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Neutron-Proton Scattering Phase Shifts in S-Channel using Phase Function Method for Various Two Term Potentials

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

Central University of Himachal Pradesh, Dharamshala, Himachal Pradesh-176206, India

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

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ABSTRACT

The scattering phase shifts for n-p scattering have been modeled using various two term exponential type potentials such as Malfliet-Tjon, Manning-Rosen and Morse to study the phase shifts in the S-channels. As a first step, the model parameters for each of the potentials are determined by obtaining binding energy of the deuteron using matrix methods vis-a-vis Variational Monte-Carlo (VMC) technique to minimize the percentage error w.r.t. the experimental value. Then, the first order ODE as given by phase function method (PFM), is numerically solved using 5th order Runge-Kutta (RK-5) technique, by substituting the obtained potentials for calculating phase shifts for the bound $^3S_1$ channel. Finally, the potential parameters are varied in least squares sense using VMC technique to obtain the scattering phase-shifts for each of the potentials in the $^1S_0$ channel. The numerically obtained values are seen to be matching with those obtained using other analytical techniques and a comparative analysis with the experimental values up to 300 MeV is presented.

1. Introduction

Modeling the n-p interaction is one of the most fundamental concepts in nuclear physics to understand the nature of nuclear force. There is large amount of experimental data available spanning energy ranges all the way upto few GeV [1-3]. The first successful theoretical description is given by Yukawa [4] which models the interaction as an exponentially decaying function with 1/r dependence, which typically only has attractive nature. Later many two term potentials, which also include a soft repulsive core, are suggested such as Modified Hulthen [5], Malfliet-Tjon (MT) [6], Manning-Rosen (MR) [7], Eckart [8], Morse [9] and Rosen-Morse [10], etc. The scattering at low energies also requires inclusion of spin and iso-spin dependent potentials for describing long-range interaction. Typically, these scattering phase-shifts are obtained analytically using either S-matrix [11] or Jost function [12] methods. Also, vast literature related to scattering phase shift calculations can be found in [13-25]. Recently there has been renewed interest in the application of phase function method (PFM) [21], [22] also called as Variable Phase Approach (VPA) which has been extensively used by Laha, et al. [5], [7]. The advantage of PFM [20], [21] over the former mentioned methods is that it requires only the potential function to obtain the scattering phase shifts without any need for determining the wave-functions.

In this paper, we utilize this technique to obtain S-channels scattering phase shifts for n-p scattering for three potentials consisting of two terms and number of parameters shown in brackets: (i) MT (4), (ii) MR (3) and (iii) Morse (3), to perform a comparative analysis to understand the various related aspects. The methodology employed is entirely based on numerical computations which have already seen to yield good results in other related problems in nuclear physics. The matrix method technique as proposed by Marsglio et al. [24] where in the potential under consideration is embedded within an infinite potential well, whose sine wave-functions are employed as basis, has been successful for obtaining the energies and corresponding wave-functions for simple central potentials such as spherical well, Coulomb and Yukawa. Our group has applied this technique to solving Harmonic Oscillator (HO) [25], Anharmonic oscillator (AHO) [26], Woods-Saxon [27] and Morse potential [28]. Here, we utilize this numerical technique to obtain the ground state energy of Deuteron for MT, MR and Morse potentials. Initially, the scattering phase-shifts are determined for MT and MR potentials with model parameters specified in [6] and [7] using PFM to ensure the obtained results are in tune with those given in

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these references. This validates that the PFM algorithm is correctly implemented using the RK-4,5 method. Then, it is applied to Morse potential which we are proposing as the model function to understand n-p interaction in this paper. In Section 2, matrix methods technique is briefly discussed within the modeling methodology framework of Hestenes [28] and simulation methodology proposed by our group [29]. The model parameters for the potentials are optimized by reducing the percentage error of the numerically obtained binding energy (BE) for the deuteron, by solving the Time Independent Schrodinger Equation (TISE), with its experimental BE using the variational Monte-Carlo (VMC) technique [26-28]. This avoids the requirement of dependence on analytical expressions, obtained from theoretical considerations, which are adjusted with experimental data to obtain the model parameters. The steps involved in implementation of VMC are communicated [27] and are briefly explained. Once, the exact potential expressions with optimized model parameters are obtained, the scattering phase shifts are obtained using PFM. The first order ODE is solved numerically using the 5th order Runge-Kutta (RK-5) method for the $^3S_1$ channel. A program is written and executed in Scilab, a Free Open Source Software (FOSS), an equivalent of MATLAB and is available on request from the author. In Section 3, the simulation results for phase shifts of $^3S_1$ are presented. Then, to compensate for the absence of spin and iso-spin dependent potentials required for obtaining the $^1S_0$ channel, which result typically in variation of depth and range of potentials [5], [7], the VMC is employed to re-optimize the parameters by obtaining the phase-shifts using PFM in the least squares minimization of 2 values w.r.t. the available experimental data. The obtained results for these three chosen potentials are discussed. Finally, conclusions are drawn in Section 4.

2. Methodology

2.1. Modeling Deuteron using Two-term Potentials

The simplest stable nucleus, Deuteron, is composed of a single neutron and single proton which are supposed to be held together by a nuclear force, is modeled via three different interactions. All of them have central character and are of exponential type, given by

i. *Malfliet-Tjon (MT) potential*: This is mathematically expressed as

$$V(r) = -V_A \frac{e^{-\mu_A r}}{r} + V_r \frac{e^{-\mu_r r}}{r} \tag{1}$$

ii. *Manning-Rosen (MR) potential*:

$$V(r) = b^{-2}\left[\frac{\alpha(\alpha-1)}{\left(1-e^{-r/b}\right)^2} e^{-2r/b} - \frac{Ae^{-r/b}}{\left(1-e^{-r/b}\right)}\right] \tag{2}$$

iii. *Morse potential:*

$$V(r) = V_0\left[e^{-2\frac{(r-r_m)}{a_m}} - 2e^{\frac{-(r-r_m)}{a_m}}\right] \tag{3}$$

This 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 model parameters of the potential are adjusted to match the bound state energy E_B to that of the experimental binding energy BE of Deuteron $E_D = -2.224589$ MeV. The central equation governing the dynamics at the microscopic domain is the Time-Dependent Schrodinger Equation (TDSE) which through separation of variables in $\vec{r}$ and t results in TISE. The radial equation governing the system for $\ell = 0$ is given by

$$\frac{-\hbar^2}{2m}\frac{d^2u(r)}{dr^2} + V(r)u(r) = Eu(r) \tag{4}$$

The first factor is kinetic energy operator T_i which together with V(r) is written as Hamiltonian H and TISE as an eigenvalue equation is 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 V of radius a, which basically defines the limits for region of interest as [0, a_0]. Now, the eigenfunctions

$$\varphi_n = \sqrt{\left(\frac{2}{a_0}\right)}\sin\left(\frac{n\pi r}{a_0}\right) \tag{5}$$

of infinite potential V_i are chosen as the basis functions to write u(r) as a linear combination:

$$u(r) = \sum_{n=1}^{N} C_n \sqrt{\left(\frac{2}{a_0}\right)}\sin\left(\frac{n\pi r}{a_0}\right) \tag{6}$$

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

$$V_{mn} = \frac{2}{a_0}\int_0^{a_0} \sin\left(\frac{m\pi r}{a_0}\right) V(r) \sin\left(\frac{n\pi r}{a_0}\right) dr \qquad (7)$$

Then, the matrix for the Hamiltonian $H_{mn} = T_{mn} + V_{mn}$ is solved using an eigen solver to obtain the energy eigen-values and corresponding eigen vectors. These eigen vectors corresponding to each eigen value are used to obtain the wave-function as in Eq. (6).

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

The parameters involved in a chosen potential need to be determined such that the ground state energy E_B, obtained from solving the TISE, matches the experimental BE i.e. E_D. To acheive the best possible values for model parameters, we ensure that the percentage error Ep = $|(E_D - E_B)/E_D|$ *100 is minimised such that convergence to 6 decimal places is met. This is done in an iterative fashion. First the parameters are initialised with certain guess values, say *oldpars* and Ep is determined, say *Epold*. Then each of the parameters is varied, using Monte-Carlo approach, one at a time by adding a random number generated in an interval *[-I,I]*. Having varied a chosen parameter, the TISE is solved using MM to obtain the ground state and *Epnew* is determined. Now, the variational principle is implemented as *"if (Epnew < Epold), then (oldpars are updated as newpars), else (newpars are discarded)"*. This procedure is repeated for a number of iterations till Ep is less than 10^{-6}.

2.4. Phase Function Method (PFM)

The mathematical foundation of PFM method is well known in theory of differential equations, that a second order linear homogeneous equation, like a Schrodinger equation, can be reduced to a nonlinear differential equation (NDE) of first order. The phase equation which was independently worked out by Calogero [20] and Babikov [21] is written in the following form.

$$\delta_l'(r) = -\left(V(r)/k\right)\left[\cos\left(\delta_l(r)\right)\hat{f}_l(kr) - \sin\left(\delta_l(r)\right)\hat{\eta}_l(kr)\right]^2 \qquad (8)$$

with initial condition $\delta_\ell(0) = 0$. The phase shift δ_ℓ 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 $\hat{f}_l$ and $\hat{\eta}_l$ are the Bessel functions. Since we are only focusing on obtaining scattering phase shifts for ℓ=0 partial wave, the Riccati-Bessel function is given by $\hat{f}_0 = \sin(kr)$ and similarly the Riccati-Neumann function is given by $\hat{\eta}_0 = -\cos(kr)$, thus reducing Eq. (8) to

$$\delta_0'(r) = \left(V(r)/k\right)\left[\sin\left(kr + \delta_0(r)\right)\right]^2 \qquad (9)$$

This NDE is numerically integrated from origin to the asymptotic region using RK-4/5 method, thereby obtaining directly the values of scattering phase shift for different values of projectile energy in lab frame. The central idea of VPA is to obtain the phase shift δ directly from physical quantities such as interaction potential V(r), instead of solving TISE for wave functions u(r), which in turn are used to determine phase shift δ.

3. Simulation of Results and Discussion

The model parameters for MT and MR potentials have been chosen from refs [13] and [14], and have been tabulated in Table 1. For the Morse potential considered in this work, they have been optimised using VMC to obtain the ground state energy to be exactly equal to the experimental BE to six decimal places.

Table 1: Model Parameters for three different potentials i.e MR, MT and Morse potential.

Malfliet-Tjon [6]				
State	**V_a(MeV-fm)**	**μ_a(fm^{-1})**	**V_r(MeV-fm)**	**μ_r(fm^{-1})**
$^3S_1$	635	1.55	1458	3.11
$^1S_0$	331.801	1.575	897.304	3.704
Manning-Rosen [7]				
State	**A**	**b(fm)**	α	
$^3S_1$	1.57	1.212542	0.005	
$^1S_0$	0.952	1.152	−0.0043	
Morse (Our work)				
State	**V_0(MeV)**	**r_m(fm)**	**a_m(fm)**	
$^3S_1$	162.309	0.658	0.3	
$^1S_0$	121.236	0.667	0.283	

The $^3S_1$ 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 1-300 MeV and are shown in Fig. 1 (a). While the MR potential does match well for energies upto 50 MeV, the scattering phase-shifts tend to saturate way higher for energies beyond. On the other hand, the results for MT potential seem to be going parallel to phase shift curve in the region

50-300 MeV. This implies subtracting a constant δ_0, may yield a good match with experimental values. But, that would mean a poor match for the phase-shifts in low energy range from 0-50 MeV. It is interesting to observe that Morse potential fares far better over the entire range and converges to the experimental data implying that it has correct characteristics required for modeling np interaction. Next, we obtain phase-shifts corresponding to $^1S_0$-channel.

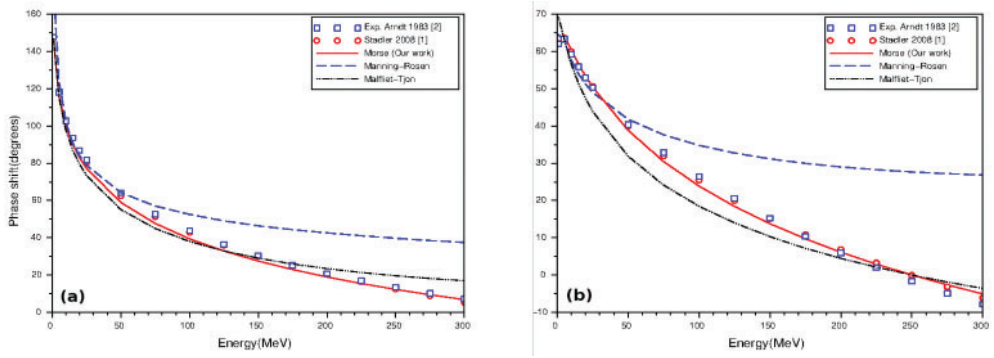

Figure 1: (n-p) scattering phase shifts for (a) $^3S_1$ and (b) $^1S_0$ channels as a function of laboratory energy.

Actually, the S-state corresponding to ℓ=0 gets split into the $^3S_1$ and $^1S_0$ states due to the coupling of the spins of neutron and proton. Since, the potentials considered here are purely central in character and the spin-dependent potential is not included, it is not possible to get the energies corresponding to both triplet and singlet state. But, the single bound state energy due to the obtained potential is attributed to the more stable triplet state. One can not obtain the scattering phase shifts using this potential description for the singlet state. To overcome this limitation, the model parameters for a chosen potential are readjusted in VMC approach by minimising the relative mean-square error

$$\chi^2 = \frac{1}{N}\sum_{i=1}^{N}\frac{\left(\delta_i^e - \delta_i^0\right)^2}{\delta_i^e} \qquad (10)$$

where δ_i^e and δ_i^o are the experimental and obtained phase-shifts. That is, the scattering phase shifts are calculated using RK4, 5 method each time a random change is made in one of the model parameters and the chisqr is determined w.r.t the available experimental data. If the obtained chisqr is less than that in the previous iteration, then the changes are accepted, else old parameter values are retained. In this way, the best possible parameters for fitting the experimental data are obtained. In Fig. 1(b), while the $^1S_0$ phase shifts for MR potential are plotted with parameters given in [14], for MT and Morse potentials they have been determined by using the VMC approach. One can once again observe that the results best match for the Morse potential as compared to MT and MR potentials. In fact this approach could be used to predict the nature of spin dependent potential, to compement the regular procedure of theoretically modeling the interaction with various mathematical functions, and could possibly result in better comprehension of experimentally observed phenomenon. The plots of MT, MR and Morse potentials for $^3S_1$ and $^1S_0$ are plotted in Fig. 2 (a) and (b) respectively. The plots of Morse potential are very much similar to those that result from one pion exchange potential (OPEP) [30].

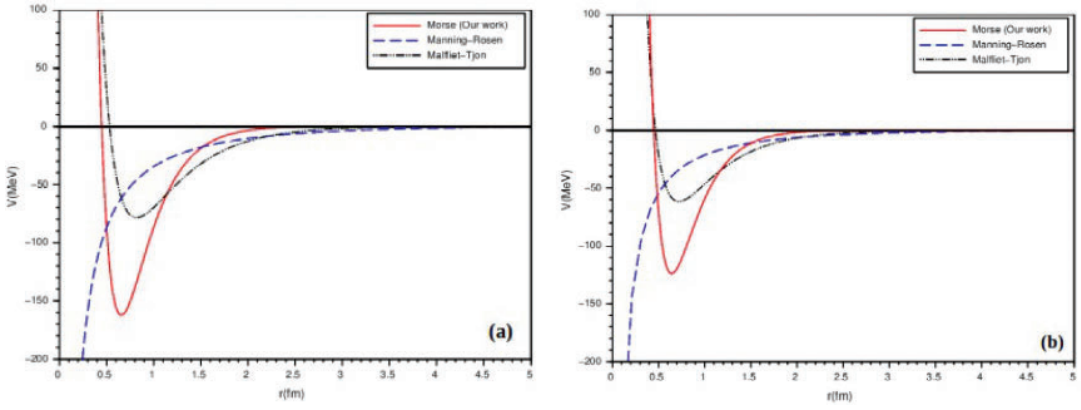

Figure 2: Plots of MT, MR and Morse potentials for np-scattering in (a) $^3S_1$ and (b) $^1S_0$ channels.

Table 2: $^3S_1$ state phase shifts (degrees) for MR, MT and Morse potential w.r.t. [1] and [2].

$E_{lab.}$ (MeV)	$\delta_{Stad.}$ [1]	$\delta_{Exp.}$ [2]	δ_{MR} [7]	δ_{MT} [6]	δ_{Morse} (This work)
1	147.644	147.71	173.191	146.795	146.138
5	117.998	118.08	123.852	114.905	115.701
10	102.408	102.76	101.811	97.552	99.804
15	–	93.55	90.808	97.552	90.039
20	–	86.92	83.878	79.286	82.915
25	80.398	81.68	78.859	73.354	77.270
50	62.498	64.23	64.247	55.156	58.975
75	51.264	52.64	57.039	44.955	47.706
100	42.838	43.71	52.546	38.064	39.469
125	36.004	36.47	49.065	38.064	32.962
150	30.222	30.44	46.381	29.080	27.581
175	25.155	25.29	44.325	25.973	22.996
200	20.573	20.83	42.610	23.448	19.004
225	16.27	16.89	41.075	21.368	15.474
250	12.471	13.36	39.716	19.640	12.311
275	8.834	10.18	38.552	18.193	9.450
300	5.441	7.27	37.554	16.973	6.840
		$\chi^2 \leq 50\ MeV$	**0.710**	**0.475**	**0.162**
		$\chi^2 > 50 MeV$	**large**	**2.573**	**0.213**

Table 3: $^1S_0$ state phase shifts (degrees) for MR, MT and Morse potential w.r.t [1] and [2].

E_{lab}(MeV)	$\delta_{Stad.}$ [1]	$\delta_{Exp.}$ [2]	δ_{MR} [7]	δ_{MT} [6]	δ_{Morse} (This work)
1	62.071	61.95	64.491	69.171	62.139
5	63.608	63.23	62.783	63.305	64.167
10	59.335	59.35	57.679	56.594	60.351
15	–	55.88	53.995	51.480	56.671
20	–	52.9	51.197	47.355	53.369
25	50.631	50.3	48.955	43.893	50.397
50	39.911	40.38	41.791	31.874	38.831
75	31.944	32.87	37.630	24.142	30.462
100	25.468	26.4	34.796	18.465	23.867
125	19.957	20.57	32.726	13.990	18.416
150	15.137	15.26	31.156	10.304	13.771

175	10.825	10.41	29.940	7.184	9.725
200	6.899	5.99	28.987	4.490	6.144
225	3.291	1.99	28.237	2.124	2.933
250	-0.05	-1.63	27.644	0.018	0.026
275	-3.16	-4.89	27.178	-1.874	-2.628
300	-6.065	-7.82	26.813	-3.587	-5.068
		$\chi^2 \leq 50MeV$	**0.051**	**0.644**	**0.015**
		$\chi^2 > 50MeV$	**large**	**1.562**	**0.498**

Conclusion

We conclude that n-p scattering phase shifts for both triplet and singlet S-channels are able to better fit the experimental data up to 300 MeV of lab energy by three parameter Morse potential as compared to three parameter Manning-Rosen and four parameter Malfliet-Tjon potential. It would be interesting to see how this Morse potential will fare in explaining the n-alpha and n-^{12}C scattering phase-shifts.

Appendix

The scattering phase-shifts obtained using RK-4/5 method for $^3S_1$ and $^1S_0$ channels using MR, MT and Morse potentials are given in Tables 2 and 3 respectively. We had to add certain constant phase value to that obtained using the MR potential using our code, to match with experimental data.

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

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