Numerical solution of deuteron potential depth using python

Adam Muhammad¹, I.A. Alnour¹, (a)

¹Department of Physics, Faculty of Pure and Applied Sciences, International University of Africa (IUA), 12223 Khartoum, Sudan

Abstract. Deuteron potential depth is hardly solvable analytically, thus this study uses a numerical method through Python programming language to calculate the depth of the potential well by coding the transcendental equation. Two different approaches were used, in which the first approach is by changing the $V_0$ (initial value) value in the code to obtain the $V_o$ values as an output, and the second, by keeping $V_0$ value constant and changing the radius $R$ values to obtain different $V_o$ values in order to find the relationship between $V_o$ and radius $R$. The mean average value of $V_o$ was found to be $-37.6$ MeV. The result was close to the typical potential value ($-36$ MeV). The relationship between the potential depth and its radius shows the potential changes with respect to the deuteron radius. Moreover, the comparison of the deuteron potential depth of the present study shows an acceptable level of consistency with those of previous studies. Among other numerical methods, Python-based solution seems to be one of the simplest and most accurate method for solving complex numerical problems.

1. Introduction
Theoretical nuclear physics is one of the most interesting and important field that scientists have been putting much effort to understand the principle of nuclear structure and its nucleons interaction [1] and in order to achieve so scientists have tried to understand the simple structure of deuteron i.e. an isotope of hydrogen consisting of one proton and one neutron, due to its simplicity as a loosely bound system of nucleon-nucleon interaction and by understanding it, many properties of the multi-nucleon system will be understood [1, 2, 3]. For nuclear physicists, a deuteron is analogous to a hydrogen atom of atomic physicists. Just like how the measured Balmer series of electromagnetic transitions between the excited states of hydrogen led to an understanding of hydrogen structure, so should the electromagnetic transitions between the excited states of the deuteron lead to an understanding of its structure. Unfortunately, there are no excited states of the deuteron; it is such a weakly bound system that the only “excited state” is the unbound system consisting of a free proton and a free neutron [1, 4, 5, 6, 7]. The deuteron is the only stable bound system of two nucleons. Experimentally it is known that the deuteron binding energy is 2.225 MeV, as it is known that the typical binding energy per nucleon is around 8 MeV. The deuteron is therefore a very weak bound system when (1.1 MeV) compared to a typical nucleon. It has a total spin quantum number of one and an orbital angular momentum of zero. The deuteron has a root-mean-square electromagnetic radius of approximately 2.1 fm [1, 4, 8, 9].

To study the properties of deuteron based on its binding energy as a weekly bound system, we will assume that we can represent the nucleon-nucleon potential as a three-dimensional square well (Spherical well) [1].

In this study, we will solve for deuteron potential depth as one of its properties necessary to be known in order to understand the nucleon-nucleon force, but we will take a different approach from what was attempted by many researchers which solved it analytically, graphically and computationally. We will use numerical method using Python programming language to solve the transcendental equation[1] as follows:
\[ K \cot KR = -L \]  

(1)

It was well established fact that the equation was hardly solvable analytically, but numerical method was proposed by Krane in 1982 [10] and some other studies, in order to solve the problem. Computational methods via Python programming has a high reputation of solving difficult and complex physics problems and it serves as the bridge between theoretical and experimental physics.

2. Calculation

2.1. Calculation of the Potential Energy \((V_o)\) of Deuteron

In the investigation of the deuteron potential almost all introductory textbooks represent the deuteron potential by a square potential well of depth \(V\) and width \(R\) as shown in Figure 1.

![Figure 1. The spherical square-potential well.](image)

The potential of deuteron can be given by writing the time-independent Schrödinger equation for any central potential \((V(r))\) [11] as:

\[
\hat{H}\psi(r) = \hat{E}\psi(r)
\]

\[
\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r)\right]\psi(r) = \hat{E}\psi(r) \tag{2}
\]

where \(V(r)\) is a central potential, \(\psi\) is the wave function, \(E\) the fundamental state binding energy, \(\hbar\) is the Planck constant and \(m\) is the reduced mass which is given by:

\[
m = \frac{m_pm_n}{m_p + m_n} \tag{3}
\]

where \(m_p\) and \(m_n\) are masses of proton and neutron respectively.

The derivation of equation (2) was made in study [1] which eventually lead to the transcendental equation below after applying the boundary conditions to Eq. (1) above,
where:

\[ K = \sqrt{\frac{2m(E + V_o)}{\hbar^2}}, \quad L = \sqrt{\frac{-2mE}{\hbar^2}} \]

\[ \sqrt{\frac{2m(E + V_o)}{\hbar^2}} \cot \left( R \sqrt{\frac{2m(E + V_o)}{\hbar^2}} \right) = -\sqrt{\frac{-2mE}{\hbar^2}} \]

(4)

The above equation (4) was then rearrange below in equation (5) to be in the form of \( V_o = f(V_{in}) \) in order to fit it into Python syntax

\[ V_o = \tan \left( R \sqrt{\frac{2m(E + V_{in})}{\hbar^2}} \right)^2 \times E - E \]

(5)

2.2. Numerical Solution of Deuteron Potential through Python

Equation (5) will be solved via coding it into Python syntax, after equation (4) has been rearranged to be in the form of \( X = f(x) \) i.e. \( V_o = f(V_{in}) \), then the algorithm is by guessing an initial \( V_{in} \) value in order to obtain the unknown \( V_o \) values, thus Python compiler iterated 10 times and it print out 10 different values among which we obtain the potential depth value \( (V_o) \) that’s closest to the typical value. The same procedure was followed to find the relationship between Deuteron distance \( (R) \) and potential depth \( (V_o) \) but this time by changing the input values of \( R \) and keeping \( V_{in} \) constant, the values of \( V_o \) will be printed out and the graph of potential depth \( V_o \) versus \( R \) will be plotted from this result.

3. Results and Discussion

3.1. Calculation results of \( V_o \)

Quite reasonable result of deuteron potential depth \( (V_o) \) has been achieved from the written program. Values of \( V_o \) for different \( V_{in} \) values ranging from 1 to 1000 are shown in Table 1. The average of \( V_o \) is \(-37.6\) MeV. The magnitude of this value shows how deep the potential well is. It is assumed that the potential depth of the deuteron only depends on the distance \( r \) between the nucleons. To be more specific it assumes that the potential has some constant value \(-V_o \) (which was the one we found in this study) up to some spacing \( r = R \). And it also assumes that the potential is zero for spacing larger than \( R \).
Table 1. The results value of deuteron potential ($V_o$).

| $V_{in}$ | $V_o$(MeV) |
|---------|------------|
| 1.0     | −36.8467   |
| 1.5     | −38.8395   |
| 10      | −22.7267   |
| 16      | −30.9610   |
| 17      | −35.5801   |
| 24      | −39.1824   |
| 26      | −59.8322   |
| 30      | −38.5322   |
| 1000    | −36.0909   |

3.2. Deuteron potential depth as a function of $R$

A graph was plotted from Table 2 to show the relationship between $V_o$ and the radius $R$ and it was made by choosing a large number i.e. 1000 as a constant $V_{in}$ value and changing the range of $R$ from 0.5 up to 4 and then printing out $V_o$ values.

Figure 2 shows depth of this potential as a function of the distance between the proton and the neutron. The curve of the graph has a minimum at $R = 1.69\ fm$. The depth of this potential implies the interaction strength of proton and neutron and the range of this interaction is that of radius $R$ which is $2.1\ fm$ and this shows how the strong force behaves between the nucleons in the potential well as the force has a repulsive and attractive part. The nuclear force started to vanishes and become negligible at some typical spacing between the nucleons where the typical range of nuclear force is roughly $1.5\ fm$ and the potential cut off $R$ is at $2.1\ fm$ (In the so-called model OPEP potential)[12]. This result is in agreement with the fact that the strong force is powerfully attractive at the range of $0.5\ fm$ but it decrease rapidly at the distance beyond $2.5\ fm$ [1], at the distance less than $0.7\ fm$ it becomes repulsive i.e. the closer the nucleons of the system are, the lower the potential energy, and the lower the potential energy, the deeper the well, and the deeper the well is, the stronger the interaction between the nucleons of that system. The fact that the potential vanishes at large nucleon spacing also appear in the wave function, which also implies that the rate of decay of the wave function at large nuclear spacing was correctly presented and this rate of decay depend only on the binding energy which is very weak. The behaviour of nuclear force became repulsive when the distance $r$ is less than $0.5\ fm$ then the potential is taken to be infinite, rather than $-V_o$. That may prevent the nucleons from getting closer to each other [1].
Table 2. Relationship between deuteron nucleon distance (R) and potential depth ($V_o$).

| R(fm) | $V_o$(MeV) |
|-------|------------|
| 0.5   | -20        |
| 1.0   | -41        |
| 1.5   | -82        |
| 2.0   | -78        |
| 2.5   | -40        |
| 3.0   | -54        |
| 3.5   | -60        |
| 4.0   | -60        |

Figure 2. The $V_o$ versus R Relationship for potentials having the deuteron as the ground state

3.3. Comparison with other results

A comparison between various studies [1, 12, 13, 14, 15, 16, 17] and our work is shown in Table 3, where the other studies used different methods and they arrived at different values which are quite close to each other. A lot of methods have been applied in our work, but the one that was successful was the numerical method (using python). Analytical solution was approached, and reasonably close values were achieved. Based on numerical method, the result achieved through our Python syntax was −37.6 MeV which is quite close to the typical potential value. Apparently, all the values in Table 3 are within the same range.

Finally, according to the above discussion, the potential depth value $V_o$ obtained from Python have up to 15 digits in value (i.e. at $V_{in}$ equals to 1; $V_o = -36.846892656974795$ MeV), which implies that the calculations via Python language seems to be reliable.
Table 3. The comparison between our study and other achieved values from other studies and methods

| Work of Researcher | Method | \( V_0 \) (MeV) |
|--------------------|--------|-----------------|
| [1]                | Numerical method | -35.0          |
| [12]               | A truncated one-pion exchange potential | -30.0          |
| [13]               | Modelling       | -33.7          |
| [14]               | A graphical and computer method | -33.4          |
| [15]               | Analytical method | -23.1          |
| [16]               | Analytical method | -59.7          |
| [17]               | Using uncertainty principle | -51.1          |
| Present Study      | Numerical method using Python | -37.6          |

3.4. Estimation of the constant value for \( K \) and \( L \) based on \( V_0 \)

Constants \( K \) and \( L \) were calculated based on the calculated value of \( V_0 \). \( K \) is found to be 0.93 \( fm^{-1} \) and \( L \) is found to be 0.23 \( fm^{-1} \). The value of \( r \) was 1.69 \( fm \) which is estimated based on the value of \( K \). The deuteron wave function is shown in Figure 3. We can see that from Figure 3, at most of the time the wave function is outside the well and it goes to the large distance which is the implication of 37% value of the exponential. The weak binding means that \( u(r) \) (wave function) is just barely able to “turn over” in the well implying that at 93% the curve started to turn down so as to connect at \( r = R \) with the negative slope of the decaying exponential, meaning the wave function extended beyond the nuclear interaction range, therefore, excited state was not expected [1].

As we can remarkably, observed Figure 2 has a relationship and connection with deuteron wave function shown in Figure 3. The maximum height value of the wave function in Figure 3 coincides with the minimum value of the potential depth graph against the deuteron radius \( R \).

4. Conclusion

The trancedental equation was coded into the Python to calculate the deuteron potential depth (\( V_0 \)), and reasonable solution to the problem was obtained; this also means that this study was limited to solving deuteron potential depth (\( V_0 \)) at the ground state based on square potential well. Compared with the other solutions from other researchers, the obtained result from this study is among the close values to the typical potential depth value (−36 MeV). The deuteron potential value that was found in this study shows the reliability of Python programming language due to its capability and simplicity.
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