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Quantum scattering approach for investigation of two interacting atoms trapped in a one-dimensional Morse potential via Lippmann-Schwinger equation

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In this work, a system including two neutral atoms confined to an external one-dimensional Morse potential was modelled. The problem can be relevant to cold atom physics, where neutral atoms may be effectively confined in radially tight tubes formed by optical lattices. The atom-atom interaction was considered as a nonlocal separable potential. Analytical expressions for wave-function as well as transition matrix were derived. The contributions of bound states and resonances in the complex energy plane were calculated. For numerical computations, the bound states in a system of argon gas confined in graphite were considered. Since the most important quantity in the low energy quantum scattering problems is “scattering length,” considering various values of Morse parameters, the behavior of this parameter was described versus the reduced energy. Published by AIP Publishing. [http://dx.doi.org/10.1063/1.4984983]

I. INTRODUCTION

Confined quantum systems are a great example of how physical problems can be explained theoretically and described based on experimental evidence. A system of one or more atoms confined in a potential well has been used to model nanopores,\textsuperscript{1,2} impurities in nanocrystals,\textsuperscript{3} semiconductors,\textsuperscript{4} etc. The advent of one-dimensional (1D) nanostructures\textsuperscript{5} such as nanowires and nanotubes was a motivation to reduce the dimensionality. The 1D scattering problems were also appeared in a vast variety of physical problems, such as ultracold highly confined atoms. Moreover, quantum scattering studies including the analytical solvable models have an important role to check the validity of theorems and occasionally to discover the new physical phenomena.

In this work, we study the quantum scattering of two interacting atoms confined to an external 1D Morse potential. The actual atom-atom interaction was replaced by a projective operator, namely, the two-body nonlocal separable potential (NLSP). Such interactions lead to the analytical solution of Lippmann-Schwinger (LS) equation. It is well-known that the non-locality in the potential interaction plays an important role in the calculation of both scattering and bound states as well as resonances. Nonlocal separable potentials have proved useful in the study of the few-body problems, in which the actual many body potential at each point is replaced by a projective two-body nonlocal potential operator. Moreover, such potentials have been studied as models for a variety of physical problems.\textsuperscript{6–14} The purpose of this article is to get the analytical solution of the LS equation for two interacting atoms with nonlocal interaction and trapped in the Morse oscillator. We calculated the transition matrix analytically and investigated the bound states and resonances. Moreover, the scattering length as the most important quantity in the low energy quantum scattering problems was obtained.

II. MATHEMATICAL MODEL

Let us consider a system of two atoms with masses $m_1$ and $m_2$ trapped in a 1D Morse potential. The Hamiltonian for the relative motion of the system is given by
\[ \hat{H} = \hat{H}_0^0 + \hat{V}_M + \hat{V}_{NL}(x), \]

where \( \hat{H}_0^0 = \hat{p}^2/2\mu \), \( \mu \) is the reduced mass, \( \hat{p} \) is the relative momentum, and \( \hat{V}_M \) is the 1D Morse potential that has the form \( \hat{V}_M = D_e \left( e^{-2\beta(x-x_0)} - 2e^{-\beta(x-x_0)} \right) \),

\[ \hat{V}_{NL} = D_e \left( e^{-2\beta(x-x_0)} - 2e^{-\beta(x-x_0)} \right) \],

where \( D_e \) is the well depth, \( x_0 \) is the distance at which the potential reaches its minimum, and \( \beta \equiv \sqrt{\frac{\hbar}{2\mu\omega}} \) controls the curvature of the potential, in which \( \omega \) is the trap frequency. In Eq. (2.1), \( \hat{V}_{NL} \) is the atom-atom interaction that we considered the two-body NLSP. It has been proved that the NLSPs are useful because of the fact that the two-body LS equation is exactly solvable and leads to the closed expressions for all scattering properties without any tedious calculations. In our model, the NLSP was considered to be with rank one \( \hat{V}_{NL} = |\chi \rangle v \langle \chi | \),

where \( |\chi \rangle \) is an arbitrary normalized state and \( v \) is the strength parameter of potential. We have chosen the Lorentzian form of the function \( \chi(p) \) so that all equations can be explicitly written as

\[ \chi(p) \equiv \langle p | \chi \rangle = \left( \frac{2a^3}{\pi} \right)^{1/2} \frac{1}{p^2 + a^2}, \]

in which the momentum parameter \( a \) plays the role of a scale factor.

The LS equation for s-wave scattering via Hamiltonian \( \hat{H} \) is given by

\[ |\psi(z)\rangle = |\varphi\rangle + \frac{1}{z - \hat{H}} \hat{V}_{NL} |\psi(z)\rangle, \]

where \( \hat{H} = \hat{H}_0^0 + \hat{V}_M \) is the Hamiltonian of one particle of mass \( \mu \) trapped in a Morse potential and \( z \equiv E + i\epsilon \) is the complex energy parameter. The vector \( |\varphi\rangle \) is the eigenvector of \( \hat{H} \) corresponding to the energy eigenvalues \( \epsilon_n \) as \( \Phi_n(X) = \left[ \frac{n! (2\lambda - 2n - 1)}{\Gamma(2\lambda - n)} \right]^{1/2} X^{\lambda - n - 1/2} e^{-X/2} L_{n}^{(2\lambda - 2n - 1)}(X/2) \), 0 < \( X < \infty \)

and

\[ \epsilon_n = \frac{D_e}{\lambda^2} \left[ 1 - \frac{1}{\lambda^2} \left( \lambda - n - \frac{1}{2} \right) \right] \]

where \( \lambda \equiv \frac{\sqrt{2\mu D_e}}{\hbar} \), \( X \equiv 2\lambda e^{-\beta(x-x_0)} \), \( L_{n}^{(2\lambda - 2n - 1)}(Y) \) is a generalized Laguerre polynomial, and \( \Gamma(x) \) is the gamma function.

Using the model potential (2.3), the LS equation can be rewritten as

\[ \langle \chi |\psi(z)\rangle = \frac{\langle \chi |\varphi \rangle}{1 - vQ(z)}, \]

where \( Q(z) \) is the matrix element of trapped particle resolvent defined as

\[ Q(z) \equiv \langle \chi \left| \frac{1}{z - \hat{H}} \right| \chi \rangle. \]

A. Matrix element of trapped particle resolvent

From Eq. (2.9), the matrix element of trapped particle resolvent may be given by

\[ Q(z) = \int_{-\infty}^{\infty} \langle \chi \left| \frac{1}{z - \hat{H}} \right| p \rangle \langle p |\chi \rangle dp. \]
Then, the matrix element of the trapped particle resolvent in the complex plane. The result is given by

\[
\langle p | \frac{1}{z - \hat{H}} | \chi \rangle \approx \left( \frac{2a^3}{\pi} \right)^{1/2} \frac{2\mu}{q^2 - p^2} \left[ \frac{1}{p^2 + a^2} - \frac{2\mu \int dp'}{(p'^2 - q^2)} \frac{\mathcal{V}_M(p,p')}{(p'^2 + a^2)} \right],
\]

where \( q = \sqrt{2\mu z} \), and \( \mathcal{V}_M(p,p') \) is the momentum representation of the Morse potential given by

\[
\mathcal{V}_M(p,p') = \frac{\hbar D_e}{\pi^2} \left[ \frac{e^{2\beta x_0}}{(p - p')^2 + 4\hbar^2 \beta^2} - \frac{e^{\beta x_0}}{(p - p')^2 + \hbar^2 \beta^2} \right].
\]

The second term of Eq. (2.11) can be obtained by contour integration via closing in the upper half of the complex plane. The result is given by

\[
\langle p | \frac{1}{z - \hat{H}} | \chi \rangle \approx \left( \frac{2a^3}{\pi} \right)^{1/2} \frac{2\mu}{q^2 - p^2} \left[ \frac{1}{p^2 + a^2} - \frac{2\mu \pi}{q^2 + a^2} \left\{ \frac{1}{a} \mathcal{V}_M(p,ia) + \frac{i}{q} \left[ \mathcal{V}_M(p,q) - \mathcal{V}_M(p,-q) \right] \right\} \right].
\]

Then, the matrix element of the trapped particle resolvent \( Q(q) \) is obtained as

\[
Q(q) = \frac{4\mu a^3}{(q^2 + a^2)^2} \left\{ \frac{(q^2 + 3a^2)}{2a^3} - 2\mu \pi \mathcal{V}_M(s,s) \left( \frac{1}{q^2} + \frac{1}{a^2} \right) + \frac{2\mu \pi \mathcal{V}_M(q,-q)}{q^2} \right\}
\]

It must be noted that from Eq. (2.12), we have

\[
\mathcal{V}_M(s,s) = \frac{D_e}{4\hbar \beta \pi^2} \left( e^{2\beta x_0} - 4e^{\beta x_0} \right)
\]

Also, we have \( \mathcal{V}_M(\mathbf{r}^*, s) = \mathcal{V}_M(s, \mathbf{r}^*) \) and \( \mathcal{V}_M(s, i\mathbf{t}) = \mathcal{V}_M^*(s, -i\mathbf{t}) \).

### B. Trapped particle wave-function

The momentum representation of the total wave-function of two-particle trapped in a one-dimensional Morse potential can be calculated using Eq. (2.5) as

\[
\psi_n(p, z) = \varphi_n(p) + \sqrt{\left| \frac{1}{z - \hat{H}} \right|} \langle \chi | \psi(z) \rangle.
\]

Inserting Eqs. (2.8) and (2.13) into Eq. (2.16), the analytic expression for the momentum representation of the total wave-function of two-particle trapped in a one-dimensional Morse potential is obtained as follows:

\[
\psi_n(p, q) = \varphi_n(p) + \sqrt{\left| \frac{1}{z - \hat{H}} \right|} \left\{ \frac{\langle \chi | \varphi \rangle}{1 - \nu Q(z)} \right\}
\]

where the momentum representation of the eigenfunctions of Hamiltonian \( \hat{H} \) is given by

\[
\varphi_n(p) = e^{-ip/\alpha a} 2^{1/2 - n} \left( \frac{2\lambda - 2n - 1}{4\pi \Gamma(2\lambda - n)} \right)^{1/2} \sum_{j=0}^{n} \frac{(-1)^j/2j}{j!} \Gamma(2\lambda - n) \Gamma(j + 1 - 2\mathbf{n}) \Gamma(2\mathbf{n} + j) \Gamma(n - j + 1) \Gamma(2\mathbf{n} + j + 1).
\]

The term \( \langle \chi | \varphi \rangle \) in Eq. (2.17) may be obtained as follows:

\[
\langle \chi | \varphi \rangle = \int_{-\infty}^{\infty} \chi(p) \varphi_n(p) dp = \frac{(2\lambda - 2n - 1)}{4\pi \Gamma(2\lambda - n)} \left[ \frac{(2\lambda - 2n - 1)}{4\pi \Gamma(2\lambda - n)} \right]^{1/2}
\]

\[
\times \sum_{j=0}^{n} \frac{(-1)^j/2j}{j!} \Gamma(2\lambda - n) \Gamma(j + 1 - 2\mathbf{n}) \Gamma(2\mathbf{n} + j) \Gamma(n - j + 1).
\]
Substituting Eqs. (2.18) and (2.19) into (2.17) allows us to obtain the momentum representation of the wave-function of two-particle trapped in a 1D Morse potential.

Of particular interest is the corresponding position representation of the two-particle wave-function trapped in a 1D Morse potential. Using the Fourier transformation of Eq. (2.17), the expression for the coordinate representation of wave-function reads

\[
\begin{align*}
\Psi_n(x, q) &= \Phi_n(x) + \left(\frac{a^3}{\hbar}\right)^{1/2} \left\{ \frac{4\mu v}{q^2 + a^2} - \frac{1}{a} \right\} \frac{1}{2a} e^{-a|x|/\hbar} - \frac{1}{q} \left(1 + \frac{2i\pi \mu}{q} V_M(q, q)\right) \sin(qx/\hbar) \\
&\quad + \frac{i\pi \nu}{qa} \left[ V_M(q, ia) e^{iqx/\hbar} - \text{complex conjugate} \right].
\end{align*}
\]

(2.20)

C. Transition matrix

As it can be seen in Ref. 11, the off-energy shell \( T \)-matrix elements are given by

\[
\hat{T}_{p\to p'} = \left\{ p \right| \hat{V}_{NL} \left( 1 - \frac{1}{z - \hat{H}} \right)^{-1} \left| p' \right\}.
\]

(2.21)

Using Eqs. (2.3) and (2.4), the transition matrix is readily found in terms of the trapped particle resolvent \( Q(q) \),

\[
\hat{T}_{p\to p'}(q) = \frac{v}{v} \chi^{*}(p) \chi(p').
\]

(2.22)

For simplicity and reducing the number of parameters, we defined the dimensionless parameters as \( \tilde{p} = \frac{p}{a} \), \( \tilde{q} = \frac{q}{a} \), \( \hat{T}_{p\to p'}(\tilde{q}) = \frac{\mu}{a} \tilde{T}_{p\to p'}(q) = \frac{\mu}{a} \hat{T}_{p\to p'}(q) \), \( \tilde{v} = \frac{v}{a} \hat{v} \), \( \tilde{V}_M = \frac{\mu V_M}{a} \hat{V}_M \), \( \tilde{D} = \frac{\mu D}{a} \hat{D} \), \( \tilde{\beta} = \frac{\beta}{a} \), and \( \tilde{x}_0 = \frac{x_0}{a} \). As a result, the dimensionless transition matrix for the scattering under the Morse potential confinement is expressed in terms of these dimensionless variables as

\[
\hat{T}_{p\to p'}(\tilde{q}) = \frac{2\tilde{v}}{\pi} \frac{1}{1 - \tilde{v}\tilde{q}(\tilde{q})} \frac{1}{(\tilde{p}^2 + 1)(\tilde{p}'^2 + 1)},
\]

(2.23)

in which the trapped reduced resolvent matrix is given by

\[
\tilde{Q}(\tilde{q}) = \frac{4}{(\tilde{q}^2 + 1)^2} \left\{ \frac{(\tilde{q}^2 + 3)}{2} - 2\pi \left\{ \frac{(\tilde{q}^2 + 1)\tilde{V}_M(s,s) - \tilde{V}_M(s,-s)}{\tilde{q}^2} \right\} \right\}
\]

(2.24)

The formulas for the transition matrix \( \hat{T}_{p\to p'}(\tilde{q}) \) and resolvent matrix \( \tilde{Q}(\tilde{q}) \) of a two-particle trapped in a Morse potential are the key result of this paper.

III. RESULTS AND DISCUSSION

In this paper, we present the scattering behavior of a system including two neutral atoms confined to an external one-dimensional Morse potential. The problem may indeed be relevant, for example, to cold atom physics, where neutral atoms may be effectively confined in radially tight tubes formed by optical lattices. This led us to study the potential of a new way of providing ultracold systems. Analytical and general expressions for the wave-function and transition matrix for such systems have been derived.

The transition matrix constructed in Eq. (2.23) may be represented the contributions of bound states and resonances in the complex energy (or momentum) plane. The “bound states” can arise when the singularities of the transition matrix appear on the positive imaginary \( \tilde{q} \)– axis, whereas the singularities on the negative imaginary \( \tilde{q} \)– axis correspond to the virtual states. Moreover, the resonances may be obtained if the two symmetrical poles about the imaginary axis with an opposite real part are located on the lower half-plane. The features of these singularities depend on the values of two reduced parameters of the Morse potential (\( \tilde{D} \) and \( \tilde{\beta} \)) and one reduced strength parameter of the nonlocal potential (\( \hat{v} \)). According to Eq. (2.23), the singularities of the transition matrix occur when the trapped reduced resolvent matrix \( \tilde{Q}(\tilde{q}) \) equals \( \hat{v}^{-1} \). For numerical computations, we selected the
values of optimized potential parameters for argon-graphite system, that is, \( \tilde{D}_e = 1.50 \) and \( \tilde{\beta} = 0.01 \). Figure 1 shows the distribution of singularities of the transition matrix in the complex momentum (\( \tilde{q} \)) plane. As shown in Fig. 1, one bound state reveals at \( \tilde{q} = 0.993 \) or \( \tilde{E} = -0.496 \) for our selected values of \( \tilde{D}_e \) and \( \tilde{\beta} \), which is independent of the selected value and sign of strong interatomic interaction. For argon gas confined in graphite, this bound-state energy equals about 0.004 eV. For positive values of \( \tilde{\nu} \), an additional bound state occurs in which the bound state energy depends on the value of \( \tilde{\nu} \).

Moreover, for \( \tilde{\nu} < 0 \), as shown in Fig. 1, there exist two symmetric poles located at \( \tilde{q} = \pm \tilde{q}_{\text{re}} - \tilde{q}_{\text{im}} \) (\( \tilde{q}_{\text{re}} \) and \( \tilde{q}_{\text{im}} \) are assumed positive) called “resonance” and “antiresonance” located in the fourth and third quadrants, respectively. The reduced resonance energy \( \tilde{E}_R \) and its corresponding reduced resonance width \( \tilde{\Gamma}_R \) are given by

\[
\tilde{E}_R = \frac{1}{2} (\tilde{q}_{\text{re}}^2 - \tilde{q}_{\text{im}}^2) ,
\]

\[
\tilde{\Gamma}_R = 2\tilde{q}_{\text{re}}\tilde{q}_{\text{im}} .
\]

The resonance width increases when the trapped potential well \( \tilde{D}_e \) becomes deeper. For weakly interacting particles, both the resonance energy and width approach to zero.

Furthermore, low energy quantum scattering problems are usually described by a single parameter, namely, “scattering length,” which for s-wave scattering in dimensionless form is defined by

\[
\tilde{a}_S = -\lim_{\tilde{p} \to 0} \frac{1}{\tilde{q}} \tilde{f}(\tilde{q}) ,
\]

where \( \tilde{f}(\tilde{q}) \) is the reduced scattering amplitude and is given by

\[
\tilde{f}(\tilde{q}) = -2\pi^2 \lim_{\epsilon \to 0^+} \left\langle \hat{\tilde{p}} \hat{\tilde{T}}(\tilde{q}) \hat{\tilde{p}} \right\rangle .
\]

![FIG. 1. Distribution of poles of the transition matrix with \( \tilde{\beta} = 0.01 \), \( \tilde{D}_e = 1.5 \), and \( \tilde{x}_0 = 0.2 \) and some different values of \( \tilde{\nu} \).](image_url)
FIG. 2. Reduced scattering length as a function of reduced energy for $\tilde{\beta} = 0.01$, $\tilde{\nu} = 0.5$, and $\tilde{x}_0 = 0.2$ and some different values of $\tilde{D}_e$.

FIG. 3. Reduced scattering length as a function of reduced energy for $\tilde{D}_e = 1.5$, $\tilde{\nu} = 0.5$, and $\tilde{x}_0 = 0.2$ and some different values of $\tilde{\beta}$. 
Applying Eqs. (2.23), (3.3), and (3.4), the reduced scattering length was calculated numerically and depicted in Figs. 2 and 3 for different values of trapped potential parameters. As shown in Fig. 2, we observe that at the lower energies, the scattering length is negative and has a minimum value depending on the well depth. At higher energies, the curves reveal the positive values for the scattering length and approach to a limiting value after passing through the maximum. Figure 3 also shows the behavior of the reduced scattering length as a function of the reduced energy for some different values of exponent parameter, $\beta$, of the trapped Morse potential. We observe that for $\beta = 0.01$ the scattering length displays a large minimum value close to the bound state.

IV. CONCLUSION

In this study, we modelled a system of two neutral atoms confined to an external one-dimensional Morse potential. Since nonlocal separable potentials lead to the analytical solution of the Lippmann-Schwinger equation and have proved useful in the study of the few-body problems, the actual atom-atom interaction potential was replaced by a projective two-body nonlocal separable potential operator. Analytical expressions for the wave-function as well as the transition matrix have been derived. The bound states and resonances were calculated via the transition matrix. For numerical computations, considering a system of argon gas confined in graphite, the bound-state energy obtained about 0.004 eV. The scattering length as an important property in the low energy quantum scattering problem was calculated and investigated as a function of the reduced energy considering different values of the Morse parameters.

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