Numerical Simulation Study of Neutron-Proton Scattering using Phase Function Method

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Abstract

In this article, we propose a numerical approach to solve quantum mechanical scattering problems, using phase function method, by considering neutron-proton interaction as an example. The nonlinear phase equation, obtained from time-independent Schrödinger equation, is solved using Runge-Kutta method for obtaining S-wave scattering phase shifts for neutron-proton interaction modeled using Yukawa and Malfliet-Tjon potentials. While scattering phase shifts of S-states using Yukawa match with experimental data for only lower energies of 50 MeV, Malfliet-Tjon potential with repulsive term gives very good accuracy for all available energies up to 350 MeV. Utilizing these S-wave scattering phase shifts, low energy scattering parameters and total S-wave cross section have been calculated and found to be consistent with experimental results. This simulation methodology can be easily extended to study scattering phenomenon using phase wave analysis approach in the realms of atomic, molecular and nuclear physics.

I. INTRODUCTION

The wavefunction obtained by solving the time-independent Schrödinger equation for various models of interaction potentials is central to understanding quantum mechanical systems. Problems involving penetration through a rectangular barrier, and bound and scattering states of finite square well are routinely performed in an undergraduate quantum mechanics course. Gamow's theory of alpha (α) particle tunneling based on extension of barrier penetration and explanation of bound state of deuteron (d) and neutron-proton (np) scattering cross section utilizing square well are part of nuclear physics course at undergraduate level. Even though Yukawa's meson exchange theory¹ to explain np-scattering is discussed at undergraduate level, corresponding time-independent Schrödinger equation for Yukawa potential is not solved. This is mainly due to non-availability of analytical solution, till recently². Thus, most textbooks on nuclear physics³⁻⁵ still rely on square well potential for obtaining binding energy of deuteron as well as discussing np scattering cross section. So, there is a need to introduce a numerical technique to solve Yukawa potential to provide a better understanding of np-scattering. This would equip students with required skills to solve two-body scattering problems in atomic, nuclear, and particle physics.

The main objective of this paper is to present a simple derivation of phase equation for S-wave (i.e. $\ell = 0$) and solve it numerically using Runge-Kutta method to obtain scattering phase shifts for neutron-proton np - interaction by choosing Yukawa potential and its modified form called Malfliet-Tjon (MT)⁶ potential.

Theoretically, scattering cross section data are obtained from scattering phase shifts (SPS) by using either effective range theory or phase shift analysis. The later approach involves determination of scattering phase shifts that arise due to scattering of incoming projectile with interaction potential of target nucleus. Theoretical modeling involves, proposing a mathematical function to represent interaction potential based on understanding of underlying physical phenomena and then solving the radial time-independent Schrödinger equation to obtain the wavefunction. Mostly, scattering phase shifts are deduced from matching the wave function within interaction region with that of asymptotic region in which interaction ceases to exist^{7–9}. This wave function approach to determining scattering phase shifts involves solving the radial time-independent Schrödinger equation numerically and is discussed in advanced computational physics book¹⁰, which is beyond the reach of many undergraduate

physics students.

Experimentally, scattering cross section data are available at different lab energies of incoming projectile, from which scattering phase shifts are deduced. The scattering phase shifts data for nucleon-nucleon [neutron-proton (np), neutron-neutron (nn) and proton-proton $(pp)^{11}$, nucleon-nucleus [neutron-deuteron (nd), proton-deuteron (pd), neutron-alpha $(n\alpha)$, proton-alpha $(p\alpha)^{12,13}$ and nucleus-nucleus $[\alpha\alpha]^{14}$ systems are available in literature.

An alternative approach to determine scattering phase shifts is variable phase approach, originally proposed by $Morse^{15}$, and later came to be known as phase function method $(PFM)^{16-18}$. This method has been utilized for obtaining scattering phase shifts for np-interaction with reasonable success¹⁹⁻²¹. In this approach, the time-independent Schrödinger equation is transformed into a first order non-linear Ricatti-type equation that directly deals with phase shifts for different ℓ values and different energies, without need for wavefunction like other methods. Thus, phase function method is an easy alternative to traditional methods like r-matrix method⁷, s-matrix method⁸ or jost function method⁹, etc.

In this work, we have solved phase equation numerically by choosing Runge-Kutta 5^{th} order²² (RK-5) method to obtain scattering phase shifts for 3S_1 and 1S_0 states in np interaction using Yukawa and Malfliet-Tjon potential. By providing best model parameters for both these potentials, RK-5 method can be easily implemented using worksheet environment such as Gnumeric, Excel or LibreOffice-Calc for determining scattering phase shifts at different energies. This would be within the reach of undergraduate physics students. The obtained scattering phase shifts are then utilized to determine total scattering cross section at various energies and scattering parameters for both singlet and triplet states.

The paper is structured based on simulation methodology 23 consisting of following four stages:

- 1. Modeling physical system²⁴
 - In next section, we will describe scattering process in detail and formulate mathematical model in terms of phase equation. Then, numerical solution is developed in three steps.
- 2. Preparation of system by choosing appropriate units, region of interest and numerical technique.
- 3. Implementation of numerical method in a computer.

These two stages are briefly touched upon in Section III. This is followed by

4. Simulation of results and discussion in Section IV and conclusions are given in last section.

II. MODELING PHYSICAL SYSTEM: DESCRIPTION AND FORMULATION

The process of scattering of a neutron with energy $E_{\ell ab}$ and a proton, which is at rest in lab frame²⁵, is represented with position vectors \vec{r}_n and \vec{r}_p . Their masses are m_n and m_p respectively. This two body system is reduced to a one body system by transformation to center of mass frame. In this process, origin is shifted to center of mass co-ordinate \vec{R}_{cm} and two particles are replaced by a single particle with reduced mass $\mu_D = (m_n m_p)/(m_n + m_p)$ which has a position vector \vec{r} , that represents relative distance between neutron and proton. The projectile energy in lab frame, $E_{\ell ab}$, would be related to centre-of-mass energy E_{cm} using standard relation^{26,27}:

$$E_{cm} = \left(\frac{m_T}{m_P + m_T}\right) E_{\ell ab} = \left(\frac{m_p}{m_n + m_p}\right) E_{\ell ab} \tag{1}$$

Where, m_P is the mass of projectile (neutron) and m_T is the mass of target (proton). For simplicity, we drop the subscript henceforth and write center of mass energy as E. The ideal choice for reference system would be spherical polar co-ordinates, $\vec{r} = (r, \theta, \phi)$, as potential has central force characteristics. The state of system, for $\ell = 0$ is described by its wavefunction $\psi(\vec{r}, t)$, and is obtained by solving the radial time-independent Schrödinger equation, given by

$$\frac{d^2u_0(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[E - V(r) \right] u_0(r) = 0 \tag{2}$$

The wavefunction must satisfy $u_0(0) = 0$ at r = 0. Further, at a distance r_0 beyond which V(r) is zero, wavefunction and its derivative both need to be continuous. That is, choosing $u_a(r)$ to be asymptotic solution of Eq. 2 for $r > r_0$, we must have

$$u_0(r)\big|_{r=r_0} = u_a(r)\big|_{r=r_0}$$
 (3)

similarly

$$\left. \frac{du_0(r)}{dr} \right|_{r=r_0} = \left. \frac{du_a(r)}{dr} \right|_{r=r_0} \tag{4}$$

These two conditions are combined together into a single equation by considering logarithmic derivative to satisfy boundary condition, obtained as

$$\frac{1}{u_0(r)} \frac{du_0(r)}{dr} \bigg|_{r=r_0} = \frac{1}{u_a(r)} \frac{du_a(r)}{dr} \bigg|_{r=r_0}$$
 (5)

A. Concept of Phase-shift:

Phase shift techniques are incredibly helpful when analyzing scattering, including nucleonnucleon scattering. The usefulness of approach to obtain phase shift using wavefunction is applied to np-scattering on a square-well potential in Krane³. Here, we are including spinspin interaction²⁸ and numerically obtain phase shifts for ${}^{1}S_{0}$ state of Deuteron. This lays foundation for deriving phase equation which is central to phase function method.

The width of square well for deuteron system is known to be $r_0 = r_D = 2.1$ fm²⁹, radius of np - system. The depth of square well can be determined to match binding energy of deuteron³. The triplet ground state has energy E = -2.2 MeV and virtual singlet state has energy E = 77 keV. Due to spin-dependence, depths V_T of triplet (3S_1) state and V_S for singlet (1S_0) state are determined to be respectively -32.5 MeV and -10 MeV²⁸.

For E > 0 singlet state, solution within region of well would be given by

$$u_0(r) = A \sin(k_0 r) + B \cos(k_0 r) = A_0 \sin(k_0 r + \phi_0)$$
(6)

where $k_0 = \sqrt{\frac{2\mu_D(E-V_S)}{\hbar^2}}$.

The boundary condition at r=0 gives $\phi_0 = 0$.

Similarly, for asymptotic solution outside the well, where there is no interaction, one obtains

$$u_a(r) = A_a \sin(k_a r + \delta_0) \tag{7}$$

where $k_a = \sqrt{\frac{2\mu_D E}{\hbar^2}}$.

The logarithmic derivatives of these two wavefunctions are matched at boundary $r = r_D$, to obtain

$$k_1 \cot(k_1 r_D) = k \cot(k r_D + \delta_0) \tag{8}$$

This equation gives us value of δ . These two solutions $u_0(r)$ and $u_a(r)$ are plotted in Fig.1 for E=50 MeV. The free particle solution $u(r)=\sin(kr)$ is also plotted in upper part to visually indicate phase shift accrued due to interaction with square well potential. This

way of obtaining numerically the phase shift associated with scattering state of deuteron is seldom done in any textbook, such an activity would enhance learning of the important concept.

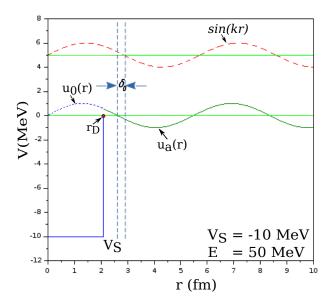


FIG. 1: The square-well potential V (MeV) is plotted w.r.t distance 'r'. The singlet state wavefunction $u_0(r)$ within the well is matched with asymptotic solution $u_a(r)$ outside it at r_D .

B. Model Interaction Potentials:

The interaction between neutron and proton is originally modeled successfully by Yukawa¹ as

$$V_Y(r) = -V_A\left(\frac{e^{-\mu_A r}}{r}\right) \tag{9}$$

where V_A is strength of interaction in MeV and μ_A fm^{-1} is screening parameter which reflects range of interaction. We will be initially solving phase equation for this potential for various lab energies to show its relevance for low energies. Then, for including role of higher energies, a repulsive part of similar form is added, as proposed by Malfliet and Tjon⁶, given by:

$$V_{MT}(r) = -V_A \left(\frac{e^{-\mu_A r}}{r}\right) + V_R \left(\frac{e^{-\mu_R r}}{r}\right) \tag{10}$$

where, they chose $\mu_R = 2\mu_A$. We will refer to it as Malfliet-Tjon (MT) potential and has three parameters.

Instead of numerically solving for wavefunction, we introduce phase function method which results in scattering phase shifts directly from interaction potential.

C. Phase function method:

Derivation of phase equation

The transformation of second order time-independent Schrödinger equation into a Ricatti type first order non-linear differential equation i.e phase equation for $\ell = 0$, was initially given by Morse and Allis³⁰. It was later generalised for higher partial waves by Babikov¹⁶ and Calegero¹⁷. Here, we present the derivation for $\ell = 0$ case³⁰ in a pedagogical manner. We now introduce the following visual explanation for the first time. Consider a general potential as shown in Fig. 2, to be a combination of extremely small square wells, of differing depths, $V_i(r_i)$.

The wavefunction for the i^{th} well between r_i to r_{i+1} would be $u_i(r) = A_i \sin(k_i r + \phi_i)$, where $k_i = \sqrt{2\mu(E - V_i(r_i))/\hbar^2}$. Here, ϕ_i is determined by matching the boundary conditions at r_i , by considering the wavefunctions in the square wells from r_{i-1} to r_i and r_i to r_{i+1} . Remember, that $\phi_0 = 0$ for the first well between r_0 and r_1 . Then, δ_i is obtained by matching wavefunction at r_{i+1} to asymptotic solution in Eq. 7. So, one would have

$$\frac{1}{u_i(r)} \frac{du_i(r)}{dr} \bigg|_{r=r_{i+1}} = \frac{1}{u_a(r)} \frac{du_a(r)}{dr} \bigg|_{r=r_{i+1}}$$
(11)

By substituting asymptotic solution from Eq. 7 and defining a function $Z_i(r_{i+1})$ as

$$Z_i(r_{i+1}) = \frac{1}{u_i(r)} \frac{du_i(r)}{dr} \bigg|_{r=r_{i+1}} = k_a \cot(k_a r_{i+1} + \delta_i(r_{i+1}))$$
(12)

As width of wells tends to 0, the approach moves from discrete to continuous. Then $u_i(r)$ is replaced by $u(r) = A\sin(kr + \phi)$, where $k = \sqrt{2\mu(E - V(r))/\hbar^2}$ and $Z_i(r_{i+1})$ becomes

$$Z(r) = \frac{1}{u(r)} \frac{du(r)}{dr} = k_a \cot(k_a r + \delta(r))$$
(13)

Derivative of Z(r), using Eq. 13 is

$$\frac{dZ(r)}{dr} = -\frac{\left(k_a^2 + k_a \frac{d\delta}{dr}\right)}{\sin^2(k_a r + \delta)} \tag{14}$$

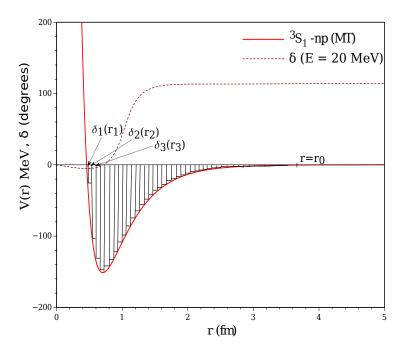


FIG. 2: MT potential for 3S_1 state, is shown as series of finite rectangular wells. The dotted line shows build up of SPS $\delta_i(r_i)$ at lab energy E = 20 MeV with distance (r).

Now, differentiating Z(r), by using first part of Eq. 13, i.e within the potential region, one obtains

$$\frac{dZ(r)}{dr} = \frac{d}{dr} \left(\frac{1}{u(r)} \frac{du(r)}{dr} \right) = \frac{1}{u(r)} \frac{d^2u(r)}{dr^2} - \frac{1}{u^2(r)} \left(\frac{du(r)}{dr} \right)^2 \tag{15}$$

From which, we obtain

$$\frac{1}{u(r)}\frac{d^2u(r)}{dr^2} = \frac{dZ}{dr} + Z^2(r)$$
 (16)

Transforming radial time-independent Schrödinger equation into phase equation:

Dividing equation Eq. 2 by u(r), we get

$$\frac{1}{u(r)}\frac{d^2u(r)}{dr^2} + \frac{2\mu}{\hbar^2}(E - V(r)) = 0$$
 (17)

In terms of Z(r), it is written as

$$\frac{dZ(r)}{dr} + Z^2(r) = \frac{2\mu}{\hbar^2} \left(V(r) - E \right) \tag{18}$$

On substituting from Eqs. 13 and 14, we have

$$-\frac{(k_a^2 + k_a \frac{d\delta}{dr})}{\sin^2(k_a r + \delta)} + k_a^2 \frac{\cos^2(k_a r + \delta)}{\sin^2(k_a r + \delta)} = \frac{2\mu}{\hbar^2} (V(r) - E)$$
 (19)

Using relation $\cos^2 \theta = 1 - \sin^2 \theta$ and $k_a^2 = \frac{2\mu E}{\hbar^2}$, it gets simplified to result in following phase equation

$$\frac{d\delta(r)}{dr} = -\frac{2\mu}{\hbar^2} \frac{V(r)}{k_a} \sin^2(k_a r + \delta(r))$$
(20)

This is a non-linear first order differential equation of Ricatti type, with initial condition $\delta(r=0)=0$. Eq. 20 can not be solved using any analytical techniques and hence we resort to numerical approach. One can obtain the wavefunctions from phase shifts¹⁷, but this is not necessary for determination of experimental scattering parameters or cross section, and hence is not attempted in this work.

III. NUMERICAL SOLUTION

A. Preparation of System:

<u>Choice of units:</u> In nuclear physics, scale of energies are in MeV and that of distances in fm. Converting J-m to MeV-fm, value of $\hbar c$ would be 197.329 MeV-fm.

Region of Interest: The potential has a certain range over which its influence is felt and dies down exponentially to zero. The limit value of distance r_f , at which $V(r_f)$ is zero is taken to be little greater than interaction radius of neutron-proton interaction. Typically, nuclear force saturates within 4 fm and hence we have chosen $r_f = 5$ fm. The interval [0, 5] for r is sampled uniformly with step-size (h) to obtain best accuracy.

Choice of Numerical technique: One must consider three key characteristics of stability, accuracy and efficiency, in that order of importance, while choosing numerical technique for solving any problem. Typically, 2^{nd} or 4^{th} order Runge-Kutta methods can be utilized for solving phase equation. But, for np-interaction, experimental SPS are known to three decimal places (See supplemental material, Table 1 in Appendix). The global error for RK-4 method is of the order h^4 and this could further add up due to propagation errors accrued with number of iterations. So, 5^{th} order Ruge-Kutta method (RK-5) is suggested for obtaining scattering phase shifts for np-interaction²⁰, even though RK-4 should suffice for implementation at undergraduate level. RK-5 is an interesting technique, that involves determination of 6 slopes even though only 5 are utilised for updating the solution at the next step.

The phase equation can be viewed as

$$\frac{d\delta(r)}{dr} = f(r, k, V, \delta) \tag{21}$$

where

$$f(r,k,V,\delta) = -\frac{2\mu}{\hbar^2} \frac{V(r)}{k} \sin^2(kr + \delta(r))$$
(22)

The method involves calculating value of $\delta(r_{i+1})$ by utilizing previous value at r_i , for i = 0, 1, ..., n-1.

$$\delta(r_{i+1}) = \delta(r_i) + \frac{h}{90}(7F_1 + 32F_2 + 12F_4 + 32F_5 + 7F_6)$$
(23)

where F_i 's are slopes of function f at different points in interval [0, h]. These function evaluations become evident on looking at algorithm presented during implementation stage.

B. Implementation of the numerical method in a computer

This stage involves writing an algorithm or pseudo code as it's first step. Broad blocks of algorithm are identified as:

- 1. Initialisation 2. Potential Definition 3. Function Definition
- **4.** RK-5 procedure **5.** Outputs.

The Scilab code for determining scattering phase shifts using RK-5 method has been given in Github³¹, which clearly delineates all steps given above.

Optimizing model parameters:

Experimental data for scattering phase shifts have been modified due to newer inputs at extended lab energies and also better accuracies at existing energies. So, one is left with a challenge of obtaining new set of model parameters that match with experimental data. There are many optimization algorithms³² for obtaining best model parameters for a chosen system. We have given our implementation^{11,33,34} based on Variation Monte Carlo technique on Github³¹.

C. Experimental Observables:

Scattering Properties:

For low energy scattering, scattering length 'a' and effective range ' r_0 ' can be calculated by

using relation³⁵

$$k \cot(\delta) = -\frac{1}{a} + 0.5r_0k^2 \tag{24}$$

Using scattering phase shifts, obtained by numerically solving phase equation, $k \cot(\delta)$ was plotted as a function of $0.5k^2$. This results in a straight line and scattering parameters r_0 and a are obtained from its slope and intercept respectively.

Partial and Total Cross section:

The partial cross section for S-wave (i.e $\ell = 0$ partial wave), is given by³:

$$\sigma(k) = \frac{4\pi}{k^2} \sin^2 \delta \tag{25}$$

Using numerically obtained scattering phase shifts for triplet 3S_1 and singlet 1S_0 states, we compute respective scattering cross section σ_t and σ_s .

The total cross section of S-wave 3,29 np scattering is calculated as

$$\sigma(k) = \frac{3}{4}\sigma_t + \frac{1}{4}\sigma_s \tag{26}$$

IV. RESULTS AND DISCUSSIONS

Experimental SPS from R. N. Pérez et.al. (Granada group)³⁶ along with 0.1 MeV data point from Nijmegen database³⁷ have been considered for both 3S_1 and 1S_0 states. Model parameters for both Yukawa and MT interaction potentials have been obtained based on an optimization procedure¹¹ given at Github³¹, and are given in Table I. The corresponding mean absolute percentage error (MAPE) are also given in Table I. Utilizing these model parameters for Yukawa and MT potentials, phase equation Eq. 20 has been solved using RK-2, RK-4 and RK-5 methods, for both triplet 3S_1 and singlet 1S_0 states. Even though mean absolute percentage error for RK-5 and RK-4 methods are exactly similar, for two data points there has been a change in phase shift values at the 3^{rd} decimal place. Hence, one can implement RK-4 method in the lab, as it is well known algorithm.

Obtained scattering phase shifts are plotted in Fig. 3. The scattering phase shifts using RK-4 method are similar to RK-5 method. Even in RK-2 method, the change in scattering phase shifts occurs in second decimal place, so they would not be visible in plots, and hence not included.

It should be emphasised that while CoM energies are used for computing scattering phase

TABLE I: Model parameters and mean absolute percentage error (MAPE) for triplet (${}^{3}S_{1}$) and singlet (${}^{1}S_{0}$) states of np interaction for Yukawa and Malfliet-Tjon potentials. For Yukawa potential, the MAPE is given up-to 50 Mev since, beyond that the MAPE value increases to a significant amount.

Potential	States	$V_r \text{ (MeV)}$	$V_a \text{ (MeV)}$	$\mu_A \ (fm^{-1})$	MAPE %
Yukawa	${}^{3}S_{1}$	_	50.25	0.37	1.65 (up-to 50 MeV)
	1S_0	_	41.79	0.61	1.52 (up-to 50 MeV)
Malfliet-Tjon	${}^{3}S_{1}$	9435.57	2134.88	2.54	0.61 (up-to 350 MeV)
	${}^{1}S_{0}$	6806.60	1522.42	2.42	$1.91~(\mathrm{up\text{-}to}~350~\mathrm{MeV})$

shifts, plots are made with laboratory energies for ease of comparison with experimental data. It is seen that scattering phase shifts for both ${}^{3}S_{1}$ and ${}^{1}S_{0}$ states, obtained using Yukawa potential match with empirical data for laboratory energies up to about 50 MeV. Then, they start to deviate and tend to saturate to values far above expected ones.

On the other hand, scattering phase shifts obtained on solving phase equation using MT potential match expected data all the way upto 350 MeV. Close match between computed and and experimental scattering phase shifts for both ${}^{3}S_{1}$ and ${}^{1}S_{0}$ states using MT potential with RK-5, RK-4 and RK-2 methods can further be observed from data compiled (See supplemental material, Table 1 in Appendix).

Plots of Yukawa and MT potentials using model parameters are shown in Fig. 4. It is interesting to observe that using MT potential, shapes of both triplet ground state and singlet scattering state are very similar except for their depths.

In order to determine low energy scattering parameters using Eq.5, we have considered energies from 0.1 - 10 MeV which results in k values from 0.035 - 0.347 fm^{-1} . Considering scattering phase shifts obtained using MT potential, we have plotted $kcot(\delta)$ w.r.t. $0.5k^2$ for both singlet and triplet states. These are shown in Fig. 5. Slopes of their regression lines give scattering length 'a' and intercepts are utilized for determining effective range ' r_0 '. Obtained values are tabulated alongside experimental ones in Table II. While there is a good overlap between ranges of calculated experimental values³⁵ for scattering length 'a', those for effective range ' r_0 ' are reasonably close. Adding more low energy data points below 0.1 MeV might further improve determination of these parameters.

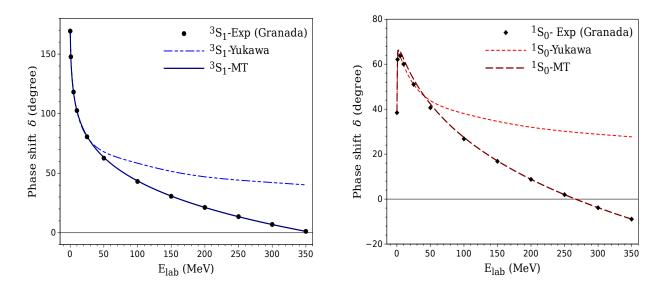


FIG. 3: Scattering phase shifts for (a) triplet 3S_1 (left) and (b) singlet 1S_0 (right) state of np scattering obtained using Yukawa and Malfliet-Tjon potentials, along with experimental data³⁶, for lab energies upto 350 MeV.

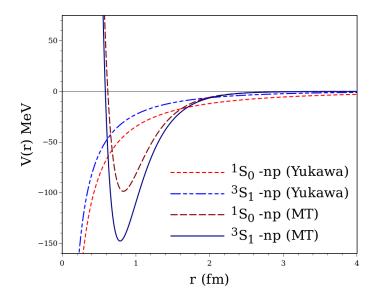


FIG. 4: Plots of Yukawa and MT potentials responsible for scattering phase shifts observed due to scattering from ${}^{3}S_{1}$ and ${}^{1}S_{0}$ states in np interaction.

Finally, partial and total scattering cross section were calculated from obtained scattering phase shifts using Eqns. 25 and 26 respectively, for experimental energies ranging from 0.1-350 MeV. Obtained total cross section is plotted along with experimental data³⁸ in Fig. 6. On extrapolating to E=0.000132 MeV, total cross section for S-wave is calculated

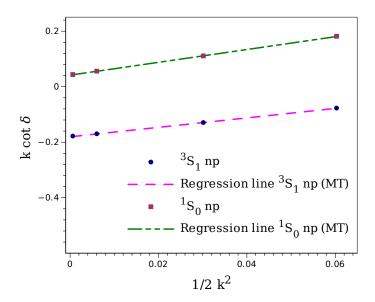


FIG. 5: Plots of $k \cot \delta$ with $0.5k^2$ for triplet and singlet states along with regression lines

to be = 20.641 b. This is in good agreement with experimental total deuteron cross section value of 20.491 b³.

Generally, interaction potentials that explain experimental scattering phase shifts of np-

TABLE II: Comparison of obtained scattering length 'a' and effective range ' r_0 ' with experimental values:

States	$a(fm) \; (\exp.)^{35}$	a(fm) (calc.)	$r_0(fm) \; (\exp.)^{35}$	$r_0(fm)$ (calc.)
${}^{3}S_{1}$	5.397 ± 0.011	5.534 ± 0.032	1.727 ± 0.013	1.705 ± 0.012
${}^{1}S_{0}$	-23.678 ± 0.028	-24.038 ± 0.045	2.44 ± 0.11	2.307 ± 0.025

scattering are utilized to determine properties of deuteron which is a weakly bound nucleus consisting of one neutron and one proton. By solving the radial time-independent Schrödinger equation using numerical technique³⁹, we have determined deuteron binding energy (BE) = -2.026 MeV for obtained 3S_1 potential. The experimental binding energy of Deuteron = -2.225 MeV³. Similarly, utilizing potential for 1S_0 , an energy value of 76 KeV has been obtained for unbound state which is very close to expected value of 77 KeV. This type of determination of certain property of a system which consists of projectile and target particles is called off-shell calculation and acts as a cross-confirmation of obtained interaction potential to be consistent with other expected data.

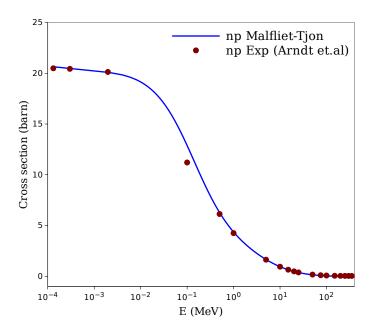


FIG. 6: Neutron-proton (np) experimental³⁸ and calculated cross section up to $E=350~{\rm MeV}.$

The proposed method for determination of scattering phase shifts for np scattering is also applicable to study $neutron - deuteron \ (nd)^{12}$ and $neutron - alpha \ (n-\alpha)^{13}$ scattering systems. One has to redetermine model parameters for chosen interaction potential by fitting simulated scattering phase shifts to match with available experimental data for these systems. Since by changing interacting particles, few physical observables i.e, reduced mass of the system, interaction potential between interacting particles and scattering phase shifts will change. Other two body scattering systems involving charged particles, such as $proton - proton \ (pp)^{11}$ and $\alpha - \alpha^{14}$ require introducing screened Coulomb potential such as Hulthen potential, a modified form of Yukawa potential.

V. CONCLUSION

The advantage of phase function method (PFM), which directly allows determination of scattering phase shifts without recourse to wavefunction, has been utilized to introduce phase wave analysis procedure to obtain scattering cross section. Phase equation for $\ell = 0$, derived from the radial time-independent Schrödinger equation, has been numerically solved using 5^{th} order Runge-Kutta (RK-5) method for determining scattering phase shifts of both

triplet and singlet states of np - interaction.

While attractive Yukawa potential was able to explain experimental scattering phase shifts data for lab energies upto about 50 MeV, MT potential consisting of an extra repulsive part performed well even at higher energies upto 350 MeV. These scattering phase shifts were utilized to obtain scattering length and effective range for both S-waves and are found to be having good match with experimental values.

Finally, total scattering cross section at various energies have been obtained from partial scattering cross section of both S-waves to very good accuracy. The methodology detailed in this paper could be easily extended to study other two body scattering phenomenon in atomic, nuclear and particle physics and hopefully is within reach of undergraduate physics students to undertake interesting projects.

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Conflict of Interest: The authors have no conflicts to disclose.

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¹ H. Yukawa, S. Sakata, M. Kobayasi, and M. Taketani. "On the Interaction of Elementary Particles. IV." Progress of Theoretical Physics Supplement 1, 46-71 (1955).

² M. Napsuciale, and S. Rodríguez. "Complete analytical solution to the quantum Yukawa potential." Physics Letters B 816, 136218 (2021).

³ K. S. Krane, *Introductory nuclear physics*. (John Wiley & Sons, 1991).

⁴ S. S. M. Wong, *Introductory nuclear physics*. (John Wiley & Sons, 2008).

⁵ H. S. Hans, Nuclear Physics: experimental and theoretical. (New Age International, 2008).

⁶ R. A. Malfliet, and J. A. Tjon. "Solution of the Faddeev equations for the triton problem using local two-particle interactions." Nuclear Physics A 127 (1), 161-168 (1969).

⁷ E. P. Wigner, and L. Eisenbud. "Higher angular momenta and long range interaction in resonance reactions." Physical Review **72** (1), 29 (1947).

⁸ R. S. Mackintosh, "Inverse scattering: applications to nuclear physics." arXiv preprint arXiv:1205.0468 (2012).

- ⁹ R. Jost, and A. Pais. "On the scattering of a particle by a static potential." Physical review 82 (6), 840 (1951).
- ¹⁰ J. Thijssen, Computational Physics. 2nd ed. Cambridge: (Cambridge University Press, 2007). doi:10.1017/CBO9781139171397.
- O. S. K. S. Sastri, A. Khachi, and L. Kumar. "An Innovative Approach to Construct Inverse Potentials Using Variational Monte-Carlo and Phase Function Method: Application to np and pp Scattering." Brazilian Journal of Physics 52 (2), 1-6 (2022).
- ¹² S. Awasthi, A. Khachi, L. Kumar and O. S. K. S. Sastri. "Triton scattering phase-shifts for S-wave using Morse potential." Journal of Nuclear Physics, Material Sciences, Radiation and Applications 9, no. 1, 81-85 (2021).
- ¹³ L. Kumar, S. Awasthi, A. Khachi and O. S. K. S. Sastri. "Phase Shift Analysis of Light Nucleon-Nucleus Elastic Scattering using Reference Potential Approach." arXiv preprint arXiv:2209.00951 (2022).
- A. Khachi, L. Kumar and O. S. K. S. Sastri. "Alpha–Alpha Scattering Potentials for Various \(\ell\)-Channels Using Phase Function Method." Physics of Atomic Nuclei 85, no. 4, 382-391 (2022).
- P. M. Morse, "Diatomic molecules according to the wave mechanics. II. Vibrational levels." Physical review 34 (1), 57 (1929).
- V. V. Babikov, "The phase-function method in quantum mechanics." Soviet Physics Uspekhi 10 (3), 271 (1967).
- ¹⁷ F. Calogero, "Variable Phase Approach to Potential Scattering by F Calogero." Elsevier, **1967**.
- ¹⁸ A. H. Kahn, "Phase-Shift method for one-dimensional scattering." Am. J. Phys. **29**, 77 (1961).
- A. Khachi, L. Kumar and O. S. K. S. Sastri. "Neutron-Proton Scattering Phase Shifts in S-Channel using Phase Function Method for Various Two Term Potentials." Journal of Nuclear Physics, Material Sciences, Radiation and Applications 9, no. 1, 87-93 (2021).
- V. Zhaba. "Calculation of phases of np- scattering up to Tlab=3 GeV for Reid68 and Reid93 potentials on the phase-function method." arXiv preprint arXiv:1604.06006 (2016).
- J. Bhoi and U. Laha. "Nucleon-Nucleon Scattering Phase Shifts via Supersymmetry and the Phase Function Method." Brazilian Journal of Physics 46, 129-132 (2016).
- ²² J. C. Butcher, "On fifth order Runge-Kutta methods." BIT Numerical Mathematics 35 (2), 202-209 (1995).
- ²³ O. S. K. S. Sastri, A. Sharma, S. Awasthi, A. Kachi, and L. Kumar. "Simulation of vibra-

- tional spectrum of diatomic molecules using Morse potential by matrix methods in gnumeric worksheet." Phys. Educ. **36**, 1-14 (2019).
- A. Sharma, S. Gora, J. Bhagavathi, and O. S. K. Sastri. "Simulation study of nuclear shell model using sine basis." Am. J. Phys. 88, 7, 576-585 (2020).
- M. Sarsour, T. Peterson, M. Planinic, S.E. Vigdor, C. Allgower, B. Bergenwall, J. Blomgren, T. Hossbach, W.W. Jacobs, C. Johansson and J. Klug. "Measurement of the absolute differential cross section for np elastic scattering at 194 MeV." Physical Review C, 74 (4), 044003 (2006).
- ²⁶ N. Zettili, 2009. Quantum mechanics: concepts and applications. (John Wiley & Sons, 2009).
- ²⁷ S.N. Paneru, "Elastic Scattering of ${}^{3}He + {}^{4}He$ with SONIK." Ohio University, (2020).
- Lecture notes on: "Applied Nuclear Physics", MIT OpenCourseWare, Massachusetts Institute of Technology. (https://ocw.mit.edu/courses/22-101-applied-nuclear-physics-fall-2003/pages/lecture-notes/).
- ²⁹ C. A. Bertulani and Pawel Danielewicz, *Introduction to nuclear reactions*. (pp. 47-48), (CRC Press, 2019).
- ³⁰ P.M. Morse, and W.P. Allis. "The effect of exchange on the scattering of slow electrons from atoms." Physical Review, **44** (4), 269 (1933).
- 31 https://github.com/Anynomous123/Phase-Function-Method-for-Neutron-Proton-np-Scattering-in-Scilab-Malfliet-Tjon-Yukawa-Potential.
- M. A. Fischler, and R. C. Bolles. "Random sample consensus: a paradigm for model fitting with applications to image analysis and automated cartography." Communications of the ACM 24, no. 6, 381-395 (1981).
- A. Sharma and O. S. K. S. Sastri. "Numerical solution of Schrödinger equation for rotating Morse potential using matrix methods with Fourier sine basis and optimization using variational Monte-Carlo approach." International Journal of Quantum Chemistry 121 (16), e26682 (2021).
- ³⁴ S. Gora, O. S. K. S. Sastri, and S. K. Soni. "Optimization of semi-empirical mass formula coefficients using least square minimization and variational Monte-Carlo approaches." European Journal of Physics 43 (3), 035802 (2022).
- ³⁵ G. Darewych, and A. E. S. Green. "Morse Function and Velocity-Dependent Nucleon-Nucleon Potentials." Physical Review 164, 1324 (1967).
- R. N. Pérez, J. E. Amaro, and E. Ruiz Arriola. "The low-energy structure of the nucleon–nucleon interaction: statistical versus systematic uncertainties." Journal of Physics G: Nuclear and

- Particle Physics 43 (11), 114001 (2016).
- ³⁷ NN-Online (https://nn-online.org/NN/).
- ³⁸ R. A. Arndt, W. J. Briscoe, A. B. Laptev, I. I. Strakovsky, and R. L. Workman. "Absolute Total np and pp Cross Section Determinations." Nuclear science and engineering 162 (3), 312-318 (2009).
- ³⁹ A. Sharma, S. Gora, J Bhagavathi, and O. S. K. S. Sastri. "Simulation study of nuclear shell model using sine basis." Am. J. Phys. 88, 7, 576-585 (2020).