Fermi pseudopotential approximation: Two particles under external confinement

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In this paper we calculate the energy levels of two trapped atoms interacting through a spherical two-body potential $V(r)$ under external confinement quantum mechanically. We then replace $V(r)$ by either a regularized *energy-independent* or an *energy-dependent* δ-function potential. A comparison shows that the use of an *energy-dependent* pseudopotential improves significantly upon the use of an *energy-independent* pseudopotential. The accuracy of the pseudopotential approximation is approximately determined by the ratio $\beta_6/a_{\rm ho}$, where β_6 and $a_{\rm ho}$ denote the characteristic length scale of the two-body interaction potential $V(r)$ and of the trapping potential, respectively.

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Recently, the experimental realization of Bose-Einstein condensation (BEC) of atomic vapors [1] has led to a revival of Fermi's pseudopotential treatment. The theoretical description of these weakly interacting atomic gases is commonly based on the mean-field Gross-Pitaevskii equation [2], which can be derived through a perturbative treatment in the small gas parameter na_0^3 (where n is the gas density and a_0 is the zero-energy s-wave scattering length) [2]. An alternative derivation starts from Schrödinger's number-conserving many-body Hamiltonian [3]. The Gross-Pitaevskii equation then follows assuming an initial Hartree-Fock (HF) state and a two-body Fermi-type contact potential, specifically a *non-regularized* δ-function potential. This contact potential is usually chosen such that it reproduces the two-body zero-energy s-wave scattering length a_0 of the ''true'' interaction potential. This alternative derivation, based on many-body Schrödinger quantum mechanics, leads to essentially the same result as the perturbative low-density treatment, except for a change from N to $N-1$ particles in the interaction parameter. For many purposes, the replacement of the ''true'' two-body interaction potential $V(r)$ by a pseudopotential is a crucial step in connecting mean-field treatments with many-body theory [2–4]. Consequently it is vital to understand the accuracy of pseudopotential approximations and its implications for the description of dilute Bose-condensed gases. Specifically, a detailed understanding of the two-particle system must be in place before applications to many-particle systems can be conducted.

Recently, Tiesinga *et al.* [5] used an *energy-independent regularized* pseudopotential

$$V_0^{(\delta)}(r)=\frac{4\pi\hbar^2 a_0}{m}\,\delta^{(3)}(\vec{r})\,\frac{\partial}{\partial r}r \tag{1}$$

to describe the interaction between two mass m particles confined in an external spherical harmonic trapping potential with trapping frequency $\nu_{\rm ho}$. Here, $\vec{r}$ denotes the distance vector between the two particles, and r the length of this vector. $\delta^{(3)}(\vec{r})$ is a three-dimensional delta function. a_0 is chosen such that the pseudopotential $V_0^{(\delta)}(r)$ has the same zero-energy scattering length a_0 as the ''realistic'' two-body interaction potential $V(r)$. In the study by Tiesinga *et al.* [5], $V(r)$ is given by the interaction potential between two Na atoms ($a_0=33$ Å), and two Cs atoms ($a_0=-370$ Å; this value has recently been refined, see Ref. [6] and Table I), respectively. Through comparison of the eigenvalues for the pseudopotential $V_0^{(\delta)}(r)$ with those for $V(r)$, they document a breakdown of the pseudopotential treatment in the regime where a_0 approaches the characteristic length $a_{\rm ho}$ of the external trapping potential, $a_{\rm ho}=\sqrt{\hbar/(\mu\omega_{\rm ho})}$ with $\mu=m/2$ and $\omega_{\rm ho}=2\pi\nu_{\rm ho}$. The present study revisits the pseudopotential approximation, and shows (i) that the validity regime of the energy-independent pseudopotential approximation is better characterized by the ratio $\beta_6/a_{\rm ho}$ than by $|a_0/a_{\rm ho}|$ [where β_6 is the characteristic length scale for the two-body potential $V(r)$ [7–13]], and (ii) that a pseudopotential with an *energy-dependent* two-body s-wave scattering length a_E leads to a highly improved description of two particles confined in a spherical trap. The energy-dependent s-wave scattering length is defined at nonzero energies by $a_E=-\tan\delta_0(E)/k$, where $k=\sqrt{2\mu E}/\hbar$. a_E approaches the usual scattering length in the limit of zero energy.

Consider two mass m particles interacting through a two-body potential $V(r)$, confined in an external trapping potential, $V_{trap}=m\omega_{\rm ho}^2(r_1^2+r_2^2)/2$. Here, $\vec{r}_1$ and $\vec{r}_2$ denote the position vector (measured with respect to the center of the trap) of atoms 1 and 2, respectively. The spherical symmetry of $V_{trap}(R)$, $\vec{R}=(\vec{r}_1+\vec{r}_2)/2$, and of $V(r)$, allow us to separate out the center-of-mass motion

$$\left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial R^2}+\frac{1}{2}M\omega_{\rm ho}^2R^2\right)\Phi(R)=E^{\rm c.m.}\Phi(R) \tag{2}$$

with eigenenergies $E^{\rm c.m.}=(3/2+n_{\rm c.m.})\hbar\omega_{\rm ho}$, where $n_{\rm c.m.}$ denotes the quantum number of the three-dimensional harmonic oscillator [Eq. (2)], and M denotes the total mass, $M=2m$. Thus, the problem reduces to solving the Schrödinger equation for the radial internal motion

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}+V(r)+\frac{1}{2}\mu\omega_{\rm ho}^2r^2\right]\psi(r)=E^{int}\psi(r). \tag{3}$$

TABLE I. Dispersion coefficient C_6, characteristic length $\beta_6=(2\mu C_6/\hbar^2)^{1/4}$, zero-energy s-wave scattering length a_0, and effective range r_{eff} for $^7Li_2$, $^{23}Na_2$, $^{39}K_2$, $^{85}Rb_2$, $^{87}Rb_2$, and $^{133}Cs_2$ interacting through $a\,^3\Sigma_u^+$ potentials (upper part), and for $^{39}K_2$ and $^{85}Rb_2$ interacting through modified potentials (lower part, see text).

	C_6 (a.u.)	β_6 (a.u.)	a_0 (a.u.)	r_{eff} (a.u.)
$^7Li_2$	1388 [a]	65	−27.3 [b]	530
$^{23}Na_2$	1472 [c]	89	77.3 [d]	62
$^{39}K_2$	3897 [e]	129	−33 [f]	2083
$^{85}Rb_2$	4700 [g]	164	−369 [g]	347
$^{87}Rb_2$	4700 [g]	165	106 [g]	143
$^{133}Cs_2$	6890 [h]	197	2400 [h]	358
M-$^{39}K_2$	3948 [i]	129	−3672	187
$M1$-$^{85}Rb_2$	4700 [j]	164	6162	223
$M2$-$^{85}Rb_2$	4700 [j]	164	10990	226

[a]Reference [28].
[b]Reference [29], analysis of photoassociation experiments on atoms in the $F=2$, $m_F=2$ state.
[c]Reference [28].
[d]Reference [30].
[e]Reference [31].
[f]Reference [32], experimental photoassociation spectroscopy, carried out in conjunction with a detailed theoretical simulation of the experiment.
[g]Reference [27], theoretical analysis of experimental elastic collision data between atoms in the $F=2$, $m_F=-2$ state.
[h]Reference [6], theoretical analysis of Feshbach resonance data for the $F=4$, $m_F=4$ state measured experimentally (see Ref. [33]); for the $F=3$, $m_F=-3$ state, Ref. [6] reports $a_0=-2770$ a.u. Note, the calculations reported in Ref. [5] (see text) use an older potential with a scattering length $a_0=-699$ a.u.
[i]The C_6 coefficient is obtained by multiplying the C_6 value given in Ref. [31] by a factor of 1.013 (see text).
[j]The short range part of the two-body potential $V_{\rm Rb}(r)$ is modified slightly, without changing C_6 from Ref. [27].

Equations (2) and (3) are derived for $L=0$ and $l=0$, where L and l denote the orbital angular momentum for the center of mass and relative motion, respectively. In the following we compare the positive eigenenergies E^{int}, for realistic alkali atom-atom potentials, with those obtained for the energy-independent pseudopotential $V_0^{(\delta)}(r)$ [Eq. (1)], and the energy-dependent pseudopotential $V_E^{(\delta)}(r)$,

$$V_E^{(\delta)}(r)=\frac{4\pi\hbar^2 a_E}{m}\delta^{(3)}(\vec{r})\frac{\partial}{\partial r}r. \tag{4}$$

Table I summarizes characteristic parameters for a series of two-body alkali systems interacting through $a\,^3\Sigma_g^+$ atom-atom potentials, namely, the dispersion coefficient C_6, the characteristic length $\beta_6=(2\mu C_6/\hbar^2)^{1/4}$ [7–13], the zero-energy s-wave scattering length a_0, and the effective range r_{eff}. The upper part of Table I reports these quantities for the two-body systems $^7Li_2$, $^{23}Na_2$, $^{39}K_2$, $^{85}Rb_2$, $^{87}Rb_2$ [14], and $^{133}Cs_2$, while the lower part summarizes these quantities for $^{39}K_2$ and $^{85}Rb_2$ interacting through modified atom-atom potentials. The potential labeled M-$^{39}K_2$ has been obtained by multiplying the K_2 potential by a factor of 1.013. This rescaling leads to a large negative scattering length a_0 for the ^{39}K isotope while changing C_6 and β_6 very little. The potentials labeled by $M1$-$^{85}Rb_2$ and $M2$-$^{85}Rb_2$ have been obtained by modifying the short-range part of the Rb_2 potential, thus leaving C_6 and β_6 unchanged, however, resulting in large positive scattering lengths a_0 for the ^{85}Rb isotope. Similar adjustments of two-body potentials are common in the presence of a Feshbach resonance.

The C_6 parameters are taken from the literature (see Table I caption), as have been the values of a_0 for some systems. For the other systems, we determined a_0 through a scattering calculation. The characteristic length β_6 is determined by the C_6 coefficient and the reduced mass μ, and determines roughly the length scale over which the radial two-body scattering wave function oscillates at zero energy. For distances larger than β_6 the scattering wave function approaches its asymptotic behavior. The effective range r_{eff} has been calculated using an expression derived by Gao [Eqs. (9) and (11) of Ref. [8], where we neglect the second term of Eq. (11), and use a_0 as input]. r_{eff} determines, for example, the energy dependence of the scattering length at low collision energies to first order,

$$-\frac{1}{a_E}\approx-\frac{1}{a_0}+\frac{1}{2}k^2 r_{eff}. \tag{5}$$

For the two-body systems considered in Table I, the absolute value of the scattering length $|a_0|$ varies from 27 a.u. to 10 990 a.u. while the characteristic length β_6 varies over a much smaller range, namely, from 65 a.u. to 197 a.u. The characteristic length β_6 is shown to primarily control the validity of the pseudopotential approximation (see below).

Figure 1(a) depicts the lowest positive eigenenergies E^{int} of Eq. (3) for two ^{39}K particles using the *realistic* K-K interaction potential $V_K(r)$ (the short-range part of the potential is taken from Ref. [15], see also Table I) (dotted lines), the *energy-independent pseudopotential* $V_0^{(\delta)}(r)$ with $a_0=-33$ a.u. (solid lines), and the *energy-dependent pseudopotential* $V_E^{(\delta)}(r)$ (dashed lines) as a function of $a_0/a_{\rm ho}$. For $V_K(r)$ we solve the radial one-dimensional Schrödinger equation, Eq. (3), for the reduced mass of the ^{39}K isotope using B splines. The lowest eigenenergy E^{int} with $E^{int}>0$ depicted in Fig. 1(a) corresponds to the vibrational state with $v=28$ and $l=0$. Note, the quantum number v of the lowest state with energy $E^{int}>0$ depends on the strength $\nu_{\rm ho}$ of the trapping potential, however, v does not change over the parameter range shown in Fig. 1(a). The eigenenergies of Eq. (3) for the energy-independent pseudopotential $V_0^{(\delta)}(r)$ can be found exactly, as solutions of the transcendental Eq. (16) of Ref. [16],

$$\frac{2\Gamma\left(-\frac{E^{int}}{2}+\frac{3}{4}\right)}{\Gamma\left(-\frac{E^{int}}{2}+\frac{1}{4}\right)}=\frac{1}{a_0/a_{\rm ho}} \tag{6}$$

(for E^{int} in units of $\hbar\omega_{\rm ho}$). Note our definition of the oscillator length $a_{\rm ho}$ differs by a factor of $\sqrt{2}$ from that used in

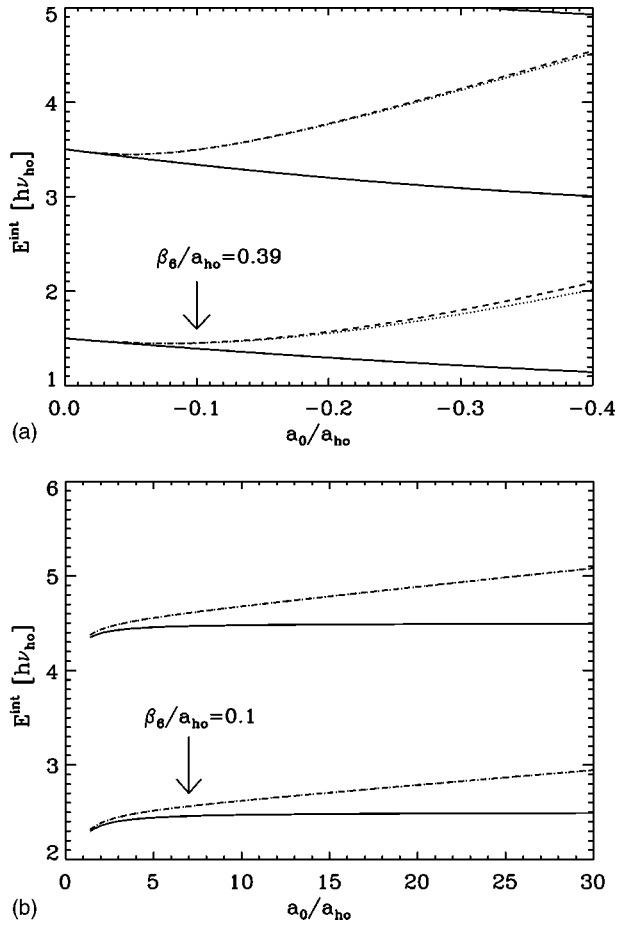

FIG. 1. Internal eigenenergies E^{int}, $E^{int}>0$, for two ^{39}K atoms (a), and two ^{85}Rb atoms (b) in a trap as a function of $a_0/a_{\rm ho}$ for the realistic shape-dependent two-body interaction potentials $V_K(r)$ and $V_{M2}(r)$ (dotted lines); the energy-dependent pseudopotential, Eq. (4) (dashed lines); and the energy-independent pseudopotential, Eq. (1) (solid lines). Arrows indicate the ratio $\beta_6/a_{\rm ho}$ at which the lowest eigenenergy with $E^{int}>0$ for the energy-independent pseudopotential deviates by 4% from the eigenenergy for the "exact" two-body interaction potential (see Table II).

Ref. [16], which leads to a different prefactor on the left-hand side of Eq. (6). Our calculations based on the energy-dependent pseudopotential $V_E^{(\delta)}(r)$ determine E^{int} iteratively. A self-consistency condition is imposed such that the energy-dependent two-body *s*-wave scattering length a_E calculated for the internal potential $V_{\rm K}(r)$ alone at a collision energy E results in exactly this energy when used in Eq. (6) (replace a_0 by a_E).

For practical reasons, it is convenient to recast this quantization condition into an energy level formula analogous to the form familiar in quantum-defect theory [17]. To see this, define the "smoothly varying" quantum-defect function $\zeta(E^{int})$ through the equation

$$\zeta(E^{int})=-\frac{1}{\pi}\arctan\left[\frac{a_0}{a_{\rm ho}}\frac{2\Gamma\left(\frac{E^{int}}{2}+\frac{3}{4}\right)}{\Gamma\left(\frac{E^{int}}{2}+\frac{1}{4}\right)}\right]. \qquad (7)$$

Inserting this expression, and using the Γ function reflection formula, results in an equivalent quantization formula

$$\sin\left[\pi\left(\frac{E^{int}}{2}+\frac{1}{4}+\zeta\right)\right]=0. \qquad (8)$$

The resulting energy levels with positive eigenenergy E^{int} now take the quantum-defect-like form

$$E_v^{int}=2(v-\zeta)+\tfrac{3}{2}, \qquad (9)$$

where $v=0,1,\ldots$ denotes the vibrational quantum number. Note that, as expected, Eq. (9) reduces to the bare harmonic oscillator energy levels if the quantum defect ζ vanishes. In general, this equation must be solved iteratively, but the iteration is highly efficient because ζ on the right-hand side is a slowly varying function of energy.

Figure 1(b) shows the lowest positive eigenenergies for the $M2$-$^{85}Rb_2$ system (see above, and also Table I) with large positive scattering length $a_0=10\,990$ a.u. for the shape-dependent "exact" potential $V_{M2}(r)$ (dotted lines), the energy-independent pseudopotential $V_0^{(\delta)}(r)$ (solid lines), and the energy-dependent pseudopotential $V_E^{(\delta)}(r)$ (dashed lines) as a function of $a_0/a_{\rm ho}$. Figures 1(a) and 1(b) show good agreement between the eigenenergies calculated for the shape-dependent realistic two-body potentials $V_{\rm K}(r)$ and $V_{M2}(r)$, and for the energy-independent pseudopotential $V_0^{(\delta)}(r)$ for $|a_0/a_{\rm ho}|<0.10$ and <7.0 for $^{39}K_2$ and $M2$-$^{85}Rb_2$, respectively. At these $|a_0/a_{\rm ho}|$ values, the deviations between the lowest eigenvalue with positive energy reach 4%. The lowest positive eigenenergies E^{int} for $V_{\rm K}(r)$ and $V_{M2}(r)$ agree to within 4% with those for $V_E^{(\delta)}(r)$, for $|a_0/a_{\rm ho}|<0.42$ [just outside of the range shown in Fig. 1(a)] and 370 [outside of the range shown in Fig. 1(b)], respectively. Note that the energy-dependent pseudopotential approximation improves significantly upon the energy-independent pseudopotential approximation. Comparison of Figs. 1(a) and 1(b) indicates that the validity of the pseudopotential approximation is not predominantly controlled by the ratio $|a_0/a_{\rm ho}|<1$, as was suggested previously [5]. Specifically, the criterion $|a_0/a_{\rm ho}|<1$ underestimates the validity regime of the pseudopotential approximation for systems having large scattering lengths a_0.

Table II summarizes our studies for $^{39}K_2$ and $M2$-$^{85}Rb_2$ together with those for $^{85}Rb_2$, $^{87}Rb_2$, M-$^{39}K_2$, and $M1$-$^{85}Rb_2$. Columns 2 and 3 report the values of $|a_0/a_{\rm ho}|$ and $\beta_6/a_{\rm ho}$ at which the eigenenergies for the energy-independent pseudopotential $V_0^{(\delta)}(r)$ differ by 4% from those for the *realistic* shape-dependent two-body potential [18]. The $|a_0/a_{\rm ho}|$ values vary from 0.10 to 7.0 (factor of 70), whereas the $\beta_6/a_{\rm ho}$ values vary over a much smaller range, namely, from 0.10 to 0.55 (factor of 5.5). Similarly, columns 4 and 5 report the $|a_0/a_{\rm ho}|$ and $\beta_6/a_{\rm ho}$ values at which the eigenenergies for the energy-dependent pseudopotential $V_E^{(\delta)}(r)$ differ by 4% from those for the realistic shape-dependent two-body potential. Here, the $|a_0/a_{\rm ho}|$ values vary from 0.42 to 370 (i.e., through a factor of 880), whereas the values of $\beta_6/a_{\rm ho}$ vary from 0.84 to 5.7 (factor of

TABLE II. Ratios $(|a_0/a_{\rm ho}|)_0$ and $(\beta_6/a_{\rm ho})_0$ at which the lowest positive eigenenergy E^{int} for the energy-independent pseudopotential, or that for the shape-dependent ''realistic'' two-body potential, deviate by 4% [18] (columns 2 and 3) for six different systems interacting through alkali atom-atom $a\,^3\Sigma_u^+$ potentials. Also shown are the ratios $(|a_0/a_{\rm ho}|)_E$ and $(\beta_6/a_{\rm ho})_E$ at which the lowest eigenenergy with $E^{int}>0$ for the energy-dependent pseudopotential, or that for the shape-dependent realistic two-body potential, deviate by 4% (columns 4 and 5).

	$(\lvert a_0/a_{\rm ho}\rvert)_0$	$(\beta_6/a_{\rm ho})_0$	$(\lvert a_0/a_{\rm ho}\rvert)_E$	$(\beta_6/a_{\rm ho})_E$
$^{39}K_2$	0.10	0.39	0.42	1.7
$^{85}Rb_2$	0.42	0.18	2.4	1.0
$^{87}Rb_2$	0.36	0.55	2.2	3.3
M-$^{39}K_2$	2.2	0.14	24	0.84
$M1$-$^{85}Rb_2$	4.0	0.11	220	5.7
$M2$-$^{85}Rb_2$	7.0	0.10	370	5.4

6.8). Roughly speaking, the energy-independent pseudopotential approximation breaks down around $\beta_6/a_{\rm ho}>0.5$. Note, however, that this value depends somewhat on the system under investigation. Table II seems to suggest that the energy-independent pseudopotential approximation breaks down at smaller values of $\beta_6/a_{\rm ho}$ for systems with large a_0.

The validity of the pseudopotential approximation can also be interpreted from a different point of view. Consider the wave function $\psi(r)$ of two ^{39}K particles in a trap interacting through the realistic two-body potential $V_K(r)$. The lowest eigenstate, with positive energy E^{int} in Eq. (3), has 27 nodes at small interparticle distances r [for the range of $\nu_{\rm ho}$ considered in Fig. 1(a), see above]. Imposing the boundary condition $\psi(r)=0$ at the outermost node and solving Eq. (3) from this last node out to large r results in the exact energy. The pseudopotential approximation, in contrast, leads to an eigenfunction $\psi(r)$ that ''ignores'' the nodal structure at small r. If the eigenfunction of the pseudopotential has a node that is identical to the outermost node of the ''exact'' wave function, then the pseudopotential approximation is exact; however, typically the boundary condition of the eigenfunction of the pseudopotential differs slightly from the exact boundary condition. The inaccuracy of the eigenenergies in the pseudopotential approximation is therefore directly related to the error in the boundary condition, and thus to the error in the phase shift, or equivalently, to the error in the scattering length. Recall that the characteristic length β_6 roughly determines the interparticle distance at which the two-body scattering wave function reaches its asymptotic behavior. With this in mind, the above interpretation implies immediately that the ratio $\beta_6/a_{\rm ho}$ rather than the ratio $a_0/a_{\rm ho}$ determines the validity of the pseudopotential approximation.

To connect our studies with commonly used mean-field treatments [2], consider the HF equation [3], which agrees with the Gross-Pitaevskii equation [2] except for a change from N to $N-1$ in the interaction parameter

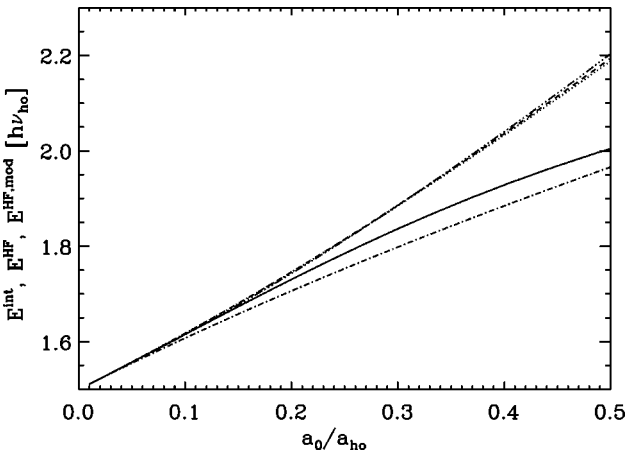

FIG. 2. Internal eigenenergies E^{int}, $E^{int}>0$, for two ^{87}Rb atoms in a trap as a function of $a_0/a_{\rm ho}$ for the realistic shape-dependent two-body interaction potential $V_{Rb}(r)$ (dotted line), the energy-dependent pseudopotential, Eq. (4) (dashed line), and the energy-independent pseudopotential, Eq. (1) (solid line). In addition, a dashed-dotted line shows the HF eigenenergy E^{HF}, and a dashed-dotted-dotted-dotted line the modified HF eigenenergy $E^{HF,mod}$. Note, the exact center-of-mass motion of $1.5\hbar\omega_{\rm ho}$ has been ''artificially'' subtracted from the HF and modified HF eigenenergies to obtain E^{HF} and $E^{HF,mod}$.

$$\left[\frac{-\hbar^2}{2m}\nabla^2+\frac{1}{2}m\omega_{\rm ho}^2\vec{r}^2+\frac{4\pi\hbar^2(N-1)a_0}{m}|\Phi_{HF}(\vec{r})|^2\right]\times\Phi_{HF}(\vec{r})=\epsilon_{HF}\Phi_{HF}(\vec{r}). \tag{10}$$

Here, Φ_{HF} denotes the Hartree-Fock orbital (normalized to 1), and ϵ_{HF} the chemical potential. The derivation of the HF equation is based on many-body wave mechanics for a Hartree-Fock initial state with a nonregularized δ-function interaction potential [i.e., Eq. (1) without the $(\partial/\partial r)r$ operator term]. Equation (10) is valid for any number of particles, particularly for the $N=2$ case considered here, and also for any density of the system (although the accuracy of the approximate treatment depends considerably on the system's density). The HF treatment does not separate out the center-of-mass motion, and thus results in the total energy, which can be obtained through evaluation of the energy functional $E_{HF}[\Phi_{HF}]$ [2]. To compare this energy with the internal eigenenergies E^{int} of Eq. (3) we ''artificially'' [19] subtract the analytically known center-of-mass energy of $1.5\hbar\omega_{\rm ho}$, and denote the resulting energy by E^{HF}.

Figure 2 depicts the lowest eigenenergy E^{int} with $E^{int}>0$ for two ^{87}Rb atoms confined in an external trap as a function of $a_0/a_{\rm ho}$. The lowest eigenenergy of Eq. (3) E^{int} with $E^{int}>0$ calculated for the energy-dependent pseudopotential (dashed line) is nearly indistinguishable from the exact eigenenergy calculated for the two-body potential $V_{\rm Rb}(r)$ (dotted line), whereas the energy-independent pseudopotential (solid line) deviates from the exact eigenenergy by 4% or more for $a_0/a_{\rm ho}\geqslant 0.36$. The HF energy E^{HF} (dashed-dotted line) deviates from the exact energy by 4% or more for $a_0/a_{\rm ho}\geqslant 0.25$, and roughly follows the eigenenergy E^{int}

of Eq. (3) for the energy-independent regularized pseudopotential. In addition to the HF equation, we also consider a modified HF equation

$$\left[\frac{-\hbar^2}{2m}\nabla^2+\frac{1}{2}m\omega_{\rm ho}^2\vec{r}^2+\frac{4\pi\hbar^2(N-1)a_0}{m}|\Phi_{HF,mod}(\vec{r})|^2 \times\left(1+\frac{32}{3\sqrt{\pi}}a_0^{3/2}(N-1)^{1/2}\Phi_{HF,mod}(\vec{r})\right)\right]\Phi_{HF,mod}(\vec{r}) = \epsilon_{HF,mod}\Phi_{HF,mod}(\vec{r}). \quad (11)$$

The total energy $E^{HF,mod}$ relevant to this modified HF equation can be obtained from the energy functional $E^{HF,mod}[\Phi_{HF,mod}]$. In the following, we denote the modified HF energy, *without* the center-of-mass energy of $1.5\hbar\omega_{\rm ho}$ by $E^{HF,mod}$. The additional mean-field term included in Eq. (11) is identical to the correction term introduced by Huang, Lee, and Yang [21–23] for the homogeneous gas. In contrast to the derivation of the Hartree-Fock equation, the derivation of the additional term within many-body wave mechanics crucially depends on the usage of the regularized pseudopotential [Eq. (1)] rather than the unregularized pseudopotential [Eq. (1) without the operator piece]. The modified HF energy $E^{HF,mod}$ (Fig. 2, dashed-dotted-dotted-dotted line) agrees very well with the exact two-body eigenenergy. We take this agreement for the $N=2$ system as another indication [20–25] that the description of a trapped atomic gas through the modified HF equation improves upon the description through the HF equation in the low- and medium-density regime. We note, however, that Eq. (11) has been derived in the large N limit [24], and thus the excellent agreement demonstrated in Fig. 2 might be somewhat fortuitous.

In summary, for $a_0/a_{\rm ho}<0.1$ Fig. 2 shows excellent agreement between the lowest positive internal eigenenergy E^{int} of Eq. (3) for $V_{\rm Rb}(r)$ and those calculated using various approximate treatments, namely, using the pseudopotentials given in Eqs. (1) and (4) in Eq. (3), and using the HF and modified HF equation. For larger interaction parameters $a_0/a_{\rm ho}$, the energy $E^{HF,mod}$ describes the eigenenergy of the system extremely well, and the accuracy for the *regularized energy-independent* pseudopotential [E^{int} of Eq. (3) for $V_0^{(\delta)}(r)$] is slightly better than that for the *nonregularized energy-independent* pseudopotential (E^{HF}).

This study of a two-particle system, the smallest system for which interactions alter the ideal-gas energy levels, provides a simple test of the validity of the mean-field HF treatment. We have shown that the positive eigenenergies of two particle systems can be described properly through the HF equation in the small interaction parameter limit, and furthermore, that a modified HF treatment improves upon the HF treatment in the medium interaction parameter regime.

Our findings contradict a recent study by Geltman and Bambini [26]. This study suggests that a significantly different effective two-body potential should be used whenever the ''realistic'' two-body potential supports one or more two-body bound states. For two ^{87}Rb atoms in a spherical trap with trapping frequency $\nu_{\rm ho}=220$ Hz, the suggested modified effective potential [Eqs. (5) and (6) of Ref. [26]] leads to such a large negative mean-field term that the HF equation does not have a solution. In contrast, for this frequency we find solutions of Eq. (3) with $E^{int}>0$ for the realistic Rb-Rb potential. Furthermore, our lowest positive eigenenergy agrees well with that obtained by solving the standard HF equation with interaction parameter $a_0/a_{\rm ho}$ (see Fig. 2). This comparison shows that modified effective potential proposed by Geltman and Bambini does not handle the BEC physics even approximately correctly. While we agree with the Geltman and Bambini criticism of the unphysical behavior of the Gross-Pitaevskii equation for large a_0, their suggested ''rectification'' is unphysical and appears to derive from an unsound interpretation of the meaning of repulsive and attractive scattering lengths [26]. Our studies in this paper suggest that the adoption of a modified two-body potential in Eq. (3), which has fewer bound states but the same scattering length a_0 as the realistic potential, can result in accurate positive eigenenergies E^{int} for interacting atoms in a trap. These eigenenergies are particularly accurate if the energy dependence of the scattering length for the modified potential resembles that for the realistic potential. This is ensured if both potentials generate comparable values of the effective range parameter r_{eff}.

Note added. Recently, a paper [34] appeared that also arrives at conclusions similar to ours.

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