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Two atoms in an anisotropic harmonic trap

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We consider the system of two interacting atoms confined in axially symmetric harmonic trap. Within the pseudopotential approximation, we solve the Schrödinger equation exactly, discussing the limits of quasi-one- and quasi-two-dimensional geometries. Finally, we discuss the application of an energy-dependent pseudopotential, which allows us to extend the validity of our results to the case of tight traps and large scattering lengths.

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Atomic interactions at ultralow temperatures are of central importance for recent research on quantum degenerate gases [1]. A typical feature of experiments on ultracold matter is the presence of a weak trapping potential, which modifies the properties of the cloud of atoms, while it does not affect the collisions of individual particles. Development of optical lattice technology, however, has created systems where the atoms are tightly confined in the wells of optical potential [2]. In addition, the experimental achievement of the Mott insulator phase [3] has allowed for a precise control over a number of atoms stored in a single well. This has opened a way for experimental studies of interactions of individual atoms in the presence of trapping potential and, together with other approaches to micromanipulation of neutral atoms such as atom chips [4,5] or tight dipole traps [6], it represents a major candidate for the implementation of quantum information processing. A theoretical understanding of the dynamics of few atoms in deformed tight-confining geometries would be of great help in all these contexts.

From the theoretical side, the analytical solution for two atoms interacting in a harmonic trap is known only for the spherically symmetric case [7,8]. The corresponding problem for axially symmetric trap was studied numerically in [9]. However, there the authors considered only the limiting regimes of quasi-one- and quasi-two-dimensional traps. In this paper we present the exact solution for the axially symmetric harmonic trap of arbitrary geometry. In particular, when the ratio of axial to radial trapping frequency is an integer, or the inverse of an integer, we give the explicit analytic form of the exact solution. In the other cases, we derive an efficient recurrence relation that allows for evaluating it. Furthermore, we study the asymptotic behavior of eigenenergies and eigenfunctions in the limit of quasi-one- and quasi-two-dimensional traps.

A standard treatment of ultracold atom interactions is based on the replacement of a real physical potential by a *s*-wave delta-function pseudopotential. To extend the validity of this model interaction to the case of tight traps and large scattering lengths, one can utilize the concept of an effective, energy-dependent scattering length [10]. We discuss this idea and show how our results can be generalized to the case of magnetically tunable Feshbach resonances.

We consider two interacting atoms of mass m confined in an axially symmetric harmonic trap with frequencies $\omega_\perp$ and ω_z. In the following we use dimensionless variables, in which all lengths are expressed in units of harmonic oscillator length $a_z=\sqrt{\hbar/m\omega_z}$, and all energies are expressed in units of $\hbar\omega_z$. In these units the trapping potential is $V_T(\mathbf{r})=\frac{1}{2}(\eta^2\rho^2+z^2)$, where $\eta=\omega_\perp/\omega_z$ and $\rho^2=x^2+y^2$. We assume that the range of the interatomic potential is much smaller than the oscillator lengths a_z and $a_\perp=\sqrt{\hbar/m\omega_\perp}$, which guarentees that the interatomic potential is not distorted by the harmonic trap. For sufficiently low energies, the scattering is purely of *s*-wave type and we model the atom-atom interaction by a Fermi pseudopotential $V(\mathbf{r})=4\pi a\delta(\mathbf{r})(\partial/\partial r)r$ with *s*-wave scattering length a [11]. For the harmonic confining potential, the total Hamiltonian

$$\hat{H}=-\frac{1}{2}\nabla_1^2-\frac{1}{2}\nabla_2^2+V_T(\mathbf{r}_1)+V_T(\mathbf{r}_2)+V(\mathbf{r}_1-\mathbf{r}_2), \quad (1)$$

can be split into a center of mass part: $\hat{H}_{\mathrm{CM}}=-\frac{1}{2}\nabla_R^2+V_T(\mathbf{R})$, and the relative motion part: $\hat{H}_{\mathrm{rel}}=-\frac{1}{2}\nabla_r^2+V_T(\mathbf{r})+V(\sqrt{2}\mathbf{r})$, where $\mathbf{r}=(\mathbf{r}_1-\mathbf{r}_2)/\sqrt{2}$ and $\mathbf{R}=(\mathbf{r}_1+\mathbf{r}_2)/\sqrt{2}$. To solve the Schrödinger equation for the relative motion, we decompose the wave function in the basis of eigenstates of the noninteracting problem, substitute this decomposition into the Schrödinger equation, and then extract the expansion coefficients by projecting onto noninteracting states [7]. This yields the wave function of $m_z=0$ states, with vanishing angular momentum along the z axis

$$\Psi(\mathbf{r})=\frac{\eta}{(2\pi)^{3/2}}\int_0^\infty \mathrm{d}t\frac{\exp\left[tE-\frac{z^2}{2}\coth t-\frac{\eta\rho^2}{2}\coth(\eta t)\right]}{\sqrt{\sinh(t)\sinh(\eta t)}}. \quad (2)$$

The harmonic oscillator states with $m_z\neq 0$ vanish at $\mathbf{r}=0$, and they are not influenced by the pseudopotential. Equation (2) represents the wave function that is not normalized, and is related with the single particle Green function of the anisotropic harmonic oscillator by $\Psi(\mathbf{r})=-2G(\mathbf{r},0)$. We note that the integral representation (2) is valid for energies

smaller than the ground-state energy of the harmonic oscillator: $E_0=1/2+\eta$. The validity of Eq. (2), however, can be extended for $E\geqslant E_0$ by means of the analytic continuation.

The presence of the trapping potential implies the discrete character of the energy spectrum. The allowed values of energy E have to be determined from the equation: $-1/(\sqrt{2}\pi a)=[(\partial/\partial r)r\Psi(\mathbf{r})]_{r=0}$, which results from derivation of Eq. (2), and expresses a boundary condition imposed by zero-range interaction. Investigation of the integral in Eq. (2) for small values of $\mathbf{r}$, shows that $\Psi(\mathbf{r})$ behaves like $1/(2\pi r)$ as $\mathbf{r}\to 0$. This divergence is removed by the regularization operator $(\partial/\partial r)r$ in the Fermi pseudopotential. Subtracting from the integral (2), the part that gives rise to the $1/r$ singularity, the condition for the eigenenergies can be rewritten as

$$-\sqrt{2\pi}/a=\mathcal{F}(-(E-E_0)/2,\eta), \tag{3}$$

where

$$\mathcal{F}(x,\eta)\equiv\int_0^\infty dt\left[\frac{\eta e^{-xt}}{\sqrt{1-e^{-t}}(1-e^{-\eta t})}-\frac{1}{t^{3/2}}\right]. \tag{4}$$

For particular values of the anisotropy parameter η, the function $\mathcal{F}(x,\eta)$ can be calculated analytically. In the case of cigar-shaped traps with $\eta=n$, where n is a positive integer, we obtain

$$\mathcal{F}(x,n)=\frac{\sqrt{\pi}\Gamma(x)\sum_{m=1}^{n-1}F\left(1,x;x+\frac{1}{2};e^{i(2\pi m/n)}\right)}{\Gamma\left(x+\frac{1}{2}\right)}-\frac{2\sqrt{\pi}\Gamma(x)}{\Gamma\left(x-\frac{1}{2}\right)}, \tag{5}$$

where $F(a,b;c;x)$ denotes the hypergeometric function and $\Gamma(x)$ is the Euler gamma function. It can be easily verified that the sum in Eq. (5) involving complex roots of unity is a real number for $x\in\mathbb{R}$. On the other hand, for pancake-shaped traps with anisotropy parameter $\eta=1/n$, the following result holds:

$$\mathcal{F}(x,1/n)=-\frac{2\sqrt{\pi}}{n}\sum_{m=0}^{n-1}\frac{\Gamma(x+m/n)}{\Gamma(x-1/2+m/n)}. \tag{6}$$

For $n=1$, we recover obviously the well-known result for the spherically symmetric trap: $\mathcal{F}(x,1)=-2\sqrt{\pi}\Gamma(x)/\Gamma(x-1/2)$ [7]. We note that Eqs. (5) and (6) are derived from the integral representation (4) applicable for $x>0$; however, their validity for $x<0$ is extended by virtue of the analytic continuation.

In the general case, when η does not meet the conditions of Eqs. (5) and (6), the energy spectrum can be determined numerically. For $E<E_0$ the function $\mathcal{F}(x,\eta)$ is given by Eq. (4), while for $E>E_0$, one can utilize the following recurrence relation:

$$\mathcal{F}(x,\eta)-\mathcal{F}(x+\eta,\eta)=\eta\sqrt{\pi}\Gamma(x)/\Gamma(x+1/2), \tag{7}$$

which can be easily derived from the definition of $\mathcal{F}(x,\eta)$.

From the practical point of view, the use of the exact results of Eqs. (5) and (6) is efficient as long as n is not too large. To determine the energy levels in the limit of quasi-one- and quasi-two-dimensional traps, we derive the asymptotic form of $\mathcal{F}(x,\eta)$ for $\eta\gg 1$ and $\eta\ll 1$.

Let us first focus on the case of $\eta\gg 1$. Performing an expansion in the integral (4) for large η and making use of the recurrence formula (7) we arrive at

$$\mathcal{F}(x,\eta)\overset{\eta\gg 1}{\approx}\sqrt{\pi\eta}\left[\zeta\left(\tfrac{1}{2},1+x/\eta\right)+\sqrt{\eta}\Gamma(x)/\Gamma\left(x+\tfrac{1}{2}\right)\right], \tag{8}$$

where $\zeta(s,a)$ denotes the Hurwitz zeta function. This asymptotic formula is valid for $x>-\eta$, which corresponds to the range of energies $E<E_0+2\eta$. For the lowest excited states $0<E-E_0\ll 2\eta$ we approximate $\zeta(1/2,1+x/\eta)$ by $\zeta(1/2,1)$ in Eq. (8), and match the resulting energy spectrum with the energy spectrum of two atoms in a one-dimensional (1D) trap. The latter is determined by $\sqrt{2}a_{1D}=\Gamma((E_0-E)/2)/\Gamma((E_0+1-E)/2)$ [7]. The two spectra are identical, provided that the one-dimensional scattering length is $a_{1D}=-1/\eta a-\zeta(1/2,1)/\sqrt{2\eta}$, which agrees with the value of the renormalized scattering length derived for a quasi-one-dimensional waveguide [12]. On the other hand, for energies $E<E_0$, we can use $\mathcal{F}(x,\eta)\approx\sqrt{\pi\eta}\zeta(1/2,x/\eta)$, which follows from Eqs. (7) and (8). This approximation, substituted into (3), leads to the condition determining the energy of a bound state

$$\sqrt{2}/a+\sqrt{\eta}\zeta(1/2,(E_0-E)/(2\eta))=0, \tag{9}$$

which is identical to the known result derived for the quasi-one-dimensional waveguide [12,13].

In the case of quasi-two-dimensional traps $\eta\ll 1$, we obtain the following approximate formula for $\mathcal{F}(x,\eta)$:

$$\mathcal{F}(x,\eta)\overset{\eta\ll 1}{\approx}-\Phi(x)-\ln(\eta)-\psi(x/\eta), \tag{10}$$

where

$$\Phi(x)=2-\ln(1+x)+2\sum_{k=1}^{\infty}\frac{(2k)!}{(2^k k!)^2}\times\left[\left(k+\frac{1}{2}\right)\ln\frac{x+k}{x+k+1}+1\right], \tag{11}$$

and $\psi(z)=(d/dz)\ln\Gamma(z)$ denotes the digamma function. This result is valid for $x>-1$, which corresponds to energies $E<E_0+2$. For the lowest excited states: $0<E-E_0\ll 2$, we approximate $\Phi(x)$ by $\Phi(0)$ in Eq. (10), and compare the resulting energy spectrum to that of the two-dimensional (2D) system. In the two-dimensional trap, the eigenenergies of two interacting atoms are given by $-\ln(2a_{2D}^2\eta)=\psi((E_0-E)/(2\eta))$ [14]. In this way we find the value of the two-dimensional scattering length a_{2D} for which both spectra are the same: $a_{2D}=\exp\left[\frac{1}{2}(\mathcal{D}-\sqrt{2\pi}/a_{3D})\right]/\sqrt{2}$, where $\mathcal{D}=\Phi(0)\simeq 1.938$. This result agrees with the value of a_{2D} derived for a quasi-two-dimensional system without confinement in the radial direction [15]. In the range of energies corresponding to a bound state, we use an asymptotic expansion of $\psi(x/\eta)$ for $x/\eta\gg 1$ in Eq. (10), which yields $\mathcal{F}(x,\eta)\approx-\Phi(x)-\ln x$. Substituting this approximation into (3), we obtain the equa-

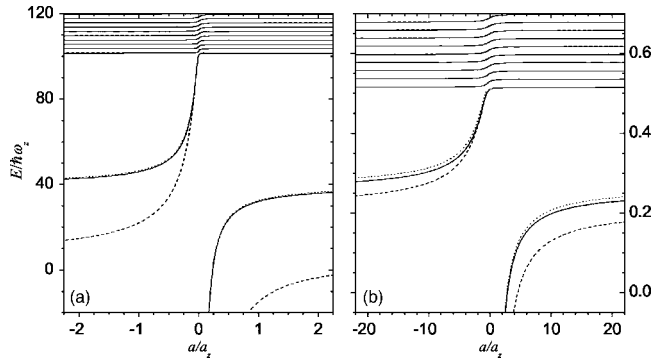

FIG. 1. Energy spectrum of two atoms interacting via regularized delta potential in a three-dimensional trap with (a) $\eta=\omega_\perp/\omega_z=100$ and (b) $\eta=0.01$ (b). Panel (a): The exact energy levels (solid lines) are compared with the energy spectrum of the one-dimensional system with renormalized scattering length (dashed lines), and with the energies of a bound state calculated from Eq. (9). (The dotted lines are almost indistinguishable from the solid ones.) Panel (b): The exact energy levels (solid lines) are compared with the energy spectrum of the two-dimensional system with renormalized scattering length (dashed lines), and with the energies of a bound state calculated from Eq. (12) (dotted lines). The scattering length a is scaled in h.o. units $a_z=\sqrt{\hbar/m\omega_z}$.

tion that determines the energy of a bound state in quasi-two-dimensional traps

$$\sqrt{2\pi}/a = \Phi((E_0-E)/2) + \ln[(E_0-E)/2]. \tag{12}$$

For a shallow bound state ($E_0-E\ll 1$) one can approximate $\Phi((E_0-E)/2)$ by $\Phi(0)$ and in this regime the binding energy is given by $E_0-E=0.288\exp(\sqrt{2\pi}/a)$ [15].

Figure 1 shows the energy spectrum of two interacting atoms calculated for (a) $\eta=100$ and (b) $\eta=0.01$. Figure 1(a) compares the exact energy levels given by Eqs. (3) and (5), with the energy spectrum of the one-dimensional system with renormalized scattering length a_{1D}, and with bound-state energies calculated from Eq. (9). Figure 1(b) presents the exact result of Eqs. (3) and (6), the energy spectrum of the two-dimensional system with renormalized scattering length a_{2D}, and bound-state energy calculated from Eq. (12). We have not included the energy levels calculated from approximations (8) and (10), which for $\eta=100$ and $\eta=0.01$ are indistinguishable from the exact result. We observe that for $E>E_0$ the one- and the two-dimensional spectra fit very well the exact eigenenergies, whereas they are incorrect with respect to the bound-state energies. The latter, however, are well described by Eqs. (9) and (12).

We now turn to the calculation of wave functions. While for $E<E_0$ they can be evaluated from the integral representation (2), in the general case, they can be determined from the following expansions

$$\Psi(\mathbf{r}) = \frac{\eta\, e^{-\eta\rho^2/2}}{2\pi^{3/2}2^{\mathcal{E}/2}}\sum_{m=0}^{\infty}\left[2^{\eta m}\Gamma\left(\frac{2\eta m-\mathcal{E}}{2}\right)L_m(\eta\rho^2)\right.$$
$$\left.\times\, D_{\mathcal{E}-2\eta m}(|z|\sqrt{2})\right], \tag{13}$$

$$\Psi(\mathbf{r}) = \frac{e^{-(\eta\rho^2+z^2)/2}}{2\pi^{3/2}}\sum_{k=0}^{\infty}\left[\frac{(-1)^k}{2^{2k}k!}H_{2k}(z)\Gamma\left(\frac{k}{\eta}-\frac{\mathcal{E}}{2\eta}\right)\right.$$
$$\left.\times\, U\left(\frac{k}{\eta}-\frac{\mathcal{E}}{2\eta},1,\eta\rho^2\right)\right]. \tag{14}$$

Here $\mathcal{E}=E-E_0$, $L_m(x)$, and $H_k(z)$ are, respectively, the Laguerre and Hermite polynomials, $D_\nu(x)$ is the parabolic cylinder function and $U(a,b,z)$ denotes the confluent hypergeometric function. As it can be easily observed, the first expansion involves the harmonic oscillator wave functions in the radial direction and the one-dimensional solution for two interacting atoms in the axial direction. We have verified that for elongated traps ($\eta\gg 1$), the first term of this series provides already a quite good approximation for the wave function of the lowest excited states. A similar feature is observed for the second series in Eq. (14) in the traps with $\eta\ll 1$. Conversely, for energies $E<E_0$ the two series involve generally several terms. In this regime, we can analyze the behavior of the wave functions on the basis of the integral representation (2). Due to the complicated form of the latter integral, we focus here only on the limiting case of quasi-one- or quasi-two-dimensional traps, and investigate only the behavior of the axial ($\rho=0$) and the radial ($z=0$) profiles of the wave functions.

Expanding the integral in Eq. (2) for $\eta\gg 1$, we obtain the axial $(\Psi_z(z)\equiv\Psi(z\hat{\mathbf{z}}))$ and radial $(\Psi_\perp(\rho)\equiv\Psi(\rho\hat{\boldsymbol{\rho}}))$ profiles of the wave function, applicable for $E<E_0$

$$\Psi_z(z) \overset{\eta\gg 1}{\approx} \frac{\eta}{2\pi}\sum_{m=0}^{\infty}\frac{\exp(-2|z|\sqrt{m\eta-\mathcal{E}/2})}{\sqrt{m\eta-\mathcal{E}/2}}, \tag{15}$$

$$\Psi_\perp(\rho) \overset{\eta\gg 1}{\approx} e^{-\eta\rho^2/2}\left[\rho^{-1}+\sqrt{\eta}\zeta\left(1/2,-\frac{\mathcal{E}}{2\eta}\right)\right]\Big/(2\pi). \tag{16}$$

For $|z|\sqrt{-\mathcal{E}}\gg 1$, the main contribution to the sum in Eq. (15) comes from the first term. In this case the wave function exhibits the exponential decay, which is similar to the behavior of a one-dimensional bound-state in a free space: $\Psi(z)\sim\exp(-\sqrt{-2\mathcal{E}}|z|)$. On the other hand, the wave function in the radial direction has a Gaussian profile, characteristic for the ground state of the harmonic oscillator, whereas the divergent term $1/(2\pi\rho)$ arises due to the interaction potential.

In quasi-two-dimensional traps, for energies $E<E_0$, we found the following radial and axial profiles of the wave functions

$$\Psi_\perp(\rho) \overset{\eta\ll 1}{\approx} \pi^{-3/2}\sum_{m=0}^{\infty}\frac{(2m)!}{(2^m m!)^2}K_0(2\rho\sqrt{m-\mathcal{E}/2}), \tag{17}$$

$$\Psi_z(z) \overset{\eta\ll 1}{\approx} \frac{e^{-z^2/2}}{2\pi}\left[\frac{1}{|z|}-\frac{\Phi(-\mathcal{E}/2)+\ln(-\mathcal{E}/2)}{\sqrt{\pi}}\right], \tag{18}$$

where $K_0(x)$ is a modified Bessel function. The asymptotic behavior of $K_0(x)$ for $x\gg 1$ is governed by $K_0(x)\sim\sqrt{\pi/2x}e^{-x}$. Hence, for $\rho\sqrt{-\mathcal{E}}\gg 1$, the sum in (17) is dominated by the first term, and the asymptotic decay of the wave function in the radial direction is similar to the one observed

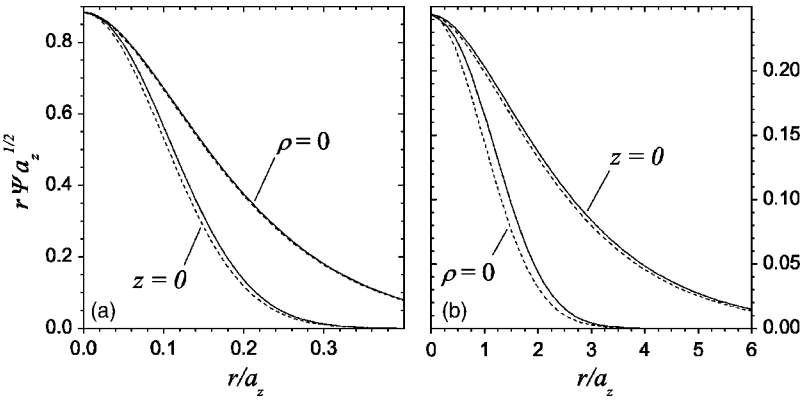

FIG. 2. The axial ($\rho=0$) and the radial ($z=0$) profiles of the ground-state wave function for two atoms interacting via a regularized delta potential with $a=\pm\infty$. The atoms are confined in a harmonic trap with (a) $\eta=\omega_\perp/\omega_z=100$ and (b) $\eta=0.01$. The exact profiles (solid lines) are compared with the approximate results of Eqs. (15)–(17) (dashed lines). All lengths are scaled to $a_z=\sqrt{\hbar/m\omega_z}$.

for a bound state in two dimensions: $\Psi(\rho)\sim K_0(\sqrt{-2\mathcal{E}}\rho)$. Along the tightly confined, axial direction, the wave function has a Gaussian profile, which is modified at short distances by the interaction potential.

The behavior of the ground-state wave function in the unitarity limit ($a=\pm\infty$) in the quasi-one-dimensional ($\eta=100$) and quasi-two-dimensional traps ($\eta=0.01$) is presented in Fig. 2. The figure compares the exact profiles evaluated from Eqs. (13) and (14) with the approximate results of Eqs. (15)–(17). We observe that all approximate curves fit quite well the exact functions.

Finally we would like to stress that our derivation can be easily supplemented to include an energy-dependent scattering length [10,16,17]. This extends the validity of the pseudopotential approximation to scattering lengths much larger than the trap size, and allows us to properly describe the entire molecular spectrum. The energy-dependent effective scattering length is defined through the *s*-wave phase shift δ_0: $a_{\mathrm{eff}}(E)=-\tan\delta_0(k)/k$, where $\hbar k$ is the relative momentum [18]. The application of this model interaction in our derivations leads to substitution of a by $a_{\mathrm{eff}}(E)$ in Eq. (3) determining the eigenenergies, and requires a self-consistent solving for the value of E. For magnetically tunable Feshbach resonances, the *s*-wave phase shift is known analytically [19], and in this case one can derive an explicit formula for $a_{\mathrm{eff}}(E)$ [10].

In summary, we solved analytically the problem of two atoms interacting in an axially symmetric harmonic trap with arbitrary trap anisotropy. For integer ratios of the trapping frequencies we gave closed formulas for the solutions. Furthermore, by introducing an effective energy dependence in the scattering length [10,16], we can find the solutions for any value of the latter. Therefore our result allows for a direct exact evaluation of the dynamics of a pair of interacting neutral atoms in very tight traps, possibly in reduced dimensionality and under an arbitrary external magnetic field, even in the presence of Feshbach resonances. Applications include a significant range of situations involving quantum control at the atomic level, from single-atom interferometry to quantum information processing.

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