SOME ASPECTS OF THE QUANTUM MECHANICS OF THE DEUTERON

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Wen-Chin Yu

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SOME ASPECTS OF THE QUANTUM MECHANICS OF THE DEUTERON

I. INTRODUCTION— IMPORTANCE OF THE DEUTERON PROBLEM IN NUCLEAR PHYSICS

The deuteron plays in nuclear physics a role similar to that of the hydrogen atom in atomic physics. It consists of two elementary particles, one proton and one neutron. In investigating the quantitative theory of nuclear forces, its crucial test is the deuteron, the simplest stable combination of heavy particles (neutrons and protons) composing the nuclei. The deuteron tests the theory without aggravating the computational situation. In spite of the comparative simplicity of the dynamical system, many phenomena of nuclear physics are known to occur in conjunction with the deuteron, such as, photodisintegration, capture of neutrons by protons, scattering of slow and fast neutrons and protons, etc. The purpose of this paper, is to consider in detail a few of the experimental and theoretical investigations of the deuteron, namely, those associated with the binding energy, spin and magnetic dipole moment, and the electric quadrupole moment.

Before proceeding further, let us briefly recall the discovery of the deuteron. The discovery of the isotope

H^2 of hydrogen was the result of very exact and careful measurement. At first it was believed that there was only one isotope of oxygen — namely O^{16}. Later, in 1929 [1], oxygen was found to be a mixture of isotope O^{16} with slight traces of O^{17} and O^{18}. Therefore it was concluded that hydrogen must also carry a trace of an isotope heavier than H^1. In 1931 Birge and Menzel [2] of the University of California estimated the relative abundance of isotope H^2 to H^1 as one part in 4500.

In 1932 Urey [3] of Columbia University, subjected a residue obtained by distilling liquid hydrogen to spectral analysis. The Balmer lines of H^1 were obtained as usual, but each line was accompanied by a faint line on its short wave-length side. The Rydberg constant for an atom with a nucleus of mass M is related to that for an atom with a nucleus of infinite mass by

$$R_m = R_\infty \frac{M}{M + m}, \tag{1.1}$$

where m is the mass of the electron. Hence

$$\frac{R_2}{R_1} = \frac{M_2(M_2 + m)}{M_1(M_1 + m)} . \tag{1.2}$$

The subscript 1 and 2 refer to H^1 and H^2 respectively. If λ_1 is the wave-length of a certain line in the spectrum of H^1 and λ_2 that of the corresponding line in the spectrum of H^2, it is seen that $\lambda_1/\lambda_2 = R_1/R_2$. Replacing the left side of Eq. (1.2) by λ_1/λ_2 and solving for M_2 we obtain

$$M_2 = \frac{M_1\ m\lambda_1}{m\lambda_1 - (M+m)(\lambda_1 - \lambda_2)}. \qquad (1.3)$$

By measuring the difference $\lambda_1 - \lambda_2$ between a Balmer line and its faint companion, Urey found the latter was due to radiation from atoms of mass 2.

Because the isotope H^2 is of great interest and importance it was given the special name of deuterium and designated by the chemical symbol D. The nucleus of deuterium is called deuteron.

The deuteron has about twice the mass of the proton, i.e., $M = 2.01472$ and carries the same electrical charge e. Its spin is 1 in units of $\hbar$ and obeys Bose statistics. Its magnetic moment is $+0.8565 \pm 0.0004$ nuclear magnetons. These values refer to the ground state of the deuteron. In the quantum mechanical description of the deuteron, it is reasonable to assume the ground state to be an S-state, i.e., a state of zero orbital angular momentum, $L = 0$. Since a free neutron and a free proton each has a spin $\frac{1}{2}$, the spin value of 1 seems to indicate that the proton and neutron have parallel spins in the deuteron.

The deuteron also possesses a small electric quadrupole moment. This interesting and surprising discovery was made by Rabi [4] and his co-workers. According to their results, the deuteron is cigar-shaped, i.e., elongated in the direction on the spin. The existence of the quadrupole moment seemed surprising, because it had been assumed that the ground state of the deuteron would be a pure S-state, for which the quadrupole moment would vanish.

To resolve this difficulty, Rarita and Schwinger [5] introduced tensor, i.e., angle-dependent, forces. The effect of this type of force causes the deuteron to spend part of its time in the S-state $(L=0)$ and part in the D-state $(L=2)$. The quadrupole moment arises from the fact that the deuteron contains a small mixture of the D-state. One of the consequences of this theory is that the magnetic moment of the deuteron will not be the sum of the magnetic moments of the free neutron and free proton. This is supported by recent measurements by Arnold and Roberts [6]. They showed that the deuteron moment is smaller than the sum of the magnetic moments of the free particles by $+0.0228 \pm 0.0016$ nuclear magnetons. Because the Rarita-Schwinger theory has been remarkably sucsessful in accounting for experimental results, a detailed discussion of their theory will be given in a later section.

In order to discuss this theory, we shall consider the deuteron binding energy from which the general characteristics of proton-neutron force can be deduced and then consider the concepts of magnetic and quadrupole moments, as they arise in classical electrodynamics.

II. BINDING ENERGY

In this section, we shall review the methods used in determining the deuteron binding energy, and point out its relation to nuclear forces.

A. EXPERIMENTAL DETERMINATION

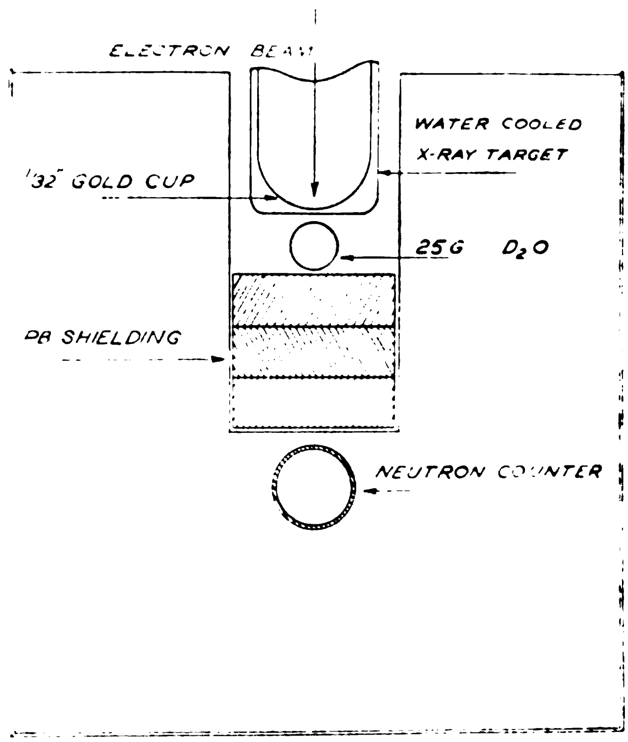
The binding energy of the deuteron was first measured by Chadwick and Golhaber in 1934 [7]. They observed the photodisintegration of deuteron produced by 2.62 Mev. γ-ray from thorium C' by means of an ionization chamber.

$$H^2 + h\nu \longrightarrow {}_1H^1 + {}_0n^1 \; . \qquad (2.1)$$

This reaction takes place when $h\nu$ which is the energy of the incident γ-ray, is greater than the binding energy of the deuteron. The difference between $h\nu$ and the binding energy appears as kinetic energy of the neutron and the proton. Because the momentum of the γ-ray is small, the momenta of the proton and neutron are almost equal but opposite. Further, since their masses are almost equal, they share the excess energy very nearly equally. The energy E of the proton can be determined by measuring its range. The binding energy is then $h\nu = 2E$.

In 1937 Chadwick, Feather and Bretscher [8] used the 2.623 Mev. γ-ray from thorium C" to disintegrate deuteron in a cloud chamber and measured the range of disintegration protons. Using Blackett and Lee's [9] range-energy curve, they gave 0.185 Mev. as the proton energy and 2.62 - 2 x 0.185 = 2.25 ± 0.05 Mev. for the binding energy. Using Parkinson, Herb, Bellamy, and Hudson's [10] more recent values of proton ranges, they estimated the proton energy as 0.2 Mev. and the binding energy as 2.22 Mev. Bethe [11] made corrections to these data and obtained a proton energy of 0.225 Mev. and the binding energy for the deuteron of 2.17 ± 0.04 Mev. One of the direct measurements of the deuteron binding energy is that done by Stetter and Jentschke [12], who measured the ionization produced by the disintegration protons in an ionization chamber and obtained the value 2.189 ± 0.022 Mev. In 1940, K. Kimura [13] obtained the deuteron binding energy 2.189 - 0.007 Mev. by estimating the energy of disintegration neutrons from RaC-D.

A more accurate determination was made by Wiedenbeck and Marhöfer [14] in 1945; (a similar method was also used by Myers and L. C. van Atta [15]). Let us describe the experiment in detail, shown in Fig. 1. They made use of the resonance absorption of neutron by rhodium or silver. It is well known from theory [16] and from experiments on the excitation of nuclei by X-rays [17], that the intensity of any isochromat in the thick target of continuous X-ray spectrum, increases linearly when the potential applied in



Schematic diagram of the apparatus used for determining the threshold voltages. The scale of the drawing is indicated by the total thickness (3") of the lead shielding.

Fig. 1

accelerating the electrons is greater than the energy of the isochromat. Therefore, in a γ-n process, the number of neutrons of a given energy should be a linear function of the applied voltage V when

$$V \geq V_t + \frac{A}{A - 1} V_n , \tag{2.2}$$

where V_t is the threshold potential, and A the atomic weight of the neutron being considered. Thus the essential features of the experiment, shown in Fig. 1, are the use of the high voltage X-rays to produce disintegration and the detector which is sensitive to only one neutron "line" energy equal to the resonance energy of the detector. The experimental result will not be affected by the faster neutrons. Thus the activity vs. accelerating-potential curve should give a straight line intersecting the abscissa at the binding potential. The detector used was an argon-ether filled counter with a rhodium cathode. Small samples of deuterium were bombarded for two minutes by X-rays produced by a beam current of 100 microamperes striking a thick gold target. The activity was taken as the number of counts above the background obtained during the two minutes after the irradiation was stopped. The activity was plotted as shown in Fig. 2. A straight line is obtained, which, when extrapolated to zero activity, gives for the deuteron binding energy the value 2.185 ± 0.006 Mev.

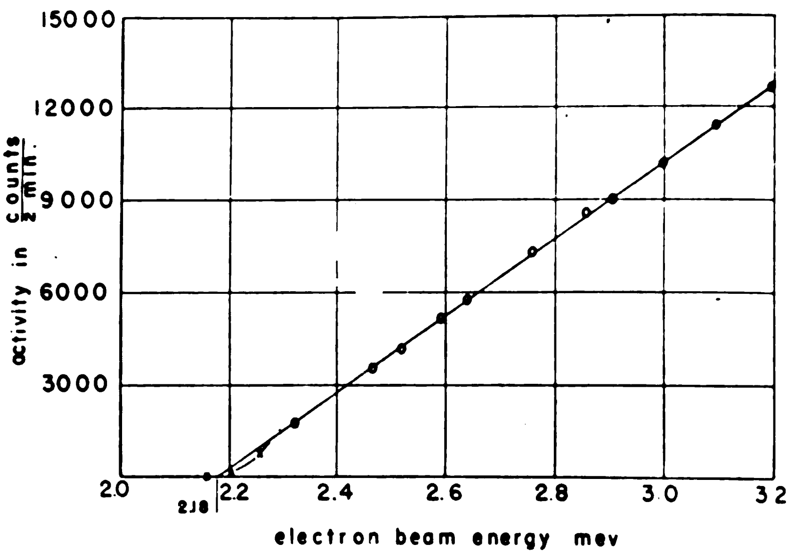


Fig. 2. Neutron counting rate versus accelerating potential.

Still another method is due to Stephens [18] who deduced the binding energy by mass considerations. The masses of deuteron and proton are known accurately from mass spectrographic data, and the mass difference of neutron and proton is known accurately from measurements on the reaction chain [19]

$$C^{13}(p,\ n)N^{13}(\beta^{+})C^{13}.$$

From the equation

$$\left[2M(p) + \left\{M(m) - M(p)\right\} - M(D^{2})\right] = \text{Binding Energy}$$

he obtains the result 2.187 ± 0.011 Mev.

B. THEORY OF NUCLEAR FORCES AND THE BINDING ENERGY

In order to account for the binding energy of the deuteron quantum mechanically, one must know or guess something about the nature of the nuclear forces holding the neutron and proton together. Since nuclear effects cannot be accounted for by known forces, such as electric and gravitational forces, it is necessary to introduce an entirely new type of force. We shall assume it to be a short range central force.

Let us now derive a few results of the type of force we have postulated. The Schroedinger equation transformed to the center of mass of the proton-neutron system is given by

$$\nabla^{2}\psi(r,\theta,\phi) + \frac{M}{\hbar^{2}}\left[E - V(r)\right]\psi(r,\theta,\phi) = 0, \qquad (2.3)$$

where r is the distance between the proton and the neutron, and m the reduced mass given by

$$m = \frac{M_1 M_2}{M_1 + M_2} \sim \tfrac{1}{2}M \;, \tag{2.4}$$

M stands for the mass of either the proton or the neutron. The quantity E occurring in Eq. (2.3) is a negative quantity and its absolute value is the binding energy as determined by experiment. Since E is a known quantity we can determine the unknown quantity V(r). For this purpose, consider the ground state. Since $L = 0$ for the ground state, ψ must be spherically symmetric. If we assume a central force, i.e., the interaction potential of neutron and proton is only a function of the distance r between the particles but independent of angles, then the wave function in Eq. (2.3) is also a function of r only. The Laplacian operator applied to the wave function $\psi = U(r)/r$ gives

$$\nabla^2\psi(r) = \nabla^2 \frac{U(r)}{r} = \frac{1}{r}\,\frac{d^2u}{dr^2}\,.$$

Eq. (2.3) then becomes

$$\frac{1}{r}\,\frac{d^2u}{dr^2} + \frac{M}{\hbar^2}\left[E - V(r)\right]\frac{u}{r} = 0,$$

i.e.,

$$\frac{d^2u}{dr^2} + \frac{M}{\hbar^2}\left[E - V(r)\right] u = 0. \tag{2.5}$$

An assumption about the shape of V(r) is necessary. One possibility is the rectangular potential well. This shape,

(Fig. 3), certainly represents a short range force and leads to a differential eqwation which can easily be solved. Here, there are two parameters, the width and depth of the well. Since the Schroedinger equation with a given E determines only one parameter, we expect to find only the relation between V and r_o, not definite values for them.

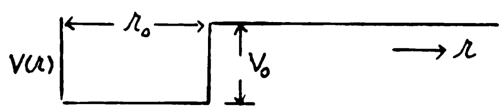


Fig. 3

With $E = -E_o$, where E_o is positive, Eq. (2.5) becomes

$$\frac{d^2u}{dr^2} + \frac{M}{\hbar^2}[V_o - E_o]\,u = 0 \qquad \text{for } r < r_o, \qquad (2.6)a$$

$$\frac{d^2u}{dr^2} - \frac{M}{\hbar^2}E_o u = 0 \qquad \text{for } r > r_o. \qquad (2.6)b$$

ψ must be continuous, finite and have a continuous first derivative everywhere. Therefore $u = r\psi$, which must have the same continuity conditions, must go to zero at $r=0$, and must not diverge faster than r as $r \to \infty$. To satisfy the conditions at zero and infinity the solution of (2.6) must be

$$u = A \sin kr \qquad \text{for } r < r_o, \qquad (2.7)a$$

$$U = Be^{-\alpha r} \qquad \text{for } r > r_o, \qquad (2.7)_b$$

where

$$k = \sqrt{M(V - E_o)}/\hbar\ , \qquad (2.8)_a$$

$$\alpha = \sqrt{ME_o}/\hbar\ . \qquad (2.8)_b$$

Now if U and its derivative are continuous then the derivative of log U must also be continuous. Applying these conditions at $r = r_o$ we obtain the result

$$k \cot kr_o = - \alpha . \tag{2.9}$$

Eq. (2.9) does not involve A and B but only the two unknowns r_o and V_o, E_o being 2.187 Mev. V_o and r_o are not restricted further. As seen from the above, E_o is small compared to V_o and can be neglected in Eq. $(2.8)_a$. Eq. (2.9) can be put in a simple and approximate form

$$\cot kr_o = - \alpha /k \approx \sqrt{E_o/V}. \tag{2.10}$$

Thus cot kr_o is negative and small in absolute value. Therefore, kr_o is only slightly larger than $\pi/2$. (We know the value of kr_o slightly larger than $3\pi/2$ is not admissible since there would be a radial node in the wave function ψ at $kr_o = \pi$, indicating that this is not the lowest energy level. This result contradicts the hypothesis.) Using $kr_o \approx \pi/2$ and again neglecting E_o in the expression for k, Eq. (2.10) gives

$$V_o r_o^2 \approx \pi^2 \hbar^2/4M. \tag{2.11}$$

Actually $(V_o r_o^2)$ is slightly greater than the quantity on the right. Thus

$$V_o r_o^2 < \frac{\pi^2 \hbar^2}{M} \quad \text{or} \quad kr_o < \pi . \tag{2.12}$$

(The expression $V_o {r_o}^2$ frequently occurs in nuclear calculation; it is not necessary to know V_o and r_o separately.)

Let us consider another result which does not depend on the detailed form of the potential (as long as the force has a short range). Such is the case for the wave function U(r). When r is greater than the range of nuclear forces, it is given by

$$U = Ce^{-\alpha r}. \tag{2.13}$$

For r less than the range of nuclear forces, the wave function should decrease as shown in the diagram (Fig. 4). However, the wave function given above is sufficiently accurate over the whole region, as to be useful in many calculation. Since the exponent α r in the above expression is a dimensionless quantity, α has the dimension of 1/cm. Therefore we can take $1/\alpha$ as a measure of the size of the deuteron.

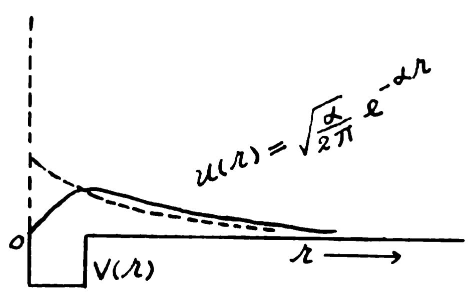


Fig. 4

Since we assume that a central force has short range, the "radius" of the deuteron is considerably larger than the range of nuclear forces. That is

$$r_0 \ll 1/\alpha \,. \tag{2.14}$$

Most of the area under U(r) occurs for $r > r_0$. The use of another shape for the potential function changes U(r) appreciably only for $r < r_0$. Therefore whatever the shape of the potential, $Ce^{-\alpha r}$ is close to the true wave function over most of space.

Let us normalize ψ so as to determine the value of C. Then

$$\int \psi^2 d\tau = 4\pi \int_0^\infty u^2 \, dr = 4\pi C^2 \int_0^\infty e^{-2\alpha r} \, dr$$
$$= 2\pi C^2/\alpha = 1,$$

or

$$C = \sqrt{\alpha/2\pi} \, .$$

Therefore, the normalized wave function is

$$u(r) = \sqrt{\frac{\alpha}{2\pi}} \; e^{-\alpha r}. \qquad (2.15)$$

Similarly if definite values are assigned to r_0 and V_0 then A and B of the true U(r) given by Eq. (2.7) can be found from the continuity and normalization conditions. B is somewhat greater than C of the approximate U(r), thus

$$B = \sqrt{\frac{\alpha}{2\pi}} \; (1 + \tfrac{1}{2}\alpha r_0). \qquad (2.16)$$

In fact Eq. (2.16) is a good approximation.

We shall conclude this section by showing that it is not possible for the deuteron to have bound excited states. Let us consider the possibility of the existence of excited states with $L = 0$. It will be assumed in this proof that the force between the neutron and the proton is the same for states of higher L as for the case $L = 0$. In order to prove our assertion we shall compute the minimum well depth V_0 required to produce a bound state, i.e., one for which the binding energy E_0 is just zero. This required well depth will be found to be considerably larger than the actual well depth, as determined above from the binding energy of the ground state. Since the actual depth is less than the minimum value required for the binding of states of non-vanishing angular momentum, such bound states can not exist. The analytical proof is as follows. For $L = 0$, the Schroedinger wave equation is

$$\frac{d^2u}{dr^2} + \frac{M}{\hbar^2}\left[E - V(r)\right]u - \frac{L(L+1)}{r^2}u = 0. \tag{2.17}$$

Assume

$$V = -V_o, \qquad r = r_o, \qquad E = -E_o.$$

Set $E_o = 0$ for minimum well depth, and let $L = 1$. The solution of Eq. (2.17) is given by

$$U = \frac{\sin kr}{kr} - \cos kr, \qquad r < r_o, \tag{2.18$_a$}$$

$$U = e^{-\alpha r}\left[\frac{1}{\alpha r} + 1\right], \tag{2.18$_b$}$$

where

$$k^2 = M(V_o - E_o)/\hbar^2, \tag{2.19$_a$}$$

$$\alpha^2 = ME_o/\hbar^2. \tag{2.19$_b$}$$

For simplicity set $E_o = 0$, and use for the outside solution

$$U = 1/r, \qquad r \geqslant r_o. \tag{2.20}$$

Using the definition of k with $E_o = 0$,

$$MV_o r_o^2/\hbar^2 = \pi^2. \tag{2.21}$$

The required depth V is almost four times as large as the actual depth in the ground state. Therefore no other bound state exists at $L = 0$.

III. EXPERIMENTAL DETERMINATION OF THE SPIN AND MAGNETIC MOMENT OF THE DEUTERON

A. THE DEUTERON SPIN

It is known that the electron possesses an intrinsic angular momentum, called the "spin", of value $\frac{1}{2}$ and a magnetic moment of 1 Bohr magneton. The simple relation between these quantitites has been pointed out by Dirac, who derived his equation by relativity arguments. For protons and neutrons and nuclei consisting of these particles, however, the relation between the spin and magnetic moment is not a simple one. So far, there is no theory of general applicability which gives this relationship. The lack of such a theory makes the problem of measuring spins and magnetic moments of nuclei very important in nuclear physics. For this purpose a number of methods have been devised: hyperfine structure, molecular beams, band spectra, etc. Since the spin of the deuteron has been determined by the band spectra method, this will be discussed in detail.

The band spectra method is very useful in determining nuclear spins, particularly for light nuclei which tend to form homonuclear molecules. The presence of a nuclear spin causes a change in the statistical weight associated with the given rotational state of a homonuclear diatomic molecule and thus causes a change in the expected intensities found in the band spectrum.

The reason for this is as follows. If the nuclear spin is zero, the statistical weight of any state for which the total angular momentum is J would be $2J+1$. The presence of a nuclear spin further increases the degeneracy of the states. A nucleus of total angular momentum I can have a component M in any prescribed direction, taking any of the values I, I - 1, $\cdots$ I, a total of $2I+1$ states. Let ψ_M represent the wave functions of these states. If a molecule contains two identical nuclei, the wave function of each being represented by $\psi_{M_1}(A)$ and $\psi_{M_2}(B)$, the total number of ways in which these functions can be combined to form the product functions

$$\psi_{M_1}(A)\,\psi_{M_2}(B) \tag{3.1}$$

is $(2I+1)^2$. Since symmetric and antisymmetric states do not combine in diatomic molecules containing identical nuclei, it is necessary to separate the $(2I+1)^2$ functions into symmetric and antisymmetric functions. We note that the product functions given by Eq. (3.1) are symmetric when $M_1 = M_2$. Of the remaining

$$(2I+1)^2 - (2I+1) = 2I(2I+1)$$

functions of the form $\psi_{M_1}(A)\,\psi_{M_2}(B)$ and $\psi_{M_2}(A)\,\psi_{M_1}(B)$, one half will be symmetric and the other half antisymmetric. Thus the total number of symmetric functions is

$$I(2I+1) + 2I+1 = (I+1)(2I+1)$$

and $(2I+1)I$, the number of antisymmetric functions. The ratio of these numbers is

$$\frac{(I+1)(2I+1)}{I(2I+1)} = \frac{I+1}{I} . \tag{3.2}$$

If the nuclei obey Bose statistics, symmetric nuclear spin functions must be combined with rotational states of even L and antisymmetric spins with those of odd L. Because of the statistical weights attached to the spin states, the intensity of even rotational lines will be $(I+1)/I$ as great as that of the neighboring odd rotational lines.

For Fermi statistics of the nuclei, the spin and the rotational states combine in a manner to make the odd rotational lines more intense, in the ratio $(I+1)/I$. Thus by determining which lines are more intense, even or odd, the nuclear statistics is determined and by measuring the ratio of intensities of adjacent lines, the nuclear spin is obtained as shown in Fig. 5.

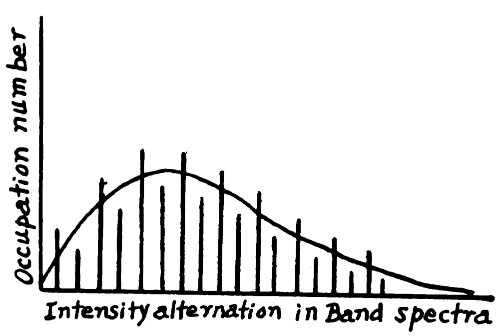


Fig. 5

The deuteron spin was investigated in 1934 by Murphy and Johnston [20], who measured photometrically the relative intensitites of 29 lines in the α bands of the molecular spectrum of deuterium. These lines correspond to the transition $3p\,\pi^3\,\Pi_\mu \rightarrow 2p\,\sigma^3\Sigma_\mu^+$ analyzed by Dicke [21]. The bands lie between 5939 and 6291 A and were photographed in the second order of a 21-foot grating. The experimental results show that the deuteron obeys Bose-Einstein statistics and that its spin is 1.

B. MAGNETIC MOMENT OF THE DEUTERON

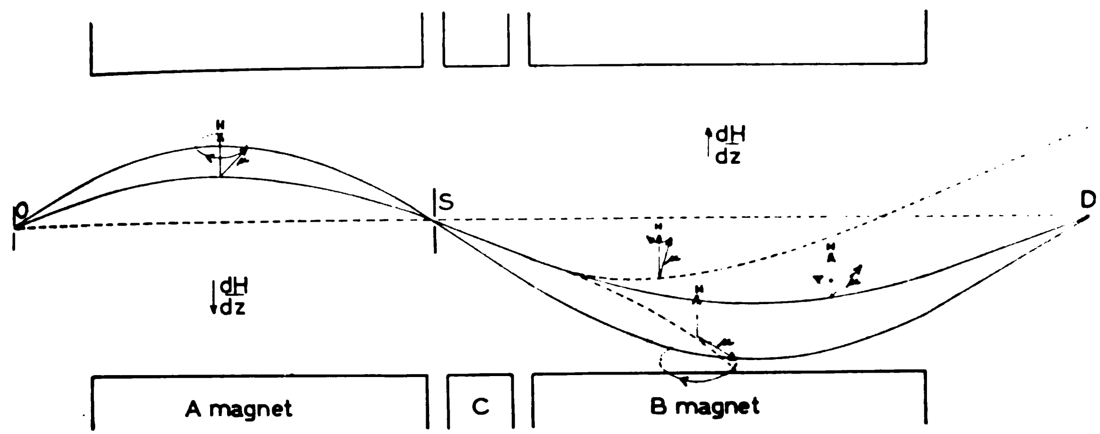
Magnetic moment of the deuteron has been determined by hyperfine structure and atomic beam methods. The latter method was used by Rabi and his co-workers [22], who measured the hyperfine structure separation by passing a beam of atomic hydrogen and deuterium through an inhomogeneous magnetic field. The magnetic moments are then calculated from the hyperfine structure separations.

The disadvantage of the above method is that the result depends on the somewhat uncertain relation between the nuclear magnetic moment and the hyperfine structure. This criticism is avoided in the molecular-beam magnetic resonance method [23] in which the nuclear moment is obtained by observing the precessional frequency of nuclei in a uniform magnetic field. Consider a system with angular momentum J, in units of $\hbar$ and magnetic moment μ, in an external magnetic field H_o. The angular momentum vector will precess about the H_o vector with the Larmor frequency given by

$$\nu = \frac{\mu H_o}{J\hbar} . \qquad (3.3)$$

Of the quantities occurring in the equation, H_o may be measured by conventional procedures and J can be determined by some one of the methods mentioned in the previous section. For the determination of ν , Rabi [24] has pointed out an ingeneous method. It is as follows. From Eq. (3.3) we see that if a nucleus of magnetic moment μ is placed in a uniform field H_o , it will continue to precess with a constant angular velocity ν and the angle which the angular momentum vector makes with H_o will remain constant. Now suppose, in addition, that a small rotating field H_1 is applied at right angles to the steady field H_o. The nucleus will then also tend to precess also about this small rotating field, thereby changing the angle which J makes with H_o. If H_1 rotates with the frequency ν this effect is cumulative and the change in the angle between H_o and J can be made large. If the frequency of revolution f of H_1 about H_o is different from ν , the net effect will be small. The smaller the ratio H_1/H_o the sharper this effect will be in its dependence on the exact agreement between the frequency of precession ν , and the resonance frequency f.

The schematic diagram of the apparatus used in detecting these reorientations is shown in Fig. 6. A stream of



Paths of molecules. The two solid curves indicate the paths of two molecules having different moments and velocities and whose moments are not changed during passage through the apparatus. This is indicated by the small gyroscopes drawn on one of these paths, in which the projection of the magnetic moment along the field remains fixed. The two dotted curves in the region of the *B* magnet indicate the paths of two molecules the projection of whose nuclear magnetic moments along the field has been changed in the region of the *C* magnet. This is indicated by means of the two gyroscopes drawn on the dotted curves, for one of which the projection of the magnetic moment along the field has been increased, and for the other of which the projection has been decreased.

Fig. 6

molecules coming from the source, O, in a high vacuum apparatus, is defined by a collimating slit, S, and detected by some suitable device at D. The magnets A and B produce inhomogeneous magnetic fields. When these magnets are turned on, molecules having magnetic moments will be deflected in the direction of the field gradient if the projection of the moment, μ_z, along the field is positive, and in the opposite direction, if μ_z is negative. The magnets A and B are adjusted so that the number of molecules arriving at D is the same whether the magnets A and B are on or off.

The molecules also pass between the poles of magnet C, which produces the uniform field H_0. Instead of a rotating field, an oscillating field (which is equivalent to two fields rotating in opposite directions) at right angles to the steady field is produced by means of a loop of wire inserted between the poles of the C magnet. (The loop is not shown in the diagram.) If the frequency of the oscilla-ting field is just right to induce reorientations of the molecules, i.e., to cause μ_z to change, magnet B will no longer be able to bring the molecules to the detector D, i.e., the deflection will be too large if μ_z increases and too small if μ_z decreases. Thus the condition of maximum reorientations is determined by noting the minimum molecular beam arriving at D.

By the use of quantum mechanics, the reorientation process is more precisely described as one in which the system, originally in some state, with a magnetic quantum number, m, makes a transition to another magnetic level m'. An exact solution for the transition probability for the case where H_1 rotates and is arbitrary in magnitude was given by Rabi [24].

For the particular case $J = \frac{1}{2}$ we have

$$P_{(\frac{1}{2},-\frac{1}{2})} = \frac{\sin^2\theta}{1+z^2-2z\cos\theta}\sin^2\pi ft(1+z^2-2z\cos\theta)^{\frac{1}{2}}, \qquad (3.4)$$

where $P_{(\frac{1}{2},-\frac{1}{2})}$ is the probability that the system, originally in the state $m = \frac{1}{2}$, is found in the state $m = -\frac{1}{2}$ after a time t; z, the ratio of the frequency of revolution f to the frequency of precession ν, given by

$$\nu = \mu(H_0^2 + H_1^2)^{\frac{1}{2}}/J\hbar, \qquad (3.5)$$

and

$$\tan\theta = H_1/H_0. \qquad (3.6)$$

For an oscillating field, when $H_1/H_0 \ll 1$, in the neighborhood of $f = \nu$ this formula becomes

$$P_{(\frac{1}{2},-\frac{1}{2})} = \frac{\Delta}{(1-z)^2+\Delta^2}\sin^2\pi ft\,[(1-z)^2+\Delta^2]^{\frac{1}{2}}, \qquad (3.7)$$

where $\Delta = H_1/2H_0$ is one half the ratio of the amplitudes of the oscillating to the static fields.

To determine the magnetic moment of the deuteron [25], the molecular beam of HD or D_2 is used. The molecule HD or D_2 is in the state with rotational angular momentum, J, equal to zero, the internuclear axis is oriented in every direction with equal probability. Therefore, if the applied steady field is large enough to decouple the particles from each other, the frequencies at which the protons or the deuterons make transitions will be effectively that of the free proton or the free deuteron. The experimental results are obtained in the following way. The radiofrequency oscillator is set at a definite constant frequency f and the molecular beam intensity is observed as a function of the homogeneous magnetic field H_0. For certain values of the magnetic field the beam intensity becomes a minimum. This occurs whenever the product hf for the oscillator is equal to the difference in energy between two molecular states. The resonance curves for deuteron in the HD and D_2 molecules are shown in Fig. 7, 8. By analyzing such curves, it is found that the magnetic moment of the deuterons is 0.855 ± 0.006 nuclear magnetons.

IV. DISCOVERY OF THE ELECTRIC QUADRUPOLE MOMENT OF THE DEUTERON

In the last section, we outlined the general procedure for determining the magnetic moments of nuclei by the magnetic resonance method and in particular, we pointed out that the very deep minima at the center of the resonance curve corresponds to the transition frequency of the free nuclear particles, such as the free proton or the free

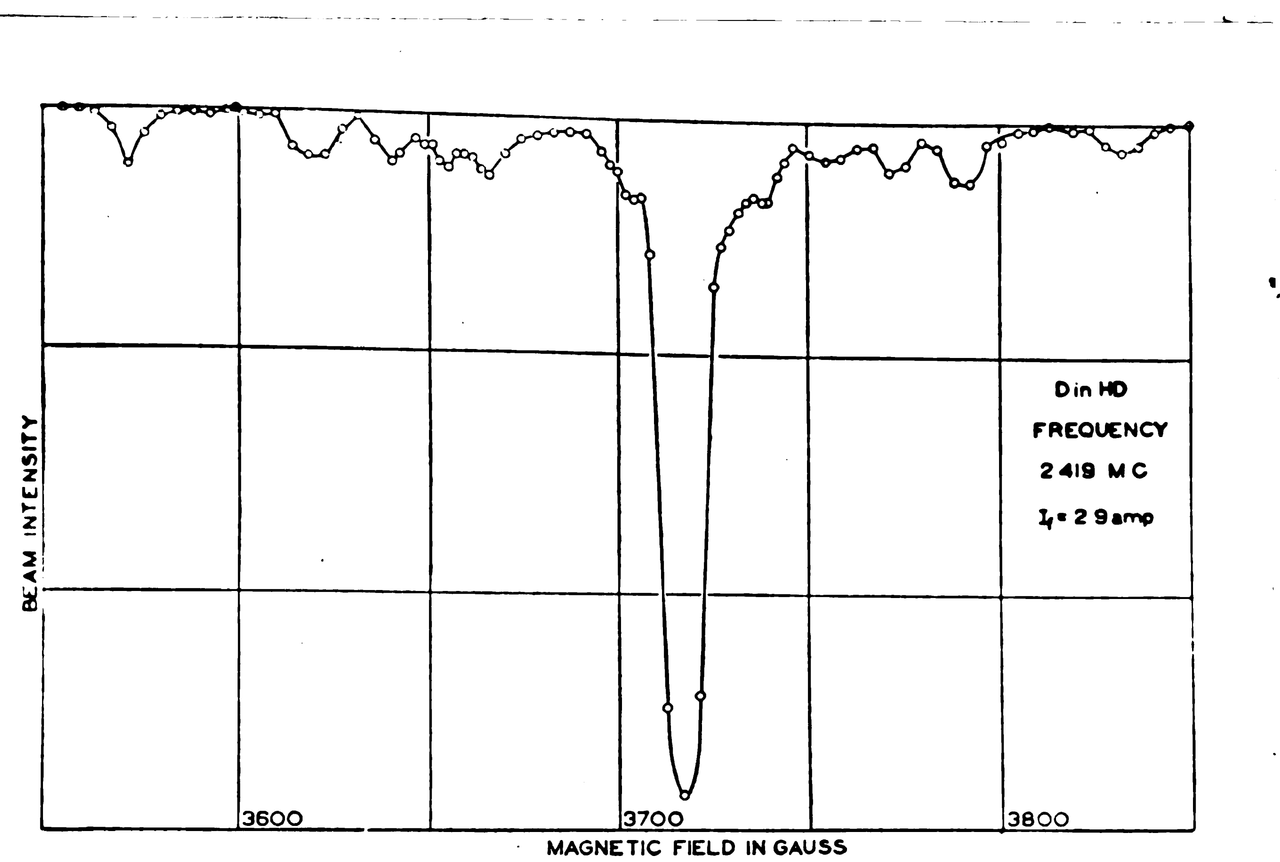


Fig. 7. Resonance curve for HD molecules chiefly showing transition of the deuteron spin for the zero rotational state.

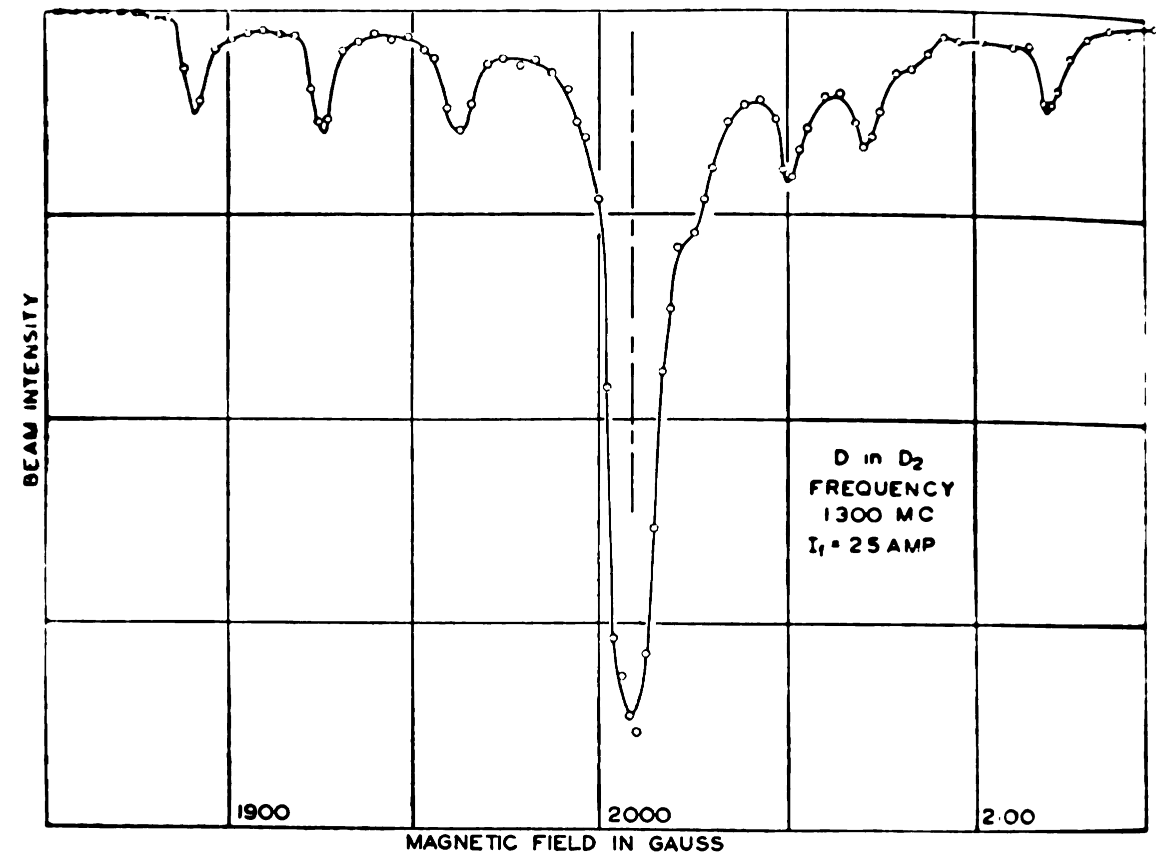


Fig. 8. Resonance curve for D_2 molecules showing transition of the resultant nuclear spin for the zero rotational state.

deuteron. However in attempting to account for the auxiliary minima flanking the central minimum, Rabi and his co-workers[4,27] noticed a fundemental difference in the spectra of H_2 and D_2 . They found that the structure of the radio-frequency spectrum of H_2 molecule could be explained by the magnetic interactions of various angular momentum vectors. They found, however, to their surprise, that a similar reasoning applied to the D_2 spectrum led to results not in agreement with the observed facts. We shall explain below the main arguments which led Rabi and his co-workers to the conclusion that the discrepancy can be attributed to the electric quadrupole moment of the deuteron.

Let us first consider the H_2 molecule. The angular momentum vectors associated with such a molecule are as shown in the diagram. The quantitites σ_1 and σ_2 are the spins of the two protons, and J is the angular momentum arising from the rotation of the H_2 molecule. It is readily seen that when such a molecule is placed in a magnetic field, its energy is given by

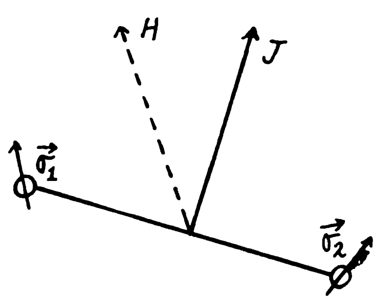


Fig. 9

$$E = -\mu_p (\vec{\sigma}_1 + \vec{\sigma}_2)\cdot\vec{H} - \mu_R \vec{J}\cdot H - \mu_p H'(\vec{\sigma}_1 + \vec{\sigma}_2)\cdot J + \frac{\mu_p^2}{r^3}\left\{\vec{\sigma}_1\cdot\vec{\sigma}_2 - \frac{3\vec{\sigma}_1\cdot\vec{r}\,\vec{\sigma}_2\cdot\vec{r}}{r^2}\right\}. \quad (4.1)$$

The quantity μ_R is the magnetic moment due to the rotation of the molecule; other terms have the usual significance. Using this as the energy expression and by analyzing the resonance curve of H_2, it is found that

$$H' = 27.2 \text{ gauss},$$

$$(\mu_P/r^3)_{av.} = 34.1 \text{ gauss.} \tag{4.2}$$

When this is combined with the value [26]

$$\langle 1/r^3 \rangle_{av.} = 2.438 \times 10^{24} \text{ cm.}^{-3}, \tag{4.3}$$

the proton magnetic moment turns out to be

$$\mu_P = \langle r^3 \rangle_{av.}(34.1) = \frac{34.1}{2.438 \times 10^{24}} = 1.403 \times 10^{-23} \text{ erg/gauss}, \tag{4.4}$$

or

$$\mu_P = 2.785 \text{ nuclear magneton.} \tag{4.4'}$$

This value is in remarkable agreement with the value of the proton magnetic moment obtained from the f/H value of the deep resonance minimum.

With the D_2 spectrum, there is no argument if one assumes only magnetic interaction between the angular momentum vectors. One would expect the spin orbit constant H' to be about ½ that of H_2 since the angular velocity of rotation of D_2 is half as large. The reason for this is that the rotational angular momentum vectors J are equal, the internuclear distances r are almost equal, but the mass of D_2 is practically twice that of H_2. One would then expect for D_2

$$H' = 13.6 \text{ gauss,} \tag{4.5}$$

$$H'' = \mu_D / \langle r^3 \rangle_{av.} = 10.5 \text{ gauss.} \tag{4.6}$$

The spectrum calculated from these constants is indicated in Fig. 10 by six short, closely spaced lines at the top. A glance at the diagram shows that there is no agreement.

In order to bring theory and experiment into agreement Kellogg [27] et al showed that it is necessary to assume the existence of the deutron quadrupole moment. The quantum theory of the effect of quadrupole moment on atomic energy levels was given by Casimir [28]. A theory for molecules can be constructed along similar lines. The part of the energy operator which concerns the quadrupole moment of a nucleus is, according to Casimir,

$$\frac{e^2qQ\{3(S.J)^2 + \frac{3}{2}(S.J) - S(S+1)J(J+1)\}}{2J(2J-1)S(2S-1)}, \tag{4.7}$$

where $Q = (3z^2 - r^2)_{av.}$ is the magnitude of the nuclear quadrupole moment. The average is taken over the nuclear charge for the state which has the largest component of the spin S in the z direction. The origin is the center of mass of the nucleus. The quantity eq is defined by

$$\left[\sum_e (3\cos^2\theta_e - 1)/r_e^3\right]_{av.}, \tag{4.8}$$

where the sum is taken over all of the molecular charges except the nucleus under consideration. This average is taken over the state of the molecule which has the greatest component along its angular momentum J, in the z direction. r_e is the distance of the e^{th} element of charge from the nucleus. J and S are the molecular and nuclear angular momentum operators, θ_e is the angle which r_e makes with the z axis. The factor ((qe) is the average of $\partial^2 V/\partial z^2$ where V is the electrostatic potential at the nucleus.

The value qQ was obtained from the D_2 resonance curve shown in Fig. 10. The quantity q was calculated from molecular wave functions by Nordsieck [39]. These values lead to

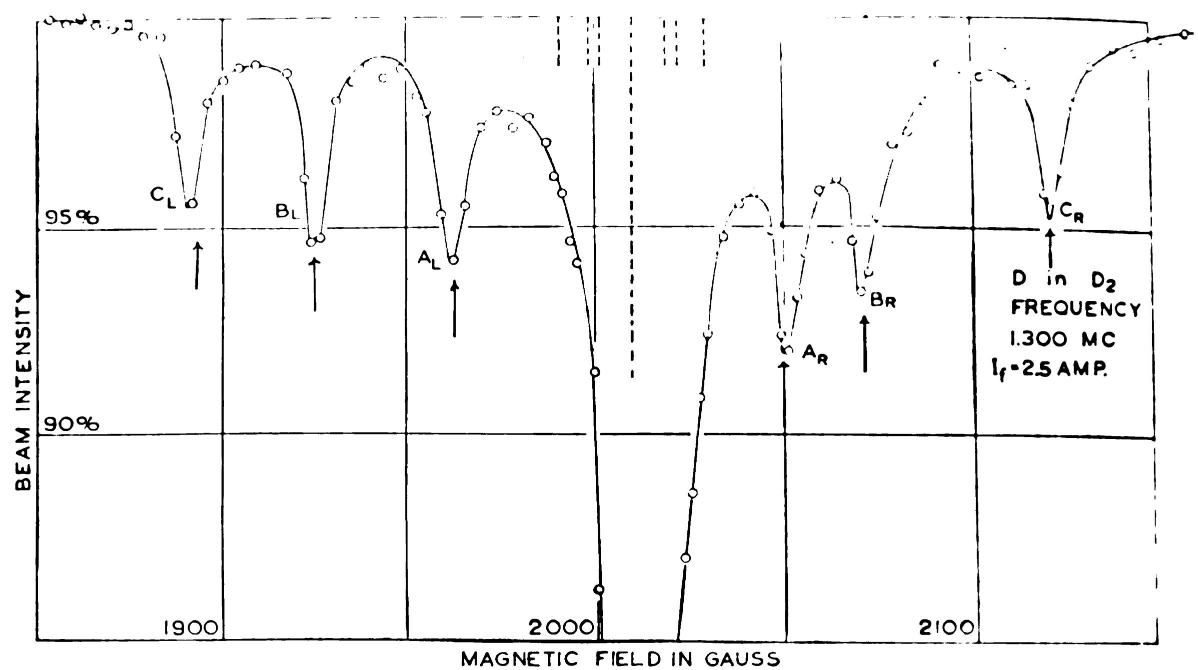
$$Q = 2.73 \times 10^{-27} \text{ cm.}^2 \tag{4.9}$$

for the deuteron quadrupole moment.

The existence of the nuclear quadrupole moment shows that the ground state of the deuteron is not a pure $^3S_1$ state, but is a mixture of states of $^3S_1$ and $^3D_1$. The effect of the mixing of such states is to result in a seeming departure from the additivity of proton and neutron magnetic moments when forming the deuteron. We shall see presently that the proton and the neutron are bound to each other not only by a central force, but also by another type of force, called tensor force.

V. ELECTROMAGNETIC INTERACTION OF THE ELECTRONS WITH THE NUCLEUS

In this section, a classical treatment of the electro-



Radiofrequency spectrum of D_2 at 80°K for $\Delta m_I = \pm 1$, with m_J unchanged. The length of the radiofrequency field is 13.5 cm. Dotted lines indicate spectrum predicted on the assumption of no quadrupole moment. Arrows indicate positions of lines predicted from the complete theory and the constants from the 2.419-MC data. Theoretical minimal half-width for any of these minima is about 6 gauss. The central minimum is not symmetrical about the central dotted line because of the method of producing the radiofrequency field.

Fig. 10

magnetic properties of the nucleus will be given. It will be shown how the concepts of magnetic dipole and electric quadrupole moments arise in classical electrodynamics. Also an important property of non-central forces will be pointed out. The reason for these discussions is that a systematic development of the classical electromagnetic properties of the nucleus is not available in the literature at present. It is hoped that the following discussion will give a better insight into the quantum-mechanical calculations that will follow in a later section.

A. ELECTROSTATIC INTERACTION—ELECTRIC QUADRUPOLE MOMENT

Let us first show that the concept of the quadrupole moment arises from the electrostatic interaction of the electrons and the nucleus. Consider then the electrostatic potential energy due to the interaction of the distributed nuclear charge density within the surface V and the distributed electron charge density ρ_e outside of V. From Fig. 11 we see that the constribution to the potential energy due to the charges in volume elements $d\tau_e$ and $d\tau_n$ is

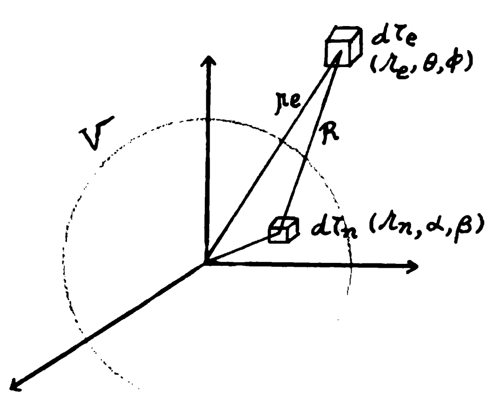


Fig. 11

$$dV = \frac{\rho_n d\tau_n \rho_e d\tau_e}{R} = \frac{\rho_n \rho_e d\tau_e d\tau_n}{|r_e - r_n|} .$$

Consequently, the total potential energy is given by

$$V = \int_{\text{outside } V} \int_{\text{inside } V} \frac{\rho_n \rho_e \, d\tau_e \, d\tau_n}{\sqrt{r_e^2 + r_n^2 - 2r_e r_n \cos\omega}}, \qquad (5.1)$$

To obtain the contribution from the various multipoles, the denominator is expanded in terms of Legendre polynominals

$$\frac{1}{\sqrt{r_e^2 + r_n^2 - 2r_e r_n \cos\omega}} = \frac{1}{r_e} \sum (r_n/r_e)^k P_k \cos\omega \quad ,$$

where $\cos\omega = \cos\theta \cos\alpha + \sin\theta \sin\alpha \cos(\phi - \beta)$. Substitution into Eq. (5.1) gives

$$V = \sum_{K=0}^{\infty} \int_{\text{outside } V} \frac{\rho_e d\tau_e}{r_e^{K+1}} \int_{\text{inside } V} r^K \rho_K P_K(\cos\omega) \, d\tau_n$$

$$= \int \frac{\rho_e d\tau_e}{r_e} \int \rho_n P_0(\cos\omega) \, d\tau_n + \int \frac{\rho_e d\tau_e}{r_e^2} \int r_n \rho_n P_1(\cos\omega) \, d\tau_n$$

$$+ \int \frac{\rho_e d\tau_e}{r_e^3} \int r_n^2 \rho_n P_2(\cos\omega) \, d\tau_n + \cdots. \qquad (5.2)$$

The first term is called the Coulomb energy and is just the energy due to a charge Ze concentrated at the center of the nucleus. The second term is the electric dipole moment term. Experiments show that the electric dipole moment does not manifest itself in atomic nuclei. Thus the contribution from this term vanishes. The third term is called the quadrupole interaction term. Let us examine this a little more closely. Since $\cos\omega$ contains both the electron and the nuclear angles, we shall separate them by using the addition-formula [28] for the Legendre polynomials.

That is

$$P_n(\cos\omega) = \sum_{K=0}^{n} (2-\delta_{oK}) \frac{(n-K)!}{(n+K)!} P_n^K(\cos\theta) P_n^K(\cos\alpha) \cos K(\phi-\beta). \qquad (5.3)$$

Substituting this into the quadrupole twem, there results

$$V_Q = \sum_{K=0}^{2} (2-\delta_{oK}) \frac{(2-K)!}{(2+K)!} \int \frac{\rho_e}{r_e^3} P_2^K(\cos\theta)\, d\tau_e \int r_n^2 \rho_n P_2^K(\cos\alpha) \cos K(\phi-\beta)\, d\tau_n . \qquad (5.4)$$

Since the nucleus is rotating rapidly about its spin axis, it is safe to assume that the nuclear charge distribution has axial symmetry. Then the charge density ρ_n is independent of β , and the only value of k for which the integral does not vanish is for $k=0$. Hence

$$\begin{aligned} V_Q &= \int \frac{\rho_e}{r_e^3} P_2(\cos\theta)\, d\tau_e \int r_n^2 \rho_n P_2(\cos\alpha)\, d\tau_n \\ &= \frac{1}{4} \int \frac{\rho_e (3\cos^2\theta - 1)}{r_e^3}\, d\tau_e \int r_n^2 (3\cos^2\alpha - 1) \rho_n\, d\tau_n , \end{aligned} \qquad (5.5)$$

where

$$eQ \equiv \tfrac{1}{2} \int r_n^2 (3\cos^2\alpha - 1) \rho_n\, d\tau_n , \qquad (5.6)$$

which is the nuclear quadrupole moment, and

$$eq \equiv \int \frac{\rho_e (3\cos^2\theta - 1)\, d\tau_e}{r_e^3} . \qquad (5.7)$$

It can be shown that this represents the second derivative of the potential, or the gradient of the electric field along the nuclear spin axis arising from the elctron charge distribution. The proof runs as follows.

$$eq \equiv \int \frac{\rho_e (3\cos^2\theta - 1)}{r_e^3}\, d\tau_e = \int \frac{\rho_e (3z_e^2 - r_e^2)}{r_e^5}\, d\tau_e .$$

The potential due to the elotron charge distribution at points inside the nucleus is

$$\int \frac{\rho_e \, d\tau_e}{|r_e - r_n|} . \tag{5.8}$$

Therefore

$$\frac{\partial^2}{\partial z^2}\int \frac{\rho_e \, d\tau_e}{|r_e - r_n|} = \int \rho_e \, d\tau_e \frac{\partial^2}{\partial z_n^2} \frac{1}{|r_e - r_n|}$$

$$= \int \frac{3(z_e - r_e)^2 - (z_e - r_n)^2}{|r_e - r_n|^5} \rho_e \, d\tau_e .$$

Hence, at the center of the nucleus

$$\left[\frac{\partial^2}{\partial z_n^2}\int \frac{\rho_e \, d\tau_e}{|r_e - r_n|}\right]_{r_n = 0} = \int \frac{3z_e^2 - r_e^2}{r_e^5} \rho_e \, d\tau_e . \tag{5.9}$$

To see how the shape of the nucleus affects the quadrupole moment, assume a nucleus to be a uniformly charged ellipsoid of revolution having total charge Ze with semi-major and semi-minor axes of a and b respectively. Assume that the spin and the major axes coincide. Since the volume of this ellipsoid of revolution is $4/3\,\pi ab^2$, the charge density is

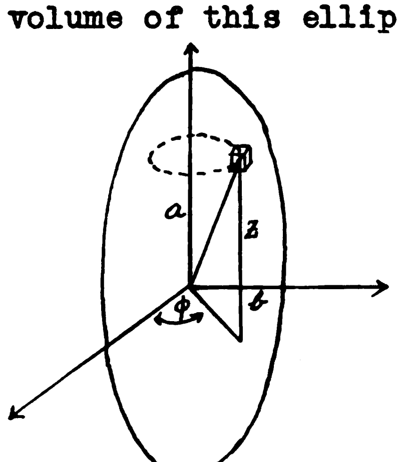


Fig. 12

$$\rho = \frac{3z_e}{4\pi ab^2},$$

$$d\tau_n = R \, d\phi \, dR \, dz,$$

$$r_n^2(3\cos^2\alpha - 1) = 3z_n^2 - r_n^2$$
$$= 2z^2 - R^2, \tag{5.10}$$

$$eQ = \int_{z=-a}^{a}\int_{y=0}^{b\sqrt{1-z^2/a^2}}\int_{\phi=0}^{2\pi} (2z^2-R^2)\frac{3ze}{4\pi ab^2} R\, d\phi\, dR\, dz$$

$$= 2\pi\int_{-a}^{a}\int_{0}^{b\sqrt{1-z^2/a^2}} (2z^2 - r^2)R\, dR\, dz$$

$$= 2\pi\int_{-a}^{a} \left[b^2z^2(1-z^2/a^2) - b^2(1 - z^2/a^2)^2/4\right] dz$$

$$= 8\pi ab^2(a^2 - b^2)/15,$$

$$eQ = \frac{3ze}{4\pi ab^2}\,\frac{8\pi}{15}\, ab^2(a^2 - b^2), \qquad (5.11)$$

$$Q = \frac{2}{5}\, z(a^2 - b^2). \qquad (5.12)$$

This verifies a remark by Mattauch [30].

Similarly in case the spin axis is the minor axis, the quadrupole moment turns out to be

$$Q = \frac{2}{5}\, z(b^2 - a^2). \qquad (5.13)$$

From these results we see that in case the nucleus is lengthened along the spin axis the quadrupole moment is positive (Fig. 13_a) and negative when flattened (Fig. 13_b).

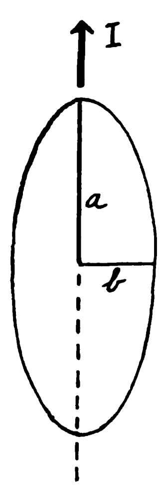


Fig. 13_a $b^2 < a^2$

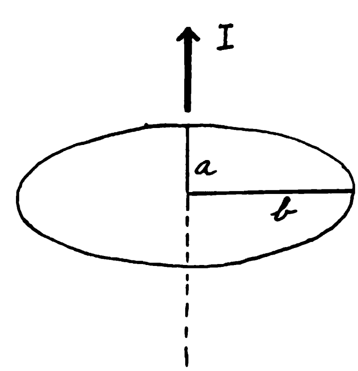


Fig. 13_b $b^2 > a^2$

The axis ratio a/b calculated according to Eq. (5.12) is plotted in Fig. 14.

B. MAGNETOSTATIC INTERACTION — MAGNETIC DIPOLE MOMENT DUE TO NUCLEAR CURRENT DISTRIBUTION

In the preceding paragraph we considered the effect of stationary distribution of charge upon the energy of an atom. Let us now consider the magnetostatic interaction energy of the atom. By this we mean the contribution to the energy of the atom due to a stationary distribution of nuclear currents, that arise from the motion of charges within the nucleus. Our purpose is to determine the effect of the internal motion of nuclear charges on the magnetic moment of the nucleus. Let us suppose that the motion of particles with-in the nucleus gives rise to an effective current of density $\vec{j}$. The vector potential [31] $\vec{A}$ due to this distribution is given by

$$\vec{A} = \frac{1}{c} \int \frac{\vec{j}(\vec{r}_n)\, d\tau_n}{|r - r_n|} . \tag{5.14}$$

Expanding the denominator, we obtain the following.

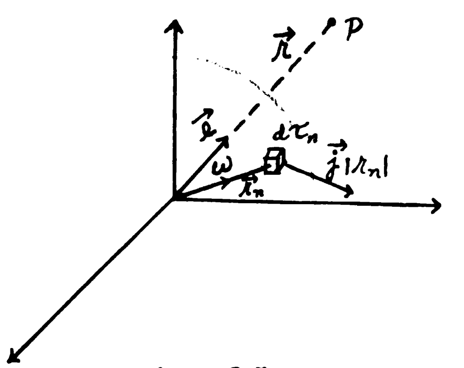
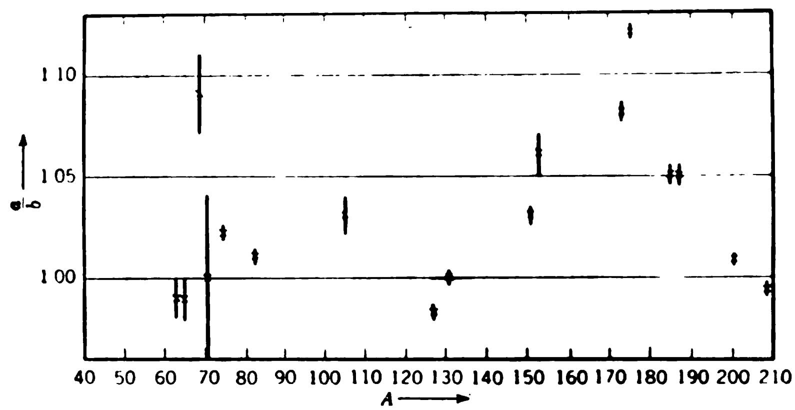


Fig. 15

$$A = \frac{1}{c}\sum_{K=0}^{\infty} \frac{1}{|\lambda|^{K+1}} \int |\lambda_n|^{K} \vec{j}(\lambda_n) P_n(\cos\omega)\, d\tau_n$$

$$= \frac{1}{c|\lambda|} \int \vec{j}(\vec{\lambda}_n)\, P_0\, d\tau_n$$

$$+ \frac{1}{c|\lambda|} \int |\lambda_K|\, \vec{j}(\lambda_n) P_1(\cos\omega)\, d\tau_n . \tag{5.15}$$



Ratio of nuclear axes when viewed as ellipsoidal, as calculated from the quadrupole moment. The arrows correspond to the limits of experimental error. A systematic dependence on mass number, A, appears to be indicated, but is uncertain because of the large scattering and the small number of experimental points.

Fig. 14.

The first term is zero. The second term is

$$\frac{1}{c}\,\frac{1}{|r|^2}\int |r_n|\,\vec{j}(\vec{r}_n)\,\cos\omega\; d\tau_n = \frac{1}{c\,|r|^2}\int \vec{e}.\vec{r}_n\,\vec{j}(\vec{r}_n)\,d\tau_n, \qquad (5.16)$$

where $\vec{e}.\vec{r}_n = |\vec{e}|\ |\vec{r}_n|\ \cos\omega$, and $\vec{e}$ is a unit vector along the vector $\vec{r}$.

From the continuity equation

$$\text{div } j + \frac{1}{c}\frac{\partial\rho}{\partial t} = 0 \qquad (5.17)$$

and from the fact that we are considering stationary distribution of charges and currents

$$\frac{\partial\rho}{\partial t} = 0, \qquad (5.18)$$

we see that the current density satisfies the relation

$$\text{div } j = 0. \qquad (5.19)$$

This means that j can be derived from the curl of some vector. Let us write therefore

$$\vec{j} = c\nabla\times\vec{m}, \qquad (5.20)$$

$$A_{dip} = \frac{1}{|r|^2}\int \vec{e}\,.\,\vec{r}_n\,\nabla\times\vec{m}\;d\tau_n. \qquad (5.21)$$

From the expansion formula [32]

$$\nabla\times(U\,\vec{V}) = \nabla U\times\vec{V} + U\nabla\times\vec{V},$$

we get

$$\begin{aligned}\vec{e}\,.\,\vec{r}_n\nabla\times\vec{m} &= \nabla\times(\vec{e}\,.\,\vec{r}_n\,\vec{m}) - \nabla(\vec{e}\,.\,\vec{r}_n)\times\vec{m}\\ &= \nabla\times(\vec{e}\,.\,\vec{A}_n\,\vec{m}) - (e.\nabla\vec{r}_n)\times\vec{m}\\ &= \nabla\times(\vec{e}\,.\,\vec{A}_n\,\vec{m}) - \vec{e}\times\vec{m},\end{aligned}$$

$$A_{dip} = -\frac{1}{|r|^2}\int \vec{e} \times \vec{m}\, d\tau_n = -\frac{\vec{e}}{|r|^2} \times \int \vec{m}\, d\tau_n, \tag{5.22}$$

since the volume integral of the first term vanishes. Comparing this with the vector potential of a dipole,

$$A_{dip} = \frac{\vec{\mu} \times \vec{r}}{|r|^3}, \tag{5.23}$$

where $\vec{\mu}$ is the magnetic dipole moment, we see that

$$\int \vec{m}\, d\tau_n = \vec{\mu} \tag{5.24}$$

is the contribution to the magnetic dipole moment due to the motion of charges in the nucleus.

We shall now obtain a more convenient expression for this orbital magnetic moment. From Eq. (5.20) we have

$$\frac{\vec{r} \times \vec{j}}{c} = \vec{r} \times \nabla \times \vec{m},$$

$$\frac{1}{c}\int \vec{r} \times \vec{j}\, d\tau_n = \int \vec{r} \times \nabla \times \vec{m}\, d\tau_n. \tag{5.25}$$

From the expansion formula [32]

$$\text{Grad}\,(U \cdot V) = V \cdot \nabla U + U \cdot \nabla V + V \text{ curl } U + U \times \text{curl } V,$$

we obtain

$$\begin{aligned} \text{Grad}\,(\vec{r}\cdot\vec{m}) &= \vec{r} \cdot \nabla m + m \cdot \nabla r + \vec{m} \times \nabla \times \vec{r} + \vec{r} \times \nabla \times \vec{m} \\ &= \vec{m} \cdot \nabla \vec{r} + m \cdot \nabla r + \vec{m} \times \nabla \times \vec{r} + \vec{r} \times \nabla \times \vec{m}. \end{aligned}$$

Then

$$\begin{aligned} \vec{r} \times \nabla \times \vec{m} &= \text{Grad}\,(\vec{r}\cdot\vec{m}) - \vec{m} \cdot \nabla \vec{r} - m \nabla \vec{r} - \vec{m} \times \nabla \times \vec{r} \\ &= \text{Grad}\,(\vec{r}\cdot\vec{m}) - m - m - \vec{m} \times \nabla \times \vec{r}. \end{aligned}$$

Substitute the above equation into Eq. (5.25)

$$\frac{1}{c}\int \vec{r} \times \vec{j}\, d\tau_n = -\int 2m\, d\tau_n \;.$$

Comparing with Eq. (5.24), we obtain

$$\frac{1}{c}\int \vec{r} \times \vec{j}\, d\tau_n = 2\vec{\mu},$$

$$\vec{\mu} = \frac{1}{2c}\int \vec{r} \times \vec{j}\, d\tau_n.$$

By means of

$$\vec{j} = \rho v \;, \tag{5.26}$$

where $\vec{j}$ is the charge density and $\vec{v}$ is the velocity, it follows that

$$\vec{\mu} = \int \frac{\rho \vec{r} \times m\vec{v}}{2mc}\, d\tau_n \;. \tag{5.27}$$

The integral of Eq. (5.27) gives the contribution of the motion of the charged nuclear particles to the nuclear magnetic moment. It can be written in the form

$$\vec{\mu} = \sum \frac{e\hbar}{2Mc} L, \tag{5.28}$$

where the summation is over all particles and L is the orbital angular momentum of the particles. For the case of the deuteron which contains a proton and a neutron,

$$\vec{\mu} = \frac{e_1 \hbar}{2M_1 c} L_1 + \frac{e_2 \hbar}{2M_2 c} L_2. \tag{5.29}$$

Since the neutron has no charge the first term is zero. Therefore

$$\vec{\mu} = \frac{e_2 \hbar}{2M_2 c} \vec{L}_2. \tag{5.30}$$

Since

$$L_1 = L_2 = L/2 \ , \tag{5.31}$$

we obtain

$$\vec{\mu}_{\text{orb}} = \frac{e\,\hbar}{2Mc}\,(\tfrac{1}{2}\,\vec{L}). \tag{5.32}$$

This is the contribution of the orbital motion of charged nuclear particles to the magnetic moment. This is also the quantum-mechanical operator for the orbital magnetic moment.

C. ANGULAR MOMENTUM CONSIDERATION FOR NON-CENTRAL FORCES

Because we find it necessary to introduce non-central or angle-dependent forces to account for the experimentally observed electric quadrupole moment, we shall discuss the classical aspects of such forces. We shall show that, although the orbital angular momentum is a constant for central forces, it is not necessarily so for non-central forces.

The fact that orbital angular momentum is conserved for central forces can be seen from the following considerations. Let us suppose that a particle is moving under the action of a central force $\vec{F}(r)$. We can then write

$$m\,\vec{a} = \vec{F} = f(r)\,\vec{r}, \tag{5.33}$$

where $\vec{r}$ is the position vector. The quantity $\vec{r}\times\vec{F}$ is known as the torque about the origin, exerted by the force F. Therefore,

$$m\,\vec{r}\times\vec{a} = \vec{r}\times\vec{F} = \vec{r}\times f(r)\,\vec{r}, \qquad (5.34)$$

since the vector product of a vector into itself vanishes. But

$$\vec{r}\times\vec{a} = \frac{d}{dt}(\vec{r}\times\vec{V}),$$

$$\frac{d}{dt}(m\,\vec{r}\times\vec{V}) = 0. \qquad (5.35)$$

So the orbital angular momentum is constant, that is

$$mr \times V = \text{constant}.$$

Thus we see that a particle in a central force field will continue to move in a fixed invariable plane, that is, the orbit of the particle will not "wobble".

On the other hand, consider two spinning dipoles each of mass m and m' and of magnetic moments M and M', as shown in Fig. 16. Consider now the moment of the force about the center of mass. Let r be their distance from each other.

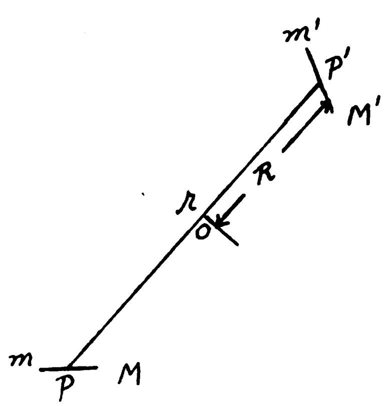


Fig. 16

The potential of the magnetic dipole [32] is

$$U = -M \cdot \nabla\, 1/r. \qquad (5.36)$$

Since the first magnet gives rise to the field

$$H = (\nabla\nabla\, 1/r) \cdot M, \qquad (5.37)$$

the potential energy of the dipole m' is

$$-M' \cdot H = -M' \cdot \left[M \cdot (\nabla\nabla 1/r)\right]. \qquad (5.38)$$

The translational force on the dipole m' is computed by the formula

$$F_{M'} = M' \cdot \nabla H = M' \cdot \nabla \left[M.(\nabla\nabla 1/r) \right] , \qquad (5.39)$$

and the torque on m' is given by

$$L_{M'} = M' \times H = M' \times (\nabla\nabla 1/r).M. \qquad (5.40)$$

But

$$\nabla\nabla \frac{1}{r} = -\nabla \frac{\vec{r}}{r^3} = -\left(\nabla \frac{1}{r^3}\right) \vec{r} - \frac{1}{r^3} \nabla \vec{r},$$

i.e.,

$$\nabla\nabla \frac{1}{r} = \frac{3\,\vec{r}\,\vec{r}}{r^5} - \frac{I}{r^3} \cdot \qquad (5.41)$$

Substitute Eq. (5.41) into Eq. (5.37). We have

$$\vec{H} = M \cdot \left\{ \frac{3\vec{r}\vec{r}}{r^5} - \frac{I}{r^3} \right\} = \frac{3M\cdot r\vec{r}}{r^5} - \frac{\vec{M}}{r^3} \cdot \qquad (5.42)$$

Substitution of Eq. (5.41) into Eq. (5.39) gives

$$\vec{F}_H = M' \cdot \nabla \left[\frac{3\vec{r}}{r^5} M\cdot r - \frac{\vec{M}}{r^3} \right] \cdot \qquad (5.43)$$

Using the expansion formula

$$\nabla (\mu \vec{V}) = \nabla \mu \vec{V} + \mu \nabla \vec{V},$$

$$\nabla (U\cdot V) = V\cdot\nabla U + U\cdot\nabla V + V \times \text{curl } U + U \times \text{curl } V,$$

we obtain the first term of Eq. (5.43)

$$\nabla \left\{ \frac{3\vec{r}}{r^5} M\cdot r \right\} = \left\{ \nabla (M\cdot r) \right\} \frac{3\vec{r}}{r^5} + M\cdot r \nabla \frac{3\vec{r}}{r^5}$$

$$= M\cdot \nabla r \frac{3\vec{r}}{r^5} + 3M\cdot r \left\{ \nabla \frac{1}{r^5} \vec{r} + \frac{1}{r^5} \nabla \vec{r} \right\}$$

$$= \frac{3\,\vec{M}\,\vec{r}}{r^5} + 3M\cdot r \left\{ -\frac{5}{r^7} \vec{r}\vec{r} + \frac{1}{r^5} I \right\}$$

$$= 3 \left\{ - \frac{5}{r^7} M\cdot r\vec{r}\vec{r} + \frac{\vec{M}\vec{r}}{r^5} + \frac{\vec{M}\cdot\vec{r}}{r^5} I \right\} \qquad (5.43)_a$$

and the second term of Eq. (5.43)

$$\nabla \frac{\vec{M}}{r^3} = \nabla \frac{1}{r^3} M = - \frac{3}{r^5} \vec{r}M. \qquad (5.43)_b$$

Substituting Eq. $(5.43)_a$ and Eq. $(5.43)_b$ into Eq. (5.43) we obtain

$$\vec{F}_{M'} = 3\left[- \frac{5}{r^3} M\cdot rM'r\vec{r} + \frac{M\cdot Mr}{r^5} + \frac{M\cdot r}{r^5}M'\right] + \frac{3}{r^5} M'\cdot rM. \qquad (5.44)$$

Therefore the moment of the translational force on m' is

$$\vec{r} \times \vec{F}_{M'} = \frac{3M\cdot r}{r^5} r \times M' + \frac{3}{r^5} M'\cdot rr \times M. \qquad (5.45)$$

If the moments are taken about the center of mass, then r' = 2R, r = - 2R. Then moment of forces on m' about the center O is

$$R \times \vec{F}_{M'} = \frac{6M\cdot R}{32R^5} R \times M' + \frac{6M'\cdot R}{32R^5} R \times M. \qquad (5.46)$$

Similarly, the moment of the translational force on m about O is

$$-R \times \vec{F}_M = \frac{6M'\cdot R}{32R^5} R \times M + \frac{6M\cdot R}{32R^5} R \times M'. \qquad (5.47)$$

Therefore the sum of the moments of the translational force on m and m' is

$$R \times \vec{F}_{M'} - R \times \vec{F}_M = \frac{12M'\cdot R}{32R^5} R \times M + \frac{12M\cdot R}{32R^5} R \times M'. \qquad (5.48)$$

Thus the sum of the moment of the translational forces does not vanish. This shows that the orbital angular momentum is not a constant of motion.

Now let us go back to the spin moments of the dipoles m and m'. Let L_M and $L_{M'}$ be the torques on m and m' respectively. Substitute Eq. (5.41) into Eq. (5.40). We have for the torque on m'

$$L_{M'} = M' \times H = M' \times \left[\frac{3}{r^5} \vec{r}\vec{r} - \frac{I}{r^3} \right] \cdot M$$

$$= \frac{12}{32R^5} M' \times RM'R - \frac{M' \times M}{8R^5}, \qquad (5.49)$$

and similarly the torque on m is given by

$$L_M = \frac{12}{32R^5} M \times RM' \cdot R - \frac{M \times M'}{8R^5}. \qquad (5.50)$$

The sum of the torques is

$$L_{M'} + L_M = \frac{12}{32R^5} M' \times RM \cdot R + \frac{12}{32R^5} M \times RM' \cdot R. \qquad (5.51)$$

Therefore the sum of moments of the translational force and the torques is

$$R \times F_{M'} + (-R) \times F_M + L_M + L_{M'} = 0. \qquad (5.52)$$

This shows that the total angular momentum of the system remains constant.

These results are true in quantum mechanics. We shall show that when tensor, i.e. non-central, forces are introduced, the orbital angular momentum L will no longer be a good quantum number, although the total angular momentum is still a constant of motion.

VI. THE THEORETICAL INTERPRETATION OF THE MAGNETIC DIPOLE AND ELECTRIC QUADRUPOLE MOMENTS OF THE DEUTERONS

In the previous section, we outlined the experimental methods used in determining nuclear multipole moments, and developed the concepts of multipole moments in classical electro dynamics. Our purpose now will be to see how these ideas can be fit into a consistent quantum mechanical scheme. One suspects this to be possible because quantum mechanics has been remarkably successful in providing a qualitative interpretation of nuclear phenomena.

It is interesting to note that the Rarita and Schwinger theory, which will be outlined below, was anticipated in 1938, in a paper by Yukawa, Sakata, and Taketani [33]. However, the physical significance of their theory of the deuteron was not fully realized until after the discovery of the deuteron quadrupole moment [34].

A. NECESSITY OF NON-CENTRAL FORCE

In order to see what must be done, let us assemble the experimental data. The moments of the deuteron are

$$\mu_D = +0.8565 \pm 0.0004 \text{ nuclear magnetons,}$$

$$Q_D = 2.73 \times 10^{-27} \text{ cm}^2.$$

The magnetic moments of the proton and neutron are

$$\mu_P = +2.7896 \pm 0.0008,$$

$$\mu_n = -1.9103 \pm 0.0012.$$

We notice that the sum of proton and neutron moments is

$$\mu_p + \mu_n = +0.8793 \pm 0.0015,$$

which differs from the deuteron moment by

$$(\mu_p + \mu_n) - \mu_p = 0.0228 \pm 0.0016.$$

Thus, the magnetic moment of the deuteron is very nearly the sum of the proton and neutron moments. In addition, as has been pointed out previously, the deuteron spin is 1, which is just the sum of the spin of the proton and the neutron. These results suggest that the ground state of the deuteron is a $^3S_1$ state. The small deviation from additivity and the small quadrupole moment is due to the presence of a small amount of $^3D_1$ state.

Let us examine the problem a little more carefully by applying the Landé formula of nuclear systems. Let $\vec{S}$ represent the intrinsic angular momenta of the particles, $\vec{L}$ the orbital angular momentum, and $\vec{J}$ the total angular momentum of the nucleus in the ground state. The eigenvalue of $\vec{J}$ is, of course, the experimentally observed nuclear spin I. Let the magnetic moments associated with the vector $\vec{S}$ and $\vec{L}$ be $\vec{\mu}_S$ and $\vec{\mu}_L$, respectively. Then, because of the Larmor precession of the vectors $\vec{S}$ and $\vec{L}$ about $\vec{J}$, the effective magnetic moment of the experimentally observable value is

$$\mu_{eff} = \mu_L \cos (L, J) + \mu_S \cos (S, J). \tag{6.1}$$

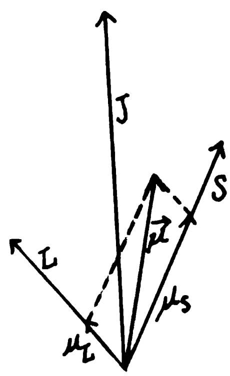


Fig. 17

Using the cosine law of trigonometry, we then get

$$\mu_{eff} = \mu_L \frac{S^2 - L^2 - J^2}{2LJ} + \mu_S \frac{L^2 - S^2 - J^2}{2SJ} . \tag{6.2}$$

Introduce the gyromagnetic ratios given by

$$\mu_L = g_L \mu_N, \tag{6.3)$_a$}$$

$$\mu_S = g_S \mu_N, \tag{6.3)$_b$}$$

$$\mu_J = g_J \mu_N, \tag{6.3)$_c$}$$

where μ_N is the nuclear magneton. Then Eq. (6.2) becomes

$$\mu_{eff} = \left[g_L \frac{S^2-L^2-J^2}{2J^2} + g_S \frac{L^2-S^2-J^2}{2J^2} \right] J \mu_N. \tag{6.4}$$

Thus the gyromagnetic ratio of the nucleus is

$$g_{eff} = -\tfrac{1}{2}(g_L + g_S) - \frac{S(S+1)-L(L+1)}{2J(J+1)}(g_S - g_L). \tag{6.5}$$

In the last step we replaced S^2 by $S(S+1)$, etc., in accordance with the results of quantum mechanics. Under the section on non-central force, we showed that $g_L = \frac{1}{2}$. The quantity g_S is just the sum of the g's of the proton and neutron. Hence

$$g_S = g_L + g_n$$
$$= 2.7896 - 1.9103 = 0.8793. \tag{6.6}$$

From Eq. (6.6) we see that if the nucleus is in the S state, ($J = S = 1$, $L = 0$), the effective magnetic moment should be

$$\mu_{\text{eff}} = \left[\tfrac{1}{2}(g_L + g_S) + \tfrac{1}{2}(g_S - g_L)\right] J\mu_N = g_S J \mu_N. \qquad (6.7)$$

Thus, if the deuteron ground state were a pure S state, its magnetic moment should be just the sum of the moments of the proton and the neutron. If the deuteron were a pure D state ($S=1$, $J=1$, $L=2$), its magnetic moment would be

$$\mu_{\text{eff}} = \left[\tfrac{1}{2}(g_L + g_S) + \frac{1(2) - 2(3)}{2(1)(2)}(g_S - g_L)\right] J\mu_N$$

$$= \left[\tfrac{1}{2}(g_L + g_S) - (g_S - g_L)\right]\mu_N$$

$$= \left[.5 + \frac{.8793}{2} - \left(\frac{.8793}{2} - .5\right)\right]\mu_N = .3104\mu_N \ . \qquad (6.8)$$

The experimentally observed value lies between these two values. Hence we are led to consider the possibility that the ground state is partly S and partly D states. If the percentage of the D state is represented by p, then the observed magnetic moment will be given by

$$\mu_D = 0.8693(1 - p) + 0.3104p, \qquad (6.9)$$

where the first term is the contribution to the magnetic moment from the S state and the second term, that from the D state. Inserting the observed value of μ_D in the above equation and solving for p we obtain $p = 4\%$. It is a remarkable result of the Rarita and Schwinger theory [6] that just this amount of D state admixture is necessary to account for the deuteron quadrupole moment.

B. PROPERTIES OF PAULI SPIN FUNCTION

In developing their theory, Rarita and Schwinger made an outright assumption that the interaction function between the proton and the neutron in the deuteron is given by

$$V(r) = \left[1 - \tfrac{1}{2}g + \tfrac{1}{2}g\,\sigma_1\cdot\sigma_2 + \gamma S_{12}\right] J(r), \tag{6.10}$$

$$S_{12} = \frac{3\,\sigma_1\cdot r_{12}\,\sigma_2\cdot r_{12}}{r_{12}^2} - \sigma_1\cdot\sigma_2\,, \tag{6.11}$$

where σ_1 and σ_2 are the neutron and proton spin operators, respectively. Also g and γ represent the strengths of spin-spin and dipole-dipole interactions, respectively. The wave equation of the proton and neutron system is

$$\left[-\frac{\hbar^2}{2M_p}\nabla_p^2 - \frac{\hbar^2}{2M_n}\nabla_n^2 + V\right]\psi = E\psi. \tag{6.12}$$

This equation can be put into a more convenient form by transforming it into a coordinate system whose origin coincides with the center of mass. The result is

$$-\frac{\hbar^2}{M}\nabla^2\psi + V\psi = E\psi. \tag{6.13}$$

This equation differs a little from wave equations treated in many text books on quantum mechanics. The difference is that the potential function V contains an angle dependent term S_{12}. Because of this term the orbital angular momentum operator L^2 will no longer commute with the Hamiltonian

$$H \equiv -\frac{\hbar^2}{M}\nabla^2 + V. \tag{6.14}$$

That is

$$[L^2, H] \neq 0. \tag{6.15}$$

The physical meaning of this is that the orbital angular momentum is not a constant of motion. Yet there are certain constants of motion. These can be determined by a method given in Rojansky [35], i.e., by finding the dynamical variables which commute with the Hamiltonian. These are S^2, J^2, J_z, and the parity. The effect of the last quantum mechanical constant of motion is to prevent the mixing of states of odd and even orbital angular momentum. Therefore the ground state solution of the wave equation can be written in the form

$$\Psi(J=1,\ S=1,\ m_J,\ \text{parity even}) = \psi(^3S_1) + \psi(^3D_1). \tag{6.16}$$

The notation used here is similar to that used in atomic spectroscopy. The symbol J represents the total angular momentum and is the observable spin of the nucleus. Let us now proceed to determine the $^3S_1$ and $^3D_1$ wave functions. For this, we assume that these functions are of the form

$$\psi(^3S_1) = c_1\, \mu(r) \chi_1^m , \tag{6.17}$$

$$\psi(^3D_1) = c_2\, \omega(r)\ S_{12} \chi_1^m, \tag{6.18}$$

where χ_1^m are the spin functions, given by

$$\chi_1^1 = \alpha(1)\alpha(2), \tag{6.19}$$

$$\chi_1^0 = \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) + \alpha(2)\beta(1)\right], \tag{6.20}$$

$$\chi_1^{-1} = \beta(1)\beta(2). \tag{6.21}$$

The above are spin functions of total spin 1 with components in the direction of quantization equal to 1, 0, -1, respectively. These remarks can be proved by showing that

$$S^2\chi_1^m = 1(1+1)\chi_1^m\ , \tag{6.22}$$

$$S_z\chi_1^m = m\chi_1^m\ , \tag{6.23}$$

where

$$S^2 = \left(\frac{\sigma_1+\sigma_2}{2}\right)^2\ , \qquad S_z = \frac{\sigma_{1z}+\sigma_{2z}}{2}\ .$$

Using these results we see that the wave functions given in Eq. (6.17) are the wave functions of a state with $J=S=1$ and $L=0$. To normalize the $^3S_1$ wave function, i.e., to determine the constant c_1 of Eq. (6.17), we write

$$c_1^2\int(\chi_1^m)^2\ d\Omega = 1.$$

Since $(\chi_1^m)^2 = 1$, $4\pi c_1^2 = 1$. Therefore

$$c_1 = \frac{1}{\sqrt{4\pi}}\ . \tag{6.24}$$

The proof that Eq. (6.18) represents a state of $J=1$, $S=1$, $L=2$ is somewhat more involved. We shall show that it represents a D state. For this we need to prove that

$$L^2(S_{12}\chi_1^m) = 2(2+1)\ S_{12}\chi_1^m\ . \tag{6.25}$$

To demonstrate this, let us first show that

$$\nabla^2(r^2\ S_{12}\chi_1^m) = 0, \tag{6.26}$$

or

$$\nabla^2(r^2\ S_{12}\chi_1^m) = \left[\nabla^2(r^2\ S_{12})\right]\chi_1^m\ .$$

since χ_1^m do not depend upon the space coordinates. Using the relation

$$S_{12} = \frac{3\sigma_1 \cdot r\sigma_2 \cdot r}{r^2} - \sigma_1 \cdot \sigma_2 ,$$

and carrying through the differentiations, we have

$$\nabla\cdot\nabla(r^2 S_{12}) = \nabla \cdot \left[3(\sigma_1 \cdot r\sigma_2 + \sigma_1 \sigma_2 \cdot r) - 2r\right]$$
$$= 3\sigma_1 \cdot \sigma_2 + 3\sigma_1 \cdot \sigma_2 - 6\sigma_1 \cdot \sigma_2 = 0.$$

The Laplacian ∇^2 can be written in the form

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial}{\partial r}) - \frac{L^2}{r^2} . \qquad (6.27)$$

Now apply the above operator to the wave function $S_{12}\chi_1^m$.

From Eq. (6.26) we have

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})(r^2 S_{12}) - \frac{L^2}{r^2}(r^2 S_{12}) = 0.$$

Therefore

$$\frac{L^2}{r^2}(r^2 S_{12}) = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial^2}{\partial r^2})(r^2 S_{12})$$
$$= \frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r})\left[3\sigma_1 \cdot r\,\sigma_2 \cdot r - r^2\sigma_1 \cdot \sigma_2\right]$$
$$= \frac{\partial}{\partial r}\left[(r^2\frac{\partial}{\partial r})\right]\left[3\sigma_1 \cdot \vec{e}_r\sigma_2 \cdot \vec{e}_r - \sigma_1 \cdot \sigma_2\right]$$
$$= 2(3)\, r^2\left\{3\sigma_1 \cdot e_r\sigma_2\, e_r - \sigma_1 \cdot \sigma_2\right\}$$
$$= 2(3)\, r^2 S_{12} = 2(2+1)\, r^2 S_{12}.$$

Consequently

$$L^2(r^2 S_{12}) = 2(2+1)(r^2 S_{12}),$$

or

$$L^2(S_{12}\chi_1^m) = 2(2+1)(S_{12}\chi_1^m). \tag{6.28}$$

Comparing this with

$$L^2\,\psi(\ell,\,m) = \ell(\ell+1)\,\psi(\ell,\,m)\ ,$$

we see that $\ell = 2$. This shows that $S_{12}\chi_1^m$ is the wave function of a state with $\ell = 2$. Let us normalize the $^3D_1$ wave function i.e., determine the constant c_2 so that

$$c_2^2\int(S_{12}\chi_1^m \cdot S_{12}\chi_1^m)\,d\Omega = 1.$$

The above integral can also be written in the form

$$c_2^2\int(\chi_1^m\,S_{12}^2\,\chi_1^m)\,d\Omega = 1.$$

Thus in order to obtain the normalizing factor, we need to evaluate S_{12}^2. This can be done in the following manner.

Since

$$S_{12} = \frac{3\,\sigma_1\cdot r\,\sigma_2\cdot r}{r^2} - 1\ ,$$

therefore

$$(S_{12}+1)^2 = \frac{9}{r^4}\,(\sigma_1\cdot r)^2\,(\sigma_2\cdot r)^2. \tag{6.29}$$

Using the relation given by Dirac [35]

$$\sigma A\,\sigma\cdot B = A\cdot B - i\,\sigma\cdot A\times B\ ,$$

Eq. (6.29) becomes

$$(S_{12}+1)^2 = \frac{9}{4}\left[r^2 + i\,\sigma_1\cdot r\times r\right]\left[r^2 + i\,\sigma_2\cdot r\times r\right] = 9\ ,$$

$$S_{12}^2 = 8 - 2S_{12}.$$

Therefore

$$c_2^2 \int \chi_1^m (8 - 2S_{12}) \chi_1^m \, d\Omega = 8c_2^2 \int \chi_1^m \chi_1^m \, d\Omega = 8c_2^2 (4\pi),$$

$$c_2^2 = \frac{1}{\sqrt{4\pi}} \frac{1}{2^{3/2}} \, . \tag{6.30}$$

For the radial part of the wave function, write $u(r)/r$ and $\omega(r)/r$ for $^3S_1$ and $^3D_1$ states, respectively. Then from Eqs. (6.16), (6.17), ~~(6.17)~~, (6.18), (6.24) and (6.30) we obtain

$$\psi = \frac{1}{\sqrt{4\pi}} \left\{ \frac{u(r)}{r} + 2^{-3/2} S_{12} \frac{\omega(r)}{r} \right\} \chi_1^m \, , \tag{6.31}$$

where

$$S_{12} = \frac{3\sigma_1 \cdot r_{12} \sigma_2 \cdot r_{12}}{r_{12}^2} - \sigma_1 \cdot \sigma_2 \, .$$

The normalization condition is

$$\int_0^\infty (u^2 + \omega^2) \, dr = 1. \tag{6.32}$$

Using the relation

$$\sigma_1 \cdot \sigma_2 = 2S(S+1) - 3 = 1, \qquad \text{when } S = 1$$

into Eq. (6.10), we obtain

$$V = -(1 + \gamma S_{12}) J(r).$$

When we substitute the above result into the deuteron wave Eq. (6.13), we obtain

$$E \psi = \frac{\hbar^2}{M} \nabla^2 \psi - \left[1 + \gamma S_{12} \right] J(r) \psi \, . \tag{6.33}$$

The differential equations which $u(r)/r$ and $\omega(r)/r$ satisfy can be found by substituting Eq. (6.31) into the deuteron wave Eq. (6.33). We get

$$\nabla^2 \frac{u(r)}{r} \chi_1^m + \frac{1}{2\sqrt{2}} \nabla^2 \left(S_{12} \frac{\omega(r)}{r} \chi_1^m\right)$$

$$+ \frac{M}{h^2}\left[E + (1+\gamma S_{12})J(r)\right]\left[\frac{u(r)}{r} + \frac{1}{2\sqrt{2}} S_{12} \frac{\omega(r)}{r}\right]\chi_1^m = 0. \quad (6.34)$$

The quantity $\nabla^2 u(r)/r$ can be evaluated easily, since $u(r)/r$ depends upon r only. Thus

$$\nabla^2 Y_2 \frac{\omega(r)}{r} = Y_2 \frac{1}{r} \frac{d^2\omega}{dr^2} + \frac{1}{r} \frac{\omega}{r} \Omega(\theta, \phi) Y_2 . \quad (6.35)_a$$

The term

$$\nabla^2 \left(S_{12} \frac{\omega(r)}{r}\right),$$

we note, can be written

$$\nabla^2 Y_2 \frac{\omega(r)}{r} = Y_2 \frac{1}{r} \frac{d^2\omega}{dr^2} + \frac{1}{r} \frac{\omega}{r} \Omega(\theta, \phi) Y_2 , \quad (6.35)_b$$

where $r^2\Omega(\theta, \phi)$ is the angular part of the Laplacian. To evaluate the last term, let us note that it contains the angular dependence of the wave function of the D state and that it is actually a linear combination of the spherical harmonics of the second degree. This can be seen by actually carrying out the operation of S_{12} on χ_1^1, i.e.,

$$S_{12}\chi_1^1 = \Big[3 \sin^2\theta\, e^{2i\phi} \chi_1^{-1} + 3\sqrt{2} \sin\theta \cos\theta\, e^{i\phi} \chi_1^0 + (3\cos^2\theta - 1)\chi_1^1\Big] . \quad (6.36)$$

The coefficient of the spin functions are $Y_2^{(2)}$, $Y_2^{(1)}$, and $Y_2^{(0)}$ respectively. Since

$$\Omega(\theta,\phi)\, Y_\ell + \ell(\ell+1)\, Y_\ell = 0,$$

therefore

$$\Omega(\theta,\phi)\, Y_2 = -\, 2(2+1)\, Y_2 = -\, 6Y_2.$$

Applying these results, we find

$$\Omega(\theta,\phi)\, Y_2 = -\, 6S_{12}\chi_1^m\,. \tag{6.37}$$

Hence Eq. (6.34) becomes

$$\Big[\frac{1}{r}\frac{d^2u}{dr^2} + \frac{1}{2\sqrt{2}}\; S_{12}\,\frac{1}{r}\,\Big(\frac{d^2\omega}{dr^2} - \frac{6}{r}\omega\Big)$$

$$+\frac{M}{\hbar^2}\Big\{E + (1+\gamma S_{12})J(r)\Big\}\Big\{\frac{u(r)}{r} + \frac{1}{2\sqrt{2}}\; S_{12}\,\frac{\omega(r)}{r}\Big\}\Big]\chi_1^m = 0. \tag{6.38}$$

Since Eq. (6.38) is identically zero the angle dependent and the angle independent parts must each be identically zero. This fact depends on the linear independence of the spherical harmonics. Making use of $S_{12}^2 = 8 - 2S_{12}$, we can separate Eq. (6.38) into

$$\frac{d^2u}{dr^2} + \frac{M}{\hbar^2}\big[E + J(r)\big]\,\frac{u(r)}{r} = -\, 2^{3/2}\,\frac{M}{\hbar^2}\gamma\omega J(r), \qquad (6.39)_a$$

and

$$\frac{d^2\omega}{dr^2} - \frac{6\omega}{r} + \frac{M}{\hbar^2}\big[E + (1-2\gamma)J(r)\big]\omega = -2^{3/2}\,\frac{M}{\hbar^2}\gamma u(r)\,\omega\,. \qquad (6.39)_b$$

C. THE EVALUATION OF THE ELECTRIC QUADRUPOLE MOMENT

The next step in the solatuon of the problem is to solve the differential equations just obtained and to apply the usual quantum mechanical continuity conditions to the wave functions. To do this, we find, unfortunately that the wave functions for points inside the potential well cannot be solved in terms of any elementary function. Rarita and Schwinger have given a power series solution, but this method involves tedious numerical work. Consequently, we shall develop a method which will enable us to ascertain the order of magnitude of the quadrupole moment arising from the presence of 4% D admixture.

The differential Eqs. (6.39) can be written in the form

$$\frac{d^2u}{dr^2} + K^2 u = -\lambda^2 V_o \omega(r), \qquad (6.40)_a$$

$$\frac{d^2\omega}{dr^2} - \frac{6\omega}{r^2} + K'^2\omega = -\lambda^2 V_o u(r), \qquad (6.40)_b$$

where

$$K^2 = \frac{M}{\hbar^2}(V_o - |E_o|) = \frac{MV_o}{\hbar^2} - \alpha^2, \qquad (6.41)_a$$

$$K'^2 = \frac{M}{\hbar^2}\left[(1 - 2\gamma)V_o - |E_o|\right] = \frac{M}{\hbar^2}(1-2\gamma)V_o - \alpha^2, \qquad (6.41)_b$$

$$\lambda^2 = 2^{3/2}\gamma \frac{M}{\hbar^2} V_o, \qquad (6.41)_c$$

$$\alpha^2 = \frac{M|E_o|}{\hbar^2}, \qquad (6.41)_d$$

and E_o, the experimentally determined binding energy 2.187 Mev. given earlier.

For points outside the potential well ($r > r_o$), V_o vanishes, and consequently, the differential equations assume the simple forms

$$\frac{d^2u}{dr^2} - \alpha^2 u = 0, \tag{6.42$_a$}$$

$$\frac{d^2\omega}{dr^2} - \frac{6\,\omega}{r^2} - \alpha^2\omega = 0. \tag{6.42$_b$}$$

The well-behaved solution of the first equation is

$$u(r > r_o) = A\, e^{-\alpha(r - r_o)}. \tag{6.43$_a$}$$

The solution of the second equation is a little more complicated; it can be shown to be

$$\omega(r > r_o) = c\sqrt{K}\, K_{5/2}\,(K'r), \tag{6.43$_b$}$$

where $K_n(r)$ is known as the modified Bessel functions [36] of the second kind. That $K_{5/2}\,(K'r)$ is a solution of the differential equation can be inferred from the fact that the solution of

$$\frac{d^2y}{dx^2} + \left\{a^2 - \frac{25/4 - \frac{1}{4}}{x^2}\right\} y = 0 \text{ [37]}. \tag{6.44}$$

is $y = \sqrt{x}\, J_{5/2}\,(ax)$. Both $J_{5/2}\,(x)$ and $K_{5/2}\,(x)$ can be expressed in terms of elementary function. These are

$$J_{5/2}(x) = \sqrt{\frac{2}{\pi x}}\left(-\sin x - \frac{3}{x}\cos x + \frac{3}{x^2}\sin x\right), \tag{6.45}$$

$$K_{5/2}(x) = \sqrt{\frac{\pi}{2x}}\,(1 + 3/x + 3/x^2)\, e^{-x}. \tag{6.46}$$

Using these results, we obtain the outside solutions

$$u(r) = A\, e^{-\alpha(r - r_o)}, \qquad r > r_o, \tag{6.47$_a$}$$

$$\omega(r) = Be^{-\alpha(r-r_0)}(1+3/\alpha r + 3/\alpha^2 r^2), \quad r > r_0, \qquad (6.47)_b$$

The inside solutions are difficult to obtain because they satisfy a pair of coupled differential equations. Therefore, let us content ourselves by a very rough method of approximating the solutions. It is to be remembered that we are here primarily interested in determining the effect of the D state on the quadrupole moment and that the effect of the D state is very small, i.e.,

$$\int_0^\infty \omega^2 \, dr = 0.04. \qquad (6.48)$$

From this fact we infer that ω is small in comparison with u. Therefore the solution of

$$\frac{d^2u}{dr^2} + K^2 u = 0$$

given by

$$u = A_0 \sin Kr \qquad (6.49)$$

is fairly close to the correct solution. Connecting this with the outside solution, we obtain

$$A_0 \sin Kr_0 = A, \qquad A_0 K \cos Kr_0 = -\alpha A,$$

or

$$\cot Kr_0 = -\alpha/K.$$

But $K \gg \alpha$, therefore $Kr_0 \approx \pi/2$ and $A \simeq A_0$.

Experiment indicates that the ground state of the deuteron is practically a S state (actually 96%). Consequently we may put

$$\int_0^\infty u^2 \, dr = 1.$$

$$\int_0^\infty u^2\,dr = \int_0^{r_0} A_0^2 \sin^2 Kr\,dr + A^2 e^{2\alpha r_0}\int_{r_0}^\infty e^{-2\alpha r}\,dr$$
$$= \frac{A_0^2}{2}\left(r_0 - \frac{1}{2K}\sin 2Kr_0\right) + \frac{A^2}{2\alpha}$$
$$\simeq \frac{A_0^2}{2} r_0 + \frac{A^2}{2\alpha} = \frac{A^2}{2\alpha}(1+\alpha r_0) = 1,$$
$$A_0^2 \approx A^2 = \frac{2\alpha}{1+\alpha r_0}\,. \tag{6.50}$$

The sine term was dropped because its argument is practically π.

The situation is a little more serious with the D state wave function. The differential equation which it satisfies is coupled to a large function u. However, let us assume that it is possible to neglect this coupling term. The differential equation then becomes

$$\frac{d^2\omega}{dr^2} - \frac{6\omega}{r^2} + K'^2\omega = 0,$$

whose solution is

$$\omega \approx B_0 \sqrt{r}\, J_{5/2}(K'r)\,. \tag{6.51}$$

To determine the relation between the amplitude B and B_0 and also the value of the parameter K', it will be necessary to apply the continuity conditions at $r = r_0$. However, this will lead to a transcendental equation which cannot be solved conveniently. Since we are interested in approximate outside results only, let us look for an approximate outside function which will lead to an easy solution. We might suspect $e^{-\alpha(r - r_0)}$ to be such a function, but the application of the continuity condition will again lead to a transcendental equation. The function $1/r$ is not admissible, since its integral will not converge. However, we will see presently that by approximating the outside solution by $1/r^2$, we can obtain an equation which can be solved easily.

Therefore, let us put

$$\omega(r < r_o) = B_o\sqrt{r}\, J_{5/2}\, (K'r), \tag{6.52a}$$

$$\omega(r > r_o) = B/r^2. \tag{6.52b}$$

Setting the logarithmic derivatives of the inside and outside solutions equal to each other, we obtain

$$\frac{d}{dr}\left[\log B_o + \frac{1}{r}\log r + \log J_{5/2}\,(K'r)\right]_{r=r_o} = \frac{d}{dr}\left[B - 2\log r\right]_{r=r_o},$$

$$\frac{r}{2} + \frac{d}{dr}\log J_{5/2}\,(K'r) = -2/r,$$

$$\frac{\frac{d}{dr} J_{5/2}\,(K'r)}{J_{5/2}\,(K'r)} = -\frac{5}{2r}. \tag{6.53}$$

Eq. (6.53) reduces to

$$J_{5/2}\,(K'r) = 0.$$

The first root of this function [39] is 4.49.

The relation between the amplitude B and B_o is given by

$$B_o\sqrt{r_o}\;\; J_{5/2}\,(K'r_o) = B/r_o^{\,2}.$$

This gives us B in terms of B_o. To evaluate B_o we need to consider

$$.04 = \int_0^\infty \omega^2\, dr = B_o^2\int_0^{r_o} rJ_{5/2}\,(K'r)dr + B^2\int_{r_o}^\infty \frac{dr}{r^4}$$

$$= B_o^2 \int_0^{r_o} r \, J_{5/2}^2 \, (K'r) \, dr + \frac{B^2}{3 r_o{}^3} \, . \tag{6.54}$$

To evaluate the remaining integral, we use the relation

$$\int_0^x x J_n^2 |x| \, dx = \tfrac{1}{2} x^2 \, (J_n{}^2 + J_{n+1}^2) - nx \, J_n \, J_{n+1}$$
$$= \tfrac{1}{2} x^2 \left\{ J_n^2(x) - J_{n-1}(x) \, J_{n+1}(x) \right\} .$$

Therefore

$$\int_0^{r_o} r \, J_{5/2}^2 \, (K'r) \, dr = \tfrac{1}{2} r_o^2 \, J_{5/2}^2 \, (K'r_o),$$

$$B_o^2 \, \tfrac{1}{2} \, r_o^2 \, J_{5/2}^2 \, (K'r) + \frac{B}{3 r_o^2} = 0.04.$$

From Eq. (6.54) we then obtain

$$\frac{B^2}{r_o^2 \, J_{5/2}^2 (K'r)} \, \tfrac{1}{2} \, r_o^2 \, J_{5/2}^2 \, (K'r) + \frac{B}{3 r_o^3} = 0.04,$$

$$B^2 = 6/5 \, (.04) \, r_o^3 \, . \tag{6.55}$$

We are now ready to estimate the value of the quadrupole moment. The quadrupole moment Q is defined as the value of $(3z^2 - r^2)$ averaged over the asymmetrical charge distribution in the magnetic sub-state $m=1$, i.e.,

$$Q = \tfrac{1}{4}(3z^2 - r^2), \quad M_J = 1.$$

Using the wave function given by Eq. (6.31), the above expression becomes

$$Q = \tfrac{1}{4} \iiint \sum_{S_{z_1}} \sum_{S_{z_2}} d\tau \, \frac{1}{\sqrt{4\pi}} \left\{ \frac{u(r)}{r} + \frac{1}{2\sqrt{2}} \, S_{12} \frac{\omega(r)}{r} \right\} \chi_1^1 \, (3z^2 - r^2)$$

$$\cdot \left\{ \frac{u(r)}{r} + \frac{1}{2\sqrt{2}} \, S_{12} \frac{\omega(r)}{r} \right\} \chi_1^1 \frac{1}{\sqrt{4\pi}} = \frac{1}{16\pi} \sum_{S_{z_1}} \sum_{S_{z_2}} \int_0^\infty dr \; r^2 \int_0^\pi d\theta \, \sin \theta$$

$$\cdot\int_0^{2\pi} d\phi \left\{ u^2(3\cos^2\theta - 1)\chi_1^{1\,2}\right\} + \frac{1}{\sqrt{2}}(3\cos^2\theta - 1)\chi_1^1 S_{12}\omega u\,\chi_1^1$$

$$+\,3(\cos^2\theta - 1)\,\frac{\omega^2}{8}\,(S_{12}\chi_1^1)^2. \tag{6.56}$$

Angular integrations give zero for the first term. For the second and third terms we use Eq. (6.36) and the orthogonality conditions of the χ's. We get for the second term $+\frac{1}{5\sqrt{2}}\int_0^\infty dr\ r^2\ u\omega$ and for the third term $-\frac{1}{20}\int_0^\infty dr\ r^2\omega^2$, upon performing the angular integration. Thus we find

$$Q = \frac{1}{5\sqrt{2}}\int_0^\infty dr\ r^2\ u\omega - \frac{1}{20}\int_0^\infty dr\ r^2\omega^2$$

$$= \frac{\sqrt{2}}{10}\int_0^\infty dr\ r^2\ \left(u\omega - \frac{1}{2\sqrt{2}}\,\omega^2\right). \tag{6.57}$$

The second term involving ω^2 is the contribution to the quadrupole moment by the D state. Since this is small, the quadrupole moment will be given practically by

$$Q = \frac{\sqrt{2}}{10}\int_0^\infty dr\ r^2\ u\omega\,.$$

Therefore,

$$Q \simeq \frac{\sqrt{2}}{10}\,A_oB_o\int_0^{r_o} r^2 \sin Kr(\sqrt{r}\ J_{5/2}(K'r))dr + \frac{\sqrt{2}}{10}\int_{r_o}^\infty ABe^{-2\alpha(r-r_o)}dr$$

$$= \frac{\sqrt{2}}{10}\,A_oB_o\int_0^{r_o} r^2 \sin Kr(\sqrt{r}J_{5/2}(K'r))dr + \frac{\sqrt{r}}{10}\,\frac{AB}{2\alpha}\,.$$

The order of magnitude of the integral is

$$\frac{\sqrt{2}}{10}A_oB_or_o^{5/2}J_{5/2}(K'r)r = \frac{\frac{\sqrt{2}}{10}ABr_o^{5/2}J_{5/2}(K'r)r_o}{r_o^{5/2}J_{5/2}(K'r)} = \frac{\sqrt{2}}{10}ABr_o .$$

This is clearly the upper limit of the value of the integral. Because the wave function vanishes at the origin, we would expect the correct value to be considerably smaller. Therefore, it will be neglected. Consequently, we obtain

$$Q \simeq \frac{\sqrt{2}}{10}\frac{AB}{2\alpha} . \qquad (6.58)$$

Squaring Eq. (6.58), we obtain

$$Q^2 \simeq \frac{2}{400\alpha^2}\frac{2}{1+\alpha r_o}\frac{6}{5}(.04)\, r_o^3$$

$$= \frac{.24}{500}\frac{1}{\alpha}\frac{r_o^3}{1+\alpha r_o} .$$

Now

$$\frac{1}{\alpha} = \frac{\hbar}{M|E_o|} = 4.36\times10^{-13}\ \text{cm}, \qquad r_o = 2.8\times10^{-13}\ \text{cm},$$

$$Q^2 \simeq \frac{.24}{500}(4.36\times10^{-13})\frac{(2.8)^3\times10^{39}}{1.64}$$

$$= \frac{23}{500(1.64)}\times10^{-52} = 2.8\times10^{-54} .$$

$$Q = 1.7\times10^{-27}\ \text{cm.}^2.$$

This result is about half the experimentally observed quadrupole moment (2.73×10^{-27}cm.). However, one should not attach too much significance to the numerical result because of the rough approximations that were made. Our calculations indicate only that a D state admixture of 4% leads to a positive quadrupole moment of the order of

10^{-27} cm^2.

VII. CONCLUSION AND DISCUSSION

In this paper, a few of the quantum mechanical problems in the theory of the deuteron were considered. In particular, it was shown that tensor forces can simultaneously account for the observed magnetic dipole and electric quadrupole moments of the deuteron.

It is to be noted, however, that the experiment, which we have discussed, does not give Q directly, but rather the product qQ. The actual value of quadrupole moment, therefore, depends to a large extent upon Nordsieck's [39] calculated value of q, which, in turn, depends upon the reliability of Wang's molecular wave functions. It would indeed be a valuable contribution to nuclear physics if a method were devised to measure the deuteron quadrupole moment directly. Recently Davis et al [40] have reported a new method by which they determined the chlorine quadrupole moment. It will be of interest to see whether their method can be adapted to give an absolute determination of the deuteron quadrupole moment.

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