



Phase Shift Analysis for Alpha-alpha Elastic Scattering using Phase Function Method for Gaussian Local Potential

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ABSTRACT

The phase shifts for α - α scattering have been modeled using a two parameter Gaussian local potential. The time independent Schrodinger equation (TISE) has been solved iteratively using Monte-Carlo approach till the S and D bound states of the numerical solution match with the experimental binding energy data in a variational sense. The obtained potential with best fit parameters is taken as input for determining the phase-shifts for the S channel using the non-linear first order differential equation of the phase function method (PFM). It is numerically solved using 5th order Runge-Kutta (RK-5) technique. To determine the phase shifts for the $\ell=2$ and 4 scattering state i.e. D and G-channel, the inversion potential parameters have been determined using variational Monte-Carlo (VMC) approach to minimize the relative mean square error w.r.t. the experimental data.

1. Introduction

Modeling the α - α interaction using local potentials in a phenomenological approach [1] has been found to be able to reproduce the scattering data [2] quite well. Buck [1] and his collaborators have argued at length as to how the microscopic resonating group methods (RGM) could be reduced to orthogonal condition model (OCM) by using simple factorization assumption, which in turn makes local potentials to be used as a plausible model. Extensive work have been carried out by various authors to understand this interaction [1-3]. Buck et al. [1] have used a single Gaussian potential with 2 parameters along with Coulomb term represented with an erf function which has one parameter and obtained the phase shift for α - α scattering for $\ell = 0, 2, 4$ and 6 partial waves. Ali and Bodmer [3] proposed a two term phenomenological potential with 4 parameters, Darriulat, Igo and Pugh [4] used four term interaction potential with 9 parameters and calculated the differential cross sections for elastic scattering of alpha particles by Helium between lab energy 53-120 MeV. Jana et al. [5] used phase function method (PFM) and calculated phase shifts for α - α using complex potential as in optical models. Myagmarjav et al. [6] calculated the scattering cross section for various potential systems for

α - α using complex scaling method (CSM). Typically, these scattering phase-shifts are obtained analytically using either S-matrix [7] or Jost function [8] methods. Recently there has been renewed interest in application of PFM [9, 10], also called as Variable Phase Approach (VPA), which has been extensively used by Laha, et al. [11-15]. They have applied this technique to study of nucleon-nucleon [11], nucleon-nucleus [14] and nucleus-nucleus [15] scattering using a variety of two term potentials such as modified Hulthen [12] and Manning-Rosen [13]. While traditional S-matrix approaches depend on wave-functions obtained by solving TISE, PFM requires only potential function to obtain the scattering phase shifts.

In this paper, our main objective is to obtain the scattering phase-shifts for alpha-alpha system using local potential as Gaussian function with two parameters and Coulomb term included as an erf function with another parameter [1]. To achieve this, we employ a methodology which is a combination of various numerical techniques. On one hand, we solve TISE for obtaining bound state energies using matrix methods (MM) with sine basis [16-19], while on the other hand, the model parameters are optimized using variational Monte-Carlo (VMC) as proposed in [16-19], in tandem.

2. Methodology

2.1. Modeling α - α using Two-term Potentials

The simplest stable nucleus, Be-8, a two alpha particle configuration is modeled by considering the interaction of Gaussian type which is mathematically expressed as

$$V(r) = -V_0 e^{-\alpha r^2} + z_1 z_2 \frac{e^2}{r} \text{erf}(\beta r) \quad (1)$$

In Eq.(1) first term is for nuclear interaction modeled as central potential and second is long range Coulomb repulsive term. Here, V_0 is well depth of the potential or interaction strength in MeV, parameter α is in fm^2 and another parameter β in units of fm^{-1} . The value of e^2 is taken as 1.45 MeVfm . The radial TISE equation governing the system is given by

$$-\frac{\hbar^2}{2m} \frac{d^2 u(r)}{dr^2} + V(r)u(r) = Eu(r) \quad (2)$$

The first factor is kinetic energy operator T_i which together with $V(r)$ is written as Hamiltonian H and the equation is written as $Hu(r) = Eu(r)$. The wave-function $u(r)$ has to satisfy the boundary condition at $r = 0$ as $u(r=0) = 0$ and should die down to zero as r tends to infinity. Further, it has to satisfy the normalization condition as well.

2.2. Numerical Solution using Matrix Methods (MM) Technique

The central idea in this method is to embed the potential of interest inside an infinite spherical well of radius a , which basically defines the limits for region of interest as $[0, a_0]$. Now, the eigenfunctions for the infinite spherical well are given by

$$\varphi_n = \sqrt{2/a_0} \sin(n\pi r / a_0) \quad (3)$$

These are chosen as the basis functions to write $u(r)$ as a linear combination:

$$u(r) = \sum_{k=1}^N c_k \varphi_k \quad (4)$$

for determining the matrix elements of K.E. operator T_i and the potential of interest $V(r)$, as follows:

$$\begin{aligned} T_{mn} &= \frac{n^2 \pi^2 \hbar^2}{2ma_0^2} \text{ and } V_{mn} \\ &= \frac{2}{a_0} \int_0^{a_0} \sin(m\pi r / a_0) V(r) \sin(n\pi r / a_0) dr \end{aligned} \quad (5)$$

Then, the matrix for the Hamiltonian $H_{mn} = T_{mn} + V_{mn}$ is solved using an eigen solver to obtain the energy eigenvalues and corresponding eigen vectors. These eigen vectors corresponding to each eigen value are used to obtain the wave-function as in eq. (4). Here, we are only interested in energies and hence the step to find wavefunctions can be avoided in the program.

2.3. Optimization of Model Parameters using Variational Monte-Carlo (VMC) Technique

For this alpha-alpha system, the known pseudo-bound state responsible for resonance is known from experiments to be $92.12 \pm 0.05 \text{ keV}$ and the $0D$ bound state to be having an energy of -22.1 MeV . The model parameters V_0 and α are set as 122.6225 MeV and 0.22 fm^2 respectively [1]. The value of β in Coulomb term [1] is chosen as 0.75 fm^{-1} . With this initialisation, the TISE is solved using matrix methods for $\ell=0$ and $\ell=2$ and the energies for $2S$ and $0D$ are compared with the experimental ones by determining mean percentage error $E_{pm} = \text{mean}(|E_d - E_b|/E_d) * 100$ where E_b and E_d are simulated and experimental energies for $2S$ and $0D$ states. Now, the values of V_0 and α are changed one after the other in each iteration by adding a random value r generated in an interval $[-b, b]$. The TISE is solved with the changed parameters and E_{pm} new is determined. If E_{pm} new is less than E_{pm} , then the changes to model parameters are accepted and hence updated, else the previous values are retained. This process is repeated with decreasing interval sizes over a large number of iterations till the mean percentage error is small enough to give us the simulated energies to required accuracy. The final optimized parameters give us the best potential that models the interaction and is utilised in PFM to obtain the scattering phase-shifts. To obtain the scattering phase-shifts for higher ℓ -channels which are unbound scattering states, the potential obtained for bound states does not yield best convergence with experimental results. In such cases, we deduce the inversion potential from the experimental data using VMC. That is, instead of solving TISE, we determine the phase shifts, say for $\ell=4$ by starting with the potential obtained for bound states using PFM which is discussed below. These are compared with experiment phase-shifts by determining the relative mean-squared error as a quantity for minimization as

$$\chi^2 = \frac{1}{N} \sum_{i=1}^N \frac{(\delta_{\text{exp}}^i - \delta_{\text{num}}^i)^2}{|\delta_{\text{exp}}^i|} \quad (6)$$

Again, the model parameters V_0 and α are varied using Monte-Carlo approach and the above parameter is minimized in the variational sense.

2.4. Phase Function Method (PFM)

Calogero [9] and Babikov [10] have treated the non-linear differential equation (NDE) that governs the phase-shifts in scattering theory. This NDE of first order is similar to the Riccati equation [20] and is given by

$$\delta'_1(r) = -(V(r)/k) \left[\cos(\delta_1) \hat{j}_1(kr) - \sin(\delta_1) \hat{\eta}_1(kr) \right]^2 \quad (7)$$

with initial condition $\delta_1(0) = 0$. The phase shift δ_1 can be seen as real function of k and characterizes the strength of scattering of any partial wave i.e. say ℓ^{th} partial wave of the potential $V(r)$. In the above equation \hat{j}_1 and $\hat{\eta}_1$ are the Bessel functions. Since we are only focusing on the scattering by the $\ell = 0, 2$ partial wave, the Riccati-Bessel function [20] is given by $\hat{j}_0 = \sin(kr)$ and similarly the Riccati-Neumann function is given by $\hat{\eta}_0 = -\cos(kr)$, thus reducing eq. (7) to

$$\delta'_0(r) = -(V(r)/k) \left[\sin(kr + \delta_0) \right]^2 \quad (8)$$

While for $\ell=2$ partial wave the Bessel functions we use are $\hat{j}_2 = \left(\sin(kr) \left(3/(kr)^2 - 1 \right) - 3 \cos(kr)/(kr) \right)$ and $\hat{\eta}_2 = \left(\cos(kr) \left(-3/(kr)^2 + 1 \right) - 3 \sin(kr)/(kr) \right)$ thus reducing eq. (7) to

$$\delta'_2(r) = -V(r)/k \left[\cos(\delta_2) \left(\hat{j}_2(kr) \right) - \sin(\delta_2) \left(\hat{\eta}_2(kr) \right) \right]^2 \quad (9)$$

and for $\ell=4$ partial wave the Bessel functions we use are $\hat{j}_4 = \left(105/(kr)^4 - 45/(kr)^2 + 1 \right) \sin(kr) + \left(-105/(kr)^2 + 10 \right) \cos(kr)/kr$ and $\hat{\eta}_4 = \cos(kr) \left(-105/(kr)^4 + 45/(kr)^2 - 1 \right) + \sin(kr)/(kr) \left(-105/(kr)^2 + 10 \right)$ thus reducing eq. (7) to

$$\delta'_4(r) = -V(r)/k \left[\cos(\delta_4) \left(\hat{j}_4(kr) \right) - \sin(\delta_4) \left(\hat{\eta}_4(kr) \right) \right]^2 \quad (10)$$

This NDE is numerically integrated from a value close to origin, typically from the point where the potential value is close to zero all the way up to asymptotic region (r is of the order of 15-20 fm) where the potential becomes zero. RK-5 method is used to obtain values of scattering phase shifts for different values of projectile energy in lab frame. The energy dependence is given by

$k = \sqrt{(2\mu E)/\hbar^2}$ where μ is the reduced mass of α - α system and $\frac{\hbar^2}{2\mu} = 10.44217 \text{ MeV fm}^2$.

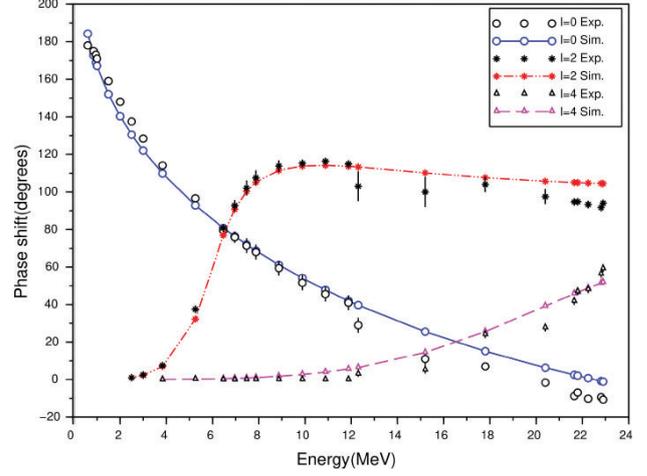


Figure 1: (α - α) scattering phase shifts for (a) $S(0^+)$, (b) $D(2^+)$ and (c) $G(4^+)$ channel as a function of laboratory energy E_{lab} .

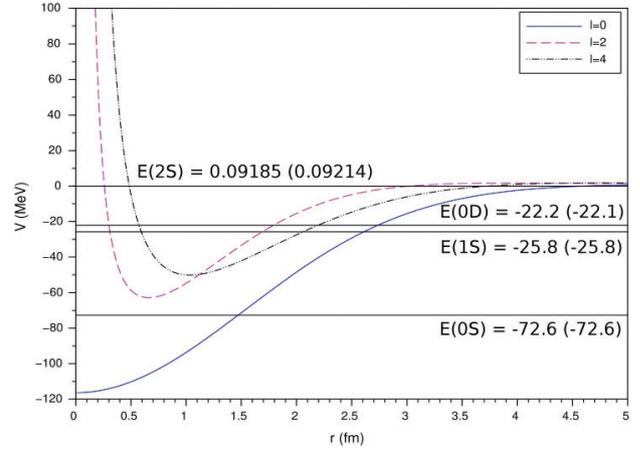


Figure 2: Potential plots Gaussian potential for $S(0^+)$, $D(2^+)$ and $G(4^+)$ channel with energy eigen value of Ref. [1] and MM.

3. Simulation of Results and Discussion

The Gaussian potential considered in this work have been optimised using VMC to obtain the ground state energy to be exactly equal to the experimental BE to five decimal places.

Table 1: Model Parameters for Gaussian potential.

State	V_0 (MeV)	α (fm $^{-2}$)	β (fm $^{-1}$)
$S(0^+)$	121.273	0.215	0.75
$D(2^+)$	96.364	0.396	0.75
$G(4^+)$	95.061	0.247	0.75

The $S(0^+)$, $D(2^+)$ and $G(4^+)$ channel scattering phase-shifts are obtained by substituting the potential functions with the choice of parameters given in Table 1 for lab energies ranging from 1-23 MeV and are shown in Fig. 1. It is interesting to observe that Gaussian potential characteristics are good for modeling α - α interaction. Next, we obtain phase-shifts corresponding to G-channel (4^+) by applying VMC in tandem with PFM.

Conclusion

We conclude that α - α scattering phase shifts for S, D and G channels are in good fit with experimental data up to 23 MeV of laboratory energy using three parameter Gaussian local potential along with Coulomb potential defined through an erf function. The present work validates that PFM is a good approach for calculation of phase shifts in scattering experiments for bound states. The higher ℓ -channel scattering states can not be obtained from the local potential as such. So, an inversion potential has been obtained by adjusting the model parameters using Monte-Carlo approach to minimize the relative mean squared error w.r.t. experimental scattering phase-shifts for the $\ell=2$ and 4 i.e. D and G-channel. The same procedure would be extended in near future to obtain the inversion potentials for other higher ℓ -channels like $\ell=6$ and 8. Hence, while the bound state S channel scattering phase shifts have been directly obtained from the potential that results from solving TISE numerically using a hybrid methodology of matrix diagonalisation and VMC, the unbound D and G-channel experimental scattering phase shifts have been utilised to obtain an inversion potential responsible for the interaction. The obtained data are found to be matching with experimental ones reasonably closely.

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