

## Beyond the Fermi pseudopotential: A modified Gross-Pitaevskii equation

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We present an effective potential and the corresponding modified Gross-Pitaevskii equation, which account for the energy dependence of the two-body scattering amplitude through an effective-range expansion. For the ground-state energy of a trapped condensate, the theory leads to what we call a shape-dependent confinement correction that improves agreements with diffusion Monte Carlo calculations. The theory illustrates, for relatively strong confinement and/or high density, how the shape dependence on atom-atom interaction can come into play in a many-atom quantum system.

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### I. INTRODUCTION

The Gross-Pitaevskii equation (GPE) has in recent years played a central role in our understanding of gaseous Bose-Einstein condensates (BECs) [1,2]. Its astonishing success has to do with the fact that in most experiments to date, both the gaseous parameter  $na^3$  (here  $n$  is the number density and  $a$  is the scattering length) and the parameter  $a/L_0$ , which characterizes the strength of confinement (with  $L_0$  being a measure of the size of the trap), have been very small. Recently, a new breed of experiments [3] have emerged that take advantage of Feshbach resonances in cold atomic collision [4] to make the scattering length  $a$  tunable through a magnetic field. Such experiments promise to take us into parameter regimes in which the validity of the GPE and its underlying assumptions, such as the shape-independent pseudopotential approximation [1,2], have to be carefully examined.

Most of the existing theories going beyond the GPE [5–7] have focused on quantum fluctuation that is responsible for the lowest-order correction in  $na^3$ . But it has become clear that eventually, a better description of atom-atom interaction, beyond the pseudopotential approximation that is the basis of the GP theory, will be required. For homogeneous systems, this has been demonstrated in a recent work by Cowell *et al.* [8], which shows that different potentials having the same scattering length  $a$  can lead to a vastly different ground-state energy for  $na^3$  of the order of 0.05 or greater. For inhomogeneous systems, recent works on two atoms in a trap have shown that the shape-independent approximation becomes less valid under strong confinement [9–11].

Neither of these results are surprising. The shape-independent approximation assumes the two-body scattering amplitude to be a constant over the momentum (or energy) range of interest. For larger  $na^3$  or stronger confinement, a greater range of momentum states become involved and this assumption becomes less applicable. This point has already been illustrated for two-atom systems under strong confinement, where it has been shown that the inclusion of the energy dependence of scattering amplitude leads to much improved results for the energy levels of the system [9–11]. The goal of this paper is to show how a similar idea can be generalized to an  $N$ -body system.

In the light of the success of the GP theory [1,2], we focus

here on a perturbative approach around the GPE. An effective potential is proposed that incorporates the energy dependence of the two-body scattering amplitude through an effective-range expansion. A corresponding modified GP equation is derived. By taking advantage of the relationship between effective range and scattering length as implied by the quantum-defect theory (QDT) [12,13], no new inputs from scattering calculations are required other than the standard scattering length and the  $C_6$  coefficient. For the ground-state energy of an inhomogeneous system, our numerical results show that the modified equation leads to better agreements with diffusion Monte Carlo (DMC) results [7] than theories that consider only the quantum fluctuation correction. More importantly, the theory introduces the concept of shape-dependent confinement correction, an origin of shape dependence on the interaction potential that is absent in a homogeneous system.

### II. MODIFIED GP EQUATION

In a second-quantization formulation, a system of  $N$  bosons in an external trapping potential  $V_{\text{ext}}(\mathbf{r})$  is described by a Hamiltonian

$$\hat{H} = \int d\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \hat{\Psi}^\dagger(\mathbf{r}_1) \hat{\Psi}^\dagger(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) \hat{\Psi}(\mathbf{r}_2) \hat{\Psi}(\mathbf{r}_1). \quad (1)$$

Here  $V$  is the interaction between particles.  $\hat{\Psi}(\mathbf{r})$  and  $\hat{\Psi}^\dagger(\mathbf{r})$  are the bosonic annihilation and creation operators that satisfy the commutation relations

$$[\hat{\Psi}^\dagger(\mathbf{r}_1), \hat{\Psi}^\dagger(\mathbf{r}_2)] = [\hat{\Psi}(\mathbf{r}_1), \hat{\Psi}(\mathbf{r}_2)] = 0, \quad (2)$$

$$[\hat{\Psi}(\mathbf{r}_1), \hat{\Psi}^\dagger(\mathbf{r}_2)] = \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (3)$$

Taking the interparticle potential  $V$  to be that of a mean field,

$$V_{\text{MF}} = g \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad (4)$$

where

$$g = \frac{4\pi\hbar^2 a}{m}, \quad (5)$$

and ignoring quantum fluctuation, one arrives at the usual GP equation [1,2]

$$i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g|\Phi|^2 \right] \Phi(\mathbf{r}, t). \quad (6)$$

Here  $\Phi = \langle \hat{\Psi} \rangle$  and is normalized by  $\int d\mathbf{r} |\Phi|^2 = N$ , with  $N$  being the total number of particles.

From a two-body scattering point of view, the mean-field potential, given by Eq. (4), is such that it gives, in the first Born approximation, the correct forward scattering amplitude at zero energy. It is a shape-independent approximation that ignores completely the energy dependence of the scattering amplitude. While this may be a good approximation for small values of  $na^3$  and for weak confinement, it becomes less valid for strong confinement and/or greater  $na^3$ . This is true even at zero temperature, as confinement and/or quantum depletion invariably involve nonzero momentum states.

For a better treatment of atomic interaction, while preserving much of the structure of the GP theory, an effective interaction is proposed here that incorporates the energy dependence of the scattering amplitude through an effective-range expansion. Specifically, we look for a  $\hat{V}_{\text{eff}}$  that gives, in the first Born approximation, the correct real part of the forward scattering amplitude,

$$-\frac{m}{4\pi\hbar^2} \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} \hat{V}_{\text{eff}} e^{+i\mathbf{k}\cdot\mathbf{r}} = \text{Re}[f(k, \theta=0)], \quad (7)$$

to the order of  $k^2$  (the first order in energy). This requirement basically ensures a better optical potential for an atom moving in the medium of others [14].

For the range of energies of interest here, only the  $s$ -wave scattering is important. In this case, the scattering amplitude can be written in terms of the  $s$ -wave phase shift  $\delta_0(k)$  as

$$f(k, \theta) = \frac{1}{k} \frac{1}{\cot \delta_0(k) - i}. \quad (8)$$

From the standard effective-range expansion

$$k \cot \delta_0(k) = -\frac{1}{a} + \frac{1}{2} r_e k^2 + \dots, \quad (9)$$

where  $r_e$  is the effective range, we have, to the order of  $k^2$ ,

$$\text{Re}[f(k, \theta)] = -a + a^2(a - \frac{1}{2}r_e)k^2. \quad (10)$$

It is straightforward to verify that the  $\hat{V}_{\text{eff}}$  satisfying Eq. (7) can be written as

$$\hat{V}_{\text{eff}} = V_{\text{MF}}(\mathbf{r}_1 - \mathbf{r}_2) + \hat{V}_{\text{mod}}(\mathbf{r}_1 - \mathbf{r}_2), \quad (11)$$

where

$$\hat{V}_{\text{mod}} = \frac{g_2}{2} [\delta(\mathbf{r}_1 - \mathbf{r}_2) \nabla_{\mathbf{r}_1 - \mathbf{r}_2}^2 + \nabla_{\mathbf{r}_1 - \mathbf{r}_2}^2 \delta(\mathbf{r}_1 - \mathbf{r}_2)] \quad (12)$$

and

$$g_2 = \frac{4\pi\hbar^2 a^2 \left( a - \frac{1}{2} r_e \right)}{m}. \quad (13)$$

This potential is consistent with the pseudopotential expansion of Huang and Yang [15], except that it is Hermitian and is represented in the coordinate space. It is worth noting that  $g_2$  is not zero for  $r_e = 0$ . This is because unlike the expansion for  $k \cot \delta_0$ , the real part of the scattering amplitude has a  $k^2$  dependence even when  $r_e = 0$ .

With this effective interaction, the many-body Hamiltonian becomes

$$\begin{aligned} \hat{H} &\equiv \hat{H}_{\text{MF}} + \hat{H}_{\text{mod}} \\ &\equiv \left\{ \int d\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \hat{\Psi}^\dagger(\mathbf{r}_1) \hat{\Psi}^\dagger(\mathbf{r}_2) V_{\text{MF}}(\mathbf{r}_1 - \mathbf{r}_2) \hat{\Psi}(\mathbf{r}_2) \hat{\Psi}(\mathbf{r}_1) \right\} \\ &\quad + \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \hat{\Psi}^\dagger(\mathbf{r}_1) \hat{\Psi}^\dagger(\mathbf{r}_2) \hat{V}_{\text{mod}}(\mathbf{r}_1 - \mathbf{r}_2) \hat{\Psi}(\mathbf{r}_2) \hat{\Psi}(\mathbf{r}_1). \end{aligned} \quad (14)$$

The term associated with  $\hat{V}_{\text{mod}}$  can be simplified in the two-body center-of-mass frame [ $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ ,  $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ ], in which  $\hat{H}_{\text{mod}}$  takes the form

$$\begin{aligned} \hat{H}_{\text{mod}} &= \frac{1}{4} g_2 \int d\mathbf{R} \int d\mathbf{r} \hat{\Psi}^\dagger\left(\mathbf{R} + \frac{\mathbf{r}}{2}\right) \hat{\Psi}^\dagger\left(\mathbf{R} - \frac{\mathbf{r}}{2}\right) [\delta(\mathbf{r}) \nabla_{\mathbf{r}}^2 \\ &\quad + \nabla_{\mathbf{r}}^2 \delta(\mathbf{r})] \hat{\Psi}\left(\mathbf{R} - \frac{\mathbf{r}}{2}\right) \hat{\Psi}\left(\mathbf{R} + \frac{\mathbf{r}}{2}\right). \end{aligned} \quad (15)$$

After integrating over  $\mathbf{r}$  and some integrations by parts,  $\hat{H}_{\text{mod}}$  can be written as

$$\hat{H}_{\text{mod}} = \frac{1}{4} g_2 \int d\mathbf{R} \hat{\Psi}^\dagger(\mathbf{R}) [\nabla^2 (\hat{\Psi}^\dagger(\mathbf{R}) \hat{\Psi}(\mathbf{R}))] \hat{\Psi}(\mathbf{R}). \quad (16)$$

Note that the Laplacian operator operates only on the

number-density operator  $\hat{\Psi}^\dagger(\mathbf{R})\hat{\Psi}(\mathbf{R})$ . Simplification of  $\hat{H}_{\text{MF}}$  follows the usual procedure, and leads finally to

$$\begin{aligned} \hat{H} = & \int d\mathbf{R} \hat{\Psi}^\dagger(\mathbf{R}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{R}) \right] \hat{\Psi}(\mathbf{R}) \\ & + \frac{1}{2} \int d\mathbf{R} \hat{\Psi}^\dagger(\mathbf{R}) \left[ g(\hat{\Psi}^\dagger(\mathbf{R})\hat{\Psi}(\mathbf{R})) \right. \\ & \left. + \frac{1}{2} g_2 \nabla^2 (\hat{\Psi}^\dagger(\mathbf{R})\hat{\Psi}(\mathbf{R})) \right] \hat{\Psi}(\mathbf{R}). \end{aligned} \quad (17)$$

From this Hamiltonian, both the static and the dynamic properties of a many-atom Bose system can be studied. We focus here on the ground-state energy of the system.

Ignoring both quantum fluctuation and  $\hat{H}_{\text{mod}}$ , Eq. (17) leads to the standard GP energy functional

$$E_{\text{GP}}[\Phi] = \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla\Phi|^2 + V_{\text{ext}}(\mathbf{r})|\Phi|^2 + \frac{1}{2}g|\Phi|^4 \right], \quad (18)$$

which corresponds to a time-independent GP equation for the ground-state wave function with a chemical potential  $\mu$ ,

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g|\Phi|^2 \right] \Phi(\mathbf{r}) = \mu\Phi(\mathbf{r}). \quad (19)$$

Inclusion of the lowest-order term due to quantum fluctuation leads to an energy functional [6,16]

$$\begin{aligned} E_{\text{MGPI}}[\Phi] = & \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla\Phi|^2 + V_{\text{ext}}(\mathbf{r})|\Phi|^2 + \frac{1}{2}g|\Phi|^4 \right. \\ & \left. \times \left( 1 + \frac{128}{15} \frac{1}{\sqrt{\pi}} a^{3/2} |\Phi| \right) \right], \end{aligned} \quad (20)$$

where the extra term due to quantum fluctuation was first derived by Lee, Huang, and Yang [16], and will be called the LHY term. This functional corresponds to a modified GP equation that we call MGPI [6,7],

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g|\Phi|^2 + g_1|\Phi|^3 \right] \Phi(\mathbf{r}) = \mu\Phi(\mathbf{r}), \quad (21)$$

where

$$g_1 = g \frac{32}{3\sqrt{\pi}} a^{3/2}. \quad (22)$$

Inclusion of both quantum fluctuation and  $\hat{H}_{\text{mod}}$  to the lowest order leads to an energy functional

$$\begin{aligned} E_{\text{MGPII}}[\Phi] = & \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla\Phi|^2 + V_{\text{ext}}(\mathbf{r})|\Phi|^2 + \frac{1}{2}g|\Phi|^4 \right. \\ & \left. + \frac{2}{5}g_1|\Phi|^5 + \frac{1}{4}g_2|\Phi|^2 \nabla^2(|\Phi|^2) \right]. \end{aligned} \quad (23)$$

The corresponding modified GP equation, which we call MGPII, is

$$\begin{aligned} & \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g|\Phi|^2 + g_1|\Phi|^3 + \frac{g_2}{2} \nabla^2(|\Phi|^2) \right] \Phi(\mathbf{r}) \\ & = \mu\Phi(\mathbf{r}). \end{aligned} \quad (24)$$

MGPII incorporates the shape dependence on the interaction potential through the effective range  $r_e$ . This additional parameter does not, however, add much extra complexity to the theory, as  $r_e$  and  $a$  are generally related. For a hard-sphere potential [ $V(r) = \infty$  for  $r \leq a$ ,  $V(r) = 0$  for  $r > a$ ], we have the well-known relation

$$r_e = (2/3)a. \quad (25)$$

For atoms with a long-range van der Waals interaction [ $V(r) \rightarrow -C_6/r^6$  for  $r \rightarrow \infty$ ],  $r_e$  can be determined from  $a$  by [12]

$$r_e/\beta_6 = \left( \frac{2}{3x_e} \right) \frac{1}{(a/\beta_6)^2} \{ 1 + [1 - x_e(a/\beta_6)]^2 \}, \quad (26)$$

where  $\beta_6 = (mC_6/\hbar^2)^{1/4}$  is a length scale associated with the van der Waals interaction, and  $x_e \equiv [\Gamma(1/4)]^2/(2\pi)$ . Similar relations for other long-range potentials should also exist, an assertion that can be deduced from a more general QDT consideration [13].

The physical meaning of the correction due to  $\hat{H}_{\text{mod}}$  can be better understood by estimating the order of magnitude of each term in Eq. (23) or (24). Consider a system of  $N$  bosons confined to a length scale  $L_0$ . The order of magnitude for the number density is  $n \sim N/(L_0)^3$ . Let  $\epsilon_{\text{MF}} \sim na^3(\hbar^2/2m) \times (1/a)^2$  to represent the energy per particle due to the mean field. It is easy to show that the LHY quantum fluctuation term is of the order of  $\epsilon_{\text{LHY}} \sim \epsilon_{\text{MF}}(na^3)^{1/2}$ , while the  $\hat{H}_{\text{mod}}$  term is of the order of  $\epsilon_{\text{mod}} \sim \epsilon_{\text{MF}}(a/L_0)^2$ . It is thus clear that the two corrections are of different origin. The  $\hat{H}_{\text{mod}}$  correction has an order of magnitude that is determined primarily by the strength of confinement. It depends also on the shape of the interaction potential through  $g_2$  and  $r_e$ . We will call this correction the shape-dependent confinement correction. It is a new source of shape dependence that is absent in a homogeneous system ( $L_0 \rightarrow \infty$  with  $n$  being fixed). In this regard, it differs substantially from the shape dependence that can come at higher densities from a two-body correlation at shorter length scales [8,17].

A further comparison of the magnitudes of the LHY and the shape-dependent confinement corrections reveals other interesting features. From the estimates above, we have  $\epsilon_{\text{mod}}/\epsilon_{\text{LHY}} \sim (a/L_0)^2/(na^3)^{1/2} \sim (a/L_0)^{1/2}/N^{1/2}$ . This means, for instance, that relative to the LHY correction, the shape-dependent confinement correction is more important for small  $N$  than for large  $N$ , a point that will be further demonstrated numerically.

We have chosen, up to this point, a formulation that most closely parallels the standard GP formulation [1,2]. For a small particle number  $N$ , a number-conserving Hartree-Fock

formulation is in fact more appropriate [2,18]. The corresponding results are easily derived. For example, at the level of MGPII, we have

$$\begin{aligned}
 E_{\text{MGPII}}[\phi] = & N \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla \phi|^2 + V_{\text{ext}}(\mathbf{r}) |\phi|^2 + \frac{1}{2} g \right. \\
 & \times (N-1) |\phi|^4 + \frac{2}{5} g_1 (N-1)^{3/2} |\phi|^5 + \frac{1}{4} g_2 \\
 & \left. \times (N-1) |\phi|^2 \nabla^2 (|\phi|^2) \right] \quad (27)
 \end{aligned}$$

and

$$\begin{aligned}
 \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g(N-1) |\phi|^2 + g_1 (N-1)^{3/2} |\phi|^3 \right. \\
 \left. + \frac{g_2}{2} (N-1) \nabla^2 (|\phi|^2) \right] \phi(\mathbf{r}) = \mu \phi(\mathbf{r}), \quad (28)
 \end{aligned}$$

where  $\phi$  is normalized according to  $\int d\mathbf{r} |\phi|^2 = 1$ . It is the Hartree-Fock formulation that we actually implement in our numerical calculations, but the difference is small for large  $N$  (between  $N$  and  $N-1$ ). Setting  $g_2$ , or both  $g_2$  and  $g_1$ , to zero in Eqs. (27) and (28) leads to the Hartree-Fock results in MGPI and GP, respectively.

### III. NUMERICAL RESULTS

We present here our numerical results for the ground-state energy of a BEC in different approximations. They are obtained using an imaginary time evolution method with alternating-direction implicit (ADI) algorithm [19]. The code has been tested by reproducing the GPE results of Ref. [20].

#### A. Results for hard spheres

A many-body system of hard spheres is an ideal test ground for various theoretical models, as accurate results for its ground-state energy are available from DMC calculations for both homogeneous [21] and inhomogeneous cases [7].

Figure 1 shows the relative differences of the energy functional between the GP and DMC for  $N$  bosons in a spherical harmonic trap characterized by a length scale  $L_0 = \sqrt{\hbar/2m\omega}$ . It is clear from these results that the ground-state energy of the system can differ substantially from those predicted by the GP theory, for either strong confinement (large  $a/L_0$ ) and/or high density (large  $N$ ).

As shown in Ref. [7], most of these differences, at least for the range of parameters considered, can be accounted for by the LHY quantum fluctuation correction [16], at a level corresponding to MGPI. This is illustrated in Fig. 2(a). In the same figure, it is also shown that a consistently better agreement with DMC is achieved by MGPII, which includes the shape dependent confinement correction. This means that of the remaining difference between MGPI and DMC, at least part of it is shape-dependent and requires a better description of atom-atom interaction. Note that in the case of hard spheres,  $g_2$  is always positive. The sign of the shape-

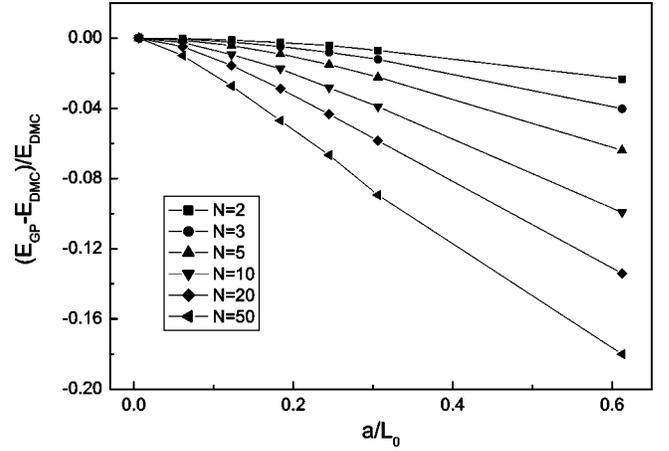


FIG. 1. Relative differences between ground-state energies predicted by the GP theory and by diffusion Monte Carlo calculations [7]. The results are for  $N$  bosons in a spherically symmetric trap of size  $L_0 = \sqrt{\hbar/2m\omega}$ . Here  $a$  is the scattering length.

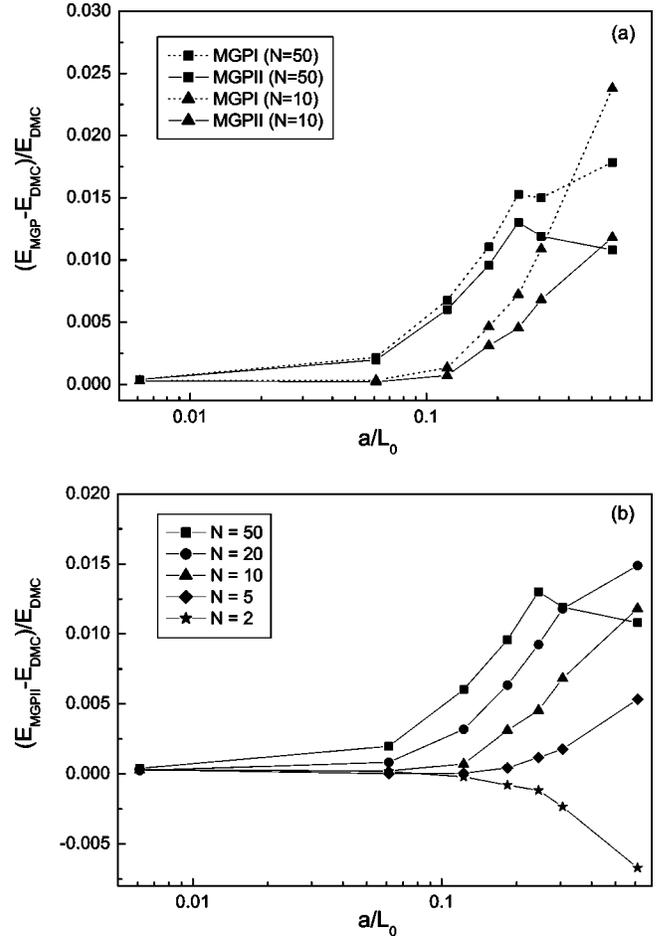


FIG. 2. Relative differences between ground-state energies predicted by modified GP theories and by diffusion Monte Carlo calculations [7]. (a) A sample comparison of MGPI and MGPII, both of which lead to much better results than the GP theory. (b) More results of MGPII. Note that the y scale of these figures are about a factor of ten smaller than that of Fig. 1.

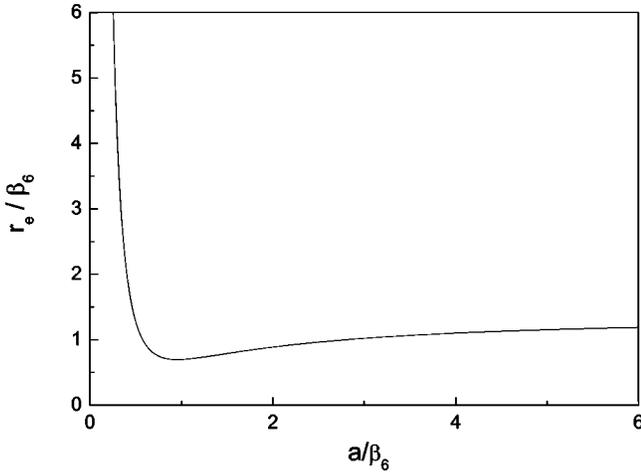


FIG. 3. The universal relationship between  $r_e/\beta_6$  and  $a/\beta_6$  for atoms with a long-range van der Waals interaction [12].

dependent confinement correction is then determined by the expectation value of  $\nabla^2(|\phi|^2)$ , which is negative for the ground state.

More results of MGPII are presented in Fig. 2(b). It shows that at the level of MGPII, the relative difference from DMC has been reduced from up to 20% for the GP theory (see Fig. 1) to less than 2% for the range of parameters considered.

### B. Results for atoms with van der Waals interaction

With the introduction of  $\hat{H}_{\text{mod}}$ , the ground-state energy becomes dependent upon the shape of the long-range potential through the relationship between  $r_e$  and  $a$ . For atoms with the van der Waals interaction,  $r_e$  and  $a$  are related by Eq. (26). Figure 3 is a graphic illustration of this relation. Note that  $r_e$  diverges for  $a=0$ , corresponding to the fact that in this particular case, the energy dependence of the scattering amplitude around zero energy cannot be described by an effective-range expansion [22]. Also note that unlike the case of hard spheres, the  $g_2$  for a van der Waals potential may become negative for sufficiently small  $a/\beta_6$ . Consequently, the shape-dependent confinement correction to the ground-state energy may, in principle, be positive. (Both points suggest that something interesting happens around  $a=0$  that may deserve a separate investigation.)

Figure 4(a) gives a comparison of ground-state energies predicted by MGPII and by the GP theory for a realistic experimental configuration. Specifically, it is for a  $^{85}\text{Rb}$  condensate in a cylindrical trap with an aspect ratio of  $\varepsilon = 6.8/17.5$  [23]. A  $C_6$  value of 4698 a.u. is used [24]. It shows that deviations from the GP theory can become substantial for either high density and/or strong confinement. With the tunability of the scattering length via a Feshbach resonance [23], such many-body effects beyond the GP theory may soon become observable. Figure 4(b) shows more explicitly the shape-dependent confinement correction. Its magnitude increases with  $a/L_0$ , as expected. For a fixed  $a/L_0$ , its relative contribution is more significant for small  $N$  than for large  $N$ , consistent with our earlier discussion. The corrections are mostly negative (except for very small  $a$ ),

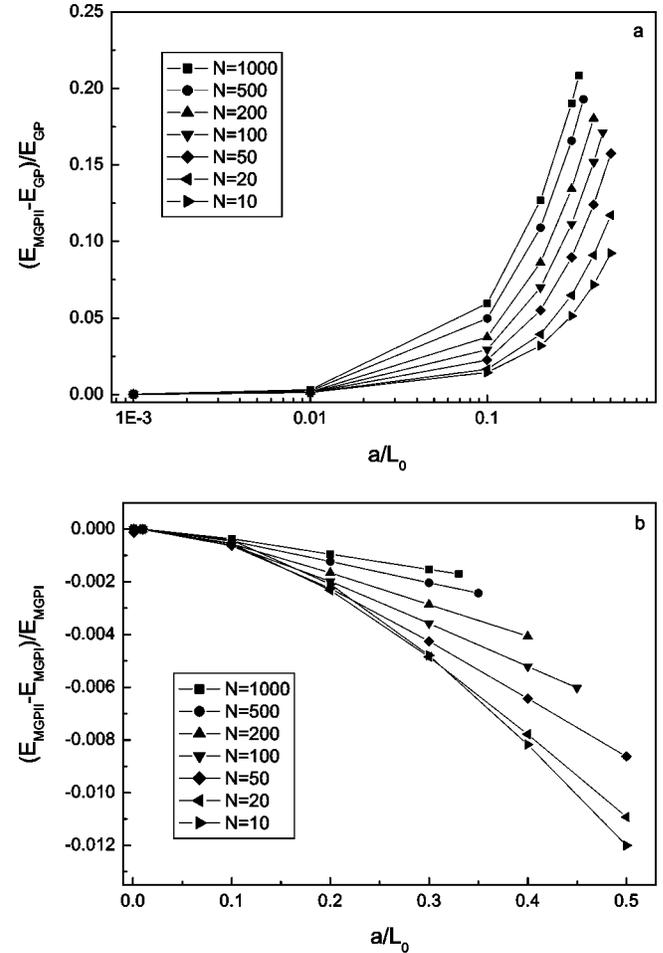


FIG. 4. (a) Relative differences between ground-state energies predicted by MGPII and by the GP theory for a  $^{85}\text{Rb}$  condensate in a cylindrical trap of aspect ratio  $\varepsilon = 6.8/17.5$ . Here  $L_0$  is defined by the transverse frequency:  $L_0 = \sqrt{\hbar/2m\omega_{\perp}}$ . (b) Relative contribution from the shape-dependent confinement correction.

since  $g_2$  is greater than zero for most of the data points shown. (Because  $L_0 = 34\,850$  a.u. is much greater than  $\beta_6 = 164.2$  a.u., most of the data points correspond to  $a/\beta_6 \gg 1$ . The  $r_e$  is then approximately a constant  $r_e \approx (3\pi)^{-1}[\Gamma(1/4)]^2\beta_6$ , and the corresponding  $g_2$ 's are positive.)

### IV. CONCLUSION

In conclusion, an effective interaction and the corresponding modified GP equation have been proposed that take into account the energy dependence of the two-body scattering amplitude through an effective-range expansion. The resulting theory, called MGPII, leads to better agreements with diffusion Monte Carlo calculations [7] than either the GP theory, or MGPI that considers only the quantum fluctuation correction. The theory expands, considerably, the parameter space (specified by  $na^3$  and  $a/L_0$ ), in which a GP type of formulation can be applied. It introduces the concept of shape-dependent confinement correction and shows that for a fixed confinement, its relative contribution is more significant for small  $N$  than for large  $N$ .

Finally, we point out that both MGPI and MGPII are perturbative expansions around the GP theory. They will eventually fail for sufficiently large  $na^3$  and/or sufficiently strong confinement. For high density, the shape dependence of a different origin will eventually emerge from two-body correlations at short length scales [8,17]. For strong confinement, the local-density approximation, implicit in both MGPI and MGPII, will eventually fail. Exploration into those regimes will require theories that differ much more substantially from the GP formulation.

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