Introduction to Radiochemistry

Lecture 7

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The Deuteron

Introduction

- The Deuteron is the "Hydrogen Atom" of nuclear physics.

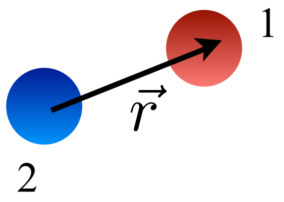
- As the study of the spectroscopic series permitted advancements in atomic physics, the study of the Deuteron permitted the understanding of many nuclear force properties.

- It is the simplest nucleon-nucleon bound state (pn).

- pp and nn are NOT bound.

- Deuterium does not have bound excited states.

Basic Properties



Its binding energy can be measured by mass spectroscopy, as we have explained in Lecture 2. But you can also measure its binding energy by bringing a p and a n together to form a d, then measure the energy of the emitted photon

$$n + p \rightarrow d + \gamma, \quad E_\gamma = E_{\text{binding}} - E_{\text{recoil}}$$

The binding energy can be measured also by the opposite reaction, by doing photodissociation

$$\gamma + d \rightarrow n + p$$

The smallest photon energy required to break the deuteron is 2.22 MeV and this corresponds to the BE.

For most nuclei, the typical case is that BE/A ~ 8 MeV.

The deuteron is a very weakly bound nucleus since for it we have BE/A=1.1 MeV.
The deuteron also has a magnetic moment, and a nonzero quadruple moment:

$$\mu = 0.8574\ \mu_N$$

$$Q = 0.28570\ \text{fm}^2$$

This means the deuteron is not a pure S-wave state

Solution of the Bound State

Now we want to theoretically solve the deuteron as a two-body problem of particles interacting with a potential in a non relativistic formalism.

In this course, we will completely neglect spin degrees of freedom, which are however important for a full treatment of nuclei.

The hamiltonian (in this case equivalent to the total energy) reads:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V\left(\vec{r_1} - \vec{r_2}\right)$$

Transforming from particle coordinates to relative and centre of mass coordinates one can simplify the problem to a one-body problem

(we now take the masses $m_1 = m_2 = m$)

$$\begin{cases} \vec{r} = \vec{r_1} - \vec{r_2} \\ \vec{R}_{CM} = \frac{\vec{r}_1 + \vec{r}_2}{2} \end{cases} \quad \text{and} \quad \begin{cases} \vec{p} = (\vec{p_1} - \vec{p_2})/2 \\ \vec{P}_{CM} = \vec{p_1} + \vec{p_2} \end{cases}$$

One obtains: $$H = \frac{P_{CM}^2}{2M} + \frac{p^2}{2\mu} + V\left(\vec{r}\right) = T_{CM} + H_{rel}$$

where $M = 2m, \ \mu = \frac{m}{2}$

Hamiltonian depending only on the relative coordinates

Solution of the Bound State

Since we are interested only in the intrinsic dynamics and we neglect the motion of the deuteron as a whole with kinetic energy T_{CM}

The Schrödinger equation we want to solve is then:

$$\left[\frac{p^2}{2\mu} + V\left(\vec{r}\right)\right]\psi\left(\vec{r}\right) = E\,\psi\left(\vec{r}\right)$$

Which is clearly a one-body problem in a three-dimensional space.

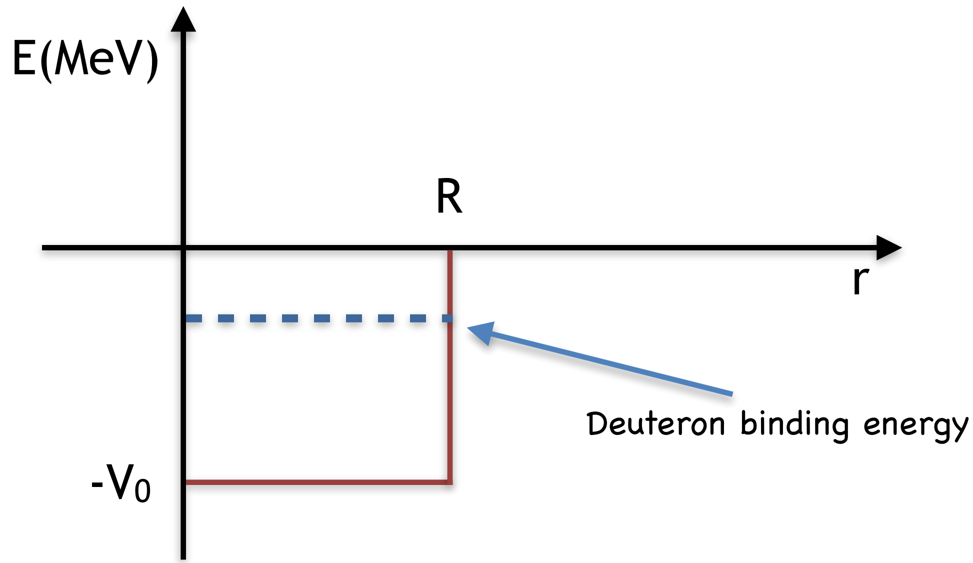
Since the problem has spherical symmetry, it is convenient to go to spherical coordinates and write the momentum squared operator p^2 in these coordinates:

$$\boxed{\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{L^2}{r^2}\right) + V\left(\vec{r}\right)\right]\psi\left(r,\theta\varphi\right) = E\,\psi\left(r,\theta\varphi\right)}$$

This is the Schrödinger equation we have to solve.

Solution of the Bound State

At this point, we need to choose the potential operator V. We know already that the nuclear force is very complex, therefore we start with a simplified square well potential.



$$V(r) = \begin{cases} -V_0 & \text{for } r \leq R \\ 0 & \text{for } r > R \end{cases}$$

In this way the potential depends only on $r = |\vec{r}\,|$ so it is purely central, orbital angular momentum is a good q.n. and we will have a zero quadrupole moment.

Solution of the Bound State

Write the wave function on a radial x spherical harmonics basis:

$$\Psi(r,\theta,\varphi) = \sum_{\ell} c_\ell \; R_\ell(r) \; Y_{\ell,m}(\theta,\varphi)$$

The ground states has l=0 : $\Psi(r,\theta,\varphi) \propto R_{\ell=0}(r) = R(r)$

Now if you introduce the modified wave function $R(r) = u(r)/r$

then the laplacian in the Schrödinger equation becomes simpler:

$$\boxed{-\frac{\hbar^2}{2\mu}\frac{d^2u(r)}{dr^2} + V(r)u(r) = Eu(r)}$$

Remember that E is negative for bound states.

For r < R $\quad V = -V_0 \quad$ and therefore: $-\frac{\hbar^2}{2\mu}\frac{du^2}{dr^2} - V_0 u = Eu \quad \Rightarrow$

$$\Rightarrow \quad \frac{du^2}{dr^2} = -\frac{2\mu(E+V_0)}{\hbar^2}u = -k_1^2 u \quad \text{with} \quad k_1 = \sqrt{(2\mu(E+V_0)/\hbar^2)}$$

The solution is: $u(r) = A\sin(k_1 r) + B\cos(k_1 r)$ Since we want r(0)=0, then B=0

Solution of the Bound State

For r > R $\quad V = 0 \quad \Rightarrow \quad \frac{du^2}{dr^2} = -\frac{2\mu E}{\hbar^2} u = k_2^2 u$ with $k_2 = \sqrt{-\frac{2\mu E}{\hbar^2}}$

This is the free Schroedinger equation with general solution:

$$u(r) = Ce^{-k_2 r} + De^{+k_2 r}$$

To keep this finite at infinite distance we have to require that D=0

Now applying the continuity condition for u and its derivative in r=R we get

$$A \sin(k_1 R) = \quad Ce^{-k_2 R}$$

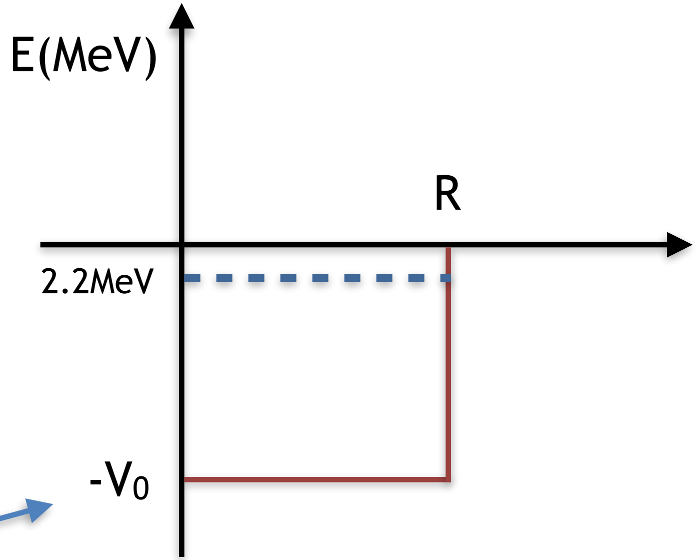
$$k_1 A \cos(k_1 R) = -k_2 Ce^{-k_2 R}$$

$$\Rightarrow \quad \boxed{k_1 \cot(k_1 R) = -k_2}$$

this gives a relation between V_0 , E and R

Solution of the Bound State

$$\boxed{k_1 \cot(k_1 R) = -k_2}$$



From electron scattering we know R~2.1 fm.

Experimentally we also know that E=-2.2 MeV

So we solve for V_0 :

It turns out that **V_0 = 35 MeV**

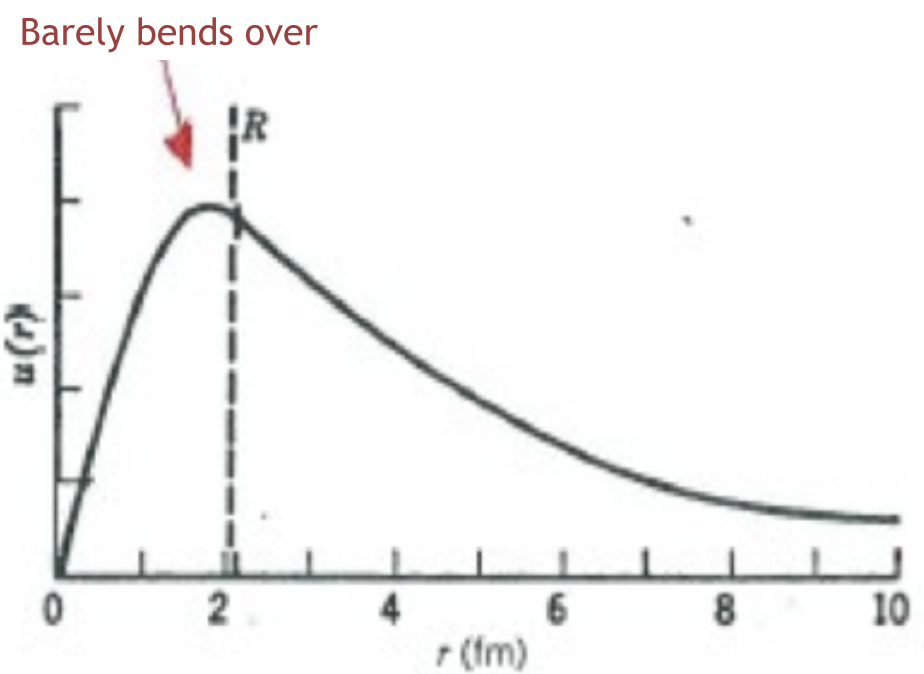
If the NN force were slightly less attractive there would be no bound state, so no deuteron.

The NN force is attractive enough, because the formation of the deuteron is the first step in the proton-proton fusion cycle in our Sun and the first step in the formation of stable matter in the Universe.

Deuteron Wavefunction

The weak binding of the deuteron translates into the wave function just barely able to turn over to match the exponential free solution outside the well.

(If the potential were more attractive, the w.f. would turn over earlier).



The deuteron ground state is so close to the top of the well that its wave function leaks way out (extended nucleus).

A more realistic description

Let's consider a more realistic potential like:

$$V(r) = V_C(r) + V_T(r)S_{12}$$

with central and tensorial parts. It turns out that the Schroedinger equation can be reduced to two second order coupled differential equations:

$$\frac{d^2}{dr^2}u(r) = -\frac{2\mu}{\hbar^2}\left(E - V_C\right)u(r) + -\frac{2\mu}{\hbar^2}V_T\sqrt{8}\omega(r)$$

$$\frac{d^2}{dr^2}\omega(r) = -\frac{2\mu}{\hbar^2}\left(E - V_C - 2V_T - \frac{6\hbar^2}{2\mu r^2}\right)\omega(r) + \frac{2\mu}{\hbar^2}V_T\sqrt{8}u(r)$$

The two functions u(r) and w(r) are connected to s- and d-states probabilities:

S-state probability

$$|a|^2 = \int_0^\infty |u(r)|^2 dr$$

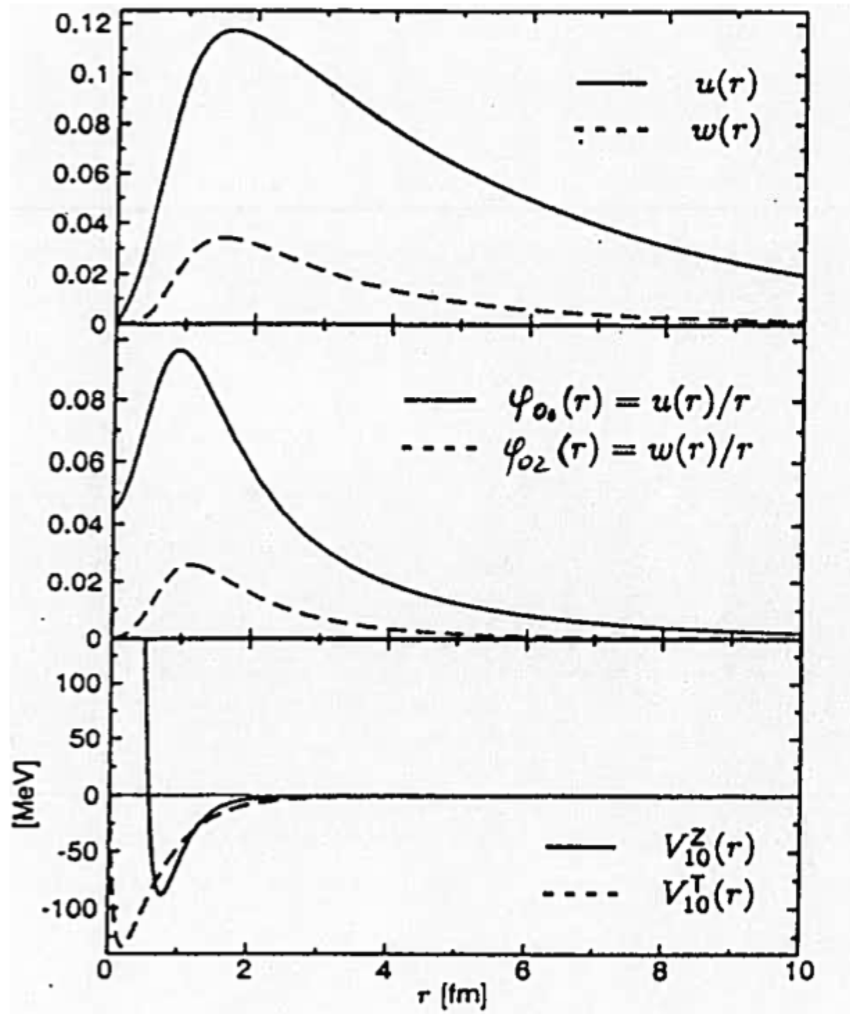
D-state probability

$$|b|^2 = \int_0^\infty |\omega(r)|^2 dr$$

A more realistic description

The previous equations are of the Rarita-Schwinger type and can be solved only numerically. The commonly used algorithm is due to B.V.Numerov (1891-1941).

From the numerical solution with the CD-Bonn-potential (includes spin-orbit) one obtains:



Summary

- How to reduce a 2-body to a 1-body problem.

- An analytical solution of the deuteron:

  spherical square-well potential : one-body problem in 1-dimension

- Realistic description of the deuteron:

  - one-body problem in 3-dimensions
  - angular part done analytically
  - radial part is found numerically as the solution of a set of two coupled second order differential equations.