Ground State of Deuteron

Deuteron is the only two nucleon bound system made up of a proton and a neutron. The two other possible two nucleon systems, the diproton and the dineutron do not exist as bound systems. The experimentally measured properties of deuteron are : (i) charge : +e

(ii) Mass : 2.014735 amu = 3.34245×10^{-27} kg

(iii) Spin : 1 (in units of $\hbar$)

(iv) statistics : Bose - Einstein

(v) Radius : RMS value of deuteron radius is 2.1 Fermi

(vi) Binding energy = 2.225 ± 0.003 MeV

(vii) Magnetic dipole moment : The magnetic dipole moment of deuteron is μ_d = 0.85736 ± 0.0003 nm

where Nuclear magneton (nm) = $\frac{e\hbar}{2m_pc}$.

By applying quantum mechanics to describe deuteron, we assume the ground state of deuteron to be an S-state for which the angular momentum L = 0. With L = 0, the wave function ψ is spherically symmetrical and also for the S-state the angular momentum quantum number l = 0. There is no contribution momentum quantum number l = 0. There is no contribution from orbital motion and so the angular momentum of the nucleus is attributed entirely to spin. The nucleons are half spin particles and deuteron is known to have a spin equal to unity. This implies that the proton and neutron spins are parallel. Experimental measurements for nucleon magnetic moments give the following values:

Magnetic moment of proton μ_p = 2.79281 ± 0.0004 nm.

Magnetic moment of neutron μ_N = −1.913148 ± 0.000066 nm

$\mu_p + \mu_N$ = 0.879662 ± 0.00005 nm.

Thus deuteron is expected to have a magnetic moment of 0.8797 ± 0.00015 nm. From experimental measurements magnetic moment is 0.85733 ± 0.0003 nm. There is a difference of 0.0223 ± 0.0002 nm between the expected and the measured values. But simplest interpretation that deuteron possesses some orbital motion and the previous assumption of l = 0 in the ground state is not correct. The ~~magtic m~~ magnetic moment measurements of deuteron establish the following conclusions:

(a) In the ground state of deuteron, the proton and neutron spins are parallel and the deuteron is in a triplet state ($^3S_1$).

Neutron is a half spin particle.

(c) In the ground state of deuteron, the orbital angular momentum quantum number is zero ($l=0$) and spin quantum number $S=1$.

(d) The electric quadrupole moment of a deuteron as measured by Rabi and other scientists in a radio-frequency molecular beam method is $Q_d = 2.82 \times 10^{-31} m^2$

$= 0.0028$ barn

where 1 barn $= 10^{-24} cm^2 = 10^{-28} m^2$

The total angular momentum is equal to the vector sum of the orbital and spin angular momentum i.e

$$J = L + S \quad \text{—— (1)}$$

In a system like deuteron which consists of one proton and one neutron, each having spin $\frac{1}{2}$, the quantum number S can have the values

$$S = \frac{1}{2} \pm \frac{1}{2} = 1 \text{ or } 0 \,; \quad \text{—— (2)}$$

The different combinations of orbital angular momentum (l) and spin angular momentum (S) can be obtained as —

(a) $l=0,\ S=1 \longrightarrow {}^3S_1$ state

(b) $l=1,\ S=0 \longrightarrow {}^1P_1$ state

(c) $l=1,\ S=1 \longrightarrow {}^3P_1$ state

(d) $l=2,\ S=1 \longrightarrow {}^3D_1$ state.

Deuteron wave function is a mixture of some of these states. We combine only parity states [${}^3S_1$ and ${}^3D_1$] or odd parity [${}^1P_1$ and ${}^3P_1$] which means that with $l=0$, only $l=2$ can be present. The wave function may be written as —

$$\psi = a_0 \psi_{1s} + a_2 \psi_{1d} \,; \quad \text{—— (3)}$$

This means that the system spends a fraction $|a_0|^2$ of its time in $l=0$ state and another fraction $|a_2|^2$ of its time in $l=2$. Therefore the ground state may be taken to be a mixture of ${}^3S_1$ and ${}^3D_1$ states. From the measurement, found that $|a_0|^2 = 0.96$ and $|a_2|^2 = .04$.

Wave equation for the Deuteron and its solution

In this section, the aim is to obtain a theoretical description of deuteron so that the experimentally observed and the theoretically predicted properties could agree.

The Schrodinger wave equation for the deuteron is

$$\nabla^2 \psi(r, \theta, \phi) + \frac{2\mu}{\hbar^2}\left[E - V(r)\right]\psi(r, \theta, \phi) = 0 \quad \text{—— (4)}$$

where $\mu = \frac{m_n m_p}{m_n + m_p} \simeq \frac{M}{2}$ is the reduced mass of the n-p system.

In the study of the nuclear interactions, the most useful co-ordinates are a set of spherical polar co-ordinates (r, θ, ϕ) which are connected to the Cartesian co-ordinates as follows:

$$\left.\begin{aligned} z &= r\cos\theta \\ y &= r\sin\theta\sin\phi \\ x &= r\sin\theta\cos\phi \end{aligned}\right\} \quad \text{—— (5)}$$

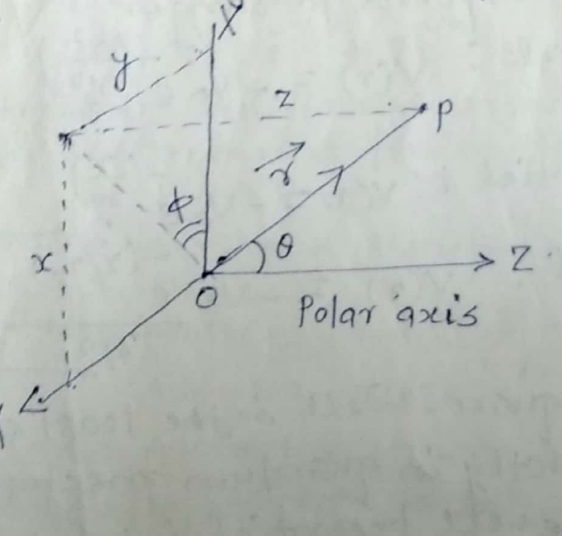
In rectangular co-ordinates, the Laplacian operator is

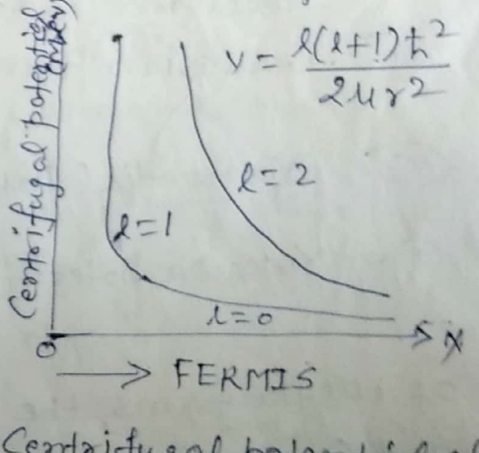
$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial}{\partial z^2}$$

Expressing ∇^2 in terms of spherical polar co-ordinates by means of equation (5), the Schrodinger equation (4) assumes the form:

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2}{\partial\phi^2}\right]\psi + \frac{2\mu}{\hbar^2}\left[E - V(r)\right]\psi = 0 \quad \text{—— (6)}$$

If the lowest stable state i.e the ground state of deuteron is taken to be purely a $^3S_1$ state, the force is central i.e depends only upon the separation r of the nucleons and not upon the relative velocity ~~and not upon th~~ or nucleon spin orientation.





Centrifugal potential of the neutron-proton-system.

The Schrodinger equation when the potential is spherically symmetric may be separated into angular and radial parts. The radial part of the wavefunction may be written as

$$\frac{d^2\psi(r)}{dr^2} + \frac{2}{r}\cdot\frac{d\psi(r)}{dr} + \frac{2\mu}{\hbar^2}\left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2}\right]\psi(r) = 0 \quad \text{—— (7)}$$

The last term $\frac{l(l+1)\hbar^2}{2\mu r^2}$ is called the centrifugal potential.
The lowest quantum mechanical state for a two nucleon system like deuteron is always an $l=0$ or an S-state.
The Schrodinger equation for S-state of deuteron ($l=0$) may therefore be written as

$$\frac{d^2\psi(r)}{dr^2} + \frac{2}{r}\frac{d\psi(r)}{dr} + \frac{2\mu}{\hbar^2}[E - V(r)]\psi(r) = 0; \quad (8)$$

The solution of equation (8) is obtained by introducing a new wave function $u(r)$ related to $\psi(r)$ as

$$\psi(r) = \frac{u(r)}{r} \quad (9)$$

Putting (9) in (8) we get

$$\frac{d^2u(r)}{dr^2} + \frac{M}{\hbar^2}[E - V(r)]u(r) = 0; \quad (10)$$

where M = neutron or proton mass and is nearly equal to 2μ.

For the solution of the above equation, various potentials can be used by assuming that nuclear forces are short range.

(a) Square-well potential: $V(r) = -V_0$ for $r \leq r_0$
$= 0$ for $r > r_0$
where V_0 is the depth of the potential well and r_0 corresponds to range. — (11a)

(b) Gaussian Potential: $V(r) = -V_0 e^{-\left(\frac{r^2}{r_0^2}\right)}$; — (11b)

(c) Exponential potential: $V(r) = -V_0 e^{-\left(\frac{r}{r_0}\right)}$ — (11c)

(d) Yukawa potential: $V(r) = -V_0 \frac{e^{-(r/r_0)}}{r/r_0}$ — (11d)

Of all the forms, the square-well is the least complicated and can be solved exactly in quantum mechanics.
For simplicity, square well potential is used for the solution of deuteron problem.
In equation (10) applied to deuteron

$$E = -E_B = -2.226 \text{ MeV}$$

where E_B is positive.
Using square well potential, equation (10) may be written as

$$\frac{d^2u(r)}{dr^2} + \frac{M}{\hbar^2}(V_0 - E_B)u(r) = 0 \quad \text{for } r \le r_0 \quad \text{———— (12a)}$$

and $$\frac{d^2u(r)}{dr^2} - \frac{M}{\hbar^2}E_B u(r) = 0 \quad \text{for } r > r_0 \quad \text{———— (12b)}$$

Writing $K = \sqrt{\frac{M}{\hbar^2}(V_0 - E_B)}$ and $\gamma = \sqrt{\left(\frac{ME_B}{\hbar^2}\right)}$ ———— (13)

Equation (12a) and (12b) may be written as —

$$\frac{d^2u(r)}{dr^2} + K^2u(r) = 0 \quad \text{for } r \le r_0 \quad \text{———— (14a)}$$

and $$\frac{d^2u(r)}{dr^2} - \gamma^2u(r) = 0 \quad \text{for } r > r_0 \quad \text{———— (14b)}$$

The general solution of equation (14a) is

$$u(r) = A\sin Kr + B\cos Kr \quad \text{———— (15a)}$$

$\psi(r)$ must be continuous and bounded and have a continuous derivative everywhere. i.e $\psi(r)$ should be finite at $r = 0$ and $\psi(r) = 0$ at $r \to \infty$. Therefore,

$u(r) = r\psi(r) \to 0$ as $r \to \infty$, ~~otherwise~~ otherwise $\psi(0)$ becomes infinite. This condition on (15a) demands that $B = 0$

Hence $u(r) = A\sin Kr \quad r < r_0$ ———— (15b)

The general solution of equation (14b) is

$$u(r) = Ce^{-\gamma r} + De^{\gamma r} \quad \text{———— (16a)}$$

and the boundary condition at infinity demands that $D = 0$ so that $u(r)$ remains finite. Hence

$$u(r) = Ce^{-\gamma r}, \quad r > r_0 \quad \text{———— (16b)}$$

At $r = r_0$, $\psi(r)$ and therefore $u(r)$ and its first derivative must be continuous.

From equation (15b) and (16b) we obtain

$$A\sin Kr_0 = Ce^{-\gamma r_0} \quad \text{———— (17a)}$$

and $$AK\cos Kr_0 = -C\gamma e^{-\gamma r_0} \quad \text{———— (17b)}$$

Dividing (17b) by (17a), we get

$$K\cot Kr_0 = -\gamma \quad \text{———— (18)}$$

The binding energy of deuteron $E_B = -2.226$ MeV and thus is small which suggests that $E_B << V_0$.

From (18) ~~and~~ with the help of (13) we get

$$\cot Kr_0 = \frac{-\gamma}{K} = -\frac{\sqrt{ME_B/\hbar^2}}{\sqrt{M(V_0 - E_B)/\hbar^2}}$$

$$= -\sqrt{\frac{E_B}{V_0 - E_B}} = -\sqrt{\frac{E_B}{V_0}}, \quad E_B << V_0 \quad \text{——— (19)}$$

Equation (19) suggests that cot Kr_0 is small and negative and therefore Kr_0 is only slightly greater than $\pi/2$.

$$Kr_0 = \frac{\pi}{2}, \frac{3\pi}{2}, \ldots \quad \text{(20a)}$$

$E_B << V_0$, Equation (13) gives

$$K = \sqrt{\frac{MV_0}{\hbar^2}} \quad \text{——— (20b)}$$

Comparing (20a) and (20b) we get

$$K = \sqrt{\frac{MV_0}{\hbar^2}} = \frac{\pi}{2r_0}, \frac{3\pi}{2r_0}, \ldots$$

or $V_0 r_0^2 = \frac{\pi^2\hbar^2}{4M}, \frac{9\pi^2\hbar^2}{4M}, \ldots$ ——— (21a)

In the ground state, $Kr_0 = \frac{\pi}{2}$,

$$\therefore V_0 r_0^2 = \frac{\pi^2\hbar^2}{4M} \quad \text{——— (21b)}$$

$$V_0 = \frac{\pi^2\hbar^2}{4Mr_0^2} = 36\,\text{MeV} \quad \text{(After calculation)}$$

* where $1\,\text{MeV} = 1.6\times10^{-13}$ J

and $r_d = \frac{1}{\gamma} = \frac{\hbar}{\sqrt{ME_B}} = 4.31\times10^{-15}\,\text{m} = 4.31$ Fermi [after calculation]

where $M = 1.67\times10^{-27}$ kg.

$E_B = 2.226$ MeV

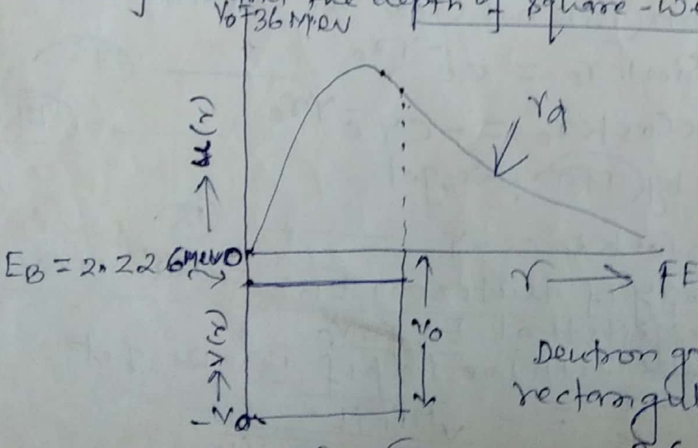
** $\hbar = 1.0545\times10^{-34}$ J. sec.

$r_0 = 2.4\times10^{-15}$ m

It infers that the nuclear force acting between a neutron and a proton depends upon whether the spins of proton and neutron are parallel or antiparallel i.e total spin S of the n-p system is 1 or 0. It is remarkable that it is spin-dependent.

The state with neutron-proton spins parallel (↑↑) is called a triplet state $^3S_1$ and that with anti-parallel spins (↑↓) is called a singlet state $^1S_0$.

The fig shown below gives a plot of the ground state wave function, the range of nuclear force and the depth of square-well potential.



Deutron ground state in the rectangular well of depth 36 MeV.

Fig (C)

* This value justifies the assumption that $E_B << V_0$. Fig c gives a plot of the ground state wavefunction, the range of nuclear force and the depth of square well potential. This potential has a depth of 36 MeV and a width of 2.4 Fermi. As compared with the depth of the potential well i.e 36 MeV, the deuteron binding energy $E_B = 2.226$ MeV, is small which means that deuteron is just barely bound.

A notable feature of the wavefunction curve is that the amplitude is appreciably large at distances beyond the range r_0 of the nuclear force. As a matter of fact the exponential decrease of $u(r)$ beyond $r = r_0$ permits us to regard $\frac{1}{\gamma}$ as a measure of radius r_d of deuteron.

** Thus the radius of deuteron is found to be much larger than the range r_0 of the nuclear force.