Computational Assessment of the Deuteron

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Contents

1 Abstract

In this computational assessment of the Deuteron graphical and computational methods were used to deduce information about the nature of the deuteron atom. The results found were in strong agreement with current theoretical predictions as well as experimental measurements of said characterises. These were chiefly the binding energy of the Deuteron, found to be 2.22MeV and the implications of a loosely bound structure through the predicted separation between proton neutron due to its low binding energy as well as the prediction of finding the nucleon within the potential well (internuclear force) as 32%, representing a greater likelihood of a separation of the n-p in the deuteron.

2 Introduction

The Deuteron consists of two nucleons, a proton and a neutron. These two particles are held together by the nuclear force alone. As such we can describe the deuteron as a two particle system. Where in reality it is truly a six particle system as each nucleons consists of three quarks however this will largely be ignored. While the time independent Schrödinger equation (TISE) is a fantastic model in most instance for this analysis we must change the equation to fit the two particle, we will call this the two particle TISE. We begin by describing the motion of the two particles where the location of the centre of mass and their motion w.r.t the centre of mass. [1]
First we begin with the TISE (eq.1), we then transform this to its radial equation (eq.2)

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+U(x)\psi(x,t)=i\hbar\frac{\partial\psi(x,t)}{\partial t} \tag{1}$$

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(\frac{r^2dR}{dr}\right)+(U(r)+\frac{\hbar^2I(I+1)}{2mr^2})R(r)=ER(r) \tag{2}$$

E is a constant and I is an integer that represents the angular momentum. The final term $\frac{\hbar^2I(I+1)}{2mr^2}$ comes from the rotation of the particles around the center of mass.
Knowing that I = 0 (in this case) and substituting $\frac{u(r)}{r}$ for R(r) simplifies to:

$$\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left(\frac{E-V_0}{2mr^2}\right)u=0$$

We now apply our boundary conditions which are provided in the diagram of our finite square well (see fig.1)

$$\begin{cases} U(r)=-V_0 & \text{for } r\leq \text{a} \quad (3)\\ U(r)=0 & \text{for } r>a \quad (4)\end{cases}$$

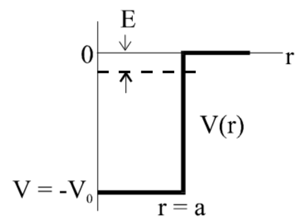

Figure 1: Finite square well of the deuteron [2]

After applying the boundary conditions in conjunction with the solutions we can use for inside and outside of the well (eq.3 & eq.4) we produce the transcendental equation when we equate U(r) for both solutions at r = a

$$U(r) = Asin(kr) + Bcos(kr) \tag{5}$$

$$U(r) = Ce^{kr} + De^{-\kappa r} \tag{6}$$

Then, applying the boundary conditions, $B = 0$ and $C = 0$ and $r = a$ will lead to the equality:

$$Asin(ka) = De^{\kappa a}$$

which can then be equated to our transcendental equation for even (p) and odd (n) solutions

$$akcot(ak) = \pm a\kappa \tag{7}$$

where $k = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$ and $\kappa = \sqrt{\frac{2mE}{\hbar^2}}$

3 Method

3.1 Graphical Methods

Transcendental equations are ones that contain a transcendental function of the variable being solves for. As such the solutions to there equations do not always have a closed form solution and must be approached differently. In this case will we be used a graphical approach to finding the roots of this equation. See below in figure 2.

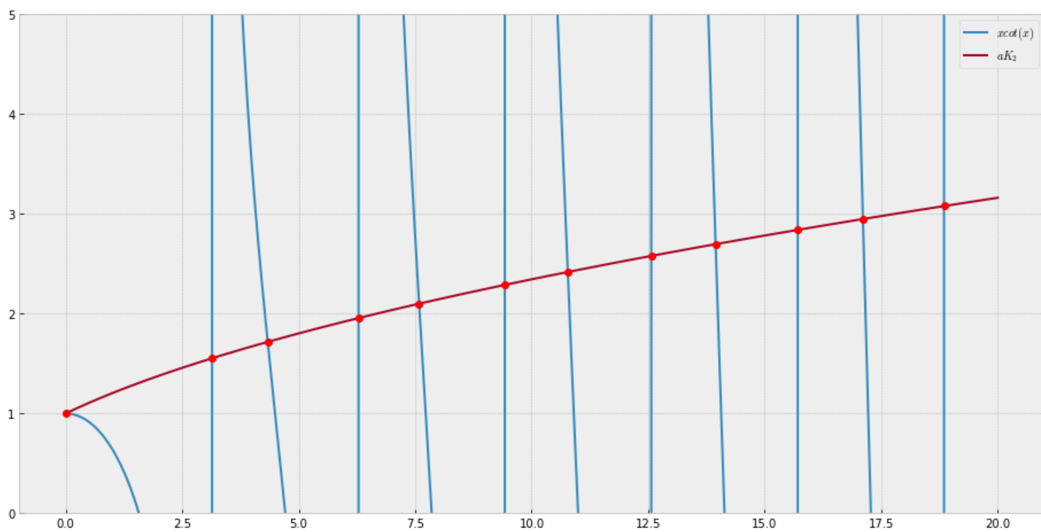

Figure 2: Graphical solution of the transcendental function (eq.7)

As you can see in the graph we have discovered a infinite range over which roots for the transcendental equation can be found, this presents a concerning projection that an infinite amount of roots exist for the transcendental equation. As such it would not be appropriate to use this method in creating estimates for N roots. However, ignoring the first root as this solution is trivial, we find that at the second root (ground state, coordinates (3.14,1.55)) we find an energy value that agrees with experimental data and theoretical predictions data that E∼2.22MeV. This is the binding energy of the deuteron.

Alternatively this can transcendental could be graphically solved by simplifying the equation into

$$tan(x) = \sqrt{\frac{x_0}{x} - 1} \tag{8}$$

Where $x_0 = \frac{a}{\hbar}\sqrt{2mV_0}$ and is used a parameter of V_0 and $x = \frac{a}{\hbar}\sqrt{2m(E - V_0)}$

This equivalence leads to a more comforting graphical solution to the transcendental equation as seen in Fig.3, however our issue with this method is that it requires the use of a varying V_0 alongside E to estimate roots. As such the results from the ground state will be taken from the first edition of NR however the latter is recommended for more general approaches to NR where experimental values need not be considered and the same constraints in this scenario are not imposed. [3]

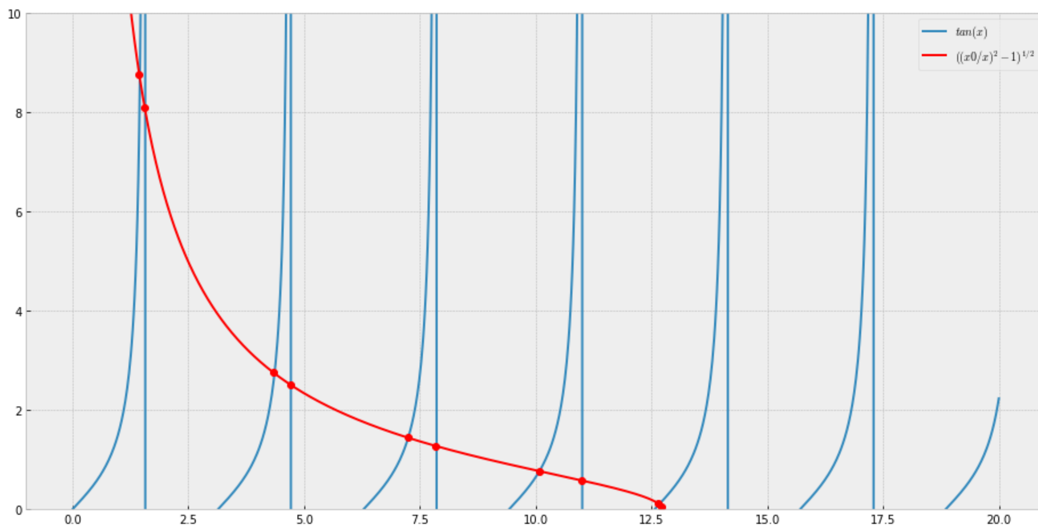

Figure 3: Graphical solution of the transcendental function (eq.8)

3.2 The Newton-Raphson Method

The Newton-Raphson method is a way of finding roots using the derivative of the function itself. The principle of this method follows the equation below:

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} \tag{9}$$

which leads to repeating the function for N iterations:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{10}$$

Using this method, with the known energy of E = +/-2.22MeV for the first root we can now calculate for the depth of the well where the variable is now V_0, our last unknown. To begin NR we must now calculate the derivative of our equation.
Starting from our equation, where we choose the first (odd) root:

$$xcot(x) = -a\kappa \Rightarrow xcos(x) + a\kappa sin(x) = f(x) \tag{11}$$

where x = ak and kappa is the same as eq.7
The derivative follows as:

$$sin(x) + xcos(x) + a\kappa cos(x) = f'(x) \tag{12}$$

Following from this we now substitute our equations into the NR method. Looking at our output from our NR routine we can see we converge upon a solution where $V_0 \sim 35MeV$. Additionally any alternate version of the transcendental equation could be used in the NR method as long as the conversion from X to V_0 is changed appropriately. As can be see in the Alternate NR section of the code if a poor intial estimate of x is used it will result in the failure of the NR method to converge to a solution. This is due the fact that the NR method relies on a strong initial estimate, x_0. If the value is too far away from the root value the difference will be too great for the method to overcome and will result in a sequentially decreasing solution.
Additionally, given the geometrically component of the equation in use, $tan(x)$. As the roots approach the asymptote the accuracy of the intial estimate will need to be more accurate. In an effort to offset this we have factorised cot(x) into $\frac{cos(x)}{sin(x)}$ and separated the values however a strong accuracy is still recommended. [4]

4 Results

4.1 Bound States of the Deuteron

While it would be nice to continue with the analysis of the deuteron through more numerical methods a concern that I mentioned earlier is still present. That is the lack of a comphrehensive consideration of the energy system involving the deuteron. The lack of consideration is visible in fig.2 and fig.3 where such an amount of bound states is clearly infeasible. As such we will be taking a step back and examining the deuteron again.
However, unlike our earlier constraints we can now use our known value for the well depth, V_0 in order to accurately deduce the existence of bound states for the deuteron. Starting again with our transcendental equation:

$$akcot(ak) = \pm a\kappa \tag{13}$$

where $k = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$ and $\kappa = \sqrt{\frac{2mE}{\hbar^2}}$.
As we know that there exists a minimum well depth and range in which we can have a bound state we must satisfy our continuity condition at r=a. This means that we require $\frac{\lambda}{4} \leq R_0$ or $\frac{\pi}{2} \leq kR_0$. Which leads to $\frac{\pi}{2k} \leq R_0$. If we know R_0, which in this case is a we can then use $\frac{\pi}{2a} \leq k$ [5]
Additionally, in order for the bound state to exist the potential energy must be greater than the kinetic energy in order to prevent separation. This results in the following condition [6]:

$$V_0 > \frac{\hbar^2\pi^2}{8ma^2} = \frac{\pi^2}{8}\frac{\hbar^2c^2}{mc^2a^2} = \frac{\pi^2}{8}\frac{(191MeVfm)^2}{469MeV(2.1fm)^2} = 23.1MeV \tag{14}$$

Thus, we find that a bound state is possible for the deuteron, where the binding energy $E_0 = E_{kin} - V_0$ is small. We know from earlier, the numerical solution to our transcendental equation involves $E_0 = -2.22MeV$. Note the interesting point that in deducing these values we started from a model of the potential that included a range of values in order to deduce the binding energy. This is the inverse to the experimental process. From scattering experiments is has been possible to determine the binding energy and from that, based on the theoretical model a value for the well depth can be found.

4.1.1 Excited states

To begin with the consideration, $l = 0$. We see that the binding energy for the ground state is small and as such exists (proof can also be seen by the existence of the atom). Looking at our next odd solution, $k = \frac{3\pi}{2a} = 3k_0$. This means that the kinetic energy is5 9 times greater than the ground state kinetic energy, $E^1_{kin} = 9E^0_{kin} = 9(32.78MeV) = 295.02MeV$.
Where $E^0_{kin} = 35 - 2.22MeV = 32.78MeV$ from our NR solution to the depth of the well. The result here shows us that the total energy has become positive, this indicates that the state of the deuteron is no longer bound. Moving to then consider $l > 0$, the potential is increased by $\frac{\hbar^2 l(l+1)}{2ma} \geq 18.75MeV$. [1]
This means that the potential thus becomes shallower and in this case the states will no longer be bound. This leads us to the conclusion that there is only one bound state of the deuteron.

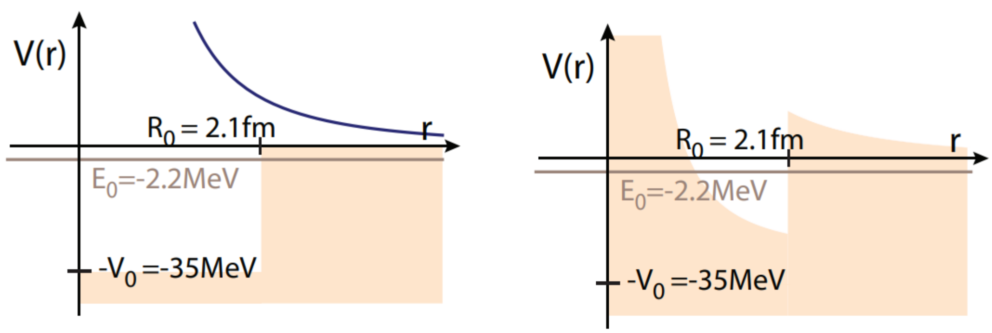

Figure 4: Nuclear potential for $l \neq 0$. Left, nuclear potential and the centrifugal potential. Right, the effective potential. [6]

As such following from these results we can conclude for a binding energy of 2.22MeV in a finite well depth of $35\tilde{M}eV$ we can say only one bound state exists. However examaning the relationship between the kinetic energies and the finite well depth we can see that for any well depths which are greater than $9E^l_k$ we can maintain a negative energy and as such is allowed.

[1] This factor comes from the radial part of the schrodinger equation $V_{eff}(r) = V_{nuc}(r) + \frac{\hbar^2 l(l+1)}{2mr^2}$

4.2 The Deuteron Wave function and Expectation Values

Now that we have determined the binding energy and the value for the well depth, $E_0 = -2.22MeV \& V_0 = 35MeV$ respectively, we can begin to construct the wave function of the deuteron in the ground state.
To begin we start with our normalised wave function for r, representing the distance between the proton and neutron of the deuteron:

$$\int_0^\infty |u^2| \, dr = 1 \tag{15}$$

Where u is the sum of the incident and outgoing wave function : $u = u_{in} + u_{out}$ This means we can expand our normalised wave function to:

$$\int_0^a |u_{in}^2| \, dr + \int_a^\infty |u_{out}^2| \, dr = 1 \tag{16}$$

Where the bounds are $0 < r < a, a < r < \infty$ for the ranges within and outside the radius of the deuteron.
Therefore we want to find a solution within these two ranges, for which we actually calculated earlier with our transcendental equation where:

$$\begin{cases} U_{in} = Asin(kr) \Rightarrow U'_{in} = Akcos(kr) & (17) \\ U_{out} = De^{-r\kappa} \Rightarrow U'_{out} = (-\kappa)De^{-r\kappa} & (18) \end{cases}$$

This leads to the equivalence of the derivatives of these two points at a of:

$$Acos(ak) = -\frac{\kappa}{k}De^{-a\kappa} \tag{19}$$

$$Asin(ak) = De^{a\kappa} \tag{20}$$

Where upon squaring and adding them:

$$A^2 = D^2(1 + \frac{\kappa^2}{k^2})e^{-2a\kappa}$$

$$A^2 = D^2 \left(\frac{K_0^2}{k^2} \right) e^{-2a\kappa} \Longrightarrow K_0^2 = k^2 + \kappa^2$$

$$D = \left(\frac{k}{K_0} \right) Ae^{a\kappa}$$

This provides us with the the ability to know describe our original wave function (eq.16) as:

$$\int_0^a |u_{in}^2|\,dr + \int_a^\infty |u_{out}^2|\,dr = A^2 \int_0^a sin^2(kr)dr + D^2 \int_a^\infty e^{-2r\kappa}dr = A^2 \left[\frac{a}{2} + \frac{k^2}{K_0^2}\left(\frac{1}{2\kappa}\right)\right] \tag{21}$$

Where $k^2 \sim K_0^2$ as $\kappa << k$ and n = 0, $k_a \sim \frac{\pi}{2}$

$$\Rightarrow \frac{A^2}{2\kappa}\left[1 + a\kappa\right] = 1 \rightarrow A = \sqrt{\frac{2\kappa}{1+a\kappa}}$$

Where A and C represent the amplitude of U_{in} and U_{out} respectively

$$D = \sqrt{\frac{2\kappa}{1+a\kappa}} e^{a\kappa}$$

Now that we know the amplitudes of the two wave functions we can begin to calculate the probability of a bound state of the deuteron.
Here we first consider the ground state where we will find a bound state within the dimension of our potential well (35MeV) and anywhere beyond the well a bound state will not exist. [7]

$$P = \int_0^a |u_{in}^2|\,dr = A^2 \int_0^a sin^2(kr)dr$$

$$\Rightarrow \frac{a\kappa}{1+a\kappa} = 0.316 \sim 32\%$$

This represents the probability of finding the nucleon within the internuclear force is small, being only 32%. So n-p stays outside the range of n-p force $\sim$ 68% of the time. This is another way to show that the deuteron is a loosely bound structure.
From that, we the outgoing wave solution is solved we find $U_{out} = Ce^{-a\kappa}$ falls to 1/e of its value at r = 0, so when there is no longer an np bound system, i.e when r ¿ a and the maximum value until the system is bound is the deuteron radius (R_d). This can be written to $R_d\kappa = 1 \rightarrow R_d = \frac{1}{\kappa} = 4.3fm$. This is the maximum value of the deuteron radius and as such is the expectation value of the radius (separation between proton neutron) of the deuteron.

5 Conclusion

In conclusion we have examined the deuteron through a number physical basis and effectively deduced core values about the atom which are in strong agreement with experimental measurements and other theoretical predictions. Where E_0, our binding energy or the energy of the atom in the ground state was found to be 2.22MeV, and in a well depth of 35MeV. These values have all been calculated and found in common methods that are widely and popularly used in scientific data analysis such as the newton-raphson method, as also illustrated earlier a prerequisite of such a technique requires a strong grasp of the initial estimates required and as such this method of deduction is only recommended in areas where there is a solid grasp of the topic and suitable deductions of existing data.

6 References

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