# Trapping effects on short-range two-body interactions

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In contrast to conventional ideal Bose and Fermi degenerate gases, atoms in experimental ultracold gases interact among themselves and are trapped by an external potential. In this work, we consider two particles of mass $m$ trapped by a $3D$ harmonic potential of frequency $\omega$, and interacting through an isotropic short range potential of intensity $V_0$ and range $b/2$, with $b/2 \ll \sqrt{\hbar/m\omega}$. Eigenfunctions and eigenenergies are obtained and compared with those resulting (a) from an effective contact interaction and (b) in the absence of the trapping potential. Concepts like zero-resonance and binding energy, usually introduced for problems that allow a continuum spectra, are discussed for trapped particles.

*Keywords:* Two body interactions; trapped systems; finite range potential effects.

En contraste con los gases degenerados de Fermi y Bose ideales convencionales, experimentalmente los gases atómicos ultrafríos interactúan entre sí además de estar confinados por medio de un potencial externo. En este trabajo, estudiamos dos partículas de masa $m$, las cuales están atrapadas por medio de un potencial armónico tridimensional con frecuencia $\omega$, e interactúan a través de un potencial de corto alcance con intensidad $V_0$ y rango $b/2$, siendo $b/2 \ll \sqrt{\hbar/m\omega}$. Se obtienen las eigenfunciones y eigenenergías, y se comparan con aquellas obtenidas: (a) a partir de una interacción de contacto; (b) en ausencia del potencial de confinamiento. Conceptos como resonancia-cero y energía de ligadura, que usualmente se introducen en problemas que pueden tener un espectro continuo, se discuten en el caso de partículas atrapadas.

*Descriptores:* Interacciones de dos cuerpos; sistemas atrapados; interactuantes; efectos de potenciales de rango finito.

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## 1. Introduction

In recent years, it has been possible to tune the interactions between atoms in dilute ultracold gases via Feshbach resonances. This is achieved by inducing slight variations on open and closed channel energies using magnetic fields [1]. For broad resonances, the binary interaction may be modeled by a single channel potential. Experiments are always performed with trapped atomic gases. The relevance of the system makes necessary to understand clearly the trapping effects on the behavior of the interacting particles.

Some general remarks must be done when comparing a collision process between interacting but otherwise free atoms, and interacting atoms trapped by an external potential. In the former case, in a single channel scenario, the scattering is usually described in terms of phase shifts. In the limit of low energies, the process is determined by the $s$-wave scattering length $a_0$ disregarding the detailed form of the interaction potential. For positive (negative) values of $a_0$ the particles experience an repulsive (attractive) effective contact interaction. In the case $|a_0| \to \infty$, a zero energy resonance occurs. This critical value of $|a_0|$ corresponds to an infinite scattering cross-section due to the presence of a virtual state of zero energy; the potential is nearly strong enough to support an $s$-wave bound state.

In the case of interacting trapped atoms, the atomic two-body wave functions correspond always to bound states both for the relative and center of mass degrees of freedom. As a consequence, the scattering $in$ and $out$ states cannot be defined and the concept of phase shift loses meaning. However, if the interaction potential has a range much smaller than the trapping natural length scale, it is still expected (and experimentally confirmed) that the scattering length defined in the absence of a trapping potential determines essential properties of the system at low temperatures.

Busch $et\ al.$ [2] studied this problem in the case of a regularized contact interaction

$$V_{contact}(\vec{r}_i,\vec{r}_j) = \frac{4\pi\hbar^2 a_0}{m}\delta^{(3)}_{reg}(\vec{r}_i-\vec{r}_j) \quad (1)$$

$$= \frac{\sqrt{2}\pi\hbar^2 a_0}{m}\delta^{(3)}(\vec{r}_i-\vec{r}_j)\frac{\partial}{\partial r}r \quad (2)$$

and a spherical trapping potential of frequency $\omega$. For the $s$-states, they found an implicit equation for the energy eigenvalues $E$,

$$\sqrt{2}\frac{\Gamma(-E/(2\hbar\omega)+3/4)}{\Gamma(-E/(2\hbar\omega)+1/4)} = \frac{\sqrt{\hbar/m\omega}}{a_0}, \quad (3)$$

and the explicit expression for the corresponding eigenfunctions

$$\varphi_0(r) = \frac{A}{2\sqrt{\pi^3}}e^{-\frac{r^2}{2}}\Gamma(\nu)U\left(-\nu,\frac{3}{2},\frac{\hbar r^2}{m\omega}\right),$$
$$\nu = \frac{E}{2\hbar\omega}-\frac{3}{4}. \quad (4)$$

The normalization constant $A$ satisfies

$$|A|^2 = \sqrt{2}\pi a_0^2\frac{\partial E}{\partial a_0} \quad (5)$$

and $U$ is the hypergeometric function in standard notation. The expression for $A$ can be found using similar procedures to those outlined in Ref. 3 and taking into account Eq. (3). Notice that at $|a_0| \to \infty$, the ground state energy is $E_0 = \hbar\omega/2$.

The purpose of this paper is to study the energy eigenvalues and eigenfunctions of two particles of mass $m$ trapped in a harmonic potential of frequency $\omega$ and interacting through an isotropic potential of finite range $b/2 \ll \sqrt{\hbar/m\omega}$. The potential is chosen so that, in otherwise free space, it would admit a finite number of bound states as its intensity is varied. We compare the results for trapped and unconfined particles, and analyze the role of the scattering length defined for a binary collision in free space. Comparison is also made with the regularized contact interaction results given above. Thus, our study complements the work by Busch $et\ al.$ where $a_0$ is directly introduced into the effective interaction. Besides, our results provide a two-body correlated basis which can be used, for example, in many-body quantum Monte Carlo simulations of atomic degenerate gases [4]. In Monte Carlo calculations, for numerical reasons and because of conceptual problems in the $|a_0| \to \infty$ limit, the contact interaction $V_{contact}$ cannot be implemented directly [4, 5].

## 2. Two-body potential

Consider a two-body interaction potential of range $b/2$ given by

$$V(r) = -V_0 e^{-2r/b}, \qquad V_0 > 0 \tag{6}$$

where $r$ denotes the relative distance between the particles. The Schrödinger equation

$$\left[\frac{\hat{\mathbf{p}}^2}{2m} + V\right]\phi = E\phi \tag{7}$$

has analytical $s$-wave solutions [6] $\phi(r) = v(r)/r$ both in the continuum

$$v(y) = c_1 J_{ib\sqrt{Em}/\hbar}(y) + c_2 J_{-ib\sqrt{Em}/\hbar}(y) \tag{8}$$

and in the bound states region

$$v(y) = c_+ J_{b\sqrt{|E|m}/\hbar}(y). \tag{9}$$

Here $y = (b\sqrt{V_0 m}/\hbar)e^{-r/b}$ and $J_\nu$ represents the Bessel function of the first kind of order $\nu$. By imposing the boundary condition at the origin,

$$c_1 J_{ib\sqrt{Em}/\hbar}(b\sqrt{V_0 m}/\hbar) + c_2 J_{-ib\sqrt{Em}/\hbar}(b\sqrt{V_0 m}/\hbar) = 0, \tag{10}$$

and the boundary condition at $r \to \infty$, $v \to \sin(kr + \delta_0)$, and considering the limit $E \to 0^+$, the following expression is found for the $s$-wave scattering length:

$$a_0 = -b\Big[\frac{\pi}{2}\frac{N_0(b\sqrt{V_0 m}/\hbar)}{J_0(b\sqrt{V_0 m}/\hbar)} - \log\big(b\sqrt{V_0 m}/2\hbar\big) - C\Big] \tag{11}$$

with $N_0$ the Bessel function of the second kind and order zero, and $C$ the Euler constant. Depending on the values of the range parameter $b$ and the intensity $V_0$, Eq. (11) illustrates the well known fact that the scattering length can be positive or negative although the two-body potential is always attractive. The scattering length diverges whenever $J_0(b\sqrt{V_0 m}/\hbar) = 0$. If $z_t, t = 0, 1, 2, \ldots$ are the zeros of this Bessel function in increasing order, the potential $V(r)$ only admits $t$-bound states for $z_t < b\sqrt{V_0 m}/\hbar < z_{t+1}$. The discrete eigenvalues are determined by the boundary condition at $r = 0$, $J_{b\sqrt{|E|m}/\hbar}(b\sqrt{V_0 m}/\hbar) = 0$.

When the two-body collision process takes place in the presence of a spherical harmonic potential of frequency $\omega$, the two-body Schrödinger equation can be separated in a center of mass equation

$$\left[\frac{\hat{\mathbf{P}}^2}{2M} + \frac{1}{2}M\omega^2\mathbf{R}^2\right]\Phi(\mathbf{R}) = E_{CM}\Phi(\mathbf{R}), \quad M = 2m, \tag{12}$$

and a relative coordinate equation

$$\left[\frac{\hat{\mathbf{p}}^2}{2\mu} + \frac{1}{2}\mu\omega^2\mathbf{r}^2 - V_0 e^{-2r/b}\right]\varphi(\mathbf{r}) = E\varphi(\mathbf{r}), \quad \mu = \frac{m}{2}. \tag{13}$$

The former is the well known harmonic oscillator equation, and the latter can be numerically solved for given $b$ and $V_0$.

In Table I, the ground energy, $E_0$, and the $s$-wave lowest eigenvalues $E_i$ of Eq. (13) are illustrated for a given value of the potential range $b/2$ and several potential depths $V_0$. We first consider $V_0$ values between zero and a maximum $V_{max}$ so that at most one bound state is admitted by the potential. The inverse of the scattering length covers the interval $(-\infty, \infty)$ once. We observe that for interaction strengths

$$V_0 < z_0^2\hbar^2/(mb^2) = \tilde{v}_0$$

the system in the absence of the trapping potential, Eq. (7), has no bound states. Meanwhile, the energies for trapped particles are lower than the noninteracting value $3/2\hbar\omega$. At $V_0 \simeq \tilde{v}_0$ the scattering length diverges and, for such a $V_0$, the confined system ground state has an energy eigenvalue near $1/2\hbar\omega$ and the $s$-wave excited states of order $n$ have energies $\sim (2n + 1/2)\hbar\omega$, as expected from Busch $et\ al.$ calculations. As $V_0$ increases the difference between the ground state energy for the particles in the presence and in the absence of the trapping potential tends to zero. Besides, the first excited state energy approaches $3/2\hbar\omega$ as $a_0 \to 0^+$. In that limit the contact interaction in free space would admit a bound state with divergent binding energy. Here the finite value of $V_0$ avoids this unphysical feature.

If the field intensity is further increased towards the second zero-energy resonance condition

$$V_0 \to z_1^2\hbar^2/(mb^2) = \tilde{v}_1$$

the $first$ excited state energy of the trapped system approaches the $1/2\hbar\omega$ eigenvalue. The other excited states are separated by a $\sim 2\hbar\omega$ factor. For even larger $V_0$, we observe that the difference between the $first$ excited state energy for trapped and unconfined atoms also tends to zero.

TABLE I. Lower discrete $s$-state relative motion energy eigenvalues of two particles interacting through the potential Eq. (6) with $b = 0.03\sqrt{\hbar/m\omega}$. When two rows are reported for a given $a_0$ the upper corresponds to the interaction in the absence of a trapping potential and the lower when it is on.

| $a_0$ $\left[\sqrt{\frac{\hbar}{m\omega}}\right]$ | $V_0$ $[\hbar\omega]$ | $E_0$ $[\hbar\omega]$ | $E_1$ $[\hbar\omega]$ | $E_2$ $[\hbar\omega]$ | $a_0$ $\left[\sqrt{\frac{\hbar}{m\omega}}\right]$ | $V_0$ $[\hbar\omega]$ | $E_0$ $[\hbar\omega]$ | $E_1$ $[\hbar\omega]$ | $E_2$ $[\hbar\omega]$ | $E_3$ $[\hbar\omega]$ |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | -0.0584 | 28848.5 | -4304.95 | | | |
| -0.0525 | 3614.504 | 1.45885 | 3.43836 | 5.42338 | -0.0584 | 28848.5 | -4304.97 | 1.45460 | 3.43261 | 5.41691 |
| | | | | | -0.1173 | 30515.2 | -4820.49 | | | |
| -0.1106 | 4720.985 | 1.41502 | 3.37331 | 5.34333 | -0.1173 | 30515.2 | -4820.43 | 1.41078 | 3.36830 | 5.33877 |
| | | | | | -0.1804 | 31403.2 | -5101.96 | | | |
| -0.1879 | 5310.566 | 1.36008 | 3.29344 | 5.24771 | -0.1804 | 31403.2 | -5101.98 | 1.36631 | 3.30455 | 5.26333 |
| | | | | | -0.5732 | 32937.2 | -5599.0 | | | |
| -0.5733 | 6017.906 | 1.14462 | 3.01448 | 4.94650 | -0.5732 | 32937.2 | -5599.0 | 1.14909 | 3.02777 | 4.96757 |
| | | | | | $\infty$ | 33857.0 | -5903.4 | | | |
| $\infty$ | 6425.786 | 0.510656 | 2.52659 | 4.53714 | $\infty$ | 33857.0 | -5903.4 | 0.520239 | 2.54982 | 4.56705 |
| 2.1035 | 6545.231 | -0.23188 | | | 2.0014 | 34152.3 | -6002.0 | -0.262403 | | |
| 2.1035 | 6545.231 | 0.00000 | 2.33058 | 4.38997 | 2.0014 | 34152.3 | -6002.0 | -0.031234 | 2.34447 | 4.41396 |
| 0.5810 | 6876.584 | -3.2487 | | | 0.5812 | 34943.3 | -6268.6 | -3.52506 | | |
| 0.5810 | 6876.584 | -3.2079 | 1.94716 | 4.07045 | 0.5812 | 34943.3 | -6268.6 | -3.48380 | 1.95525 | 4.08711 |
| 0.1952 | 7933.069 | -34.580 | | | 0.1954 | 37779.3 | -7250.0 | -44.8408 | | |
| 0.1952 | 7933.069 | -34.576 | 1.66094 | 3.73393 | 0.1954 | 37779.3 | -7250.1 | -44.8365 | 1.66185 | 3.73652 |
| 0.1170 | 9253.132 | -115.04 | | | 0.1176 | 41798.7 | -8704.85 | -177.821 | | |
| 0.1170 | 9253.132 | -115.04 | 1.59568 | 3.64153 | 0.1176 | 41798.7 | -8704.9 | -177.819 | 1.59631 | 3.64283 |
| 0.0524 | 14458.02 | -774.04 | | | 0.0524 | 56857.6 | -14699.7 | -1334.76 | | |
| 0.0524 | 14458.02 | -774.04 | 1.54230 | 3.55782 | 0.0524 | 56857.6 | -14699.6 | -1334.73 | 1.54229 | 3.56315 |

All these numerical results are compatible with Eq. (3) valid for a range zero interaction, the comparison between our numerical solutions for the eigenenergies and those obtained by Busch $et\ al.$ is shown in Fig. 1. It can be seen that the positive eigenvalues are always very similar for potential ranges $b/2 < 0.03\sqrt{\hbar/m\omega}$. As for the negative eigenvalues, the comparison between the ground state energy of the zero-range potential and of a potential with finite range $b/2$ is poorer as the depth of the latter potential increases. Let us choose, for instance, $a_0 = 0.581\sqrt{\hbar/m\omega}$ the Busch $et\ al.$ equation gives the ground state energy $E_0 = -2.9217\hbar\omega$. For the exponential potential trapped system, $E_0 = -3.2\hbar\omega$ if $b = 0.03\sqrt{\hbar/m\omega}$ (see Table I), $versus$

$$E_0 = -2.96\hbar\omega = -\hbar^2/ma_0^2$$

for the contact interaction in free-space. Taking again $b = 0.03\sqrt{\hbar/m\omega}$, for $a_0 = 0.117011\sqrt{\hbar/m\omega}$ the energy for the trapped system and a regularized delta potential is $E_0 = -73.04\hbar\omega$, $versus$ $E_0 = -115.0389\hbar\omega$ for the $b = 0.03\sqrt{\hbar/m\omega}$ exponential potential (see Table I), $versus$

$$E_0 = -73.04\hbar\omega = -\hbar^2/ma_0^2$$

for the contact interaction in free-space. In order to get results closer to contact interaction, shorter ranges must be considered. For instance, if $a_0 = 0.117011\sqrt{\hbar/m\omega}$, for different values of the parameter $b$ in the limit $b \to 0$ we found: for $b = 0.02\sqrt{\hbar/m\omega}$, it turns out that $E_0 = -99.261418\hbar\omega$, while for $b = 0.015$, it results $E_0 = -91.940596\hbar\omega$. A numerical fit of the energy as a function of $b$ using a second order polynomial predicts $E_0 = -72.25\hbar\omega$ in good agreement with the zero-range energy reported above ($E_0 = -73.04\hbar\omega$). If one is interested in obtaining results closer to the contact interaction ones, it is necessary to take into account more significant figures for the scattering length. For the potential ranges illustrated in the second column of Table I, excited states energies $E_i$, $i \geq 1$ coincide at least within the first three figures with the analytical result for the regularized delta function.

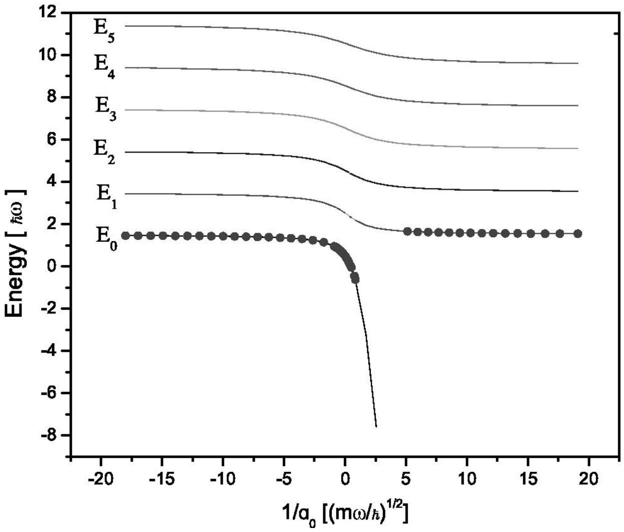


FIGURE 1. Lowest $s$-wave relative energy eigenvalues in units of $\hbar\omega$ for two colliding trapped particles, Eq. (13), around the first resonance. They were evaluated by considering a potential range $b/2 = 0.015\sqrt{\hbar/m\omega}$ and a strength $V_0$ starting from $V_0 \sim 0$ to the lowest $|V_0|$ yielding $a \rightarrow 0^+$. The scattering length is measured in units of $\sqrt{\hbar/m\omega}$. Circles show the energy obtained by Busch *et al*.

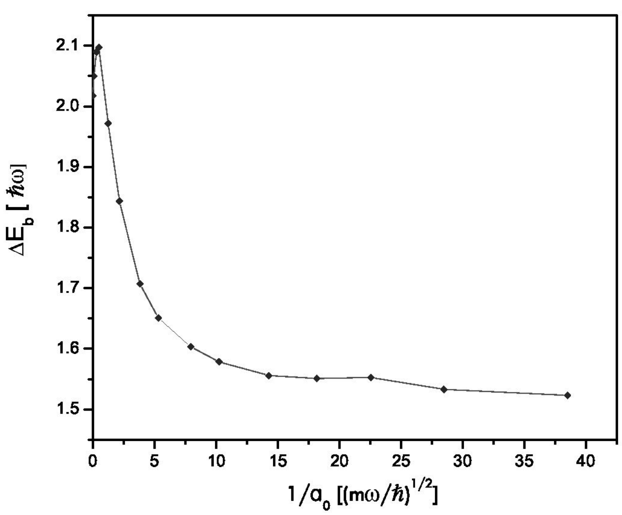


FIGURE 2. Difference between the binding energies as estimated with interacting trapped atoms and with interacting atoms in otherwise free space. The dots give the numerical values with errors smaller than the symbols used to plot them and the line is a numerical interpolation. The interaction intensity is chosen so that just one bound state is allowed for the free space system. The parameter $b = 0.03\sqrt{\hbar/m\omega}$ was used for the numerical calculations.

All these results confirm $a_0$ as the relevant parameter for determining the general features of the interaction. That is, $a_0$ determines the eigenvalues $E > 1/2\hbar\omega$ regardless of the number of states with $E < 1/2\hbar\omega$; it seems that the states with $E > 1/2\hbar\omega$ inherit the free space "scattering" states role, and the state with $E = 1/2\hbar\omega$ replaces the zero-energy resonance at $a_0 \rightarrow \infty$. Notice that in the confined two-body system the concept of binding energy must be revisited. For particles in free space, it is defined as the energy necessary to reach the continuum. According to the previous discussion, for trapped atoms it could be defined as the difference between the energy eigenvalue of the state under consideration and the lowest eigenvalue $E > \hbar\omega/2$. The scenario behind measuring such energies would be the dissociation of the molecule keeping the trapping potential on. In Fig. 2, the difference between the binding energies measured with and without harmonic trapping, as a function of the inverse of the scattering length, is illustrated.

The general behavior of the radial $s$-eigenfunctions $v_{a_0}$ and $u_{a_0}$ is illustrated for unconfined particles in Fig. 3 and for trapped particles in Fig. 4. For an interaction in otherwise free space, the zero-energy resonant function $v_\infty(r)$

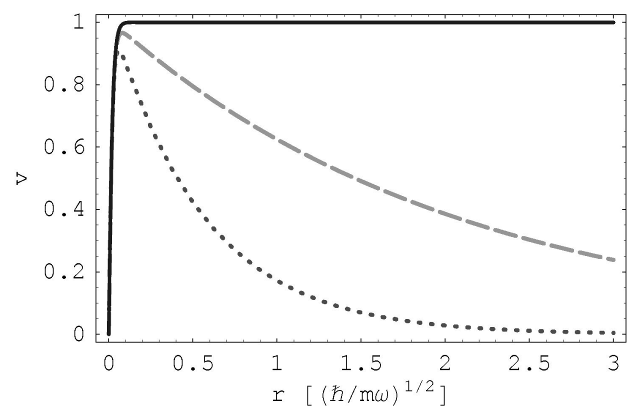


FIGURE 3. Radial function $v_{a_0}(r)$, $\phi_a(r) = u_a(r)/r$, for interacting particles in otherwise free space, Eqs.(8-9). The zero-energy resonant function $v_\infty(r)$ (solid line) tends to a nonzero constant as $r \rightarrow \infty$, while $v_{2.1}(r)$ (dashed line) and $v_{0.58}(r)$ (dotted line) correspond to increasingly bound states.

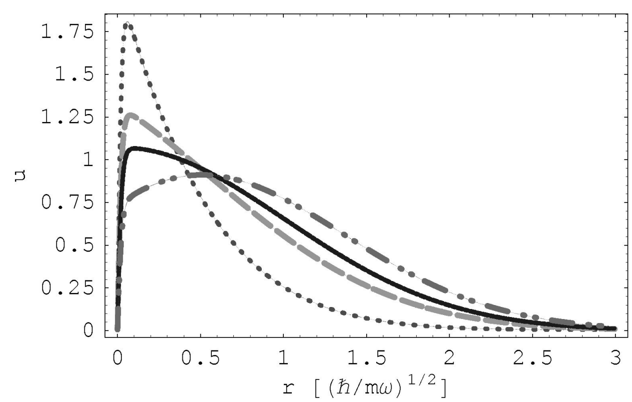


FIGURE 4. (Color online) Radial function $u_{a_0}(r)$, $\varphi_{a_0}(r) = u_{a_0}(r)/r$, for two interacting particles in the presence of the trapping potential, Eq. (13). The dot-dashed curve corresponds to the ground $s$-state for a negative scattering length $u_{-0.6}(r)$, and the resonant function $u_\infty$(r) is given by the solid curve, while $u_{2.1}(r)$ by the dashed one and $u_{0.58}(r)$ by the dotted line correspond to positive scattering lengths. In this figure the wave functions have been properly normalized. Distances are measured in units of $\sqrt{\hbar/m\omega}$.

(solid line) goes to a nonzero constant as $r \to \infty$, meanwhile $v_{2.1}(r)$ (dashed line) and $v_{0.58}(r)$ (dotted line) correspond to increasingly bound states. For trapped particles, before the zero-resonance condition is achieved the wave functions have, in general, a structure in which three regions are recognized, as illustrated by the dot-dashed line in Fig. 3. Very close to the origin, the slope of $u_{-0.6}(r)$ is positive and large, so that for $r \sim b/2$ it becomes positive but less than one until it reaches an extremum at $1 > r \gg b/2$ and becomes negative. At the zero-resonance condition the intermediate region shrinks so that the extremum is reached at $r \sim b/2$; nevertheless the function decays directly as the harmonic oscillator factor $\exp(-m\omega r^2/\hbar)$.

In the region of positive scattering lengths, an $ansatz$ for the ground state function is:

$$\varphi(r) = v(y(r)) \exp(-m\omega r^2/\hbar) g(r)/r \qquad (14)$$

with $v$ defined in Eq. (9) for bound states in the absence of a trapping potential, it is numerically found that the values of the function $g(r)$ are in the interval $(0.99, 1.01)$ for $b \leq 0.03\sqrt{\hbar/m\omega}$. The structure of Eq. (14) for the eigenfunctions at $|a_0| \to \infty$ allows us to understand the origin of the eigenvalue $\sim 1/2\hbar\omega$. In this case, $v(y(r))$ takes care of the boundary condition $v(0) = 0$ so that the effective equation for $\psi(r) =: \varphi(r) \cdot r/v$ is almost identical to that of the one-dimensional harmonic oscillator without the requirement of becoming null at $r = 0$, thus admitting the possibility $E \sim 1/2\hbar\omega$.

For negative values of the scattering length, we found that the numerical solution to the ground state problem can be approximated using the following analytical compact representation:

$$\varphi_{apx}(r) = J_0(z_0 e^{-r/b}) e^{-m\omega r^2/4\hbar} \times (1 + c e^{-2r/b}) P(r/b)/r \qquad (15)$$

with c independent of $r$ and $P(r/b)$ a polynomial of fourth order, both of which depend on $V_0$ and $b$. The coefficients of the polynomial and the parameter $c$ were obtained using standard numerical fitting methods. For $|V_0| \ll (z_0/b)^2\hbar\omega$, the polynomial $P(r/b)$ is almost linear while for $|V_0| \leq (z_0/b)^2\hbar\omega$, it turns out that $c \approx 0$. The accuracy of this approximation was measured by evaluating the ratio $\varphi_{apx}(r)/\varphi_{num}(r)$ between the analytical approximate expression Eq. (15) and the numerical solution. This ratio yielded $1 \pm 0.0001$ over the entire interval $0 \leq r \leq 3\sqrt{\hbar/m\omega}$ for $b/2 \leq 0.015\sqrt{\hbar/m\omega}$.

All the results discussed above are just an illustration of what we have found numerically for all values of the parameter $b$ that we studied within $b < 0.05\sqrt{\hbar/m\omega}$.

## 3. Conclusions

We have shown that even an extremely short range interaction between particles trapped in a harmonic potential, may significantly alter both the spectra and eigenfunctions in comparison with (i) noninteracting trapped particles and (ii) unconfined interacting particles. Our results are compatible with previous findings for $s$-states and a regularized $\delta$ potential [2]. They allow us to establish a more clear relationship between contact interaction and finite range results for trapped interacting dilute gases.

Notice that states with higher angular momenta can also be analyzed and compared to pseudopotential contact interaction predictions. In those cases, the scattering is characterized by other parameters, $e.\ g.$, the $p$-scattering volume. It must also be emphasized that our results show the need to take trapping effects into account when binding energies are measured particularly near the limit $a_0 \to \infty$.

Although all calculations were presented for a particular potential $V(r)$, the qualitative features of our results are expected to apply in general for short range interaction potentials.


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