PHYSICAL REVIEW VOLUME 94, NUMBER 5 JUNE 1, 1954

Magnetic Moment of K^{40} in Intermediate Coupling

G. E. TAUBER* AND TA-YOU WU
National Research Council, Ottawa, Canada
(Received January 15, 1954)

The K^{40} nucleus is of interest since its spin $I=4$ forms a notable exception to Nordheim's rule while the observed value $\mu=-1.29\mu_N$ for the magnetic moment seems to favor the $j-j$ coupling. The theory of intermediate coupling is applied to the configuration $d^{-1}f$ with the view of accounting for the spin and the observed magnetic moment. It is found that a small spin-orbit interaction will lead to a negative magnetic moment. A central nucleon-nucleon interaction of the form $(mP+nQ)V(r_{12})$, where P denotes the Majorana and Q the Bartlett operator, is assumed and calculations have been carried out for the exponential, Yukawa and Gaussian types of potential $V(r_{12})$ with various "ranges." For a suitable choice of the spin-orbit interaction parameter ζ, the observed magnetic moment can be obtained, the exact value of ζ depending on the type of potential and range used.

1. INTRODUCTION

THE spin $I=4$ of the ground state of the K^{40} nucleus forms a notable exception to Nordheim's empirical rule[1] and might indicate that pure j, j coupling does not hold for that nucleus. On the other hand, the negative magnetic moment $\mu=-1.29\mu_N$ observed[2] for K^{40} seems to favor the j, j coupling, since none of the L, S states having the observed spin $I=4$, namely, ${}^3H_4$, ${}^3G_4$, ${}^3F_4$, and ${}^1G_4$, gives rise to a negative magnetic moment, whereas of the four configurations $(d_{5/2})^{-1}f_{5/2}$, $(d_{3/2})^{-1}f_{5/2}$, $(d_{5/2})^{-1}f_{7/2}$, and $(d_{3/2})^{-1}f_{7/2}$ in j, j coupling, the last does give rise to a negative magnetic moment $\mu=-1.70\mu_N$.[3] It was suggested by Feenberg[3] that a possible explanation of the observed moment might be found in an intermediate coupling. In the present note, calculations of the energy levels and the magnetic moment for intermediate coupling have been carried out in the manner of a previous work of the authors.[4]

2. ENERGY LEVELS OF THE $d^{-1}f$ CONFIGURATION

It is reasonable, on the nuclear shell model, to take the proton-neutron configuration of the incomplete shell in the nucleus K^{40} to be $d^{-1}f$, i.e., one d particle missing from a closed shell and an f particle. The 140 states of this configuration can be grouped in the L, S limit into the levels

$$ {}^3H_{6,5,4},\quad {}^3G_{5,4,3},\quad {}^3F_{4,3,2},\quad {}^3P_{2,1,0},\quad {}^1H_5,\quad {}^1G_4,\quad {}^1F_3,\quad {}^1D_2,\quad {}^1P_1. \tag{1}$$

The matrix elements of the particle-particle interaction can be calculated with the aid of the theorem of trace invariance for the case of a d and an f particle, if for the d particle one uses the m_l and m_s value of the "missing" particle in the complete shell and changes the sign of the resulting matrix element.[5] This will give the correct matrix element up to an additive constant. Consider, for example, a state in the m_l, m_s representation in which the missing d particle from the closed shell d^{10}, denoted by d' for the moment, has the quantum numbers m_l', m_s'. The matrix elements of the particle-particle interactions in the configuration $d^{-1}f$, $d^{10}f$ are related by

$$E(d^{-1}f)=E(d^9f),$$
$$E(d^9f)=E(d^{10}f)-E([d^9]d')-E(d'f),$$

where $E([d^9],d')$ means the interaction energy between the d' particle and the other nine d particles. This may be written

$$E(d^9f)=E(d^{10}f)-E(d^{10})+E(d^9)-E(d'f).$$

Since the first 3 terms on the right are independent of the m_l', m_s' of the missing d particle, we may write

$$E(d^9f)=\text{const}-E(d'f), \tag{2}$$

in so far as relative energies of the various states in (1) are concerned.

A general nucleon-nucleon interaction of the form

$$V_{12}=(mP+nQ)V(|\mathbf{r}_1-\mathbf{r}_2|) \tag{3}$$

has been assumed, where P and Q are the Majorana and Bartlett operators, respectively, and V is a central potential. As we are dealing only with central interactions, the potential can be expanded in a series of Legendre polynomials and the resulting interaction expressed in terms of the Slater integrals defined by

$$F^k(a_1,a_2)=\int\int R_{a_1}{}^2(r_1)R_{a_2}{}^2(r_2)f_k(r_1r_2)dr_1dr_2$$

$$G^k(a_1,a_2)=\int\int R_{a_1}(r_1)R_{a_2}(r_2)f_k(r_1r_2)R_{a_1}(r_2)R_{a_2}(r_1)dr_1dr_2$$

where

$$f_k=\frac{2k+1}{2}\int V(|\mathbf{r}_2-\mathbf{r}_1|)P_k(\cos\omega_{12})d\cos\omega_{12}. \tag{4}$$

* National Research Laboratories Postdoctorate Fellow.
[1] L. W. Nordheim, Phys. Rev. **78**, 294 (1950); A. de Shalit, Phys. Rev. **91**, 1479 (1953).
[2] P. F. Klinkenberg, Revs. Modern Phys. **24**, 63 (1952); Eisinger, Bederson, and Feld, Phys. Rev. **86**, 73 (1952) give $\mu=-1.30\mu_N$.
[3] E. Feenberg, Phys. Rev. **76**, 1275 (1949); I. Talmi, Phys. Rev. **83**, 1248 (1951); H. M. Schwarz, Phys. Rev. **89**, 1293 (1953).
[4] G. E. Tauber and Ta-You Wu, Phys. Rev. **93**, 295 (1954).
[5] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, Cambridge, 1951), second edition.

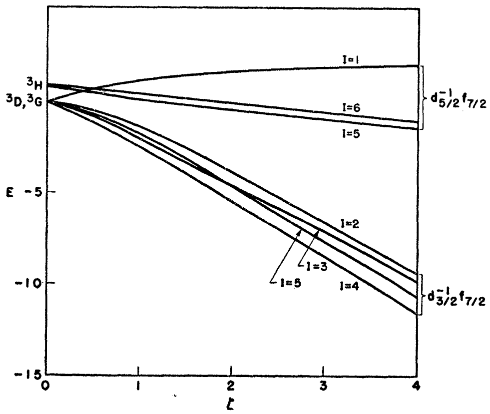

FIG. 1. Energy levels of K^{40} as a function of spin-orbit parameter ζ for Yukawa potential, $r_0=1.0\times10^{-13}$ cm. Scales in Mev. Only the lowest levels are shown.

The energies of the various states in the $L-S$ limit for the $d^{-1}f$ configuration are given in Table I. The accidental degeneracy of some of these states (and vanishing matrix elements) is due to the fact that on introducing the missing particle all triplet states $(m_1m_s, m_1'm_s'|Q|m_1m_s, m_1'm_s')$ vanish on account of the spin wave functions, and that the sum of $(m_1m_s, m_1'm_s'|P|m_1m_s, m_1'm_s')$ is the same for a given value of M and S.[6]

To evaluate the integrals F_i and G_i, we shall assume for the radial wave functions R the harmonic oscillator wave functions. The Slater integrals can be expressed in terms of the Talmi integrals I_l for harmonic oscillator wave functions,[7]

$$I_l=N_l^2\int_0^\infty \exp(-\nu r^2)r^{2l+2}V(r)dr, \qquad (5)$$

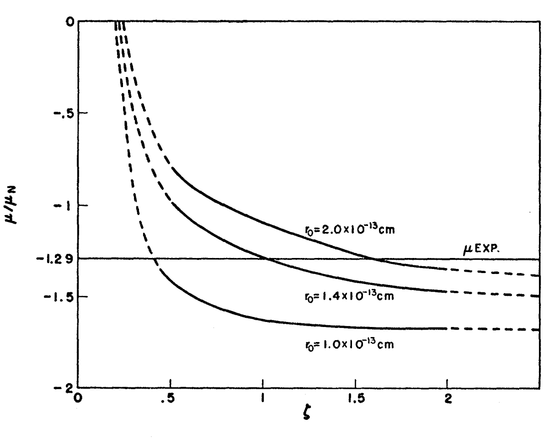

FIG. 2. Magnetic moment of K^{40} as a function of spin-orbit parameter ζ for exponential potential and various ranges. Magnetic moment in units of μ_N. The parameter ζ is in Mev. Dotted parts of the graphs indicate results near L, S and j, j limits.

[6] See reference 5, Chapter 6, Table I.
[7] I. Talmi, Helv. Phys. Acta **25**, 185 (1952).

as follows:

$$\begin{aligned}
160\,G^1&=99(I_0-I_5)+9(I_1-I_4)+38(I_2-I_3), & G_1&=G^1/35,\\
160\,G^3&=21[11(I_0-I_5)-19(I_1-I_4)+2(I_2-I_3)], & G_3&=G^3/315,\\
160\,G^5&=363[(I_0-I_5)-5(I_1-I_4)+10(I_2-I_3)], & G_5&=G^5/1524.6,\\
160\,F^0&=33(I_0+I_5)+21(I_1+I_4)+26(I_2+I_3), & F_0&=F^0,\\
160\,F^2&=15[11(I_0+I_5)-5(I_1+I_4)-6(I_2+I_3)], & F_2&=F^0/105,\\
160\,F^4&=297[(I_0+I_5)-3(I_1+I_4)+2(I_2+I_3)], & F_4&=F^4/693.
\end{aligned} \qquad (6)$$

A general method for obtaining the coefficients in (6) in any problem of this kind is given in Appendix I.[8]

TABLE I. Energy states for $d3^1f$ configuration in $L-S$ limit.

State	P	Q
^3H	$-210G_5$	0
^1H	$-210G_5$	$-2F_0-20F_2-6F_4$
^3G	0	0
^1G	0	$-2F_0+30F_2+44F_4$
^3F	$-60G_3$	0
^1F	$-60G_3$	$-2F_0+22F_2-132F_4$
^3D	0	0
^1D	0	$-2F_0-12F_2+198F_4$
^3P	$-35G_1$	0
^1P	$-35G_1$	$-2F_0-48F_2-132F_4$

To carry out the calculation, we have confined ourselves to the following types of potentials:[4]

$$\begin{aligned}
&\text{(i)} \quad \text{Exponential} \quad V(r)=V_0^E e^{-r/r_0},\\
&\text{(ii)} \quad \text{Yukawa} \quad V(r)=V_0^Y e^{-r/r_0}(r_0/r),\\
&\text{(iii)} \quad \text{Gaussian} \quad V(r)=V_0^G \exp(-r^2/r_0^2),
\end{aligned} \qquad (7)$$

where V_0 is the depth and r_0 the "range" of the potential. These constants and m and n appearing in the interaction can be estimated from the data of two free nucleons.[9] With these values the Talmi integrals I_l for the various interactions and ranges can be calculated, and finally the energies of the various states (Table I) can be obtained by inserting the appropriate expressions for the F's and G's.

In order to obtain the energy levels for any intermediate coupling between the L, S and j, j limits, the secular equations must be solved. From (1) it is seen that there are three equations of order 4 ($I=4$, 3 and 2), two of order 3 ($I=5$ and 1) and two linear ones ($I=6$ and 0). The spin-orbit matrices for two nucleons are known[10] and can be given in terms of two parameters

[8] A more general method, but not as readily adaptable for numerical calculations, has been given by E. H. Kronheimer, Phys. Rev. **90**, 1003 (1953).
[9] See reference 4, Table II.
[10] G. Racah, Physica **16**, 651 (1950).

$\zeta_1 = \zeta_d$ and $\zeta_2 = \zeta_f$. As in the shell-model of Mayer *et al.*[11] the spin-orbit interaction is to be assumed negative for particles and positive for "holes," one can write

$$\zeta_d = \zeta, \quad (\zeta > 0), \qquad \zeta_f = -a\zeta, \tag{8}$$

where a is an arbitrary positive constant $a \geq 1$. The secular equations are particularly simple for $a = 1$ and already give a splitting of the correct order for the d and f levels;[12] they are given in Appendix II. The energy levels as functions of the spin-orbit parameter ζ for the various ranges and potentials considered can then be obtained by inserting the corresponding values of the $L-S$ energies and solving them numerically. Figure 1 shows the energy levels for one range in the Yukawa potential. It is seen that the lowest level has the spin $I = 4$ in agreement with observation. The levels for the other types of interactions and ranges are similar.

3. MAGNETIC MOMENT OF K[40]

The magnetic moment is given by the expectation value of the operator

$$\mu = \sum_{i=P,N} (m_l^i g_l^i + m_s^i g_s^i)\mu_N, \tag{9}$$

where m_l^i and m_s^i are the orbital and spin angular momentum operators of the nucleons, respectively, and g_l^i and g_s^i are the gyromagnetic ratios of orbit and spin, respectively, and are given by

$$g_l^P = 1, \quad g_l^N = 0,$$
$$g_s^P = 5.58, \quad g_s^N = -3.82.$$

In order to adapt (9) to a hole-particle configuration, it is again sufficient to consider only the missing particle instead of the nearly completed shell, provided the eigenvalues of the operators m_l^P and m_s^P are replaced by their negatives. The appropriate wave function is found from the solution of the secular equation. For $I = 4$ it is a linear combination of the (zeroth-order) wave functions corresponding to the states $^3H_4$, $^3G_4$, $^3F_4$, and $^1G_4$ and can be written as

$$\psi(4_14) = \alpha\psi(^3H_4) + \beta\psi(^1G_4) + \gamma\psi(^3F_4) + \delta\psi(^3G_4), \tag{10}$$

where the coefficients α, β, γ, δ are obtained from the appropriate solution of the secular equation for $I = 4$, and satisfy the requirement that $\alpha^2 + \beta^2 + \gamma^2 + \delta^2 = 1$. The (zeroth-order) wave functions are obtained by properly combining the states corresponding to the various values of M_l and M_s into multiplets and are given in Appendix III. The phases have been so chosen as to give the known expressions for the spin-orbit matrices.[10]

Applying the operator μ in (9) to the wave function (10) one obtains for the magnetic moment:

$$\langle\mu\rangle/\mu_N = 1.47\alpha^2 + 1.4\beta^2 + 1.63\gamma^2 + 1.51\delta^2 + 0.43\alpha\delta - 8.41\beta\delta + 0.645\gamma\delta. \tag{11}$$

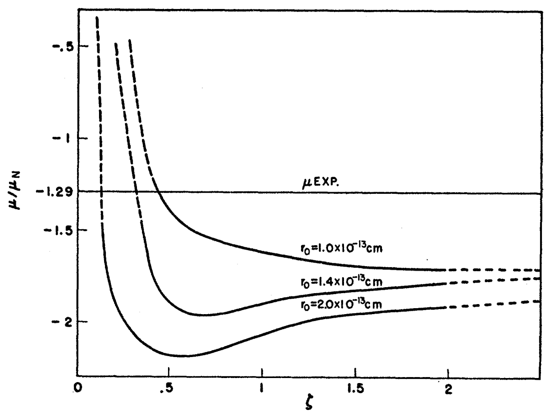

FIG. 3. Magnetic moment of K[40] as a function of spin-orbit parameter ζ for Yukawa potential and various ranges. For scale and notation see Fig. 2.

The magnetic moment as a function of the spin-orbit parameter ζ has been plotted for the various potentials and ranges considered (Figs. 2–4). From these figures it is seen that for large values of the spin-orbit parameter the $j-j$ coupling value $\mu = -1.70\mu_N$ is obtained as an asymptotic limit, and also that a comparatively small amount of spin-orbit coupling is sufficient to give the (observed) negative magnetic moment $\mu = -1.29\mu_N$. This is due to the appearance of cross terms in Eq. (11) which do not appear in the $L-S$ limiting case.[13]

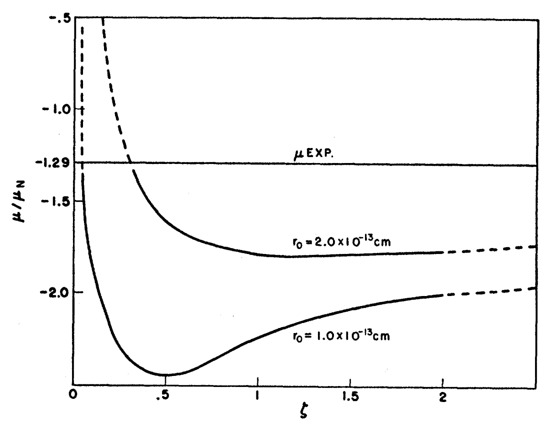

FIG. 4. Magnetic moment of K[40] as a function of spin-orbit parameter ζ for Gaussian potential and various ranges. For scale and notation see Fig. 2.

ACKNOWLEDGMENT

We wish to express our appreciation to Miss E. Motard for carrying out the numerical calculations involved.

[11] M. G. Mayer, Phys. Rev. **74**, 235 (1948); **75**, 1969 (1949); **78**, 16 (1950). Haxel, Jensen, and Suess, Phys. Rev. **75**, 1766 (1949).

[12] The case for $a = 2$ has also been considered without changing the final results materially.

[13] In the L, S limit, the lowest level $^3G_4$ has $\mu = 1.51\mu_N$.

APPENDIX I. CALCULATION OF SLATER INTEGRALS IN TERMS OF TALMI INTEGRALS

The Slater integrals occuring in calculations of $L-S$ limit matrix elements are given by Eq. (4) of the test, where for the radial wave function we use harmonic oscillator wave functions

$$R_{a1}(r)=N_{l_1}r^{l_1+1}\exp(-\tfrac{1}{2}\nu r^2),\quad n=0,$$
$$R_{a2}(r)=N_{l_2}r^{l_2+1}\exp(-\tfrac{1}{2}\nu r^2).$$

The Legendre polynomials P_k can be expressed in terms of a power series in $\cos\omega_{12}$ for which the coefficients are well known.[14]

$$P_k(\cos\omega_{12})=\sum_{a=0,1}^{m}C_a\cos^a\omega_{12},\quad a=\begin{cases}\text{even for } k \text{ even,}\\ \text{odd for } k \text{ odd,}\end{cases}\tag{12}$$

the upper limit m being $m=k/2$ or $(k-1)/2$ according as k is even or odd.

If one now introduces two new integrals, A^a and B^a, defined by

$$\begin{aligned}A^a&=\tfrac{1}{2}N_{l_1}^2N_{l_2}^2\int\int\int(r_1r_2)^{l_1+l_2+2}\exp[-\nu(r_1^2+r_2^2)]\\&\qquad\times V(|\mathbf{r}_1-\mathbf{r}_2|)\cos^a\omega_{12}d\cos\omega_{12}dr_1dr_2,\\B^a&=\tfrac{1}{2}N_{l_1}^2N_{l_2}^2\int\int\int r_1^{2l_1+2}r_2^{2l_2+2}\exp[-\nu(r_1^2+r_2^2)]\\&\qquad\times V(|\mathbf{r}_1-\mathbf{r}_2|)\cos^a\omega_{12}d\cos\omega_{12}dr_1dr_2,\end{aligned}\tag{13}$$

F and G can be expressed as sums involving the new integrals

$$F^k=(2k+1)\sum_{a=0}^{m}C_aB^a,\quad G^k=(2k+1)\sum_{a=1}^{m}C_aA^a.\tag{14}$$

Following Talmi one now introduces new coordinates defined by

$$\mathbf{r}=\mathbf{r}_2-\mathbf{r}_1,\quad 2\mathbf{R}=\mathbf{r}_1+\mathbf{r}_2,\quad \cos\vartheta=(\mathbf{r}\cdot\mathbf{R})/rR.$$

The R and ϑ integration can be done immediately, and one finally obtains for A and B the series

$$A^a=\sum_{s=0}^{L}K_sb_s^aI_s,\quad B^a=\sum_{s=0}^{L}K_sd_s^aI_s,\tag{15}$$

where

$$K_s=2^{-L}(1+2s)!!(2p-1)!!/(1+2l_1)!!(1+2l_2)!!;$$

b_s^a is the coefficient of y^s in the sum

$$\sum_{\sigma=0}^{(L-a)/2}\binom{(L-a)/2}{\sigma}\frac{2^{2\sigma}}{2\sigma+1}(-1)^\sigma x^\sigma y^\sigma(x+y)^{L-a-2\sigma}(x-y)^a;$$

d_s^a is the coefficient of y^s in the sum

$$\sum_{\sigma}^{L_1}\sum_{\tau}^{L_2}\binom{L_1}{\sigma}\binom{L_2}{\tau}\frac{2^{2\rho}}{2\rho+1}(-1)^\sigma x^\rho y^\rho(x+y)^{L-a-2\rho}(x-y)^a,\quad 2\rho=\sigma+\tau;$$

$n!!=n(n-2)\cdot(n-4)\cdots2$ or 1, according as n is even or odd; $L=l_1+l_2$, where l_1 and l_2 are the angular momenta, $L_1=l_1-\frac{1}{2}a$, $L_2=l_2-\frac{1}{2}a$, and $p=L+1-s$.

On combining (4) and (5), F and G can be expressed in terms of the Talmi integrals by tabulating the required coefficients, which are obtainable by inspection without having to do any integration. It should be noted that $B^a=A^a$ (and hence $F^k=G^k$) if both angular momenta are the same, i.e., $l_1=l_2$. The method can also be extended to the case for which the radial quantum number $n\neq0$.

[14] See, e.g., E. Jahnke and F. Emde, *Tables of Functions* (Dover Publications, New York, 1943).

APPENDIX II. SECULAR EQUATIONS FOR $d^{-1}f$ CONFIGURATION [FOR $a=1$ IN (8)]

$$I=6,\qquad E={}^3H-\tfrac{1}{2}\zeta$$

$$I=5,\qquad \begin{vmatrix}{}^1H-E & 0 & -\frac{1}{2}\zeta\sqrt{30}\\ 0 & {}^3G-\frac{3}{5}\zeta-E & 6\zeta/5\\ -\frac{1}{2}\zeta\sqrt{30} & 6\zeta/5 & {}^3H+\zeta/10-E\end{vmatrix}=0,$$

$$I=4,\qquad \begin{vmatrix}{}^3H+3\zeta/5-E & 0 & 0 & \zeta\sqrt{88}/\sqrt{75}\\ 0 & {}^1G-E & 0 & -\zeta\sqrt{5}\\ 0 & 0 & {}^3F-3\zeta/4-E & \zeta\sqrt{125}/\sqrt{48}\\ \zeta\sqrt{88}/\sqrt{75} & -\zeta\sqrt{5} & \zeta\sqrt{125}/\sqrt{48} & {}^3G+3\zeta/20-E\end{vmatrix}=0,$$

$$I=3,\qquad \begin{vmatrix}{}^3G+3\zeta/4-E & 0 & 0 & 15\zeta/\sqrt{112}\\ 0 & {}^1F-E & 0 & -\zeta/\sqrt{3}\\ 0 & 0 & {}^3D-\zeta-E & \zeta\sqrt{24}/\sqrt{7}\\ 15\zeta/\sqrt{112} & -\zeta/\sqrt{3} & \zeta\sqrt{24}/\sqrt{7} & {}^3F+\zeta/4-E\end{vmatrix}=0.$$

$$I=2,\qquad \begin{vmatrix}{}^3F+\zeta-E & 0 & 0 & \zeta\sqrt{12}/\sqrt{5}\\ 0 & {}^1D-E & 0 & -\sqrt{6}\zeta/2\\ 0 & 0 & {}^3P-3\zeta/2-E & \sqrt{18}\zeta/\sqrt{5}\\ \zeta\sqrt{12}/\sqrt{5} & -\zeta\sqrt{6}/2 & \zeta\sqrt{18}/\sqrt{5} & {}^3D+\zeta/2-E\end{vmatrix}=0,$$

$$I=1,\qquad \begin{vmatrix}{}^3P+3\zeta/2-E & 0 & \sqrt{2}\zeta\\ 0 & {}^1P-E & -\zeta/\sqrt{2}\\ \sqrt{2}\zeta & -\zeta/\sqrt{2} & {}^3P+3\zeta/2-E\end{vmatrix}=0,$$

$$I=0,\qquad E={}^3P+3\zeta.$$

Here ${}^3H$ stands for the energy in the L, S limit in Table I, etc.

APPENDIX III. WAVE FUNCTIONS FOR $d^{-1}f$ CONFIGURATION

The 140 wave functions can be grouped together in states of definite M_l and M_s enumerated in Eq. (1) in the text. The corresponding wave functions are linear combinations of the above and can be found either by direct diagonalization or using the operators[15]

$$\mathfrak{L}_\pm=L_x\pm iL_y,\quad \mathcal{S}_\pm=S_x\pm iS_y,\quad \mathcal{J}_\pm=J_x\pm iJ_y.$$

The wave functions required in calculating the magnetic moment are those for which $I=M=4$ and are given in the following:[16]

$$\begin{aligned}\psi({}^3H_4)=&\Big\{\frac{3}{\sqrt{20}}[\sqrt{6}(-2^-,2^-)+\sqrt{6}(-2^+,2^+)\\&-2(-1^-,3^-)-2(-1^+,3^+)]-3\sqrt{5}(-2^+,3^-)-\frac{1}{\sqrt{30}}\\&\times[\sqrt{10}(-2^-,1^+)-4(-1^-,2^+)+2(0^-,3^+)]\Big\}\Big/\sqrt{55},\\ \psi({}^1G_4)=&-[\sqrt{2}(-2^-,2^-)+\sqrt{3}(-1^-,3^-)\\&-\sqrt{2}(-2^+,2^+)-\sqrt{3}(-1^+,3^+)]/\sqrt{10},\\ \psi({}^3F_4)=&-[\sqrt{2}(-2^-,1^+)+\sqrt{5}(-1^-,2^+)+\sqrt{5}(0^-,3^+)]/\sqrt{12},\\ \psi({}^3G_4)=&\{2\sqrt{2}[\sqrt{2}(-2^-,2^-)+\sqrt{2}(-2^+,2^+)\\&+\sqrt{3}(-1^-,3^-)+\sqrt{3}(-1^+,3^+)]-[\sqrt{10}(-2^-,1^+)\\&+(-1^-,2^+)-3(0^-,3^+)]\}/10.\end{aligned}$$

[15] N. M. Gray and L. A. Wills, Phys. Rev. **38**, 248 (1931).

[16] The first figure in each parenthesis gives the m value of the "missing" proton, with the + or − denoting the z component of the spin equal to $+\frac{1}{2}$ or $-\frac{1}{2}$, respectively. The second figure gives the corresponding information for the neutron.