Simple Potential Wells in $\mathbb{R}^3$ as a Model for the Deuteron

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Abstract. We construct the wave function $\psi(x)$ for a simple model of the deuteron. We see that, in this model, the nucleons have a greater probability of lying outside the potential well than in it, as noted in nuclear physics texts. However, our calculations yield for the ratio of these probabilities a figure closer to 1 than what these texts say. We speculate on an explanation for this discrepancy. We then consider a modified potential, incorporating hard core repulsion.

1. First model – a simple well

Given $a, V_0 \in (0,\infty)$, $x \in \mathbb{R}^3$, set

$$V(x) = -V_0, \quad |x| < a, \qquad 0, \quad |x| > a. \tag{1.1}$$

We consider whether $-\Delta + V$ has negative eigenvalues, and if so, how its ground state behaves. Our motivation is to clarify some calculations presented on pp. 44–47 of [BM] (and on pp. 115–116 of [F] and pp. 448–449 of [S]).

If $-\Delta + V$ has negative eigenvalues, denote by $-E$ the one with largest absolute value. We must have $E \in (0, V_0)$, and the ground state will be given by a function $\psi \in C^1(\mathbb{R}^3)$, rapidly decreasing at infinity, positive and radially symmetric, satisfying

$$\Delta\psi = [V(x) + E]\psi \quad \text{on} \ \ \mathbb{R}^3. \tag{1.2}$$

In particular, with $r = |x|$,

$$\psi(x) = \frac{u(r)}{r}, \tag{1.3}$$

where $u \in C^1((0,\infty))$ satisfies

$$u''(r) = [V(r) + E]u(r). \tag{1.4}$$

The properties of E and ψ detailed above demand that, for some $A, B \in (0,\infty)$,

$$u(r) = A \sin kr, \quad r \le a, \qquad Be^{-\gamma r}, \quad r \ge a, \tag{1.5}$$

with

$$k = \sqrt{V_0 - E}, \quad \gamma = \sqrt{E}. \tag{1.6}$$

The fact that $u \in C^1((0,\infty))$ yields the relations

$$A \sin ka = Be^{-\gamma a}, \quad kA \cos ka = -B\gamma e^{-\gamma a}, \tag{1.7}$$

hence

$$B = Ae^{\gamma a} \sin ka, \quad k \cot ka = -\gamma. \tag{1.8}$$

Also

$$\begin{aligned} \psi > 0 &\Longrightarrow 0 < ka < \pi \\ &\Longrightarrow (V_0 - E)a^2 < \pi^2. \end{aligned} \tag{1.9}$$

Note that A is a positive multiple of B; hence the second part of (1.7) yields

$$\cos ka < 0, \quad \text{so} \ \ ka > \frac{\pi}{2}. \tag{1.10}$$

Comparison with (1.9) gives

$$\frac{\pi}{2} < ka < \pi, \quad \text{hence} \ \ \frac{\pi^2}{4} < (V_0 - E)a^2 < \pi^2. \tag{1.11}$$

In particular:

Proposition 1.1. *If $-\Delta + V$ has a negative eigenvalue, then*

$$V_0 a^2 > \frac{\pi^2}{4}. \tag{1.12}$$

Given that there is a negative eigenvalue $-E$ with largest absolute value, we next strive for a formula: $E = E(V_0, a)$. To get this, it is convenient to set

$$\begin{aligned} E = \delta^2 V_0, &\quad 0 < \delta < 1, \\ ka = \frac{\pi}{2} + \varepsilon, &\quad 0 < \varepsilon < \frac{\pi}{2}, \end{aligned} \tag{1.13}$$

and get formulas relating these quantities. Note that

$$\cot ka = \cot\Big(\frac{\pi}{2} + \varepsilon\Big) = -\tan \varepsilon, \tag{1.14}$$

and bringing in (1.8) we have

$$\tan\varepsilon = \frac{\gamma}{k} = \sqrt{\frac{E}{V_0 - E}} = \sqrt{\frac{\delta^2}{1-\delta^2}}, \quad \delta \in (0,1). \tag{1.15}$$

Equivalently,

$$\delta = \sin\varepsilon, \quad 0 < \varepsilon < \frac{\pi}{2}. \tag{1.16}$$

To continue, we have

$$\begin{aligned} &(V_0 - E)a^2 = (ka)^2 && \text{by (1.6)} \\ &\Rightarrow (1-\delta^2)V_0 a^2 = \Big(\frac{\pi}{2} + \varepsilon\Big)^2 && \text{by (1.13)} \\ &\Rightarrow V_0 a^2 = \frac{(\pi/2+\varepsilon)^2}{1-\delta^2} = \frac{1}{\cos^2\varepsilon}\Big(\frac{\pi}{2}+\varepsilon\Big)^2 && \text{by (1.16).} \end{aligned} \tag{1.17}$$

This gives the sought-after relation:

Proposition 1.2. *Given $V_0 a^2 > \pi^2/4$, we have*

$$\begin{aligned} V_0 a^2 &= \frac{1}{\cos^2\varepsilon}\Big(\frac{\pi}{2}+\varepsilon\Big)^2, \quad 0 < \varepsilon < \frac{\pi}{2} \\ \Longrightarrow E &= V_0 \sin^2\varepsilon, \end{aligned} \tag{1.18}$$

where $-E$ is the negative eigenvalue of $-\Delta + V$ of largest absolute value.

Remark. Given $\varepsilon << 1$, we have

$$V_0 a^2 \approx \frac{\pi^2}{4} + \pi\varepsilon, \quad E \approx V_0\varepsilon^2. \tag{1.19}$$

Having this calculation, we desire to compute the integral of $|\psi(x)|^2$ over the respective regions $\{|x| < a\}$ and $\{|x| > a\}$. We have

$$\begin{aligned} \int\limits_{|x|<a} |\psi(x)|^2\,dx &= 4\pi \int_0^a u(r)^2\,dr \\ &= 4\pi A^2 \int_0^a \sin^2 kr\,dr \\ &= \frac{4\pi A^2}{k} \int_0^{\pi/2+\varepsilon} \sin^2 s\,ds \\ &= \frac{4\pi A^2}{\sqrt{V_0 - E}}\Big(\frac{\pi}{4} + \int_0^\varepsilon \cos^2 t\,dt\Big) \\ &= \frac{1}{\cos\varepsilon}\Big(\frac{\pi}{4} + \int_0^\varepsilon \cos^2 t\,dt\Big)\frac{4\pi A^2}{\sqrt{V_0}}, \end{aligned} \tag{1.20}$$

and

$$
\begin{aligned}
\int\limits_{|x|>a} |\psi(x)|^2\,dx &= 4\pi \int_a^\infty u(r)^2\,dr \\
&= 4\pi B^2 \int_a^\infty e^{-2\gamma r}\,dr \\
&= \frac{4\pi B^2}{2\gamma} e^{-2\gamma a} \\
&= \frac{4\pi A^2}{2\gamma} \sin^2 ka \\
&= \frac{4\pi A^2}{2\sqrt{E}} \sin^2\Bigl(\frac{\pi}{2}+\varepsilon\Bigr) \\
&= \frac{\cos^2\varepsilon}{2\sin\varepsilon}\,\frac{4\pi A^2}{\sqrt{V_0}}.
\end{aligned}
\tag{1.21}
$$

The quantity A (which we need not compute) is the normalizing constant, making the two integrals above sum to 1. We see that, as $\varepsilon \searrow 0$,

$$
\begin{aligned}
\int\limits_{|x|<a} |\psi(x)|^2\,dx &\approx \frac{\pi^2 A^2}{\sqrt{V_0}}, \\
\int\limits_{|x|>a} |\psi(x)|^2\,dx &\approx \frac{2\pi A^2}{\varepsilon\sqrt{V_0}},
\end{aligned}
\tag{1.22}
$$

so the integral over $\{|x|>a\}$ is much larger than the integral over $\{|x|<a\}$, for ε small enough.

As for how small ε is, we note that (1.18) plus the identity $E=\gamma^2$ yield

$$
\Bigl(\frac{\pi}{2}+\varepsilon\Bigr)\tan\varepsilon = \gamma a. \tag{1.23}
$$

Information on a and on E (hence on γ) would allow one to solve for ε, and then for $V_0 = E/\sin^2\varepsilon$.

We next see how this plays out for the deuteron, for which (1.2) arises as a crude model for the ground state. Actually, (1.2) is the nondimensionalized form. The physical form is

$$
\Delta\psi = \frac{2m}{\hbar^2}[\widetilde{V}(x)+\widetilde{E}]\psi, \tag{1.24}
$$

where, with $m = m_p m_n/(m_p+m_n) \approx m_p/2$ and $c \approx 3\times 10^8$ m/sec,

$$
\begin{aligned}
2m &\approx \text{mass of a proton} \approx 938\ \text{MeV}/c^2, \\
\hbar &= \text{Planck's constant} \approx 6.6\times 10^{-22}\ \text{MeV-sec},
\end{aligned}
\tag{1.25}
$$

and $\widetilde{V}(x)$ and $\widetilde{E}$ are measured in MeV. This leads to (1.2) with

$$V(x) = \frac{2m}{\hbar^2}\widetilde{V}(x), \quad E = \frac{2m}{\hbar^2}\widetilde{E}, \tag{1.25A}$$

where $\widetilde{V}(x) = -\widetilde{V}_0$ on $|x| < a$, and $V_0 = (2m/\hbar^2)\widetilde{V}_0$. Experiments shooting gamma rays at deuterium show that

$$\widetilde{E} \approx 2.225 \text{ MeV}. \tag{1.26}$$

This corresponds via $\gamma = \sqrt{E} = \sqrt{2m\widetilde{E}}/\hbar$ to

$$\gamma^{-1} \approx 4.32 \text{ fm}, \tag{1.27}$$

where 1 fm$=10^{-15}$ m. The meson model of nuclear forces suggests

$$a \approx 2.8 \text{ fm}. \tag{1.28}$$

Cf. [S], p. 449. This gives

$$\gamma a \approx 0.648, \tag{1.29}$$

and solving (1.23) then gives

$$\varepsilon \approx 0.329. \tag{1.30}$$

Hence

$$\delta \approx 0.323, \tag{1.31}$$

so

$$\widetilde{V}_0 = \delta^{-2}\widetilde{E} \approx 21.34 \text{ MeV}. \tag{1.32}$$

Referring to (1.20)–(1.21), we see that in this case

$$\int\limits_{|x|<a} |\psi(x)|^2\, dx \approx (1.165)\frac{4\pi A^2}{\sqrt{V_0}} \tag{1.33}$$

and

$$\int\limits_{|x|>a} |\psi(x)|^2\, dx \approx (1.387)\frac{4\pi A^2}{\sqrt{V_0}}. \tag{1.34}$$

The figure (1.30) for ε is not terribly consistent with the hypothesis that $\varepsilon << 1$, though the figure (1.32) for $\widetilde{V}_0$ is consistent with $\widetilde{V}_0 >> \widetilde{E}$. The figures for γ and $\widetilde{V}_0$ given in (1.27) and (1.32) agree with those given in [S] (p. 449). We note however that the integral (1.34) is only a little larger than (1.33). This disagrees with the statement in [S] that it is "about twice as large."

In more detail, the ratio of (1.34) to (1.33) is

$$R \approx \frac{1.387}{1.165} \approx 1.191, \tag{1.35}$$

which is not close to 2. On the other hand, if we take ε as in (1.30) and plug it into the "small ε approximation" (1.22), we get the "approximation"

$$R \approx \frac{2}{\pi\varepsilon} \approx 1.935, \tag{1.36}$$

in close agreement with the assertion in [S].

Coincidence? Who can say?

2. Second model – well with hard core repulsion

We now consider a model in which the two nucleons experience a hard core repulsion when their centers are at a distance b, for some $b \in (0, a)$. Then (1.1) is replaced by

$$
\begin{aligned}
V(x) &= -V_0, \quad b < |x| < a, \\
&\quad\; 0, \qquad\quad\; |x| > a,
\end{aligned}
\tag{2.1}
$$

and we solve (1.2) on $\mathbb{R}^3 \setminus B_b(0)$, with boundary condition $\psi(x) = 0$ for $|x| = b$. Taking u as in (1.3), we solve (1.4) on $r \in (b, \infty)$, with $u(b) = 0$. Thus, in place of (1.5), we have

$$
\begin{aligned}
u(r) &= A\, \mathrm{sin} k(r-b), \quad b \le r \le a, \\
&\quad\; Be^{-\gamma r}, \qquad\qquad r \ge a.
\end{aligned}
\tag{2.2}
$$

We again have (1.6), i.e.,

$$
k = \sqrt{V_0 - E}, \quad \gamma = \sqrt{E}. \tag{2.3}
$$

Since $u \in C^1([b, \infty))$, we have the following analogue of (1.7),

$$
A \sin k(a-b) = Be^{-\gamma a}, \quad kA \cos k(a-b) = -B\gamma e^{-\gamma a}, \tag{2.4}
$$

yielding the following analogue of (1.8):

$$
B = Ae^{\gamma a} \sin k(a-b), \quad k \cot k(a-b) = -\gamma. \tag{2.5}
$$

Also, parallel to (1.9),

$$
\begin{aligned}
\psi > 0 &\Longrightarrow 0 < k(a-b) < \pi \\
&\Longrightarrow (V_0 - E)(a-b)^2 < \pi^2.
\end{aligned}
\tag{2.6}
$$

As in §1, A must be a positive multiple of B, so the second part of (2.5) yields

$$
\cos k(a-b) < 0, \quad \text{so} \;\; k(a-b) > \frac{\pi}{2}. \tag{2.7}
$$

Comparison with (2.6) gives

$$
\frac{\pi}{2} < k(a-b) < \pi, \quad \text{hence} \;\; \frac{\pi^2}{4} < (V_0 - E)(a-b)^2 < \pi^2. \tag{2.8}
$$

Thus, parallel to Proposition 1.1, we have that, if $-\Delta+V$ has a negative eigenvalue, then

$$V_0(a-b)^2 > \frac{\pi^2}{4}. \tag{2.9}$$

Given that there exists a negative eigenvalue $-E$, with largest absolute value, we seek a formula, $E = E(V_0, a, b)$. Parallel to (1.13), we set

$$\begin{aligned} E &= \delta^2 V_0, \quad 0 < \delta < 1, \\ k(a-b) &= \frac{\pi}{2} + \varepsilon, \quad 0 < \varepsilon < \frac{\pi}{2}, \end{aligned} \tag{2.10}$$

and seek formulas relating these quantities. Parallel to (1.14), we have

$$\cot k(a-b) = \cot\Bigl(\frac{\pi}{2} + \varepsilon\Bigr) = -\tan\varepsilon, \tag{2.11}$$

and then (2.5) yields

$$\tan\varepsilon = \frac{\gamma}{k} = \sqrt{\frac{E}{V_0 - E}} = \sqrt{\frac{\delta^2}{1-\delta^2}}, \quad 0 < \delta < 1, \tag{2.12}$$

or equivalently

$$\delta = \sin\varepsilon, \quad 0 < \varepsilon < \frac{\pi}{2}, \tag{2.13}$$

as in (1.16). We then get the following variant of (1.17):

$$\begin{aligned} &(V_0 - E)(a-b)^2 = k^2(a-b)^2 && \text{by (2.3)} \\ &\Rightarrow (1-\delta^2)V_0(a-b)^2 = \Bigl(\frac{\pi}{2} + \varepsilon\Bigr)^2 && \text{by (2.10)} \\ &\Rightarrow V_0(a-b)^2 = \frac{(\pi/2+\varepsilon)^2}{1-\delta^2} = \frac{1}{\cos^2\varepsilon}\Bigl(\frac{\pi}{2} + \varepsilon\Bigr)^2 && \text{by (2.13)} \end{aligned} \tag{2.14}$$

This gives the following analogue of Proposition 1.2.

Proposition 2.1. *Given $V_0(a-b)^2 > \pi^2/4$, we have*

$$\begin{aligned} &V_0(a-b)^2 = \frac{1}{\cos^2\varepsilon}\Bigl(\frac{\pi}{2} + \varepsilon\Bigr)^2, \quad 0 < \varepsilon < \frac{\pi}{2} \\ &\Longrightarrow E = V_0 \sin^2\varepsilon, \end{aligned} \tag{2.15}$$

where $-E$ is the negative eigenvalue of $-\Delta + V$ with largest absolute value.

We then have the following analogue of (1.20)–(1.21):

$$
\begin{aligned}
\int_{b<|x|<a} |\psi(x)|^2\,dx &= 4\pi \int_b^a u(r)^2\,dr \\
&= 4\pi A^2 \int_b^a \sin^2 k(r-b)\,dr \\
&= \frac{4\pi A^2}{k} \int_0^{\pi/2+\varepsilon} \sin^2 s\,ds \\
&= \frac{1}{\cos\varepsilon}\Big(\frac{\pi}{4} + \int_0^{\varepsilon} \cos^2 t\,dt\Big)\frac{4\pi A^2}{\sqrt{V_0}},
\end{aligned} \tag{2.16}
$$

and

$$
\begin{aligned}
\int_{|x|>a} |\psi(x)|^2\,dx &= 4\pi \int_a^\infty u(r)^2\,dr \\
&= 4\pi B^2 \int_a^\infty e^{-2\gamma r}\,dr \\
&= \frac{4\pi B^2}{2\gamma} e^{-2\gamma a} \\
&= \frac{4\pi A^2}{2\gamma} \sin^2 k(a-b) \\
&= \frac{\cos^2\varepsilon}{2\sin\varepsilon}\,\frac{4\pi A^2}{\sqrt{V_0}}.
\end{aligned} \tag{2.17}
$$

Hence the ratio

$$
R = \Big(\int_{|x|>a} |\psi(x)|^2\,dx\Big)\Big(\int_{b<|x|<a} |\psi(x)|^2\,dx\Big)^{-1} \tag{2.18}
$$

satisfies

$$
\frac{1}{R} = \frac{\pi}{2}\,\frac{\sin\varepsilon}{\cos^3\varepsilon}\Big(1 + \frac{4}{\pi}\int_0^{\varepsilon} \cos^2 t\,dt\Big). \tag{2.19}
$$

As for finding ε, note that (2.15) plus the identity $E = \gamma^2$ yield

$$
\Big(\frac{\pi}{2} + \varepsilon\Big)\tan\varepsilon = \gamma(a-b). \tag{2.20}
$$

Now, parallel to (1.24)–(1.32), we have

$$
V_0 = \frac{2m}{\hbar^2}\widetilde{V}_0, \quad E = \frac{2m}{\hbar^2}\widetilde{E}, \tag{2.21}
$$

with m and $\hbar$ as in (1.25), and

$$\widetilde{E} \approx 2.225 \text{ Mev}, \tag{2.22}$$

as in (1.26), hence

$$\gamma^{-1} \approx 4.32 \text{ fm}, \tag{2.23}$$

as in (1.27). We also continue to take $a \approx 2.8$ fm, as in (1.18). As for b, we take a cue from Fig. 3.2 on p. 23 of [CG], and set

$$b \approx 0.8 \text{ fm}, \quad \text{hence} \ \ a - b \approx 2.0 \text{ fm}, \tag{2.24}$$

which leads to the following variant of (1.29):

$$\gamma(a - b) \approx 0.463. \tag{2.25}$$

Now solving (2.20), via Newton's method, yields

$$\varepsilon \approx 0.249, \tag{2.26}$$

in contrast with (1.30), hence

$$\delta \approx 0.247, \tag{2.27}$$

so

$$\widetilde{V}_0 = \delta^{-2} \widetilde{E} \approx 36.47 \text{ MeV}, \tag{2.28}$$

in contrast with (1.32). Also, we get from (2.16) and (2.26) that

$$R \approx 1.786, \tag{2.29}$$

which is somewhat closer to 2 than (1.35).

References

[BM] H. Bethe and P. Morrison, Elementary Nuclear Theory, J. Wiley, New York, 1956 (Dover, 2006).

[CG] W. Cottingham and D. Greenwood, An Introduction to Nuclear Physics, Cambridge Univ. Press, Cambridge, 1986.

[F] E. Fermi, Nuclear Physics, Univ. of Chicago Press, 1949.

[S] E. Segre, Nuclei and Particles, Benjamin, New York, 1977.