J. Nucl. Phys. Mat. Sci. Rad. A. Vol. 9, No. 1 (2021), pp.81–85

CHITKARA

Journal of Nuclear Physics, Material Sciences, Radiation and Applications
Journal homepage: https://jnp.chitkara.edu.in/

Triton Scattering Phase-Shifts for S-wave using Morse Potential

Shikha Awasthi, Anil Khachi, Lalit Kumar and O.S.K.S. Sastri*

Central University of Himachal Pradesh, Dharamshala, Himachal Pradesh - 176215, India

*sastri.osks@hpcu.ac.in (Corresponding Author)

ARTICLE INFORMATION

Received: February 9, 2021
Accepted: May 27, 2021
Published Online: August 31, 2021

Keywords:
n-d Scattering, Matrix Method, Phase Function Method (PFM), Variational Monte-Carlo (VMC), RK4,5 Method, Triton

DOI: 10.15415/jnp.2021.91014

ABSTRACT

In this paper, the phase-shifts for neutron-dueteron (n-d) scattering have been determined using the molecular Morse potential as theoretical model of interaction. The Triton (n-d) $^2S_{1/2}$ ground state initially has been chosen as -7.61 MeV to determine the model parameters using variational Monte-Carlo technique in combination with matrix methods numerical approach to solving the time independent Schrodinger equation (TISE). The obtained potential is incorporated into the phase function equation, which is solved using Runge-Kutta (RK) 4,5 order technique, to calculate the phase-shifts at various lab energies below 15 MeV, for which experimental data is available. The results have been compared with those obtained using another molecular potential named Manning-Rosen (MR) and have been observed to fare better. Finally, the Triton ground state has been chosen as its binding energy (BE), given by -8.481795 MeV, as determined from experimental atomic mass evaluation data and the calculations are repeated. It has been found that these phase-shifts from BE data are slightly better matched with experimental ones as compared to those obtained using -7.61 MeV ground state for Triton (n-d two-body system) modeled using Morse potential.

1. Introduction

Understanding the nucleon-nucleon and nucleon-nucleus interactions for very light nuclei are of importance to gaining insights into various aspects of two-particle and three-particle interactions that might be the underlying reasons for stability of nuclei. For instance, the binding energy of Triton is observed to be 1-2 MeV under-estimated [1] by considering two nucleon interactions alone. It becomes necessary to include three nucleon interactions [2], especially for scattering data above 100 MeV. So, at small lab energies below 15 MeV, it should be typically sufficient to consider the three body Triton as being a combination of neutron and deuteron two-body system modeled by a local central potential for explaining phase-shifts observed in their scattering experiments. One would have to consider Bargmann type potentials [3] as the choice for local potential to model the three-body problem to represent similar treatment as in two-particle scattering especially for the S-wave. The phenomenological potentials modeling the Nucleon-Nucleon(NN), N-Deuteron and N-Nucleus or Nucleus-Nucleus interactions at low energy must be able to reproduce the experimental scattering parameters such as scattering length and effective range. Recently [4], the molecular Manning-Rosen potential has been tried for obtaining the scattering phase-shifts in n-d using phase-function method. An important aspect to keep in mind is that, a potential that results in correct scattering phase-shifts for various lab energies must also simultaneously give the correct binding energy for the bound state and vice-versa. Another feature that is looked for as per Amado et al. [2] is quoted here: "*the scattering length and binding energy together are sufficiently restrictive to distinguish potential forms and that local potentials must result in smaller scattering lengths for the same binding*". These features help us distinguish as to which model parameters, obtained through a procedure like variational Monte-Carlo that we implement in this work, really represent physically meaningful results.

In this paper, the interaction between the neutron and deuteron has been modeled using the molecular Morse potential. The premise for considering this potential is that, it has all the required characteristics of a potential to properly represent the interaction. It is generally found to be fading away as the distance between the neutron and deuteron increases and increases with decreasing inter nucleon-nucleus distance suggesting an attractive potential with an exponentially decaying tail and has a repulsive core. This is very much what one observes in molecular interactions between neutral atoms where in the secondary interactions of Vander-walls (VW) type come into picture. It is now almost accepted that the strong interaction is a consequence of internal quark structure and the nucleons themselves only experience a secondary interaction. These

ISSN No.: 2321-8649(Print) ISSN No.: 2321-9289(Online); Registration No. : CHAENG/2013/51628

VW type interactions are best modeled using Lennard-Jones (LJ) in case of periodic solids and by Morse function and its variations in case of molecular systems. It has been shown [5] that these two potentials have a near perfect relationship even though LJ uses only two parameters while Morse has three parameters. The later has better capability in describing the non-bonded interaction as compared to former and hence chosen for modeling the neutron-deuteron interaction. Recently, our group has implemented this Morse potential for describing the neutron-proton interaction as in the deuteron ground state S-wave scattering phase analysis with successful results.

In the next section, we give a brief description of simulation methodology given by D. Hestenes [6], utilising the numerical method of matrix diagonalisation [7] in tandem with variational Monte-Carlo [8] to obtain the ground state of Triton, thus abstracting the Morse potential with best fit parameters that model the interaction. This is utilised in the non-linear differential equation [NDE] governing the scattering phase-shifts as obtained from variable phase approach (VPA) [9, 10] or equivalent phase function method (PFM) [11, 12]. The RK-4,5 numerical method is implemented in Scilab, a free open source software (FOSS) to solve the NDE and obtain the scattering phase-shifts at various lab energies. The results have been presented and discussed in Section 3. Finally, we draw our conclusions and give suggestions for future work that could further enhance the study of Triton.

2. Methodology

2.1. Modeling Triton using Two-term Potentials

The three body Triton system, at small lab energies below 15 MeV, is modeled as being a combination of neutron and deuteron two-body system which are supposed to be held together by a nuclear force. Here the molecular Morse potential is considered as theoretical model of interaction, which is given by [13]

$$V(r) = V_0\left[e^{-2\frac{(r-r_m)}{a_m}} - 2e^{\frac{-(r-r_m)}{a_m}}\right] \tag{1}$$

The modeling helps in reducing the two-body problem into a one-body, wherein the reduced mass of the system is obtained as a bound state of the central potential, which is better represented in spherical polar co-ordinates due to its inherent symmetry. The central equation governing the dynamics at the microscopic domain is the Time-Dependent Schrödinger Equation (TDSE) which through separation of variables in $\vec{r}$ and t results in Time-Independent Schrödinger Equation (TISE). The radial equation governing the system for l=0 is given by

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

The TISE is also written as an eigenvalue equation Hu(r) = Eu(r), where H is Hamiltonian operator and its wave-function u(r) is governed by u(r=0) = 0 and dies down to zero as r tends to infinity, thus making it normalisable.

2.2. Matrix Methods (MM) using Sine Basis

Typically, Morse potential dies down to zero very quickly and hence the region of interest could be limited to [0, w_0]. This is equivalent to embedding it within an infinite spherical-well potential (ISP) of width a_0. The eigen-functions of ISP are given by

$$\varphi_k = \sqrt{\left(\frac{2}{w_0}\right)}\sin\left(\frac{k\pi r}{w_0}\right) \tag{3}$$

The wave-functions u(r) as a linear combination of these ISP eigen functions:

$$u(r) = \sum_{n=1}^{N} C_n\sqrt{\left(\frac{2}{w_0}\right)}\sin\left(\frac{n\pi r}{w_0}\right) \tag{4}$$

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

$$T_{mn}u(r) = \frac{n^2\pi^2\hbar^2}{2mw_0^2}u(r) \tag{5a}$$

$$V_{mn} = \frac{2}{w_0}\int_0^{w_0}\sin\left(\frac{m\pi r}{w_0}\right)V(r)\sin\left(\frac{n\pi r}{w_0}\right)dr \tag{5b}$$

Hamiltonian (H_{mn} = T_{mn} + V_{mn}) matrix is diagonalised using eigen solvers routinely available in many software environments such as Scilab, Matlab, Python, Maple and Mathematica.

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

The idea involved is to determine those parameters that result in minimum percentage error for the simulated ground state energy (say E_G), obtained from solving the TISE, w.r.t experimental BE (i.e. E_B = *-7.61 MeV*). The parameter values from Morse potential optimized for n-p system [14], deuteron, are considered as initial values to detremine E_G. Then, perentage error is calculated as

$$E_P = \frac{|E_B - E_G|}{|E_B|}\times 100 \tag{6}$$

The value of V_0 is varied by adding a random number generated in an interval *[-0.1, 0.1]* and the ground state E_{Gnew} is determined and corresponding E_{Pnew} is calculated. If E_{Pnew} is less than E_p, then V_0 is updated with new value, else old value is retained. Then, the paramter α is varied by adding a random number generated in *[-0.1, 0.1]* interval and same procedure is repeated. This completes one iteration. Now, the process is repeated for a large number of iterations till not much variation in E_p is noticed. Then, the interval size is reduced to *[-0.01, 0.01]* and code is run to further reduce E_p. Finally, the best parameters are obtained when E_p is far less than 10^{-6}.

2.4. Phase Function Method (PFM)

The PFM method is based on solving a second order linear homogeneous equation by using Green's function approach that results in a nonlinear differential equation (NDE) of first order. The phase equation for Schrödinger equation, has been independently derived by Calogero [11] and Babikov [12] to be in terms of Bessel functions $\hat{j}_l$ and $\hat{\eta}_l$ as

$$\delta_l'(r) = -\left(V(r)/k\right)\left[\cos\left(\delta_l(r)\right)\hat{j}_l(kr) - \sin\left(\delta_l(r)\right)\hat{\eta}_l(kr)\right]^2 \tag{7}$$

with $\delta_l(0) = 0$. It gives the scattering phase-shifts at given energy k for l^{th} partial wave. One can observe that it depends only on potential V(r) and not wave-function u(r). In the above equation. For l=0, we have $\hat{j}_0 = \sin(kr)$ and $\hat{\eta}_0 = -\cos(kr)$, thus reducing eq. (7) to

$$\delta_0'(r) = -\left(V(r)/k\right)\left[\sin\left(kr + \delta_0(r)\right)\right]^2 \tag{8}$$

We have written a code in Scilab to solve this NDE numerically using RK-4,5 method to obtain phase-shifts for a given set of lab energies.

3. Simulation of Results and Discussion

Considering the Triton's ground state energy as -7.61 MeV, the model parameter for MR potential have been worked out in [4]. The corresponding parameters for Morse potential have been worked out using VMC and are presented in Table 1. Alongside we have also worked out the best model parameters for Morse potential by considering binding energy obtained from atomic mass evaluation data as -8.48175 MeV. These obtained potentials are used to calculate the phase-shifts at various lab energies below 15 MeV, for which experimental data [15] is available and the relative mean-square error is determined in each case by using

$$\chi^2 = \frac{1}{N}\sum_{i=1}^{N}\frac{\left(\delta_i^e - \delta_i^0\right)^2}{\delta_i^e} \tag{9}$$

Here δ_i^e and δ_i^o are the experimental and obtained phase-shifts. Another important way to compare the obtained scattering phase-shifts with experimental data is by determining the scattering and effective range parameters. The S-wave phase shifts for any potential at low energies is given by [13]:

$$k\cot(\delta) = \frac{-1}{a} + \frac{1}{2}r_0k^2 \tag{10}$$

where a is scattering length and r_0 is effective range which corresponds to size range of potential.

These parameters *a* and r_0 have been determined, for different scattering phase-shifts obtained using various potentials considered, from the slopes and intercepts of their respective *kcot(δ) vs 0.5k²* plots, shown in Fig. 1. The obtained values are given in Table 1. The experimental data taken from [15] is utilized to calculate the experimental scattering length *a* and effective range r_0.

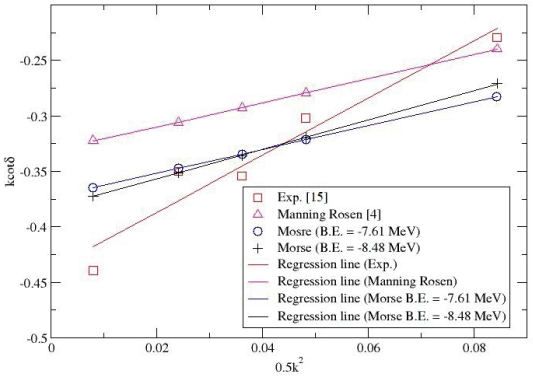

Figure 1: kcot (δ) vs $0.5k^2$ for scattering phase-shifts of n-d sytem, obtained using MR[4] potential, Morse potential (-7.61 MeV and -8.48 MeV)[Current work] w.r.t Experimental data [15].

In Fig. 2, the scattering phase shifts for $^2S_{1/2}$ channel of n-d system for MR potential with parameters given in [4] and Morse potential; obtained by using VMC technique for ground state -7.61 MeV and by using the obtained BE data (-8.481795 MeV), are plotted as a function of laboratory energy. It is observed that the phase-shifts obtained by using the obtaied BE data (-8.481795 MeV) are matching better with the plot obtained by using experimental data [15].

Table 1: Model Parameters for MR [4] and Morse potentials for different binding energies of Triton. Alongside, the scattering parameters in each case are given.

		Model Parameters		Scattering Parameters	
				a (fm)	r_0 (fm)
State $^2S_{1/2}$		MR Potential [4]			
B.E (MeV)	A	b(fm)	α		
-7.61	2.1054	1.106897	0.005	3.02	1.08
Morse Potential [Current work]					
	V_0 (MeV)	rm (fm)	am (fm)		
-7.61	254.503	0.600	0.300	2.68	1.07
-8.481795	258.006	0.915	0.300	2.61	1.07
				2.28 (Exp. [15])	2.58

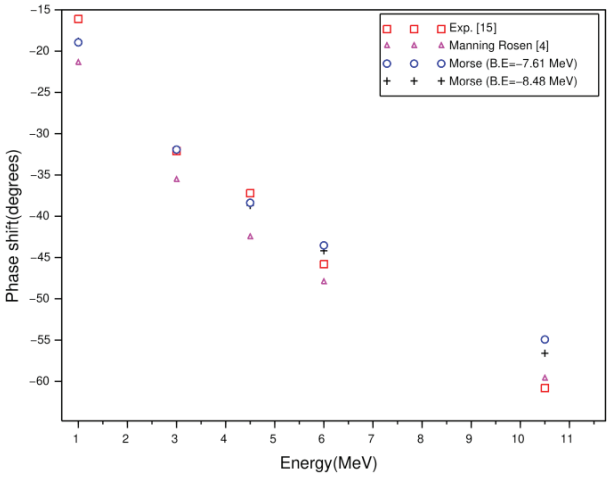

Figure 2: (n-d) Scattering phase shifts for $^2S_{1/2}$ channel as a function of laboratory energy.

The scattering phase-shifts obtained using RK-4,5 method for $^2S_{1/2}$ channel using Morse potentials (for both BEs considered) along with the experimental phase-shifts and that obtained using MR potential [4] are presented in Table 2 and are also shown in Figure 2.

Table 2: The scattering phase-shifts for $^2S_{1/2}$ state of n-d system for different lab energies.

[Exp.] [15]		MR Potential [4] (BE = -7.61 MeV)		Morse Potential (BE = -7.61 MeV)		Morse Potential (BE = -8.481795 MeV)	
Elab. (MeV)	$\delta_{Exp.}$ (degree)	δ_{MR} (degree)	% error	δ_{morse} (degree)	% error	δ_{morse} (degree)	% error
1.0	-16.1	-21.467	33.3	-19.180	19.1	-18.8	16.8
3.0	-32.1	-35.642	11.0	-32.297	0.6	-32.0	0.3
4.5	-37.2	-42.573	14.4	-38.795	4.3	-38.7	4.0
6.0	-45.8	-48.022	4.9	-43.991	3.9	-44.18	3.5
10.5	-60.8	-59.702	1.8	-55.448	8.8	-56.59	6.9
		X^2=0.617	$<E_p>$=13.08	X^2=0.240	$<E_p>$=7.34	X^2=0.173	$<E_p>$=6.30

It can be observed that scattering-phase shifts otained by using BE data (-8.481795 MeV) are in better agreement with experimental data [15] with $\chi^2 = 0.173$, as compared to those obtained for BE of -7.61MeV, which are $\chi^2 = 0.240$ [current work] again better than that obtained from MR which is 0.617 [4].

Conclusion

The phase-shifts for n-d scattering of Triton $^2S_{1/2}$ ground state have been determined using the molecular Morse potential, which has been used as theoretical model of interaction. The obtained phase-shifts from BE data are slightly better matched with experimental ones as compared to those obtained using

-7.61 MeV ground state for neutron-deuteron (n-d) two-body system, as modeled using Morse potential.

References

[1] R. Aaron et al., Physical Review **5B**, 140 (1965). https://doi.org/10.1103/PhysRev.140.B1291

[2] R. D. Amado, Annu Rev. Nucl. Sci. **19,** 61 (1969). https://doi.org/10.1146/annurev.ns.19.120169.000425

[3] M. Vallieres and Y. Nogamin, Revista Brasileira de Flsica **7**, 3 (1977). http://www.sbfisica.org.br/bjp/download/v07/v07a32.pdf

[4] B. Khirali et al., J. Phys. G. Nucl. Part. Phys. **46**, 115104 (2019). https://doi.org/10.1088/1361-6471/ab4118

[5] T. C. Lim, V. Z. Naturforsch **58a**, 615 (2003). https://doi.org/10.1515/zna-2003-1104

[6] D. Hestenes, American Journal of Physics **55**, 440 (1987). https://doi.org/10.1119/1.15129

[7] B. A. Jugdutt and F. Marsiglio, American Journal of Physics **81**, 343 (2013). https://doi.org/10.1119/1.4793594

[8] A. Sharma and O. S. K. S. Sastri, (2020). https://doi.org/10.35543/osf.io/5a6by

[9] J. Bhoi and U. Laha, Brazilian Journal of Physics **46**, 129 (2016). https://doi.org/10.1007/s13538-015-0388-x

[10] A. K. Behera, J. Bhoi, U. Laha and B. Khirali, Communications in Theoretical Physics **72**, 075301 (2020). https://orcid.org/0000-0003-4544-2358

[11] F. Calogero, American Journal of Physics **36**, 566 (1968). https://doi.org/10.1119/1.1975005

[12] V. V. Babikov, Soviet Physics Uspekhi **10**, 271 (1967). https://doi.org/10.1070/PU1967v010n03ABEH003246

[13] G. Darewych and A. E. S. Green, Physical Review **164,** 1324 (1967). https://doi.org/10.1103/PhysRev.164.1324

[14] A. Khachi, L. Kumar and O. S. K. S. Sastri, Submitted in Proceedings of the Online International Conference on Theoretical Aspects of Nuclear Physics, (2021).

[15] D. Huber, J. Golak, H. Witala, W. Gloeckle and H. Kamada, Few-Body Systems **19**, 175 (1995). https://doi.org/10.1007/s006010050025

CHITKARA

Journal of Nuclear Physics, Material Sciences, Radiation and Applications

Chitkara University, Saraswati Kendra, SCO 160-161, Sector 9-C, Chandigarh, 160009, India

Volume 9, Issue 1 **September 2021** **ISSN 2321-8649**