A model study on atom-atom interactions with large scattering length in quasi-two dimensional traps

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Abstract

We carry out a model study on two-atom interactions and bound states in quasi-two dimensional traps. The interactions are modeled by two-parameter potentials with parameters being the range $r_0$ and the $s$-wave scattering length $a_s$. We show that one can make use of two forms of finite-range model potentials, one for $a_s > 0$ and the other for $a_s < 0$. Both potentials reduce to same form in the limits $a_s \to \pm \infty$.

We investigate into the dependence of the binding energies and the wave functions of two-atom trap-bound states on $a_s$ and $r_0$. In particular, we study the effects of $a_s$ ranging from large negative to large positive values on the bound state properties. Our results show that long-range interactions with infinite scattering length significantly alter the ground-state energy of the two atoms in a quasi-two or two dimensional trap. In contrast, short-range interactions can not significantly change the ground-state energy of two atoms in a 2D harmonic trap.

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1 Introduction

It is well established that the many-body properties of one or two dimensional systems \cite{1} are qualitatively different from those of three dimensional ones. Generally, interacting systems in low dimensions exhibit intriguing properties, for example, exotic phenomena such as quantum Hall effect and high temperature superconductivity occur in electrons in two dimensions (2D). Over the last three decades, low dimensional phenomena have been extensively studied in condensed matter systems. With the recent advent of ultracold atoms in highly anisotropic traps, new perspectives of low dimensional physics with trapped atoms have arisen \cite{2}. An ensemble of harmonically trapped noninteracting ultracold atoms becomes kinematically two dimensional in $x$ and $y$ directions (one dimensional in $z$ direction) when the temperature and the chemical potential of the ensemble are much lower than the harmonic trapping frequency in the tightly confining $z$ direction (frequencies in $x$ and $y$ directions).

In such a 2D (1D) trap, the atoms essentially occupy the ground states (state) of the harmonic oscillators in the tightly confining directions (direction). Then, the deviations from the purely 2D (1D) physics are expected to arise only from interatomic interactions. The effects of tight trapping or lower dimensions on Bose-Einstein condensates (BEC) have attracted a great deal of research interests, both theoretically \cite{3} and experimentally \cite{4}, ever since the first realization of atomic Bose-Einstein condensation in 1995.

One unique advantage for research with ultracold atoms is that one can alter interactions between the atoms over a wide range by a magnetic Feshbach resonance \cite{5,6,7}. This provides an opportunity for exploring many-body physics with tunable interactions \cite{8}. Though, most of the recent experimental works on ultracold atomic gases with tunable $s$-wave scattering length are carried out in 3D traps, it is possible to study tunable two-body interactions in highly anisotropic or lower dimensional traps \cite{9}. The effects of confinement due to tight anisotropic trapping on atom-atom cold collision are an interesting topic of research in cold atom science. Confinement induced resonances in quasi-one dimension due to strong confinement along transverse directions for any value of 3D scattering length has been discussed theoretically by Olshanii \cite{10}. It has been experimentally demonstrated by Moritz et al. \cite{11} that, cold atoms trapped in quasi-1D form confinement induced dimers. Petrov and Shlyapnikov have discussed quasi-2D and 3D regimes of atom-atom scattering in a trap that is tightly confined in axial direction \cite{12}.

Usually, two-body interaction in dilute atomic gases at low temperatures is modeled with a zero-range contact potential. In such an approach, the actual two-body interaction is replaced by a delta-type pseudo-potential

$$ V_{\text{pseu}} = \frac{4\pi\hbar^2a_s}{2\mu} \delta(r) \quad (1) $$
Table 1: Ground-state energy eigenvalue $E_{g}^{3D}$ (in unit of $\hbar\omega$) of two atoms interacting with the model potentials with $a_s = \pm \infty$ in an isotropic 3D harmonic oscillator for different values of $r_0$ (in unit of $l_0 = \sqrt{\hbar/m\omega}$, where $\omega$ is the frequency of the isotropic harmonic oscillator) applying Numerov method in one case and Hamiltonian matrix diagonalisation method in another case.

| $r_0$ | $E_{g}^{3D}$ (Numerov) | $E_{g}^{3D}$ (Matrix) |
|-------|------------------------|------------------------|
| 10.0  | 1.4622                 | 1.4622                 |
| 6.0   | 1.4045                 | 1.4045                 |
| 4.0   | 1.3162                 | 1.3163                 |
| 2.0   | 1.0742                 | 1.0747                 |
| 1.0   | 0.82220                | 0.8507                 |

where $a_s$ represents the energy-independent $s$-wave scattering length, $\mu$ is the reduced mass of two colliding atoms and $r$ denotes the separation between the two particles. This is valid for a class of two-body potentials which have finite $a_s$ in the zero energy limit. The essential idea behind this approach is to deal with a simple potential that is capable of reproducing the total two-body elastic scattering amplitude in the limit of the collision energy going to zero. The $s$-wave scattering amplitude $f_k$ for collision wave number $k$ is related to the $s$-wave scattering phase shift $\delta(k)$ by

$$f_k = \frac{1}{k \cot \delta_k - ik}$$  \hspace{1cm} (2)

and $a_s$ is related to $\delta_k$ by the well-known Bethe’s expansion formula \[13\]

$$\lim_{k \to 0} k \cot[\delta(k)] = -\frac{1}{a_s} + \frac{1}{2} r_0 k^2 + ...$$  \hspace{1cm} (3)

where $r_0$ is the effective range. Near a scattering resonance, $a_s$ diverges and so the potential, shown by expression $11$, becomes ill-defined. This means that the delta function potential can not rigorously describe the phenomena that occur near a scattering resonance. However, an improved treatment of resonant phenomena can be done in terms of the regularised delta function potential derived by Lee, Yang and Huang \[14\]. Busch et al. \[15\] have obtained an exact solution and bound-state energy spectrum for two ultracold atoms interacting via zero-range regularized delta potential in an isotropic 3D harmonic trap. Idziaszek and Calarco \[16\] have found an exact solution of two interacting particles in an axially symmetric trap within pseudopotential approximation. Tiesinga et al. \[17\] have argued that the applications of the exact solutions of \[15\] are limited to the sufficiently weak traps the width of which is much larger than $|a_s|$. To circumvent this limitation, Bolda and coworkers \[9\] have used an energy-dependent scattering length in regularised pseudopotential and developed a self-consistent method to calculate two-atom bound state in an isotropic trap, and to study $s$-wave collisions in an optical lattice with quasi-one and two dimensional harmonic confinement \[18\]. Peach et al. \[19\] have theoretically studied ultracold collisions between metastable helium atoms in tight harmonic traps using energy-dependent scattering length based self-consistent as well as quantum defect theoretic numerical integration methods.

The purpose of our investigation is to understand how a finite-range resonant two-body interaction can affect two-body bound states in low dimensional traps. To this end, we use a class of finite-range model potentials which do not diverge as $a_s \to \pm \infty$ and do not require any regularisation. To treat the effects of large scattering length in a tightly confined trap, our model potentials does not require any assumption of an energy-dependent scattering length. These model potentials are based on the expansion \[3\] and derivable by the method of Gelfand and Levitan \[20\]. We show that there exists two such finite-range model potentials - one for $a_s > 0$ and the other for $a_s < 0$. In the limits $a_s \to \pm \infty$, both potentials reduce to the same form. The finite-range model potential for $a_s = -\infty$ is well-known, and used earlier by Carson et al. \[21\] for quantum Monte Carlo simulation of a homogeneous superfluid Fermi gas, and by also Shea, van Zyl and Bhaduri \[22\] to study the energy spectrum of two interacting cold atoms in an isotropic harmonic trap. Following the work of Jost and Kohn \[23\], we introduce an analytical form of the potential for $a_s > 0$ that can smoothly match with the other potential for $a_s \to -\infty$ in the limit $a_s \to +\infty$. This means that these two potentials can account for the entire regime of low-energy interactions from large positive to the large negative scattering length for any arbitrary range of interactions.

Here we study the effects of the scattering length and the range of the potentials on the two-atom bound-state properties in quasi two-dimensional (quasi-2D) traps. Our results illustrate that, as the positive scattering length
Table 2: Six low-lying energy eigenvalues $E_{\nu,m}$ (in unit of $\hbar \omega$) of two-atom bound states in quasi-2D harmonic oscillator traps ($\eta = 100$ and $\eta = 1000$) and different values of $a_s$ (in unit of $Z_0$) keeping $r_0 = 1Z_0$.

| $\eta$ | $a_s$ | $E_{0,0}$ | $E_{1,0}$ | $E_{2,0}$ | $E_{0,1}$ | $E_{1,1}$ | $E_{2,1}$ |
|--------|-------|-----------|-----------|-----------|-----------|-----------|-----------|
| 100    | 4     | 0.9055    | 2.9125    | 4.9173    | 1.999380  | 3.998790  | 5.998230  |
| 100    | 10    | 0.9153    | 2.9209    | 4.9247    | 1.999530  | 3.999080  | 5.998640  |
| 100    | $\infty$ | 0.9201    | 2.9250    | 4.9285    | 1.999590  | 3.999264  | 5.998910  |
| 1000   | 4     | 0.9715    | 2.9721    | 4.9725    | 1.999999  | 3.999960  | 5.999940  |
| 1000   | 10.0  | 0.9743    | 2.9748    | 4.9751    | 1.999980  | 3.999970  | 5.999950  |
| 1000   | $\infty$ | 0.9757    | 2.9761    | 4.9764    | 1.999980  | 3.999970  | 5.999960  |
| 100    | -0.1  | 0.9918    | 2.9918    | 4.9919    | 1.999989  | 3.999989  | 5.999980  |
| 100    | -1.0  | 0.9623    | 2.9634    | 4.9642    | 1.999899  | 3.999800  | 5.999700  |
| 100    | -10   | 0.9321    | 2.9357    | 4.9383    | 1.999398  | 3.999910  | 5.999900  |
| 100    | $\infty$ | 0.9245    | 2.9289    | 4.9320    | 1.999627  | 3.999264  | 5.998910  |
| 1000   | -0.1  | 0.9974    | 2.9974    | 4.9974    | 1.999999  | 3.999999  | 5.999999  |
| 1000   | -1.0  | 0.9880    | 2.9880    | 4.9880    | 1.999996  | 3.999993  | 5.999990  |
| 1000   | -10.0 | 0.9782    | 2.9785    | 4.9788    | 1.999989  | 3.999979  | 5.999960  |
| 1000   | $\infty$ | 0.9757    | 2.9761    | 4.9765    | 1.999980  | 3.999980  | 5.999960  

increases, the probability amplitude for finding the two particles at the centre of the trap decreases, while that in the case of negative scattering length increases. The ground-state energy of two-particle bound state in the trap approach the same value for both limits $a_s \to \pm \infty$. Our results further demonstrate that the long-ranged interactions most significantly affect two-atom bound states in quasi-2D while short or zero-ranged interactions have rather small effects on such bound states.

The paper is organized in the following way. In section 2 we present and discuss two-parameter model interaction potentials. In section 3 we describe the method of calculating quasi 2D bound states of two particles interacting via the model potentials. We present and analyze numerical results in section 4. The paper is concluded in section 5.

2 Model potentials

The model interaction potentials we consider are two-parameter potentials. The two parameters are the range $r_0$ of the potential and the $s$-wave scattering length $a_s$. These potentials are derived making use of the effective range expansion of equation (3). The procedure for deriving a finite-ranged effective potential from the experimental data of phase shift $\delta_0(E)$ was first demonstrated long ago by Fröberg [24]. This was followed by the work of Gelfand and Levitan [20] who gave the mathematical method for the derivation of finite-range model potentials. This method was then used by a number of workers in deriving model potentials for various physical systems and parameter regimes.

For an appropriate form of a finite-range potential for negative $a_s$, we use the potential introduced by Jost and Kohn [25]. This has the form

$$V_-(r) = \frac{-4\hbar^2}{\mu r_0^2} \frac{\alpha^2 \beta^2 \exp(-2\beta r/r_0)}{[\alpha + \exp(-2\beta r/r_0)]^2}$$

where $\alpha = \sqrt{1-2r_0/a_s}$, $\beta = 1 + \alpha$ and $\mu$ is the reduced mass. This potential is valid for $|\delta_0(E)| < \pi/2$ in the limit $E \to 0$.

For positive $a_s$, we make use of the three-parameter potential derived again by Jost and Kohn [23] from an adaptation of the mathematical method of Gelfand and Levitan [20]. Among the three parameters, two are $r_0$ and $a_s$, the third one ‘$\lambda$’ (as denoted in Ref.[23]) is related to the binding energy of a bound state that the potential may support. If we use the particular choice $\lambda = -\sqrt{1-2r_0/a_s}$ with $a_s > 2r_0$, then the potential given by equation (2.29) of Ref. [23] reduces to a two-parameter potential of the form

$$V_+(r) = \frac{-4\hbar^2}{\mu r_0^2} \frac{\alpha^2 \beta^2 \exp(-2\beta r/r_0)}{[1 + \alpha \exp(-2\beta r/r_0)]^2}.$$
Figure 1: Quasi-2D ground state wave function in unit of $\rho_0^{-1}$ for $a_s = -0.1Z_0$ (solid black line), $a_s = -1.0Z_0$ (dashed red lines) and $a_s = -10.0Z_0$ (dotted blue lines) for the fixed parameters $\eta = 100$ and $r_0/Z_0 = 1$.

This choice of $\lambda$ corresponds to the binding energy $E_{\text{bin}} \approx \hbar^2/(2\mu a_s^2)$ for $2r_0/a_s << 1$. If a potential supports a bound state, $a_s$ is positive. However, positivity of $a_s$ is not sufficient for a potential to support a bound state. As discussed in Ref. [23], the experimental data on phase shift and the range of a two-body interaction are not enough to construct a model potential that can support a bound state. In order to construct such a potential it is necessary to add another term making use of the bound state wave function. This results in a four-parameter potential, the fourth parameter being the normalization constant of the wave function. Here we do not consider such bound-state supporting interaction potentials.

In the limit $a_s \to \pm \infty$, both the potentials of equations (4) and (5) reduce to the same form

$$V_\infty = -\frac{4\hbar^2}{\mu r_0^2 \cosh^2(2r/2r_0)}$$

Thus the two potentials of equations (4) and (5) smoothly connect to the resonance point as $a_s$ is varied through $\pm \infty$.

3 Bound states in a harmonic trap

The question is how to treat resonant interaction in a highly anisotropic or low dimensional trap. In the case of atoms inside traps, two-body interaction can not be described from the traditional scattering point of view. Because, atoms are bound in a trap, and the interaction between two atoms inside the trap can change the properties of trapping states of atoms. In case of two atoms in a harmonic trap, the centre-of-mass and the relative motions between the two atoms become separable. As a result, only the relative motion will be affected by an isotropic interaction. The effects of interactions will then be manifested through the changes in the properties of trap-induced two-atom bound states. In this context, it is worth noting that, very recently variable interatomic interaction induced shifts in the bound-state energy of two ultracold atoms in the microtraps of a 3D optical lattice have been used to experimentally demonstrate Feshbach resonance between excited- and ground-state atoms [26]. In case of highly anisotropic harmonic traps, lowering of spatial dimensions is possible. Then it is necessary to discuss the effects of low dimensionality on the bound states.

A harmonic trap is anisotropic if trapping frequencies in all three directions are not same. Let us consider axially symmetric case i.e $\omega_x = \omega_y = \omega_\rho \neq \omega_z$. If $\omega_\rho >> \omega_z$ i.e. if the trapping frequency $\omega_\rho$ in radial direction is much greater than that in axial direction, we get a cigar-shaped one dimensional (1D) trap. On the other hand, if $\omega_z >> \omega_\rho$ then we have pancake like quasi-two dimensional trap.

Since the relative and centre-of-mass motions between two atoms in a harmonic trap are separable, and the model interaction potentials we consider are isotropic, we henceforth consider only the relative motion between two atoms in an axially symmetric harmonic trap. In case of a many-particle system in a harmonic trap, the system effectively becomes two dimensional if the chemical potential and thermal energy are smaller than the energy gap in strongly confined axial direction. Our aim here is to elucidate how finite-range interaction between a pair of atoms in a quasi-2D or 2D trap affects bound states between the atoms. Denoting the position...
coordinates of atom 1 and 2 by \((x_1, y_1, z_1)\) and \((x_2, y_2, z_2)\), respectively; the cylindrical coordinates for the relative motion between the two atoms are given by \(\rho = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}\) and \(z = z_1 - z_2\). Schrödinger equation for relative motion can then be written as

\[
\begin{align*}
-\frac{\hbar^2}{2\mu} & \left( \frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} - \frac{|m|^2}{\rho^2} + \frac{d^2}{dz^2} \right) \psi_s(\rho, z) \\
+ & \ V_s(\rho, z) \psi_s(\rho, z) = E \psi_s(\rho, z)
\end{align*}
\]

where the subscript \(s\) stands for either ‘+’ or ‘-’. \(\mu\) is the relative mass and \(m\) is the magnetic quantum number. Due to interaction, radial and axial modes cannot be separated out. However, in case of two noninteracting particles in an axially symmetric harmonic oscillator trap, the radial and axial modes. Let \(\psi_{n\rho, m, n_z}(\rho, z)\) denote the wave function of relative motion between a pair of noninteracting particles in the trap, where \(n_\rho\) and \(n_z\) are the radial and axial principal quantum numbers, respectively. This wave function is separable in axial and radial coordinates as

\[
\psi_{n\rho, m, n_z}(\rho, z) = R_{n\rho, m}(\rho) \times f_{n_z}(z)
\]

where

\[
R_{n\rho, m}(\rho) = \left[ \frac{n_\rho!}{\pi \Gamma(n_\rho + |m| + 1)} \right]^{\frac{1}{2}} \frac{1}{\rho_0^{|m|+1}} \rho^{|m|} \exp \left[ -\frac{\rho^2}{2 \rho_0^2} \right] \mathcal{L}_{n_\rho}^{[m]} \left( \frac{\rho^2}{\rho_0^2} \right)
\]

and

\[
f_{n_z}(z) = \frac{\pi^{-\frac{1}{2}}}{\sqrt{2^{n_z} n_z!}} H_{n_z} \exp \left[ -\frac{z^2}{2 Z_0^2} \right].
\]

\(R_{n\rho, m}(\rho)\) and \(f_{n_z}(z)\) are 2D and 1D harmonic oscillator wave functions, respectively. Here \(\mathcal{L}_n^{[m]}\) and \(H_n\) are Laguerre and Hermite polynomials, respectively; \(\rho_0 = \sqrt{\frac{\hbar}{\mu \omega_\rho}}\) and \(Z_0 = \sqrt{\frac{\hbar}{\mu \omega_z}}\) are the 2D and 1D harmonic oscillator length scales, respectively. These two length scales are related by \(\rho_0 = \sqrt{\eta Z_0}\). The energy \(E = (2n_\rho + |m| + 1)\hbar \omega_\rho + (n_z + 1/2)\hbar \omega_z\) is the sum of 2D and 1D harmonic oscillator eigen energies. The aspect ratio of an axially symmetric trap is defined by \(\eta = \omega_z/\omega_\rho\).

**Quasi 2D or 2D regime**

We now return to the problem of two interacting atoms in an axially symmetric anisotropic potential. A quasi 2D or 2D regime may be reached when the two atoms are strongly confined in axial direction i.e. \((\omega_z = \omega_y = \omega_\rho << \omega_z)\), so that the axial ground state is not affected much by the interaction. We call a trap quasi 2D if \(\eta\) is relatively large and typically of the order of 100, for which the effects of axial motion at low energy is small.
The 2D case is characterized with $\eta$ of the order of or greater than 1000, consistent with the recent experimental explorations [27, 28] of 2D physics with trapped cold atoms with tight confinement along the axial direction. For 2D atom traps, typically value of $\omega_r$ is a few Hertz or of the order of 10 Hz while $\omega_z$ typically ranges between 10 to 100 kHz. This means that the harmonic oscillator radial length scale $\rho_0$ is in the micrometer regime while the axial length scale $Z_0$ is in the nanometer or even sub-nanometer regime. Since $a_s$ of alkali atoms currently used for cold atom research is typically a few nanometer, the value $Z_0$ of a 2D trap is comparable with $a_s$.

Since the model interaction potentials are isotropic, the magnetic quantum number $m$ is a good quantum number. Let $\psi^{(x)}_{\nu,m}$ denote an eigenfunction that satisfy the equation (7), where $\nu$ is the principal quantum number of the interacting system. Expanding this wave function in terms of the wave functions of noninteracting one, we have

$$\psi^{(x)}_{\nu,m}(\rho, z) = \sum_{n_\rho, n_z} c_{n_\rho, n_z} \psi^{0}_{n_\rho, n_z, n_z}(\rho, z)$$

(11)

Substituting $\psi(\rho, z)$ of equation (7) by $\psi^{(x)}_{\nu,m}(\rho, z)$, multiplying both sides by $\psi^{0}_{n_\rho, n_z, n_z}(\rho, z)$ of equation (8) and then integrating over $z$ and $\rho$, we obtain

$$\sum_{n_\rho, n_z} (2n_\rho + |m| + 1) c_{n_\rho, n_z} \hbar \omega_\rho + \sum_{n_\rho = 1}^{\infty} \sum_{n_z} V^{(m)}_{s, n_\rho, n_z, n_z, n_z} c_{n_\rho, n_z} = \tilde{E} c_{n_\rho, n_z}$$

(12)

where

$$V^{(m)}_{s, n_\rho, n_z, n_z, n_z} = \int d^2 \rho dz R^{0}_{n_\rho, m}(\rho) f^{0}_{n_z}(z) f^{0}_{n_z}(z) V_s(\rho, z) R^{0}_{n_\rho, m}(\rho)$$

(13)

and $\tilde{E} = E^{\text{trap}} - \hbar \omega_z (n_z^2 + 1)/2$, where $E^{(\text{trap})}$ denotes an eigenenergy $E$ of for the relative motion of the two interacting atoms in the anisotropic trap including both radial and axial modes. The equation (12) can be cast into a matrix form which can be diagonalised to evaluate the coefficients $c_{n_\rho, n_z}$.

We first consider the ground state of our quasi 2D or 2D system with $n_z = n_z^* = 0$, that is, we assume that the atoms occupy only the ground state of their relative motion in the axial direction. By solving the equation (12), we obtain a 2D eigenfunction

$$\psi_{\nu,m}(\rho) = \sum_{n_\rho} c_{n_\rho, 0} R^{0}_{n_\rho, m}(\rho)$$

(14)

with 2D energy eigenvalue $E_{\nu,m} = E^{(\text{trap})} - \hbar \omega_z/2$. We then consider corrections to the ground state energies and wave function due to the finite probability of excitations to the higher levels of axial modes ($n_z \neq 0$). For calculating corrections to the ground state energy and wave function, we consider possible couplings of unperturbed states with $n_z = 0$ with the states with $n_z \neq 0$ due to the interaction. Now, since the potential $V_s$
is an even function of \( z \), the matrix element \( V^{(m)}_{s,n';n,n'} \) will couple states with either even or odd \( n_z \). Since we are primarily interested in ground state energy and wave function we consider coupling between even states only for our numerical work. Let the minimum number of radial states required in order to get convergent results is \( N_\rho \). Considering coupling between \( n_z = 0 \) and \( n_z = 2 \) and introducing two vectors

\[
X_0 = \begin{pmatrix} c_{10} \\ c_{20} \\ \vdots \\ c_{N_\rho 0} \end{pmatrix} \quad (15)
\]

\[
X_2 = \begin{pmatrix} c_{12} \\ c_{22} \\ \vdots \\ c_{N_\rho 2} \end{pmatrix} \quad (16)
\]

we can write the eigenvalue equation in the form

\[
\begin{pmatrix} H_0 & 0 \\ 0 & H_2 \end{pmatrix} \begin{pmatrix} X_0 \\ X_2 \end{pmatrix} + \begin{pmatrix} V_0 & V_{02} \\ V_{20} & V_2 \end{pmatrix} \begin{pmatrix} X_0 \\ X_2 \end{pmatrix} = E \begin{pmatrix} X_0 \\ X_2 \end{pmatrix} \quad (17)
\]

where both \( H_0 \) and \( H_2 \) are \( N_\rho \times N_\rho \) diagonal matrices with elements \( (H_0)_{nn} = (2n + |m| + 1)\hbar \omega_\rho + \hbar \omega_z / 2 \) and \( (H_2)_{nn} = (2n + |m| + 1)\hbar \omega_\rho + 5\hbar \omega_z / 2 \); \( V_{02} \) is a \( N_\rho \times N_\rho \) matrix that describes couplings between different radial wavefunctions with \( n_z = 0(2) \). An element of the \( N_\rho \times N_\rho \) matrix \( V_{02} \) or \( V_{20} \) is the cross coupling between one state with \( n_z = 0 \) and another with \( n_z = 2 \). Here \( E \) represents a diagonal matrix for the eigenvalues.

4 Results and discussions

Before we present our results on the effects of \( r_0 \) and \( a_s \) on the bound state properties of two trapped atoms in a quasi-2D or 2D trap (\( \eta \gg 1 \)), we wish to see how these two parameters affect the ground-state energy for the isotropic case, that is \( \eta = 1 \) or equivalently \( \omega_x = \omega_y = \omega_z = \omega \) where \( \omega \) denotes the frequency of the isotropic harmonic trap. The results for finite-range potential with \( a_s = -\infty \) for the isotropic case are given in Ref. [22]. We would like to reproduce the known ground-state energy for the isotropic case with our model potentials in the limit \( a_s \to \pm \infty \) as a consistency check of our numerical method. The eigenstates and eigenvalues of two noninteracting atoms in an isotropic trap are well-known and can be characterised by 3 quantum numbers which are the principal, orbital angular momentum and and the magnetic quantum numbers. We calculate the ground-state energy by two methods: One is diagonalisation of the Hamiltonian matrix constructed in the basis of these eigenstates and the other is direct numerical integration of Schroedinger equation by Numerov method.
Table 3: Ground state energy eigenvalues $E_{0,0}$ (in unit of $\hbar \omega_0$) of two-atom bound states in a quasi-2D ($\eta = 100$) and 2D ($\eta = 1000$) harmonic oscillator trap for different values of $a_s$ (in unit of $Z_0$) keeping $r_0 = 1Z_0$ considering $n_z = 0$ in one case and $n_z = 0, 2$ in another case.

| $\eta$ | $a_s$ | $E_{0,0}$ $(n_z = 0)$ | $E_{0,0}$ $(n_z = 0, 2)$ |
|--------|-------|-----------------------|------------------------|
| 100    | 4     | 0.9055                | 0.99996                |
| 100    | 10    | 0.9153                | 0.99997                |
| 100    | $\infty$ | 0.9201                | 0.99998                |
| 1000   | 4     | 0.9715                | 0.99999                |
| 1000   | 10    | 0.9743                | 0.99999                |
| 1000   | $\infty$ | 0.9757                | 0.99999                |

We have found that to get convergent value of the ground-state energy by diagonalisation method, at least 7 lowest basis functions need to be considered for $r_0 > l_0$, where $l_0 = \sqrt{\hbar/\mu \omega}$ is the harmonic oscillator length scale. In table-1, some representative values of the ground-state energies (for different values of $a_s$) obtained by diagonalisation with 7 basis functions are given and compared with those obtained by Numerov method. From this table we notice that when $r_0$ is much greater than $l_0$, the two methods yield almost the same results, but when $r_0$ becomes comparable to $l_0$, the two results start to deviate considerably. This is because as $r_0$ decreases towards or below $l_0$, the two particles start to interact or collide more strongly at or near the trap center. As a result, a larger number of harmonic oscillator states can be coupled by the interaction necessitating the use of a larger number of basis functions for convergence of the eigenvalue. We find that the ground-state energy for $r_0 > l_0$ and $a_s \to \pm \infty$ agree quite well with the results of [22]. We have checked by Numerov method that as $r_0$ decreases below 0.6 $l_0$, the ground-state energy tends to 0.5 $\hbar \omega$ consistent with the earlier results for zero-ranged pseudo-potential [19]. This indicates that in the limit $r_0 \to 0$, our model potentials are capable of reproducing the results of the two atoms interacting with zero-ranged pseudopotential in an isotropic harmonic trap.

We now provide results for quasi-2D trap. In our numerical illustration, in order to compare readily with the minimum length scale of trapping potential, we express all length scales in unit of $Z_0$. However, all energies are expressed in unit of $\hbar \omega_0$. We first set $n_z = n_z' = 0$ and obtain bound-state wave functions and bound-state energies by numerically solving the equation (12). The results for the ground state ($\nu = 0, m = 0$) converge when the matrix dimension $n_\rho$ is equal or greater than 4. For low lying energy eigenvalues ($\nu \leq 2, m \leq 2$), we have found convergent results for $n_\rho \geq 6$. The radial part of the ground state wave function in case of quasi-2D trap are displayed in figures 1 and 2 for different positive and negative values of scattering length $a_s$, respectively; for the fixed $r_0 = 1Z_0$. Figure 1 shows that the ground state amplitude at the trap centre increases with the increase of negative scattering length, exactly opposite effect occurs in the case of positive scattering length as figure 2 shows. As can be noticed from these two figures, the interactions affect the bound state most significantly near the trap centre rather than near the edge of the trap. This is due to the fact that at the trap centre trapping potential vanishes. In contrast, at the edge of the trap, trapping potential dominates over the atom-atom interactions and consequently the interactions with short or finite range have practically no effect on the bound state near the edge of the trap.

Figure 3 exhibits the effects of $r_0$ of $V_{\pm \infty}$ on the the radial probability density $P_{2D}(\rho) = |\psi_{00}(\rho)|^2$ at $\rho = 0$. From this figure, we observe that as $r_0$ increases the probability amplitude of relative motion between the two particles at the centre ($\rho = 0$) of the 2D or quasi-2D trap increases first up to a certain range $r_0 \sim 3Z_0$ and then decreases. The effect is more prominent in case of quasi-2D rather than in 2D case ($\eta$ very large).

In figure 4 we show the effects of the range of the potential $V_{\infty}$ for infinite scattering length on the ground-state energy of two-particle bound states in a quasi-2D or 2D harmonic trap. We notice that when $r_0 \to 0$ the ground state energy is close to unity implying that the interaction has hardly any effect on ground state energy. However, as $r_0$ increases the energy decreases by a few percent - the decrease is more prominent if the aspect ratio is relatively smaller. In case of $\eta = 1000$, that is $\omega_z = 1000 \omega_\rho$, the ground-state energy decreases by about 4% as $r_0$ increases from zero to $10Z_0$; while in the case $\omega_z = 100 \omega_\rho$ the energy decreases by about 10% as $r_0$ increases reaching a minimum at $r_0 \approx 3Z_0$ and then the energy increases as $r_0$ increases past $3Z_0$. We can infer from these results that the long-ranged interactions have significant effects on ground state energy of a pair of interacting particles in quasi-2D or 2D traps.

In Table-2 we display a few low lying energy eigenvalues with magnetic quantum numbers $m = 0$ and $m = 1$
of eigenstates of two interacting particles in a quasi-2D ($\eta = 100$) and 2D ($\eta = 1000$) traps for different values of $a_s$ but for fixed $r_0 = 1Z_0$. From this table several inferences can be drawn. First, the deviation of the ground-state energy in the interacting case with positive $a_s$ from that in the noninteracting case ($\hbar \omega_\rho$) is more prominent compared to the similar case with negative $a_s$. In contrast, as we have observed from figures 1 and 2, the modification in ground-state wave function at or near the centre of the 2D trap ($\rho = 0$) due to an increased negative scattering length is larger than that due to an increase in positive scattering length by the same amount. This means that an attractive interaction (negative scattering length) has more prominent effect on the central probability density than on the ground-state energy, while the reverse is true for repulsive interaction (positive scattering length). Second, as the positive $a_s$ increases, the energies increase while for increasing negative $a_s$ the energies decrease. For both the limits $a_s \to +\infty$ and $a_s \to -\infty$, the energies approach to the same value. Third, the decrease of energies with lowering of $\eta$ as can be noticed from this table can be attributed to the deviation from 2D nature. Fourth, the change in $a_s$ alters ground state energies more prominently than the excited state energies implying that the interactions have most significant effects on the ground state. Fifth, this table shows that the interactions have quite small influence on the bound states with $m = 1$. In contrast, the interactions have pronounced effects on bound states with $m = 0$. Since 2D harmonic oscillator wave functions for $m \neq 0$ go to zero as $\rho \to 0$, short range interactions between two atoms can hardly affect those oscillator states.

Now, we discuss how good are the conditions of large $\eta$ that we have used to describe quasi-2D or 2D regime of the traps. We numerically solve equation (16) to know how significant are the effects of axial excitation with $n_z = 2$ on the ground-state energy and wave function. In table-3 we compare ground-state energies for the two cases $n_z = 0$ and $n_z = 0, 2$ with $\eta = 100$ and $\eta = 1000$ for 3 values of $a_s$. We notice that for $\eta = 100$ the ground-state energy for $n_z = 0, 2$ case deviates by more than 7% that for $n_z = 0$, while the corresponding deviation in case of $\eta = 1000$ is about 2%. We display the effects of this axial excitation on the ground-state wave function in figures 5 and 6 for $\eta = 100$ and $\eta = 1000$, respectively. We observe that in both the cases the deviation of the wave function are small near the trap centre and near the edges, while in the intermediate radial separations the deviation for $\eta = 100$ is quite significant but for for $\eta = 1000$ the deviation is small and may be ignored for all practical purposes. From this analysis, we may infer that while for $\eta \leq 100$ one can not ignore axial excitations and has to consider full 3D picture, in case $\eta \geq 1000$ the effects of axial excitations on the ground-state properties are quite small. For $\eta >> 100$, one may describe a quasi-2D regime where one can approximately calculate the ground state eigenenergy by ignoring the effects of axial excitations.

5 conclusion

In conclusion we have presented the results of a microscopic model study on the effects of the range and the scattering length of a class of two-parameter model potentials on the properties of trapping bound-state of two atoms in a quasi-2D trap. As discussed in the introduction part, the range $r_0$ of atom-atom interaction in the
Figure 6: 2D ground state wave function in unit of $\rho^{-1}$ for $a_s = \infty Z_0, \eta = 1000$ considering $n_z = 0, 2$ (solid black line) and $n_z = 0$ (dashed red line).

pseudo-potential approximation is usually neglected. However, when $a_s \rightarrow \pm \infty$ which is identified as “unitarity limit” in current cold atom literature, the only length scale available for expansion given in equation (3) is the effective range $r_0$. In this limit, the range of interaction and the momentum dependence of s-wave scattering amplitude may not be negligible. Finite range of two-body interactions is also important in the context of dipolar systems such as magnetic dipolar atoms or electrically polar molecules which have long-range and anisotropic interactions. Recently, physics of cold polar molecules have attracted tremendous research interests because of the long-range nature of their intermolecular interactions. Furthermore, ultracold polar molecules in 2D trap may serve as an intriguing system for exploring new physics with anisotropic interactions. In view of these recent developments in the frontier areas of ultracold atoms and molecules, the results of this study may be useful to develop an understanding on microscopic picture about those finite-ranged interactions in 2D trap the counterpart of which in 3D corresponds to the tunable Fano-Feshbach resonances.

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