Numerical Methods for the Deuterium Problem

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The nucleus of the deuterium atom is called the deuteron (^{2}H) and it is the lightest nucleus in nature, composed of only one proton and one neutron. Because of the simplicity of its two-body bound state, the structural study of this n-p system can act as the basis for future explorations of nuclei with more complex nuclear structure. In this current work, by using the Julia programming language and a matrix representation of the iterative Numerov's method, we solve the problem of the coupled differential equations for an Argonne v18 potential. We calculate the binding energy, dipole and quadrupole moments and matter radius that are in agreement with the experimentally observed values.

I. INTRODUCTION AND THEORY

The deuteron nucleus has been studied extensively experimentally in the past and many attempts have been made to solve the problem using calculations. Because of its simplicity of its two-body bound state, it can act as a platform to explore more complex nuclei in the future. In this work, we will not focus on the theory behind the deuteron model, as has been done in numerous other projects in the past. A useful review of the topic is done in Ref. [1]. Instead we will focus on the numerical methods of solving the wave functions of the deuteron.

The deuteron wave function can be written as a superposition of s and d waves. Then, by using the Schrödinger equation and a potential of the form $V_c(r) + V_t(r)\, S_{12}$, where $V_c(r)$ is the scalar term and $V_t(r)\, S_{12}$ is the tensor term, accounting for the spin-spin interaction between the two nucleons, we get the following pair of coupled differential equations :

$$u''(r) - \gamma(E + V_0(r))\, u(r) = \gamma\sqrt{8} V_t(r)\, w(r) \tag{1}$$

$$w''(r) - \gamma(E + V_2(r) + \frac{6}{\gamma\, r^2} - 2V_t(r))\, w(r) = \gamma\sqrt{8} V_t(r)\, u(r) \tag{2}$$

$$\gamma \equiv \frac{2\mu}{\hbar^2} \tag{3}$$

In order to solve the coupled differential equations, we used the Argonne potential, a N-N interaction potential shown in Fig. 1, which is one of the best candidates to approach this problem and match the experimental results. The configuration of the parameters used when calling the Argonne potential within the code, are shown in Table I. Subsequently, regarding the validation of our calculations with the chosen potential, we compare the values obtained for the magnetic dipole and quadrupole moments, with the experimentally observed ones. For the dipole moment of the deuteron, the dipole vector has the form:

TABLE I. The configuration of the n-p two body system used when calling the Argonne Potential subroutine av18pw.

L	S_{total}	J_{total}	I_{total}	τ_1^z	τ_2^z
0	1	1	0	1 (p)	-1 (n)

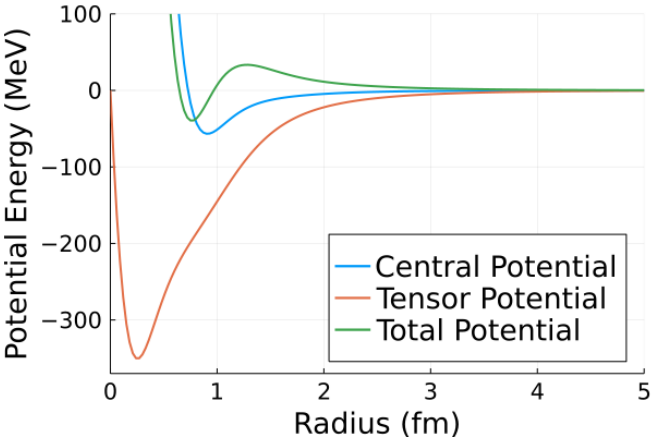

FIG. 1. The Argonne potentials for the n-p deuterium system. There are three plots signifying the l=0 central potential, l=2 central potential and a tensor component.

$$\vec{\mu_d} = g_p \vec{s_p} + g_n \vec{s_n} + \frac{1}{2}\vec{l} \tag{4}$$

where $\vec{s_p}$ and $\vec{s_n}$ are the spins and g_p and g_n are the g-factors for the proton and neutron, respectively. After the proper manipulation and by taking the z projection of the dipole moment, we can express the expectation value of the dipole magnetic moment as a function of the magnetic moments μ_p of the proton and μ_n of the neutron :

$$\mu_d = <\mu_z> = (\mu_p + \mu_n) + (\frac{1}{2} - \mu_p - \mu_n)\frac{3}{2} W_d \tag{5}$$

where W_d is the d-wave weight :

$$W_d = \int w^2\, dr \tag{6}$$

Similarly, after a proper manipulation we reach the expression for the expectation value of the quadrupole magnetic moment Q_z in the z direction as a function of u_0 and u_2 :

$$Q_d =< Q_{zz} >= \frac{e}{5}\int \left(\frac{2\,u\,w}{\sqrt{8}} - \frac{w^2}{4}\right) r^2 dr \qquad (7)$$

Another quantity that we can calculate using the radial wave function is the characteristic size of the deuteron. This matter radius is defined as half the rms distance between two nucleons.

$$r_d^2 = \frac{1}{4}\int (u^2 + w^2)\, r^2\, dr \qquad (8)$$

II. NUMERICAL METHODS

The previous work predominately utilized the FORTRAN programming language to solve the coupled differential equations. This is mainly due to the speed of FORTRAN computations and the fact that many of the NN-interaction potentials are written as FORTRAN subroutines. However, there has been a lot of progress and interest in scripting languages such as python. Python was considered for this project based on the wide availability of libraries such as numpy, scipy and matplotlib. Unfortunately there was some difficulty calling the argonne potential subroutine in python. Ultimately, the Julia Language was chosen for this project and can be downloaded here: Julia. This programming language was built with numerical computations in mind and has native methods for calling FORTRAN subroutines which are utilized often.

Many students have attempted to solve the deuteron problem, using a coupled fourth order Runge-Kutta routine with a shooting method, in order to determine the energy eigenvalue. But, unable to get the equations to converge, the groups typically turned to a different approach. The most common was a matrix diagonalization using the finite difference approximation of the second order wave function. The difficulty likely arises from the extreme variation of the potential at low radii.

To solve the differential equation in Sec. I we utilize a matrix representation of the Numerov's (or Cowell's) method [2], which solves the follow form

$$y''(r) + g(r)y(r) = s(r) \qquad (9)$$

For this problem, s(r) is equal to zero and we only need to calculate the g(r) matrix :

$$g(r) = \begin{pmatrix} \gamma\,(E + V_0) & \gamma\, V_t \\ \gamma\, V_t & 6/r^2 + \gamma\,(E + V_2) \end{pmatrix} \qquad (10)$$

The above g(r) matrix differs slightly from the differential equation discussed in the introduction. When the $\sqrt{8}$ and the $2V_t$ are included our equations cease to converge. Fortunately, the simplified set of equations produce excellent results.

To determine the binding energy, the Numerov method is called twice, alternating the initial conditions between 1e-6 and 0 to see the central and tensor contribution of the wave functions. Then instead of using the common secant method to find the root we utilize the asymptotic solutions, f_s and f_d, of the wave functions discussed in class [3].

$$f_s \approx e^{-\sqrt{\gamma E}} \qquad (11)$$

$$f_d \approx e^{\sqrt{\gamma E}}\,(1 + \frac{3}{(\gamma E)} + \frac{3}{(\gamma E)^2}) \qquad (12)$$

We construct a 4x4 matrix of the asymptotic solutions, the numerical values and their derivative at the maximum radius, which has the form:

$$M = \begin{pmatrix} u_c & u_t & f_s & 0 \\ w_t & w_c & 0 & f_d \\ u_c' & u_t' & f_s' & 0 \\ w_t' & w_c' & 0 & f_d' \end{pmatrix} \qquad (13)$$

The determinant of this matrix has its minimum at the location of a solution for the coupled differential equations shown in Fig. 2. Finally, with our known binding energy, we need to combine our central and tensor components of our radial wave functions, to form the total radial solution.

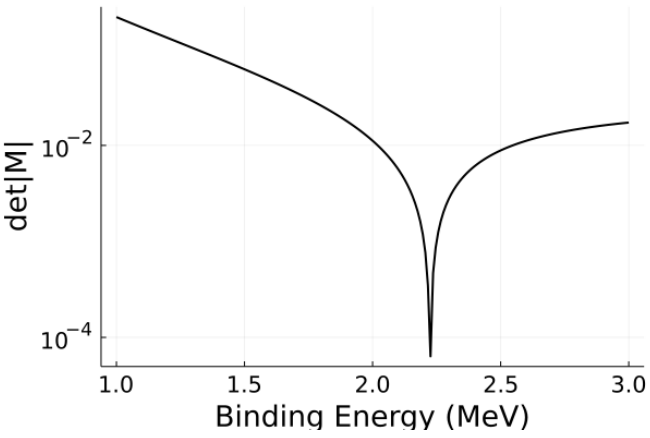

FIG. 2. This plot shows the determinant of the 4x4 matrix M, constructed using the numerical and asymptotic values as well as their derivatives as a function of the binding energy.

TABLE II. Comparison of the theoretically calculated values with the experimental results from Ref. [4].

	Experiment	Theory/this work	% Difference
Binding energy (MeV)	-2.224575	-2.224564	0.0005
Dipole moment, μ_d (μ_N)	0.857406	0.84699	1.22
Quadrupole moment, Q_d (e fm^2)	0.2859	0.26845	6.10
D-State probability, W_d	0.068	0.0576	15.29
Matter radius, r_d (fm)	1.953	1.9672	0.73

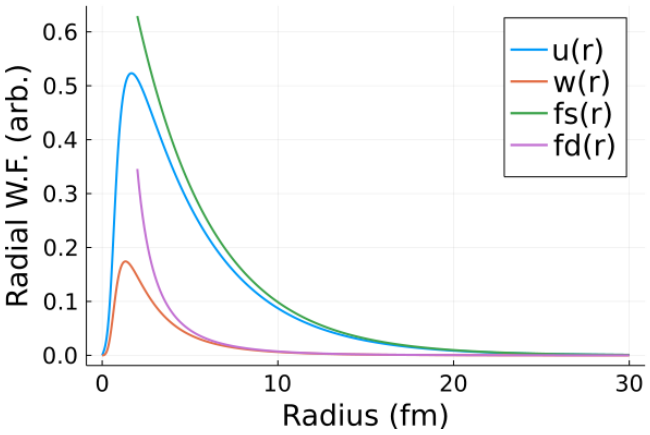

FIG. 3. The numerically determined radial wave functions plotted alongside the asymptotic solutions of the deuteron.

III. RESULTS

The radial wave functions are calculated using the previously mentioned methods in Sec. II and are shown in Fig. 3. The deuteron properties discussed in Sec. I are shown in Table II. Overall, the results of our numerical solution match the experimentally observed values.

IV. CONCLUSION

It is evident that the method that we used, utilizing the Argonne potential, gives us a good agreement with the experimentally observed values. The binding energy has almost 0% difference between the experimental and the calculated value and both the dipole and quadrupole moments, have equal or less than 6% difference, between theory and experiment. The deuteron matter radius has a 1% difference from the measured value. Lastly the D-State probability has the largest error of 15%. Future investigation is required to determine the source of this error. In order to do that, the source code and instructions will be available at `https://github.com/eli-temanson/Nuc1-Deuteron-Project.git`.

Ultimately, the method implemented in this work produced excellent results and provides one of the first iterative solutions to the deuteron wave functions presented in this class.

ACKNOWLEDGMENTS

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