Improved large-N limit for Bose-Einstein condensates from perturbation theory

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We present a perturbation solution of a model Bose-Einstein Hamiltonian derived by Bohn, Esry, and Greene. In our solution we use $1/N$ as the perturbation parameter, where N is the number of particles in the condensate. Ground-state energies are reported for parameters approximating the Joint Institute for Laboratory Astrophysics ^{87}Rb experiments. We predict the critical number of atoms with negative scattering lengths that can be trapped using the effective trap frequency of the first-order equation. The $N\rightarrow\infty$ perturbation limit, which retains a single term beyond the conventional Thomas-Fermi limit, gives ground-state energies that agree to three digits with converged results, thus providing a much improved limit for large N. [S1050-2947(99)00305-4]

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I. INTRODUCTION

Using ordinary Schrödinger quantum mechanics, Bohn, Esry, and Greene [1] have derived effective potentials for dilute Bose-Einstein condensates. The many-atom problem is reduced to a linear Schrödinger equation by identifying a single coordinate, R, the mean condensate radius. Bohn *et al.* use hyperspherical coordinates to define R, expand in hyperspherical harmonics, and then retain only a single term in this expansion. They refer to this as the ''K-harmonic'' approximation following terminology from nuclear theory. The resulting one-dimensional linear Schrödinger equation gives quite good results for ground-state energies in a trap roughly approximating the JILA ^{87}Rb experiments [2], faring slightly better than other variational approaches. Their effective potential is also able to predict reasonably well the critical number of bosons with negative scattering lengths that can be condensed, as well as other characteristics of the condensate such as low-lying excitation frequencies, peak densities, and decay rates from two- and three-body processes.

We chose this model Hamiltonian to test a perturbation formalism which uses $1/N$ as the perturbation parameter, where N is the number of particles in the condensate. This formalism is analogous to the dimensional perturbation methods used successfully in many areas of physics [3–8]. In particular, we use a matrix method developed for atomic systems to solve the perturbation equation [9]. We find that this perturbation approach takes advantage of the simplicity of the Thomas-Fermi limit which is valid for N large, but improves on this limit significantly for the zeroth-order starting point by including a single additional term beyond Thomas-Fermi.

II. FORMALISM

The derivation of Bohn *et al.* begins with the full N-body Hamiltonian:

$$H=-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2+\sum_{i=1}^{N}\frac{1}{2}m\omega^2 r_i^2+\sum_{i<j}^{N}U_{\rm int}(\vec{r}_i-\vec{r}_j), \quad (1)$$

where $U_{\rm int}$ is the two-body atomic interaction potential. All three-body and higher interactions are ignored under the assumption of a dilute gas. The mean condensate radius of the atoms from the trap center is

$$R=\left(\frac{1}{\sum_{i=1}^{N}m_i}\sum_{i=1}^{N}m_i r_i^2\right)^{1/2}=\left(\frac{1}{N}\sum_{i=1}^{N}r_i^2\right)^{1/2}, \quad (2)$$

where we assume all the particles in the condensate are identical. The remaining $3N-1$ coordinates are then given in terms of hyperangles collectively denoted by Ω [10]. Using the transformation $(\vec{r}_1,\ldots,\vec{r}_N)\rightarrow(R,\Omega)$ and assuming $U_{\rm int}(\vec{r}_1-\vec{r}_2)=(4\pi\hbar^2 a/m)\delta(\vec{r}_1-\vec{r}_2)$, where a is the s-wave scattering length, yields a transformed Schrödinger equation:

$$\left\{-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial R^2}-\frac{(3N-1)(3N-3)}{4R^2}-\frac{\Lambda^2}{R^2}\right)+\frac{1}{2}M\omega^2R^2+\sum_{i<j}^{N}\frac{4\pi\hbar^2 a}{m}\delta(\vec{r}_i-\vec{r}_j)-E\right\}R^{(3N-1)/2}\psi(R,\Omega)=0, \quad (3)$$

where Λ^2 is a ''grand angular momentum operator'' [11]. Expanding in hyperspherical harmonics and retaining a single term results in the final equation

$$\left\{-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial R^2}+V_{\rm eff}^{\rm Bohn}(R)-E\right\}F(R)=0, \quad (4)$$

where

$$V_{\rm eff}^{\rm Bohn}=\frac{\hbar^2}{2M}\frac{(3N-1)(3N-3)}{4R^2}+\frac{1}{2}M\omega^2R^2+\zeta\sqrt{\frac{1}{2\pi}}\frac{\hbar^2 aN^2(N-1)}{MR^3}, \quad (5)$$

$$\zeta = \frac{\Gamma(3N/2)}{\Gamma((3N-3)/2)N^{3/2}}. \tag{6}$$

is the effective potential. Bohn and co-workers solve this equation numerically using a *B*-spline approach.

In our solution of this equation we use a perturbation approach where $1/N$ is the perturbation parameter. We transform the equation using scalings that give a stable $N\to\infty$ limit:

$$R = N^2\hat{R}, \quad \omega = N^{-4}\hat{\omega}, \quad a = N\hat{a}, \quad E = N^{-3}\epsilon,$$

and then change to scaled oscillator units: $\hat{R} = \sqrt{(\hbar/m\hat{\omega})}\overline{R}$, $\hat{\epsilon} = \hbar\hat{\omega}\overline{\epsilon}$, which yields

$$\left\{ -\frac{1}{2}\delta^2\frac{\partial^2}{\partial\overline{R}^2} + \left(\frac{(9-12\delta+3\delta^2)}{8\overline{R}^2}\right) + \frac{1}{2}\overline{\omega}^2\overline{R}^2 + \zeta\frac{\hat{a}}{\sqrt{2\pi}}\sqrt{\frac{m\hat{\omega}}{\hbar}}\frac{(1-\delta)}{\overline{R}^3} - \overline{\epsilon}\right\}\hat{\Phi}(\overline{R}) = 0, \tag{7}$$

where $\delta = 1/N$ and $\overline{\omega} = 1$ in scaled oscillator units. To obtain a zeroth-order starting point we let $N\to\infty$, i.e., $\delta\to 0$. In this limit the derivative term and part of the centrifugal potential drop out and the problem reduces to finding the minimum of the effective potential, $V^{\infty}_{\rm eff}$:

$$[V^{\infty}_{\rm eff}(\overline{R}_m) - \overline{\epsilon}]\hat{\Phi}(\overline{R}_m) = 0, \tag{8}$$

$$V^{\infty}_{\rm eff}(\overline{R}) = \frac{9}{8\overline{R}^2} + \frac{1}{2}\overline{\omega}^2\overline{R}^2 + \frac{\lambda}{\overline{R}^3}, \tag{9}$$

$$\lambda = \frac{\zeta\hat{a}}{\sqrt{2\pi}}\sqrt{\frac{m\hat{\omega}}{\hbar}} = \frac{N\zeta a}{\sqrt{2\pi}}\sqrt{\frac{m\omega}{\hbar}}. \tag{10}$$

Note that this effective potential retains an additional term, $9/(8\overline{R}^2)$, compared to the Thomas-Fermi limit of Eq. (4). This additional term comes from the centrifugal part of the effective potential which originates in the kinetic energy. The Thomas-Fermi limit of Eq. (4) drops the entire kinetic energy including the centrifugal potential. Note also that all the terms in Bohn's effective potential are included at least in part. The importance of including a term from the centrifugal potential is obvious from Fig. 1, where we compare our $N\to\infty$ effective potential, $V^{\infty}_{\rm eff}$, for $a<0$ and $a>0$ to the Thomas-Fermi limit of Bohn's potential using the same values of a. In contrast to the Thomas-Fermi potential, our $V^{\infty}_{\rm eff}$ retains the correct features for both positive and negative scattering lengths. For $a>0$, $V^{\infty}_{\rm eff}$ gains a repulsive contribution from the interaction term increasing the strength of the effective trap, compared to the Thomas-Fermi limit, which is too deep. For $a<0$, the competition between the positive centrifugal term, $9/8\overline{R}^2$, and the negative term, $\lambda/\overline{R}^3$, which contains the negative scattering length, creates a potential barrier for small $\overline{R}$ and a metastable well in our $V^{\infty}_{\rm eff}$, while for the Thomas-Fermi potential no metastable region exists.

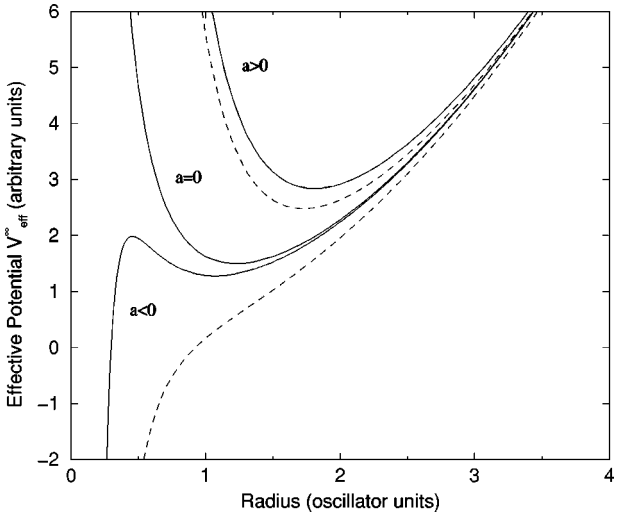

FIG. 1. Comparison of $V^{\infty}_{\rm eff}$ for different values of the scattering length, a. The solid lines are our $N\to\infty$ effective potential, $V^{\infty}_{\rm eff}$, for $a>0$, $a=0$, and $a<0$. The short dashed lines are the Thomas-Fermi limit of the Bohn potential for $a>0$ and $a<0$.

Equation (9) can be solved for the $\overline{R}=\overline{R}_m$ which yields the minimum energy $\overline{\epsilon}_{\infty} = V^{\infty}_{\rm eff}(\overline{R}_m)$. The perturbation series is then generated by defining a scaled displacement coordinate, r, by $\overline{R} = \overline{R}_m + \delta^{1/2}r$ and expanding,

$$\hat{\Phi}(r) = \sum_{j=0}^{\infty}\hat{\phi}_j(r)\delta^{j/2}, \quad \overline{\epsilon} = \overline{\epsilon}_{\infty} + \delta\sum_{j=0}^{\infty}\epsilon_{2j}\delta^j. \tag{11}$$

The first-order equation in δ is harmonic:

$$\left\{ -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{1}{2}\omega^2_{\rm eff}r^2 + v_0\right\}\hat{\phi}_0(r) = \epsilon_0\hat{\phi}_0(r), \tag{12}$$

$$\epsilon_0 = (\nu + \tfrac{1}{2})\omega_{\rm eff} + v_0, \tag{13}$$

$$\hat{\phi}_0(r) = (\omega_{\rm eff})^{1/4}h_{\nu}(\omega^{1/2}_{\rm eff}r), \tag{14}$$

where

$$v_0 = -\frac{3}{2\overline{R}^2_m} - \frac{\lambda}{\overline{R}^3_m}, \tag{15}$$

$$\omega^2_{\rm eff} = \frac{27}{4\overline{R}^4_m} + \frac{12\lambda}{\overline{R}^5_m} + \overline{\omega}^2, \tag{16}$$

and h_{ν} is a harmonic-oscillator solution. This equation defines the harmonic basis functions that are used to solve the higher-order equations. Note that the harmonic frequency, $\omega_{\rm eff}$ [Eq. (16)], automatically adapts as the trap frequency and/or scattering length changes, essentially folding these interactions into an effective trap. Thus this first-order equation provides basis functions that are sensitive to the interplay between the trap frequency, ω and the scattering length, a. For $a<0$, $\omega^2_{\rm eff}$ shows the gradual ''softening'' of the effective trap, $\frac{1}{2}\omega^2_{\rm eff}r^2$, due to the attractive potential, $\lambda/\overline{R}^3$, which increases as N increases [see Eqs. (9) and (10)]. As the

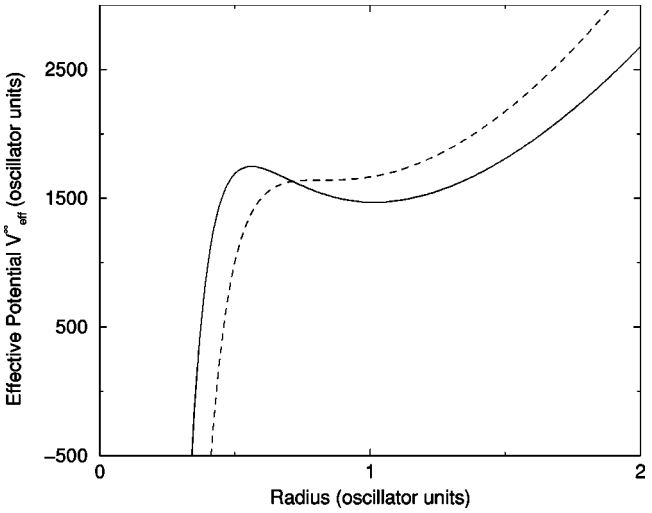

FIG. 2. Plots of our $N\rightarrow\infty$ effective potential, $V^{\infty}_{\rm eff}$, for $a=-27.3$ bohr and $\nu=144.6$ Hz. The solid curve represents the case where the number of particles, N, is just less than the critical number, N_c. The dashed curve shows the case where $N>N_c$ resulting in no metastable region.

metastable well slowly disappears, the minimum and maximum of $V^{\infty}_{\rm eff}$ coincide in an inflection point where $\partial^2 V^{\infty}_{\rm eff}/\partial\overline{R^2}=0$. This occurs at $R_c=(1/5)^{1/4}(3/2)^{1/2}$ and corresponds to $\omega^2_{\rm eff}=0$ (since $\omega^2_{\rm eff}=\partial^2 V^{\infty}_{\rm eff}/\partial\overline{R^2}$), i.e., no effective trap exists. The resulting critical number, N_c, of negative scattering length atoms that can be trapped is found to be

$$N_c=0.671\sqrt{\frac{\hbar}{m\omega}}\frac{1}{|a|}, \tag{17}$$

which is the same N_c obtained by Bohn *et al.* from his effective potential. (This is not unexpected since Bohn *et al.* assume that $N\gg 1$ in their alternative derivation of N_c [see Ref. [1], Eq. (4.4)].) This result is also in excellent agreement with the results obtained from several variational treatments [13–16]. Figure 2 shows the change in our $V^{\infty}_{\rm eff}$ as the number of particles changes from slightly below N_c to slightly above this value. (For this graph we use trap parameters that approximate the ^{7}Li experiments at Rice University [12].)

Higher-order terms bring in coupling between the higher-order terms in the centrifugal potential and the atomic interaction term. The external harmonic trap is included entirely in the first-order harmonic equation.

The infinite set of differential equations for the $\hat{\phi}_j(r)$ and the ϵ_{2j} are computed using a linear algebraic method that expands the $\hat{\phi}_j(r)$ in terms of the harmonic-oscillator functions h_ν and represents the displacement coordinate r as a matrix in this basis. A recursion relation yields the wave function and energy coefficients [9].

III. RESULTS AND DISCUSSION

Our results for this one-dimensional problem using values of $a=100$ bohr and $\nu=200$ Hz, roughly approximating the JILA ^{87}Rb experiments [2], are extremely encouraging. Our converged results, of course, compare quite well to the results of Bohn *et al.*, agreeing to five digits. (See Table I.) Table I also compares our zeroth-order results to converged results. The agreement is striking. Our zeroth-order results agree to three or four digits with the converged results (100.02% of the converged value). The Thomas-Fermi results, which are obtained from the effective Hamiltonian of Bohn *et al.* [see Eq. (4)] by dropping the full kinetic energy including the centrifugal potential, and finding the minimum of the remaining potential, are 45% of the converged results at $N=500$, improving to 97% agreement at $N=10\,000$. (Bohn *et al.* compare their results to the results from the Gross Pitaevskii equation as well as to the Thomas-Fermi limit of the Gross Pitaevskii equation. See Ref. [1], Fig. 2.) Our zeroth-order equation retains just a single additional term beyond the Thomas-Fermi limit of the Schrödinger equation used by Bohn *et al.*, a term from the centrifugal potential. This is an impressive improvement over Thomas-Fermi since the zeroth-order perturbation term is obtained from a trivial calculation. The first-order term brings in the interplay between the trap and the interatomic interaction term and adds two more decimal places of accuracy. Table II shows the extremely rapid convergence to five or six digits by first order and ten or more digits by sixth order for three condensates. This is obtained by a simple summing of the

TABLE I. Results for ground-state energies in oscillator units, tabulated in the form $E/N-\frac{3}{2}\hbar\omega$ for a condensate with $a=100$ bohr and $\nu=200$ Hz. We compare our zeroth-order and our converged results (10th order) to the results of Bohn *et al.* We also compare the Thomas-Fermi limit of the effective Hamiltonian of Bohn *et al.* to our zeroth-order results.

N	TF limit of Eq. (4)	Zero order	Converged	Bohn *et al.*
500	0.37509	0.83749	0.83732	0.83732
1000	0.97643	1.33807	1.33784	1.33783
2000	1.76914	2.04852	2.04828	2.04827
3000	2.34534	2.58465	2.58443	2.58441
4000	2.81462	3.02877	3.02857	3.02855
5000	3.21766	3.41402	3.41382	3.41380
6000	3.57472	3.75759	3.75741	3.75738
7000	3.89759	4.06975	4.06958	4.06955
8000	4.19382	4.35719	4.35702	4.35700
9000	4.46857	4.62454	4.62439	4.62436
10000	4.72555	4.87518	4.87503	4.87500

TABLE II. Partial sums for the ground-state energy using $a=100$ bohr and $\nu=200$ Hz for condensates with 500 particles, 5000 particles, and 10 000 particles in oscillator units, tabulated in the form $E/N-\frac{3}{2}\hbar\omega$.

Order	$N=500$	$N=5000$	$N=10\,000$
0	0.837 487 821 79	3.414 016 707 69	4.875 183 724 38
1	0.837 324 621 72	3.413 825 082 25	4.875 032 178 85
2	0.837 323 748 09	3.413 824 807 49	4.875 032 077 37
3	0.837 323 665 36	3.413 824 805 36	4.875 032 076 83
4	0.837 323 663 03	3.413 824 805 33	4.875 032 076 83
5	0.837 323 662 93	3.413 824 805 33	4.875 032 076 83
6	0.837 323 662 93	3.413 824 805 33	4.875 032 076 83

series rather than Padé summation reflecting the excellence of the zeroth-order starting point. We obtain similar agreement with the excitation energies of Bohn *et al.* (See Ref. [1], Fig. 3.) By first order our results agree to four or more digits with the converged results of Bohn *et al.* [17].

Our $V_{\rm eff}^{\infty}$ potential is quite similar in form to several other effective potentials [13–16] in the literature, which have been obtained using variational approaches. Our method, which is based on a rigorous perturbation analysis of the Hamiltonian with a perturbation parameter of $1/N$, offers the possibility of systematic improvement by including higher-order terms.

IV. CONCLUSIONS

For the model Bose-Einstein Hamiltonian of Bohn, Esry, and Greene, this perturbation theory treats the physics in a very advantageous way. The zeroth-order term takes advantage of the Thomas-Fermi limit to simplify the solution for large N, but improves on this limit by retaining a term from the centrifugal potential which stabilizes the $N\rightarrow\infty$ limit. The first-order equation is harmonic with a frequency that reflects not only the trap frequency but also the interatomic interaction.

The harmonic-oscillator basis set (obtained from the first-order equation) is expanded about the point R_m which is the minimum of the $N\rightarrow\infty$ effective potential, $V_{\rm eff}^{\infty}$. This value of R_m is thus sensitive to the balance between the trap potential and the interatomic potential [see Eq. (9)]. For example, for the case of no interaction between the particles ($a=0$), $\overline{R}_m=\sqrt{3/2}$ (in oscillator units), which is the value of the uncertainty, ΔR, for the ground state of a harmonic oscillator. $V_{\rm eff}^{\infty}$ at this minimum is $\frac{3}{2}\hbar\omega$ corresponding to an ideal Bose condensate. For $a>0$, $\overline{R}_m>\sqrt{3/2}$, due to the repulsive interaction of the particles with a positive scattering length while for $a<0$, $\overline{R}_m<\sqrt{3/2}$, due to the attractive interaction of the particles with a negative scattering length. Thus, the basis set is not only chosen with a frequency that is responsive to both the trap frequency and the scattering length, but this basis set is also expanded about a point, R_m, which adjusts to changes in these two parameters.

The zeroth-order energy, E_0, is quite close to the converged result reflecting the excellent starting point provided by the $N\rightarrow\infty$ effective potential which retains terms from all parts of the full effective potential.

Most importantly, this $1/N$ perturbation approach suggests that a new $N\rightarrow\infty$ limit, which retains part of the kinetic energy, will provide a much improved limit over the conventional Thomas-Fermi limit. The extension of this approach to the Gross-Pitaevskii equation is planned.

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