theory (AQDT) [25–28] has led both to a systematic understanding of atomic interaction of the types of $-C_n/r^n$ with $n \geq 3$, and to a methodology for uncovering and studying universal properties at different length scales for two-atom, few-atom, and many-atom systems [22,23,27,29]. This work illustrates how this method can be implemented in a variational Monte Carlo (VMC) formulation that gives basically exact results for the N-atom universal equations of state at length scale β_6 [22,23]. Explicit numerical results are presented for three and five Bose atoms in a symmetric harmonic trap. They provide both samples of benchmark (basically exact) results for few atoms in a trap and a quantitative understanding of the shape-dependent confinement correction [24]. In the process of achieving these results, we also show that atoms in a trap have long-range correlation that becomes important under strong confinement.

Our VMC formulation for N Bose atoms in an external potential, which differs from existing formulations [7] in its choice of correlation function, is presented in Sec. II. The universal equations of state at length scale β_6 are discussed in Sec. III, with explicit numerical results for three and five Bose atoms in a symmetric harmonic trap presented in Sec. IV. Conclusions are given in Sec. V.

II. VMC TREATMENT OF N BOSE ATOMS IN AN EXTERNAL POTENTIAL

The relative merit of different Monte Carlo methods are well documented [4]. We choose here the variational Monte Carlo method (VMC) for a number of reasons (a) VMC always works, for bosons, fermions, or excited states, provided one picks the right trial wave function. (b) VMC provides the most transparent understanding of the many-body wave function, and is thus the best for conceptual purposes. (c) The advantages of other Monte Carlo methods [4], such that

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being a "black box," mostly disappear when applied to fermions or to the excited states of a many-body system. (d) The result of VMC can always be used as the starting point upon which further adjustment or relaxation of wave function can be allowed, if at all necessary. More specifically, it can be used to fix the nodal structure and provide the importance sampling [3].

The difficulty, or the challenge of VMC, is in choosing a proper trial wave function. Otherwise no converged result would be obtained, as reflected in the fact that the variance of energy would be of the same order of, or greater than, the average value being evaluated. The same challenge can, however, also be regarded as an opportunity, as it forces one to understand the wave function.

Consider an N-atom Bose system described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i=1}^{N}V_{\text{ext}}(\mathbf{r}_i) + \sum_{i<j=1}^{N}v(r_{ij}), \tag{1}$$

where V_{ext} describes the external "trapping" potential, and $v(r)$ represents the interaction between atoms that has a behavior of $v(r)\rightarrow -C_6/r^6$ in the limit of large r.

Such an N-atom Bose system has of course many different states. We focus ourselves here on the lowest gaseous Bose-Einstein condensate (BEC) state, which can be defined as the state that evolves from the lowest N-free-particle state in a trap as one turns on an atomic interaction with positive scattering length. For this particular state, we take the variational trial wave function to be of Jastrow form [30]

$$\Psi = \left(\prod_{i=1}^{N}\phi(\mathbf{r}_i)\right)\prod_{i<j=1}^{N}F(r_{ij}). \tag{2}$$

It is straightforward to show that the expectation value of energy for such a state can be written as

$$E = \frac{\int d\tau\Psi^* H\Psi}{\int d\tau\Psi^*\Psi} = \frac{\int d\tau\Psi^*\Psi E_L(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)}{\int d\tau\Psi^*\Psi}, \tag{3}$$

where the integrations are over all N-atom coordinates, and E_L is a local energy that can be written as the sum of three terms whose contributions to the energy depend on the one-body, two-body, and three-body correlation functions, respectively,

$$E_L = E_L^{(1)}(\mathbf{r}_1) + E_L^{(2)}(\mathbf{r}_1,\mathbf{r}_2) + E_L^{(3)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3). \tag{4}$$

Here

$$E_L^{(1)} = \frac{1}{\phi(\mathbf{r}_1)}\left(-\frac{\hbar^2}{2m}\nabla_1^2\phi(\mathbf{r}_1)\right) + V_{\text{ext}}(\mathbf{r}_1), \tag{5}$$

$$E_L^{(2)} = E_{L1}^{(2)} + E_{L2}^{(2)}, \tag{6}$$

with

$$E_{L1}^{(2)} = (N-1)\frac{1}{2}\left[\frac{1}{F(r_{12})}\left(-\frac{\hbar^2}{m}\nabla_1^2 F(r_{12})\right) + v(r_{12})\right], \tag{7}$$

$$E_{L2}^{(2)} = -(N-1)\left(\frac{\hbar^2}{m}\right)\frac{1}{\phi(\mathbf{r}_1)F(r_{12})}[\nabla_1\phi(\mathbf{r}_1)]\cdot[\nabla_1 F(r_{12})], \tag{8}$$

and

$$E_L^{(3)} = -\frac{1}{2}(N-1)(N-2)\left(\frac{\hbar^2}{m}\right) \times \frac{1}{F(r_{12})F(r_{13})}[\nabla_1 F(r_{12})]\cdot[\nabla_1 F(r_{13})]. \tag{9}$$

Once ϕ and F are chosen, Eq. (3) can be evaluated using Metropolis Monte Carlo method (see, e.g., Ref. [31]), and the variational parameters are then varied to find the stationary energies.

The success, or the failure, of a VMC calculation depends exclusively on the proper choice of the wave function. The choice of ϕ is fairly standard and is based on the independent-particle solution in the external potential. The choice of F is less obvious, and depends on the understanding of atom-atom correlation in a trap. Our choice of F is based on the following physical considerations. (a) Atom-atom correlation at short distances is determined by two-body interaction. (b) Atoms in a trap can have long-range correlation that becomes important under strong confinement, as suggested by our recent work on two atoms in a trap [19]. Specifically, we choose our F as

$$F(r) = \begin{cases} Au_\lambda(r)/r, & r < d, \\ (r/d)^\gamma, & r \geq d. \end{cases} \tag{10}$$

Here $u(r)$ satisfies the Schrödinger equation

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + v(r) - \lambda\right)u_\lambda(r) = 0, \tag{11}$$

for $r<d$. γ is the parameter characterizing the long-range correlation between atoms in a trap, with $\gamma=0$ (meaning $F=1$ for $r>d$) corresponding to no long-range correlation. Both d and γ are taken to be variational parameters, in addition to the variational parameters associated with the description of ϕ. The parameters A and λ are not independent and are determined by matching F and its derivative at d.

The key difference between our choice of F and the standard choices [7], in addition to the systematic treatment of atomic interaction to be discussed in the next section, is the allowance for the long-range correlation characterized by parameter γ [19]. One can easily verify that regardless the model potential used for v (such as the hard sphere potential), a choice of F without long-range correlation, such as [7]

$$F(r) = 1 - a_0/r, \tag{12}$$

would not have led to converged VMC results under strong confinement. This explains why the existing Monte Carlo

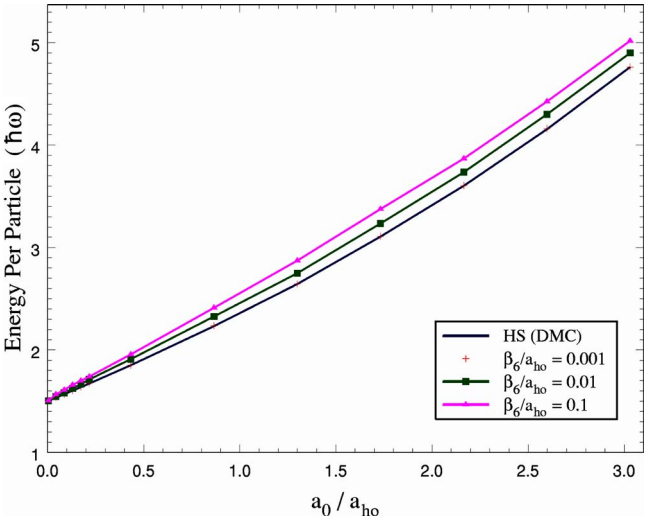

FIG. 1. (Color online) The universal equation of state for three atoms in a symmetric harmonic trap as a function of a_0/a_{ho}, compared to the DMC results of Blume and Greene for hard spheres [6].

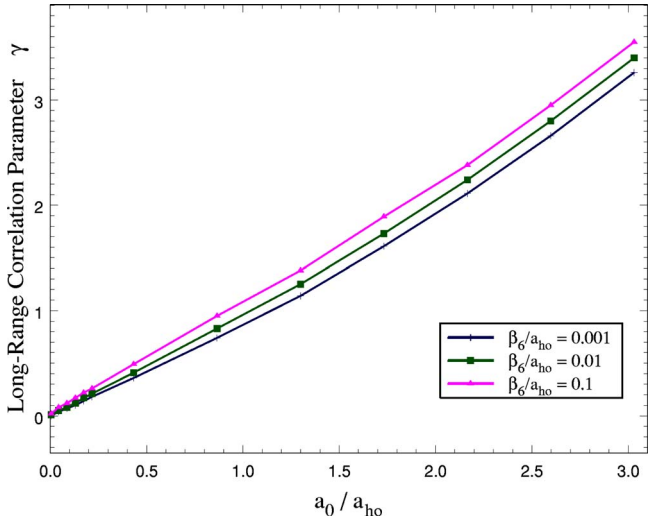

FIG. 2. (Color online) The parameter γ, characterizing the long-range atom-atom correlation, for three atoms in a symmetric harmonic trap, as a function of a_0/a_{ho}.

results for few atoms under strong confinement have come from diffusion Monte Carlo (DMC) [6], but not from VMC, which was successful for weak confinements [7].

III. UNIVERSAL EQUATION OF STATE AT THE VAN DER WAALS LENGTH SCALE FOR N BOSE ATOMS IN A SYMMETRIC HARMONIC TRAP

For any state in which the atomic interaction at the average atomic separation is well represented by $-C_6/r^6$, which for N Bose atoms in a trap implies $\rho\beta_6^3 \sim N(\beta_6/a_{ho})^3 < \sim 10$, its energy follows a universal behavior [22,23] that is uniquely determined by the trapping and the van der Waals potentials, independent of the interactions at short distances except through a parameter that can be taken either as the short range K matrix K^c [25] or the s wave scattering length a_0. Within the VMC formulation, this can be understood by noting that for such diffuse states, the solution $u_\lambda(r)$ of Eq. (11), wherever it has an appreciable value [29], is given by [22,23,25,27]

$$u_{\lambda_s}(r_s) = B[f^{c(6)}_{\lambda_s l=0}(r_s) - K^c g^{c(6)}_{\lambda_s l=0}(r_s)]. \tag{13}$$

Here B is a normalization constant. $f^{c(6)}_{\lambda_s l}$ and $g^{c(6)}_{\lambda_s l}$ are universal AQDT reference functions for $-C_6/r^6$ type of potential [22,25,32]. They depend on r only through a scaled radius $r_s = r/\beta_6$, and on energy only through a scaled energy $\lambda_s = \lambda/s_E$, where $s_E = (\hbar^2/m)(1/\beta_6)^2$ is the energy scale associated with the van der Waals interaction. K^c is a short-range K matrix [25] that is related to the s wave scattering length a_0 by [27,29]

$$a_0/\beta_6 = \left(b^{2b}\frac{\Gamma(1-b)}{\Gamma(1+b)}\right)\frac{K^c + \tan(\pi b/2)}{K^c - \tan(\pi b/2)}, \tag{14}$$

where $b = 1/(n-2)$, with $n = 6$. Note that while K^c and a_0 are related to each other, by propagating the wave function in the van der Waals potential from small to large distances [27,33], they have considerably different physical meanings. K^c is a short-range parameter that is directly related to the logarithmic derivative of the wave function coming out of the inner region, a region where atomic interaction may differ from $-C_6/r^6$ [25]. a_0 is determined by the asymptotic behavior of the wave function at large distances. The universal behavior is conceptually easier to understand in terms of K^c, as it simply implies that for any state in which the probability for finding particles in the inner region is small, the only role of the inner region is in determining the logarithmic derivative of the wave function coming out of it. Our results are presented in terms of a scaled a_0 parameter only to facilitate connections with existing models and understandings.

When u_λ, as given by Eq. (13), and therefore F, depend on the interactions of shorter range than β_6 only through K^c or a scaled a_0, so do the overall wave function and the energy of the N-atom Bose system. For an inhomogeneous system of atoms in a trap, the energy depends of course also on the trap configuration. To be specific, we consider here atoms in a symmetric harmonic trap, characterized by

$$V_{\text{ext}}(r) = \tfrac{1}{2}m\omega^2 r^2, \tag{15}$$

where ω is the trap frequency. The corresponding independent-particle solution suggests

$$\phi(\mathbf{r}) = \exp[-\alpha(r/a_{ho})^2], \tag{16}$$

where α is chosen as one of the variation parameters, in addition to parameters d and γ used to characterize the correlation function F. From this combination of ϕ and F, the resulting VMC energy per particle, properly scaled, can be written as

$$\frac{E/N}{\hbar\omega} = \Omega(a_0/a_{ho}, \beta_6/a_{ho}), \tag{17}$$

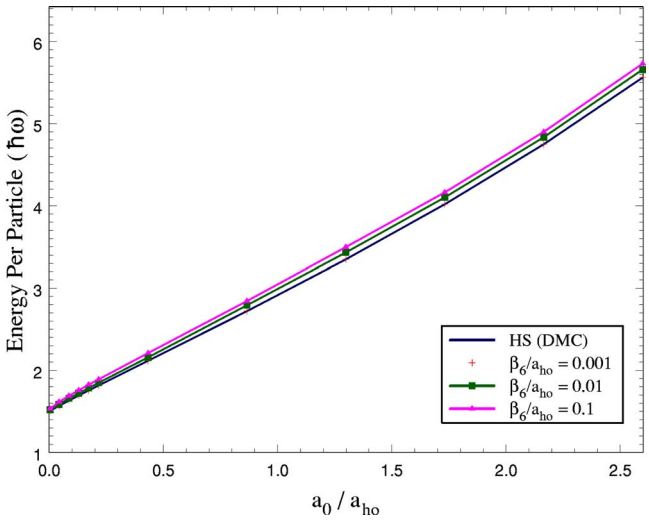

FIG. 3. (Color online) The universal equation of state for five atoms in a symmetric harmonic trap as a function of a_0/a_{ho}, compared to the DMC results of Blume and Greene for hard spheres [6].

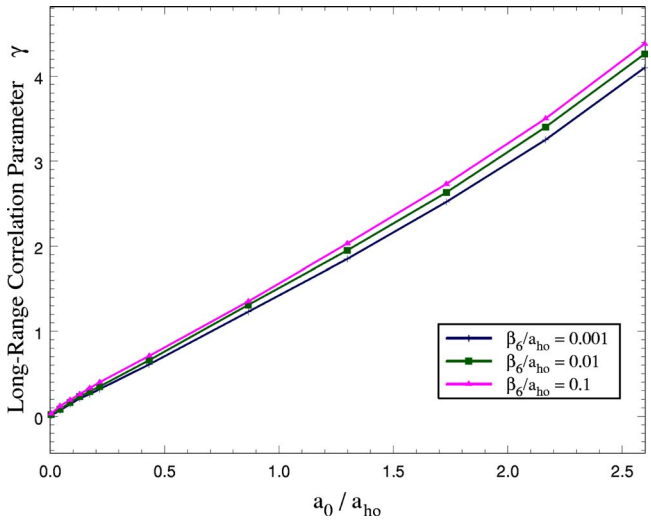

FIG. 4. (Color online) The parameter γ, characterizing the long-range atom-atom correlation, for five atoms in a symmetric harmonic trap, as a function of a_0/a_{ho}.

where Ω is a universal function that is uniquely determined by the number of particles, the exponent of the van der Waals interaction ($n=6$), and the exponent of the trapping potential (2 for the harmonic trap). The strengths of interactions, as characterized by C_6 and ω, play a role only through scaling parameters such as β_6 and a_{ho}.

Equation (17), which is one example of what we call the universal equation of state at length scale β_6, can also be defined, independent of the VMC formulation, using the method of effective potential as in Ref. [22]. It is a method of renormalization in the coordinate space to eliminate all length scales shorter than β_6. The same procedure in VMC corresponds simply to using Eq. (13) for all $r<d$ (see the Appendix). The function Ω, following this procedure, is rigorously defined for all values of a_0/a_{ho} and for all $\beta_6/a_{ho}>0$. An N-atom Bose system in a symmetric harmonic trap and in the lowest gaseous BEC state can be expected to follow this universal behavior for $\beta_6/a_{ho}<\sim 2/N^{1/3}$, beyond which the interactions of shorter range, such as $-C_8/r^8$, can be expected to come into play.

It is worth noting that the parameter β_6/a_{ho} in Eq. (17) plays a similar role, for atoms in a trap, as $\rho\beta_6^3$ for homogeneous systems [22,23]. The latter parameter is not used here obviously because ρ is not uniform, but its order of magnitude is still related to β_6/a_{ho} by $\rho\beta_6^3\sim N(\beta_6/a_{ho})^3$. When either parameter goes to zero, the universal equations of state at length scale β_6 can be expected to go to the shape-independent results as obtained by Blume and Greene [6] for particles in a trap and by Giorgini *et al.* [5] for homogeneous systems [22,23].

IV. RESULTS FOR FEW BOSE ATOMS IN A SYMMETRIC HARMONIC TRAP

The formulation in the preceding sections is applicable to any number of atoms. We present here explicit numerical results for few Bose atoms in a symmetric harmonic trap. This is not only because such calculations are less numerically intensive than for larger number of atoms, but also because before N gets sufficiently large that $\rho\beta_6^3\sim 1$, the shape-dependent confinement correction is actually more important for smaller number of particles [24].

Figure 1 illustrates the equation of state for three atoms in a symmetric harmonic trap. It is a function of two variables that we plot here as a set of functions of a_0/a_{ho} for different values of β_6/a_{ho}. The results for $\beta_6/a_{ho}=0.001$ show that, as expected, the universal equation of state at length scale β_6 does *eventually* approach a shape-independent result in the limit of $\beta_6/a_{ho}\to 0$, and are in excellent agreement with the DMC results of Blume and Greene for hard spheres [6]. The results for $\beta_6/a_{ho}=0.01$ and $\beta_6/a_{ho}=0.1$ illustrate the shape

TABLE I. Selected data of energy per particle, in units of $\hbar\omega$, as a function of a_0/a_{ho} for three atoms in a symmetric harmonic trap. The number in the parentheses represents the variance in the last digit.

a_0/a_{ho}	HS[a]	$\beta_6/a_{ho}=0.001$	$\beta_6/a_{ho}=0.01$	$\beta_6/a_{ho}=0.1$
0.433	1.851	1.851(2)	1.911(2)	1.957(1)
0.866	2.233	2.237(1)	2.327(1)	2.411(1)
1.732	3.107	3.110(1)	3.235(1)	3.375(1)
2.598	4.154	4.162(1)	4.301(2)	4.426(1)

[a]DMC results for hard spheres from Ref. [6].

TABLE II. Selected data of energy per particle, in units of $\hbar\omega$, as a function of a_0/a_{ho} for five atoms in a symmetric harmonic trap. The number in the parentheses represents the variance in the last digit.

a_0/a_{ho}	HS[a]	$\beta_6/a_{ho}=0.001$	$\beta_6/a_{ho}=0.01$	$\beta_6/a_{ho}=0.1$
0.433	2.115	2.116(1)	2.159(1)	2.210(1)
0.866	2.720	2.722(1)	2.791(1)	2.844(1)
1.732	4.018	4.019(2)	4.101(2)	4.163(1)
2.598	5.560	5.561(1)	5.657(2)	5.729(1)

[a]DMC results for hard spheres from Ref. [6].

dependence of the equation of state due to the van der Waals interaction. They show that even for relative small $\rho\beta_6^3$, which is of order of 10^{-6} for $\beta_6/a_{ho}=0.01$, the shape-dependent correction can become quite appreciable under strong confinement. This correction, which we call the shape-dependent confinement correction [24], can be understood qualitatively as due to energy dependence of the two-body scattering amplitude [16–19,24],which becomes significant for large scattering lengths. To put our results in perspective, we note that a recent experiment on two atoms in a symmetric harmonic trap is already exploring the region close to $\beta_6/a_{ho}\sim 0.1$ [2].

Figure 2 shows the parameter γ, characterizing the long-range atomic correlation, for three atoms in a symmetric harmonic trap. It is clear that γ can become quite large under strong confinement, $a_0/a_{ho}\sim 1$. Not surprisingly, a variational wave function that does not incorporate this long-range correlation explicitly would fail under such conditions.

Figure 3 shows the equation of states for five atoms in a symmetric harmonic trap. Compared to the results for three atoms, the shape-dependent corrections can be seen to be less significant, confirming the conclusion from Ref. [24] that the shape-dependent confinement correction is more important for smaller number of particles than for larger number of particles. The long-range atom-atom correlation is again very important, as shown in Fig. 4.

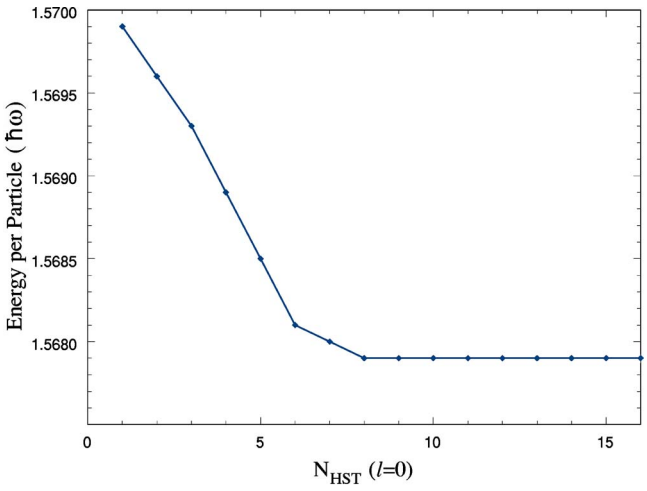

FIG. 5. (Color online) Energy per particle for three atoms in a trap, with $a_0/a_{ho}=0.0866$ and $\beta_6/a_{ho}=0.001$, as a function of the number of s wave bound states supported by a HST effective potential.

Some specific data points shown in Figs. 2 and 4 are tabulated in Tables I and II for the convenience of future comparisons. They represent samples of basically exact results for few Bose atoms in a symmetric harmonic trap. The effects of atomic interactions with shorter ranges than β_6 would come into play only for states with energies that are much further away from the threshold (either below or above). If the scattering length parameter used here is achieved by tuning around a Feshbach resonance [34,35], the same results would apply, provided it is a broad Feshbach resonance with a width much greater than the energy scale, s_E, associated with the van der Waals potential [36–39].

V. CONCLUSIONS

In conclusion, we have presented a VMC formulation for the universal equations of state at the length scale β_6 for N Bose atoms in a symmetric harmonic trap. We have also shown that atoms under strong confinement have significant long-range correlation of the form of r_{ij}^{γ}. Since an independent-particle model, such as the Hartree-Fock approximation, corresponds to a variational method based on a wave function with $F\approx 1$, the fact that F, for atoms under strong confinement, deviates significantly from 1 everywhere implies that any independent-particle model is likely to fail for such systems. The results for $N=3$ and 5 provide a quantitative understanding of the shape-dependent confinement correction, which is important for a small number of particles under strong confinement [24].

We are extending our calculations to larger number of particles to study universal behaviors, for both homogeneous and inhomogeneous systems, in the region of $\rho\beta_6^3\sim 1$, where shape dependence is obviously important [22,23]. We are also extending our methodology to other states of few-atoms and many-atoms systems. They include not only the excited states with higher energies than the lowest gaseous BEC states, but also the liquid states with lower energies [22,23].

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APPENDIX: FURTHER COMMENTS ON IMPLEMENTATION

We make a few additional comments here on the computational procedure leading to the universal equation of state at length scale β_6, as it is slightly different depending on whether one has the capability of computing the reference functions $f^{c(6)}_{\lambda_s l}$ and $g^{c(6)}_{\lambda_s l}$.

Mathematically, the universal equation of state is rigorously defined using the method of effective potential, in a limit that eliminates all length scales shorter than β_6 [22]. The short range behavior of the effective potential is not important, provided that it is sufficiently repulsive and gives rise to the desired K^c, or a_0/β_6, which are related to each other by Eq. (14). For most purposes, the most conveniently effective potential is simply a hard sphere with an attractive tail (HST):

$$v_{\text{eff}}(r) = v_{\text{hst}}(r) = \begin{cases} \infty, & r \le r_0, \\ -C_6/r^6, & r > r_0, \end{cases} \tag{A1}$$

for which the scattering length, the short-range K^c parameter, and the number of bound levels for any partial wave l, can all be found analytically [29].

With this choice of effective potential, the limit that eliminates all length scales shorter than β_6 is denoted by $r_0 \to 0+$, and defined as r_0 taking on a *discrete set* of successively smaller, but never zero, values [22]. The corresponding effective potentials all have the same K^c or a_0/β_6, with the only difference being that the ones with smaller r_0 support a greater number of bound states [29]. Figure 5 illustrates this limiting process, and shows how the energy per particle for a three-atom system becomes independent of r_0 in the limit of $r_0 \to 0+$, which is equivalent to the limit of a large number of s wave bound states. Numerically, this limit is simply realized by taking a r_0 that is sufficiently small that the energy has become independent of r_0.

For each set of parameters a_0/a_{ho} and β_6/a_{ho}, their ratio determines a parameter a_0/β_6. Without the capability for computing the reference functions $f^{c(6)}_{\lambda_s l}$ and $g^{c(6)}_{\lambda_s l}$, one would proceed to pick a sufficiently small r_0/β_6, either by using the analytic results of Ref. [29] or numerically, such that the effective potential yields the desired a_0/β_6. The correlation function is then found by integrating Eq. (11) with v replaced by the effective potential and matching to the outer behavior at d, which is typically of the order of a_{ho} for few atoms in a trap.

For people with the capability of computing the reference functions $f^{c(6)}_{\lambda_s l}$ and $g^{c(6)}_{\lambda_s l}$, no integration of Eq. (11) is necessary, as its solution is simply given by Eq. (13) with K^c determined from a_0/β_6 by Eq. (14). There is also a greater freedom in picking r_0/β_6. It must be sufficiently small, but it no longer must be determined from a_0/β_6, because the correlation function is determined from a_0/β_6 directly, not through r_0/β_6 as is the case in the first approach. For sufficiently small r_0, the possible inconsistency between r_0/β_6 and a_0/β_6 in such an approach has no computational consequence because the correlation function goes to zero in the limit of small r_0. Our calculations are carried out using this second approach with a r_0 sufficiently small that the corresponding effective potential supports at least 32 s wave bound states.

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