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Solution of a two-dimensional time-dependent Schrödinger equation describing two interacting atoms in an optical trap

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Abstract. We introduce a numerical method to solve the two-dimensional time-dependent Schrödinger equation, which characterizes a system of two atoms with a finite-range interaction potential confined within a harmonic oscillator trap. We choose a Gaussian-shaped potential for the interaction potential. Such a system has been previously studied analytically, except that a zero-range interaction potential was used instead. We observe a strong agreement between the results for the two types of interactions. Also, we investigate the one-dimensional time-dependent Schrödinger equation for the relative motion and compute the ground state energy level as a function of the coupling strength.

Key words and phrases: split operator method, finite differences, time-dependent Schrödinger equation, quantum harmonic oscillator, Gaussian interaction potential, zero-range interaction, pseudopotential, cold atoms, optical trap

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1. Introduction

The physics of ultracold atoms has become one of the most intriguing fields of research. Due to the ability to precisely control the interaction between particles, the dimensions of the system, and its quantum state, researchers can explore a diverse range of phenomena with wide-ranging applications [1]. It is now even possible to experimentally realize systems with only a few atoms, or even just two atoms [2, 3]. This opens up a pathway for experimental verification of few-body models, highlighting the significant importance of solving the Schrödinger equation that describes such systems [4–12].

In this study, we present the solution of the two-dimensional time-dependent Schrödinger equation that describes two interacting atoms subject to the external harmonic oscillator confinement. We assume the bosonic symmetry for the particles. We choose the short-range Gaussian interaction potential to describe the interaction between the particles. Similar system, only for the zero-range interaction potential, or pseudopotential, has been studied previously [13–15]. It is a common practice to represent the interaction potential in terms of the coupling strength or scattering length. In this regard, we adjust the parameters of the Gaussian interaction potential to match the ground state energy level of the pseudopotential. This allows us to effectively analyze the system in the context of coupling strength.

Because of the harmonic trap potential, the system can be separated into relative and center-of-mass motions. First, we compute the ground state energy for the relative motion as a function of the coupling strength, Gaussian interaction depth and the correlation between these two parameters. Next, we compare the evolution of the wave function with the solutions derived from the pseudopotential, both for the relative motion and when including the center-of-mass motion. Our comparison reveals a strong agreement with the zero-range interaction potential in both of these cases.

The presented method has been employed for anharmonic trap potentials and various scenarios in the works [16–20]. In our present study, however, we illustrate that fitting the energy for the short-range Gaussian interaction with that of the zero-range potential yields an almost exact match of both wave functions within the designated range of the Gaussian interaction. Notably, in the vicinity of the origin, where the range is less than that of the Gaussian interaction, discernible distinctions between the two interaction types become evident. This contrast is even more pronounced in the two-dimensional case within the same region.

The remainder of this paper is organized as follows. Section 2 describes the Hamiltonian of two atoms in the harmonic oscillator potential. The interaction between the particles is modeled using a Gaussian-shaped function with a fixed interaction width. We also consider the system with zero-range interaction, for which the analytical solution is known. Section 3 presents the ground state energy results as a function of the interaction parameters. We then proceed to study the dynamics of the wave function for both relative motion and the total Hamiltonian. Section 4 provides a summary of the results obtained.

2. Model Hamiltonian and the method

2.1. Gaussian interaction

The Hamiltonian describing two interacting atoms in the harmonic trap reads:

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + V(x_1) + V(x_2) + V_{\text{int}}(x_1 - x_2),$$

where the $V(x)$ stands for the trapping potential:

$$V(x) = \frac{1}{2}m\omega x^2,$$

and V_{int} represents the interaction potential, which we have selected in the Gaussian form:

$$V_{\text{int}}(x_1 - x_2) = -V_0 \exp\left\{-\frac{(x_1 - x_2)^2}{2r_0^2}\right\}.$$

In the following, we use oscillator units, wherein length is given by $\ell = \sqrt{\frac{\hbar}{m\omega}}$, energy by $\hbar\omega$, and time by ω^{-1} units. We set the interaction range of (2) to a fixed value of $r_0 = 0.1$. This value provides a good approximation for the contact interaction between the atoms [11, 12, 20, 21].

Next, it is convenient to switch to the relative and center-of-mass motion coordinates given by:

$$\begin{cases} r = \dfrac{x_1 - x_2}{\sqrt{2}} \\ R = \dfrac{x_1 + x_2}{\sqrt{2}} \end{cases}, \tag{3}$$

where the factor $\sqrt{2}$ ensures that the kinetic operators and trapping potentials have equal coefficients. Thus, the Hamiltonian in these variables is represented as:

$$H(r, R) = H_r + H_R, \tag{4}$$

where

$$H_r = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{1}{2}r^2 + V_{\text{int}}(r),$$

and

$$H_R = -\frac{1}{2}\frac{\partial^2}{\partial R^2} + \frac{1}{2}R^2.$$

The dynamics of the system are governed by the time-dependent Schrödinger equation:

$$i\frac{\partial \Psi(r, R, t)}{\partial t} = H(r, R)\Psi(r, R, t).$$

Due to the separability of the Hamiltonian, the evolution operator can be factorized. Therefore, the dynamics of the wave function can be expressed as:

$$\Psi(r, R, t + \Delta t) = \exp\{-i\Delta t H_r\} \exp\{-i\Delta t H_R\}\, \Psi(r, R, t). \tag{6}$$

The operators on the right-hand side of (6) are approximated using the Crank–Nicolson formula:

$$\exp\left(-i\Delta t\hat{A}\right) = \left(1 + \frac{i}{2}\Delta t\hat{A}\right)^{-1}\left(1 - \frac{i}{2}\Delta t\hat{A}\right), \tag{7}$$

where $\hat{A}$ represents the operators in (6). The equation (7) is accurate up to third order in terms of $\mathcal{O}(\Delta t^3)$. The partial derivatives are approximated using finite differences of sixth-order accuracy. The system of linear equations thus obtained is of a band diagonal type and is solved using the sweep method.

We employ the imaginary-time propagation method to compute the stationary states, i.e., $\Psi(r, R, t = 0)$, and the bound energy levels.

2.2. Zero-range interaction

For the purpose of comparison, we also consider an analytical model for two bosons with zero-range interaction. In this approach, the total Hamiltonian (in oscillator units) is given by:

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + \frac{1}{2}x_1^2 + \frac{1}{2}x_2^2 + \sqrt{2}g\delta(x_1 - x_2), \tag{8}$$

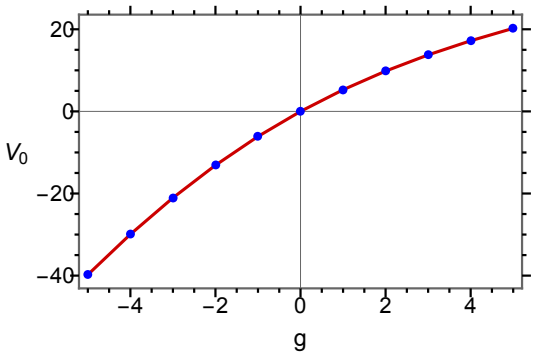

Figure 1. The relationship between the depth of the Gaussian interaction and the coupling strength g of the pseudopotential (data points with a guiding line)

where $\delta(x_1 - x_2)$ is the Dirac Delta function, and the factor $\sqrt{2}$ is used for convenience. Applying the transformation (3), the Hamiltonian decouples into the form given by (4), where the relative motion part is expressed as:

$$H_r = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{1}{2}r^2 + g\delta(r). \tag{9}$$

The solution to (9) is established through the work of Busch et al. [13, 14]. Specifically, the energy levels are determined as the roots of the transcendental equation:

$$-g = 2\frac{\Gamma\left(-\frac{E_r}{2} + \frac{3}{4}\right)}{\Gamma\left(-\frac{E_r}{2} + \frac{1}{4}\right)}, \tag{10}$$

and the wave functions are given as:

$$\psi_r(r) = \mathcal{N}e^{-r^2/2}U\left(\frac{1}{4} - \frac{E_r}{2}, \frac{1}{2}, r^2\right).$$

Here $\mathcal{N}$ is the normalization constant and $U(a, b, z)$ are the Kummer functions. The solutions of the center-of-mass motion Hamiltonian H_R are the well-known solutions of the harmonic oscillator.

The time-dependent solution for the zero-range interaction of equation (5) can then be expressed as follows:

$$\Psi(r, R, t) = e^{-itE}\Psi(r, R, t = 0), \tag{11}$$

where E is the eigenenergy of the total Hamiltonian (8).

3. Results

Further on, we will focus solely on the ground state solutions. To represent the results of solving (5) for the Gaussian interaction, we adjust the depth of $V_{\text{int}}(r)$ such that the ground state energy level matches that of the pseudopotential in (10). This way we can directly compare the outcomes obtained for the Gaussian interaction potential with those of the zero-range interaction potential. The result of this adjustment is depicted in Fig. 1. From Fig. 1, it is evident that negative values of g correspond to attractive interactions between the particles, while positive values indicate repulsion.

Figure 2 illustrates the dependence of the ground state energy on the parameters for both the Gaussian interaction potential (Fig. 2(a)) and the zero-range interaction potential (given by (10), Fig. 2(b)).

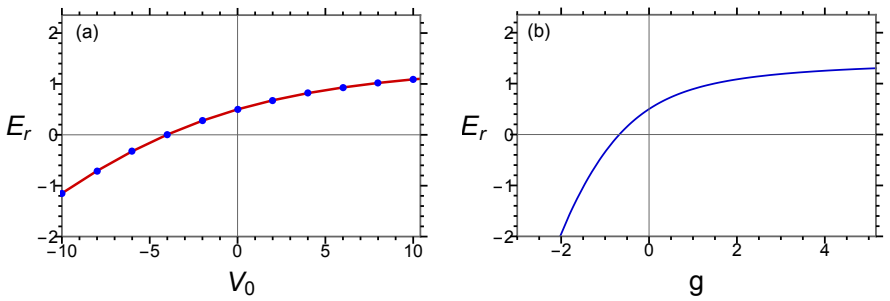

Figure 2. (a) Ground state energy for the relative motion as a function of the Gaussian interaction depth V_0 (data points with a guiding line). (b) Ground state energy for the relative motion as a function of the coupling strength g

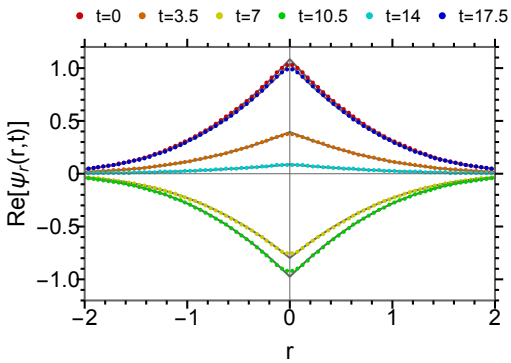

Figure 3. The real part of the wave function for the relative motion at various time points, calculated numerically (data points) and analytically (gray lines), for the coupling strength $g = -1$

3.1. Relative motion

First, we consider the Hamiltonian of the relative motion and compare the dynamics of the real part of the wave function (data points) with that of the zero-range interaction (gray lines), as shown in Fig. 3. We focus on the case where the coupling strength is $g = -1$. In Fig. 3, one can observe that the wave functions differ mainly in the region close to the origin, approximately $r \sim 0.1$, which corresponds to the length of the Gaussian interaction potential. Apart from that region, both solutions are in excellent agreement.

3.2. Relative and center-of-mass motions

Here, we incorporate the center-of-mass motion component of the Hamiltonian (4) into our analysis. We numerically calculate the dynamics of the wave function $\Psi(r, R, t)$ for the Gaussian interaction potential using (6) and for the pseudopotential using (11). Our focus is on the case where the coupling strength is $g = -1$. The results are presented in Fig. 4. In this figure, differences become noticeable around the region close to the origin, once again attributed to the width of the Gaussian interaction $r_0 = 0.1$. However, the discrepancy between the two types of interaction is slightly more pronounced.

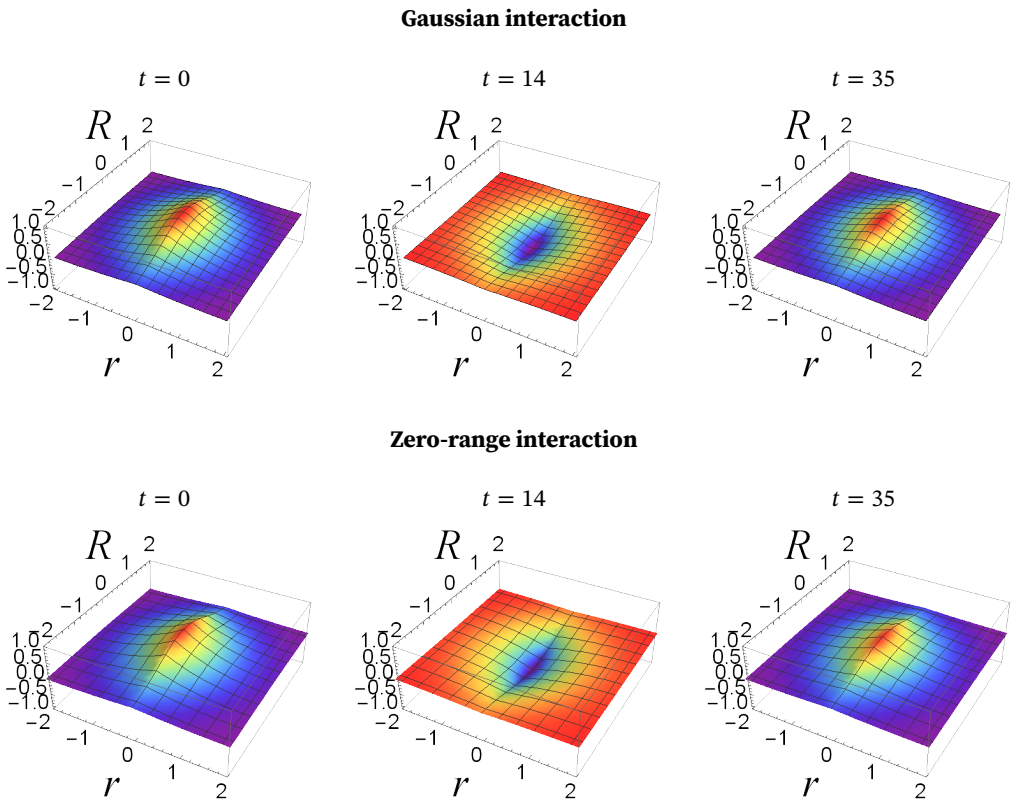

Figure 4. Real part of the wave function, $\mathrm{Re}\,[\Psi(r,R,t)]$, is shown at different time moments for both the Gaussian interaction (upper graphs) and the zero-range interaction (lower graphs), for the coupling strength $g=-1$

4. Summary

We studied the solutions of the two-dimensional Schrödinger equation for Gaussian and zero-range interaction potentials. The trap potential has the form of a harmonic oscillator, which results in the separability of the relative and center-of-mass motions. The solution for the Gaussian interaction potential was numerically obtained using the Crank-Nicolson approximation for the evolution operator and sixth-order finite differences for the spatial derivatives. The solution for the zero-range interaction is known analytically [13, 14].

The comparison between the two types of interaction potentials for the relative motion revealed that the discrepancy manifests around the region where $r \sim 0.1$, corresponding to the width of the Gaussian interaction potential. In the case where the center-of-mass motion is included, the difference becomes even more noticeable.

The provided method can be extended to more complex interaction and trap potentials [16, 17], as well as to systems involving more particles and/or higher dimensions [20].

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formal analysis, I.S. Ishmukhamedov, A.S. Ishmukhamedov and Zh.E. Jalankuzov; investigation, I.S. Ishmukhamedov, A.S. Ishmukhamedov and Zh.E. Jalankuzov; resources, I.S. Ishmukhamedov, A.S. Ishmukhamedov and Zh.E. Jalankuzov; data curation, I.S. Ishmukhamedov, A.S. Ishmukhamedov and Zh.E. Jalankuzov; writing—original draft preparation, I.S. Ishmukhamedov, A.S. Ishmukhamedov and Zh.E. Jalankuzov; writing—review and editing, I.S. Ishmukhamedov, A.S. Ishmukhamedov and Zh.E. Jalankuzov; visualization, I.S. Ishmukhamedov, A.S. Ishmukhamedov and Zh.E. Jalankuzov; supervision, I.S. Ishmukhamedov; project administration, I.S. Ishmukhamedov; funding acquisition, I.S. Ishmukhamedov. All authors have read and agreed to the published version of the manuscript.

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Решение двумерного нестационарного уравнения Шрёдингера, описывающего два взаимодействующих атома в оптической ловушке

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Аннотация. Мы представляем численный метод решения двумерного нестационарного уравнения Шредингера, которое характеризует систему двух атомов с потенциалом взаимодействия конечного радиуса действия, заключенную в ловушку гармонического осциллятора. В качестве потенциала взаимодействия мы выбираем гауссовский потенциал. Такая система ранее изучалась аналитически, с той лишь разницей, что вместо нее использовался нулевой потенциал взаимодействия. Мы наблюдаем хорошее согласие между результатами для двух типов взаимодействий. Кроме того, мы исследуем одномерное нестационарное уравнение Шредингера для относительного движения и вычисляем уровень энергии основного состояния в зависимости от константы связи.

Ключевые слова: метод расщепления, конечные разности, нестационарное уравнение Шрёдингера, квантовый гармонический осциллятор, гауссов потенциал взаимодействия, взаимодействие нулевого радиуса, псевдопотенциал, холодные атомы, оптическая ловушка