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The Magnetic Moment of the Li^7 Nucleus. II

J. H. BARTLETT, JR., J. J. GIBBONS, JR. AND R. E. WATSON, *Department of Physics, University of Illinois, Urbana, Illinois*

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Calculation of the magnetic moment of the Li^7 nucleus, using the experimental data of Fox and Rabi and a wave function due to James and Coolidge, results in the value 3.33 nuclear magnetons.

THE magnetic moment of a nucleus is at present determined in a rather indirect way. The hfs splitting of some atomic level is found experimentally (either spectroscopically or by the molecular beam method) and the computed interaction of nucleus with the electron cloud is then used to evaluate the magnetic moment. To compute the interaction for many electrons, one must make an assumption as to the interaction operator, which is then averaged over configuration space. The averaging process requires some knowledge of the electronic wave function. One usually assumes the form of this function, and then determines its constants by the Ritz variational method.

Until quite recently, there has been no opportunity to obtain a fairly accurate check of the hyperfine structure theory, since variational wave functions were not available. The value of the magnetic moment of the lithium nucleus as calculated from the normal atom with a Fock function was shown to be in disagreement with the value calculated from ionized lithium with a Hylleraas-type function.[1, 2] If the latter type of function be assumed to be the more accurate (since there is closer agreement with the experimental values of energy), and the theory of hfs supposed to be correct, then one must conclude that Fock functions are inadequate for calculation of nuclear moments.

However, the situation for lithium has been changed considerably with the computation by James and Coolidge[3] of a ground state wave function involving the interelectronic distances. It seemed, therefore, of some interest to see what the corresponding value of the magnetic moment would be.

HYPERFINE STRUCTURE FORMULA

We have extended the theory of Breit and Doermann[2] to the three-electron case. For one electron, the perturbing part of the Hamiltonian may be written as

$$H'=\frac{(e/mc)(M\cdot\mu)}{1+(E-mc^2+eA_0)2mc^2}\cdot\frac{1}{r^3}+\frac{hec/2\pi}{E+mc^2+eA_0}\left\{-\frac{(\mu\cdot\sigma)}{r^3}+\frac{3(r\cdot\sigma)(r\cdot\mu)}{r^5}\right\}$$

$$+\frac{(hec/2\pi)(e|\mathcal{E}|)}{(E+mc^2+eA_0)^2}\left\{\frac{(\mu\cdot\sigma)}{r^2}-\frac{(r\cdot\sigma)(r\cdot\mu)}{r^4}\right\}$$

$$=(B\cdot\mu)+(A\cdot\sigma).$$

It is assumed that the perturbation for three electrons is simply the sum of three such terms, each pertaining to a particular electron, i.e.

$$\sum H'=\mu\cdot\sum_{j=1}^{3}B_j+\sum_{j=1}^{3}A_j\cdot\sigma_j.$$

To find the hfs splitting for normal lithium, it is sufficient to calculate the energy displacement w for the state of highest f, and to apply the interval rule. The wave function for this state may be

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[1] Results on the basis of a Fock function were obtained by Bartlett and Gibbons, Phys. Rev. **49**, 552 (1936).

[2] Breit and Doermann, Phys. Rev. **36**, 1732 (1930).

[3] H. M. James and A. S. Coolidge, Phys. Rev. **49**, 688 (1936).

written $\mu = N_{\frac{3}{2}}\Phi$, where Φ is the electronic function for $m_s = \frac{1}{2}$, and N is the nuclear function. Since μ_z is the only component of μ with diagonal elements, we may, for the present purpose, confine our attention to it. The perturbation is, effectively:

$$\mu_z \sum_{j=1}^{3} (B_j)_z + \sum_{j=1}^{3} (A_j)_z (\sigma_j)_z.$$

Now

$$(B_j)_z = \frac{(e/mc)}{1+[E-mc^2+e(A_0)_j]/2mc^2} \cdot \frac{1}{r_j^3} \cdot \frac{\hbar}{i} \frac{\partial}{\partial \varphi_j}.$$

The wave function of James and Coolidge is of the form:

$$\Phi = F(123)S(12\bar{3}) + F(231)S(23\bar{1}) + F(312)S(31\bar{2})$$

where the F's are space functions, the S's spin functions, and the bar denotes the electron with β-spin. This is not a function of ϕ_1, ϕ_2 or ϕ_3, but only of the mutual distances. Therefore, there will be no contribution from the B_j's. The above displacement is, then,

$$\begin{aligned} w &= \int \Phi^* (A_{1z}\sigma_{1z} + A_{2z}\sigma_{2z} + A_{3z}\sigma_{3z}) \Phi d\tau \\ &= 3 \int [F(123)]^2 \{A_{1z} + A_{2z} - A_{3z}\} d\tau \\ &= 3 \{ \int [F(123)]^2 A_{1z} d\tau + \int [F(213)]^2 A_{1z} d\tau - \int [F(321)^2] A_{1z} d\tau \}, \end{aligned}$$

since the spin functions above are mutually orthogonal. Here,

$$(A)_z = \frac{hec/2\pi}{E+mc^2+eA_0} \left(-\frac{1}{r^3} + \frac{3z^2}{r^5} \right) \mu_z + \frac{(hec/2\pi)e|\mathcal{E}|}{(E+mc^2+eA_0)^2} \left(\frac{1}{r^2} - \frac{z^2}{r^4} \right) \mu_z.$$

The first term involves P_2 (cos θ), so that there is no contribution to the integral from this. Effectively, then,

$$A_z = \frac{(hec/2\pi)e[dA_0/dr]}{(E+mc^2+eA_0)^2} \frac{\mu_z}{r^2} \cdot \frac{2}{3}, \quad \text{since} \quad \frac{z^2}{r^2} = \frac{1}{3}(P_0 + 2P_2).$$

We have to evaluate integrals such as $\int f^2 A_z dt$, where f is a known function.

$$\begin{aligned} \int f^2 A_z dt &= -4\pi \int f^2 \left(\frac{hec}{2\pi} \right) \cdot \frac{2}{3} \left(\frac{d}{dr} \frac{1}{E+mc^2+eA_0} \right) dr \cdot \mu \\ &= +\frac{8\pi}{3} \mu \int 2ff' \frac{(hec/2\pi)}{2mc^2} dr \\ &= \frac{8\pi}{3} \mu \frac{hec/2\pi}{2mc^2} f^2(0) = \frac{8\pi}{3} \mu\mu_0 f^2(0). \end{aligned}$$

The function $F(123)$ is antisymmetric in electrons 1 and 2, hence

$$w = (8\pi/3)\mu\mu_0 \cdot 3 \int [2F^2(000,\ x_2,\ y_2,\ z_2,\ x_3,\ y_3,\ z_3) - F^2(x_3y_3z_3,\ x_2y_2z_2,\ 000)] d\tau_2 d\tau_3. \tag{A}$$

This represents the energy referred to the center of gravity of the hfs multiplet. [For comparison with the simple theory (wave function separable), put $F(123) = (1/6)^{\frac{1}{2}} \{1s(1)2s(2) - 2s(1)1s(2)\} 1s(3)$, etc.

Then

$$\int F(023)^2 d\tau_2 d\tau_3 = 1/6 \{ [1s(0)]^2 + [2s(0)]^2 \}.$$

Combining, one finds that $w = \frac{1}{3} 8\pi\mu\mu_0 [2s(0)]^2$, which is the ordinary formula.] The doublet separation is, according to the interval rule, $\Delta s = w(2I+1)/I$. (I denotes the nuclear spin.)

WAVE FUNCTION

The wave function to be used is

$$\Phi = F(123)S(12\bar{3}) + F(231)S(23\bar{1}) + F(312)S(31\bar{2}),$$

where

$$F(123) = (1/\pi)^{\frac{3}{2}}\{\sum A_{kmnp}f_{kmnp}(123) + \sum B_{kmnp}g_{kmnp}(123) + \sum C_{kmnp}h_{kmnp}(123)\},$$

$$f_{kmnp}(123) = \psi_{kmnp}(123) - \psi_{kmnp}(213),$$

$$g_{kmnp}(123) = \varphi_{kmnp}(123) - \varphi_{kmnp}(213),$$

$$h_{kmnp}(123) = \chi_{kmnp}(123) - \chi_{kmnp}(213),$$

and

$$\psi_{kmnp}(123) = e^{-(\gamma r_1+\delta r_2+\delta r_3)}r_1{}^k r_2{}^m r_3{}^n r_{12}{}^p,$$

$$\varphi_{kmnp}(123) = e^{-(\gamma r_1+\delta r_2+\delta r_3)}r_1{}^k r_2{}^m r_3{}^n r_{23}{}^p,$$

$$\chi_{kmnp}(123) = e^{-(\gamma r_1+\delta r_2+\delta r_3)}r_1{}^k r_2{}^m r_3{}^n r_{31}{}^p.$$

Here r_1 refers to the $2s$ electron, r_2 to the $1s$ electron with the same spin as the $2s$ electron, r_3 to the other $1s$ electron. James and Coolidge give the following coefficients for the approximate function $F(123)$:[3]

$$B_{1000} = 1.088500, \qquad B_{1001} = 0.583191,$$

$$B_{1010} = 0.058054, \qquad B_{1002} = -0.075465,$$

$$B_{1100} = 0.058054, \qquad B_{0^*000} = -0.970781,$$

$$B_{1020} = B_{1200} = 0.468163, \qquad B_{0^*010} = B_{0^*100} = -0.232377,$$

$$B_{1110} = -0.281807, \qquad A_{0001} = 0.196518,$$

$$C_{0001} = 0.241624.$$

The coefficients marked by the asterisk belong to terms in which the constant γ is to be replaced by γ^*. For example, -0.970781 is the coefficient of g_{0^*000} which is $[e^{-(\gamma^* r_1+\delta r_2+\delta r_3)} - e^{-(\gamma^* r_2+\delta r_1+\delta r_3)}]$. The values of the constants in the exponentials are: $\delta = 3$, $\gamma = 0.65$, $\gamma^* = 1.5$.

For brevity, write $F(123)_{r_1=0} = F(023)$, etc., and $e^{-(\gamma r_1+\delta r_2+\delta r_3)} = (123)$.

Then

$$\begin{aligned} F(203) = (1/\pi)^{3/2}[&(-1.285018 r_2 - 0.641245\, r_2r_3 - 0.392698\, r_2r_3{}^2)(203) - 0.970781\{(0^*23) \\ &- (2^*03)\} + 0.232377\, r_3(2^*03) + 0.009247\, r_3(023) - 0.241624\, r_{23}(203) \\ &- 0.035859\, r_2(023)], \end{aligned}$$

$$F(230) = f(23) - f(32),$$

$$\begin{aligned} \text{where } f(23) = (1/\pi)^{3/2}\{&(230)[1.330124\, r_2 + 0.641245\, r_2r_3 + 0.392698\, r_2r_3{}^2 + 0.196518\, r_{23}] \\ &- (2^*30)[0.970781 + 0.232377\, r_3]\}. \end{aligned}$$

INTEGRALS

Since $\int f^2(23)d\tau_2 d\tau_3 = \int f^2(32)d\tau_2 d\tau_3$, the calculation simplifies. For purposes of checking, we present the results in tabular form. Table I contains the contributions to $\int F(023)^2 d\tau_2 d\tau_3$, Table IIa the contributions to $\int f^2(23)d\tau_2 d\tau_3$, and Table IIb those to $\int f(32)f(23)d\tau_2 d\tau_3$ (except for a factor $(16/\pi)$, which multiplies everything). The entry at the head of a column gives the multiplicand, that at the left of a row the multiplier. The integral of their product is the entry in the table itself. The square

TABLE I. *Contributions to* $\int F(023)^2 d\tau_2 d\tau_3$.

	−1.285018 $(203)r_2$	−0.641245 $(203)r_2r_3$	−0.392698 $(203)r_2r_3{}^2$	−0.970781 (2^*03)	0.970781 (2^*03)	0.232377 $(2^*03)r_3$	−0.035859 $(023)r_2$	0.009247 $(023)r_3$	−0.241624 $(203)r_{23}$
−1.285018 $(203)r_2$	0.0988301								
−0.641245 $(203)r_2r_3$	0.0246589	0.0082035							
−0.392698 $(203)r_2r_3$	0.0100674	0.0041865	0.0025638						
−0.970781 (0^*23)	0.0003905	0.0000974	0.0000398	0.0000808					
0.970781 (2^*03)	−0.0032434	−0.0008093	−0.0003304	−0.0001915	0.0006438				
0.232377 $(203)r_3$	−0.0003882	−0.0001291	−0.0000659	−0.0000229	0.0000774	0.0000123			
−0.035859 $(023)r_2$	0.0000158	0.0000039	0.0000016	0.0000015	−0.0000047	−0.0000006	0.0000000		
0.009247 $(023)r_3$	−0.0000019	−0.0000006	−0.0000003	−0.0000004	0.0000009	0.0000002	0.0000000	0.0000000	
−0.241624 $(023)r_{23}$	0.0188871	0.0047559	0.0019656	0.0000881	−0.0006571	−0.0000821	0.0000033	−0.0000005	0.0036583

TABLE IIa. *Contributions to* $\int f(23)^2 d\tau_2 d\tau_3$.

	1.330124 (230)r_2	0.641245 (230)r_2r_3	0.392698 (230)$r_2r_3^2$	0.196518 (230)r_{23}	−0.970781 (2*30)	−0.232377 (2*30)r_3
1.330124 (230)r_2	0.1058900					
0.641245 (230)r_2r_3	0.0255445	0.0082035				
0.392698 (230)$r_2r_3^2$	0.0104208	0.0041865	0.0025638			
0.196518 (230)r_{23}	0.0158872	0.0038371	0.0015987	0.0024199		
−0.970781 (2*30)	−0.0033573	−0.0008093	−0.0003304	−0.0005344	0.0006464	
−0.232377 (2*30)r_3	−0.0004018	−0.0001291	−0.0000659	−0.0000668	+0.0000774	+0.0000123

TABLE IIb. *Contributions to* $\int f(23)f(32) d\tau_2 d\tau_3$.

	1.330124 (230)r_2	0.641245 (230)r_2r_3	0.392698 (230)$r_2r_3^2$	0.196518 (230)r_{23}	−0.970781 (2*30)	−0.232377 (2*30)r_3
1.330124 (320)r_3	+0.0020218					
0.641245 (320)r_3r_2	+0.0010682	+0.0005643				
0.392698 (320)$r_3r_2^2$	+0.0008961	+0.0004734	+0.0003972			
0.196518 (320)r_{32}	+0.0005082	+0.0002263	+0.0001709	+0.0001177		
−0.970781 (3*20)	−0.0009581	−0.0003079	−0.0001676	−0.0001877	+0.0004540	
−0.232377 (3*20)r_2	−0.0002513	−0.0000808	−0.0000440	−0.0000442	+0.0000724	+0.0000116

arrays are symmetrical about the main diagonal, so that only about half of the total number of entries need be given.

The integration of $F^2(123)$, etc. was straightforward for terms not involving r_{23}. For example, the first term in $\int F(023)^2 d\tau_2 d\tau_3$ is

$$(1/\pi)^3(1.285018)^2\int_0^\infty e^{-2\gamma r_2}r_2^4dr_2\int_0^\infty e^{-2\delta r_3}r_3^2dr_3\int_0^\pi \sin\theta_2 d\theta_2\int_0^\pi \sin\theta_3 d\theta_3\int_0^{2\pi}d\varphi_2\int_0^{2\pi}d\varphi_3$$
$$=(16/\pi).09883008.$$

For terms involving $r_{23}^2=r_2^2+r_3^2+2r_2r_3$ (cos θ_2 cos θ_3+ sin θ_2 sin θ_3 cos $(\phi_2-\phi_3)$ the angular parts integrate to zero, leaving the integral of $(r_2^2+r_3^2)$. The terms involving r_{23} are integrated most easily with a transformed volume element,[4] in which r_{23} appears as variable of integration, between the limits $|r_2-r_3|$ and (r_2+r_3):

$$r_2^2r_3^2 \sin\theta_2 \sin\theta_3 d\theta_2 d\theta_3 d\phi_2 d\phi_3 dr_2 dr_3 = r_2r_3r_{23}dr_{23} \sin\theta' d\theta' d\phi' d\phi dr_2 dr_3,$$

where $\theta'=\theta_2$, $\phi'=\phi_2$, and ϕ is the angle between r_2 and r_3. The range of integration falls into two parts, one for $r_2<r_3$, and the other for $r_3<r_2$. It was found that certain terms cancel out when one integrates first from $r_3=0$ to $r_3=\infty$. For illustration, in Table IIa the entry 0.0158872 represents, except for the factor $16/\pi$, the value of,

$$(0.196518)(1.330124)\int e^{-2\gamma r_2}r_2^2dr_2\int e^{-2\delta r_3}r_3dr_3\int_{|r_2-r_3|}^{r_2+r_3} r_{23}^2dr_{23}. \tag{B}$$

The last integral in this expression is $2r_2^2r_3+(2/3)r_3^3$ if $r_3<r_2$, and $2r_2r_3^2+(2/3)r_2^3$ if $r_2<r_3$. Integrating as above, we obtain the result

$$\int_0^\infty e^{-2\gamma r_2}r_2^2\left(2r_2^2\int_0^{r_2} e^{-2\delta r_3}r_3^2dr_3+(2/3)\int_0^{r_2} e^{-2\delta r_3}r_3^4dr_3+2r_2\int_{r_2}^\infty e^{-2\delta r_3}r_3^3dr_3+(2/3)r_2^3\int_{r_2}^\infty e^{-2\delta r_3}r_3dr_3\right)dr_2.$$

The integrals appearing within the parenthesis are of the form

$$\int_0^r e^{-ar}r^ndr=(n!/a^{n+1})-\sum_{\nu=0}^{n}\frac{n!}{(n-\nu)!}\frac{r^{n-\nu}}{a^\nu} \quad\text{and}\quad \int_r^\infty e^{-ar}r^ndr=\sum_{\nu=0}^{n}\frac{n!}{(n-\nu)!}\frac{r^{n-\nu}}{a^\nu}.$$

Let us write
$$[b]_n=\frac{n!}{b^{n+1}}=\int_0^\infty e^{-br}r^ndr.$$

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[4] Cf. E. A. Hylleraas, Zeits. f. Physik **48**, 475 (1928).

Then all the integrals in question which involve r_{23} can be evaluated as:

$$[a]_{m+3}[b]_{n+2}+(1/3)[a]_{m+1}[b]_{n+4}-(2/b^4)[a+b]_{m+n+2}-(8/b^5)(n+1)[a+b]_{m+n+1}$$
$$-(20/b^6)(n+1)n[a+b]_{m+n}-(40/b^7)(n+1)(n)(n-1)[a+b]_{m+n-1}$$
$$-(70/b^2)(n+1)n(n-1)(n-2)[a+b]_{m+n-2}-\cdots$$

where m and n are the powers, less one, of r_2 and r_3 appearing in the first two integrands of (B). For our integrals, this seven term formula suffices. In the example above, $a=2\gamma$, $b=2\delta$, $m=1$, $n=0$. We have then,

$$16/\pi(0.196518)\{(1.330124)[2\gamma]_4[2\delta]_2+(1/3)[2\gamma]_2[2\delta]_4-\{2/(2\delta)^4\}[2\gamma+2\delta]_3$$
$$-8(2\delta)^{-5}[2\gamma+2\delta]_2\}=(16/\pi)(0.0158872).$$

The values of the two integrals are:

$$\int F(023)^2 d\tau_2 d\tau_3=(16/\pi)0.232590, \quad \int F(230)^2 d\tau_2 d\tau_3=(16/\pi)0.450318.$$

If the second be subtracted from twice the first, the result is $(16/\pi)$ 0.014862.

THE MAGNETIC MOMENT

Let us substitute in Eq. (A), and use $\Delta s=0.0267$ as determined by Fox and Rabi.[5]

$$0.0267=[8\pi(8/3)(g/1838)\mu_0^2(16/\pi)0.014862]/[(0.528\times10^{-8})^3(19.662\times10^{-17})]; \quad \mu_0=0.9174\times10^{-20}.$$

This gives $g=3.33$ nuclear magnetons for the value of the magnetic moment. This is to be compared with that of 3.29 given by Granath[6] (from measurements of hfs in Li$^+$ and the theory of Breit and Doermann).

DISCUSSION

The excellent agreement between the two values of the magnetic moment, one determined from measurements on Li$^+$ and the other from normal Li data, would ordinarily be acceptable as strong evidence that the true value is in the immediate neighborhood. However, there are certain factors which require one to be rather cautious in drawing such a conclusion.

In the first place, our calculation involves the subtraction of two large, approximately equal, quantities. The contribution of the r_{23} terms to $\int[F(023)]^2 d\tau_2 d\tau_3$ is $(16/\pi)0.049889$; that to $\int[F(230)]^2 d\tau_2 d\tau_3$ is $(16/\pi)0.080317$. Subtracting the second from twice the first, one obtains $(16/\pi)0.019461$, which is larger than the corresponding result for all the terms i.e. $(16/\pi)$ 0.014862. This indicates the sensitiveness of the calculation to terms involving the interelectronic distances. It is quite possible that such terms could be modified in such a way that their influence on the energy would be small, but so that the nuclear moment would be changed appreciably.

Secondly, it is not known how good either the Breit-Doermann function or the James and Coolidge function is. A function may give good energy values, but yet be considerably in error near the singularities of the wave equation.

For these reasons, we prefer for the present to regard the value of the magnetic moment of the lithium nucleus as a quantity which has not been determined with great accuracy. If it should prove feasible to measure this moment in a more direct manner, then such a procedure would be much to be preferred, and it would give us more information about electronic wave functions as well.

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[5] Fox and Rabi, Phys. Rev. **48**, 746 (1935).

[6] Granath, Phys. Rev. **42**, 44 (1932).