that $\theta_0 = 1$ implies $\gamma = (t + q_0)\nu$. The possibility remains, however, that in the Ising model the $\tilde{q}_0(\vec{r}, \kappa)$ given by Eq. (8) behaves like a nonzero constant only for r near 1 with $\tilde{q}_0(\vec{r}, \kappa) \approx 0$ for $1 \ll r \ll \Lambda$. In this case Eq. (9) would no longer define a Λ_0 that would manifest itself in any tangible way in the structure of $\hat{F} - \hat{F}_c$. This is precisely the situation in the spherical-model case, where if $d \geq 4$, both $\tilde{q}(\vec{r}, \kappa)$ and $\tilde{q}_0(\vec{r}, \kappa)$ for small κ are $d - 4$ for $r \approx 1$ but zero for $r \gg 1$. Although we do not believe that the situation is similar in the 3-d Ising case, there is surely room for further clarification on this point. What is strongly suggested to us by our analysis is the application of the numerical methods of Ref. 2 to the 5-d spherical model, for which one knows that $\tilde{q}_0 \approx 0$ for $r \gg 1$ but $\tilde{q}_0 \approx 1$ for $r \approx 1$. The question is: Will the numerical analysis reveal that strong scaling of $\hat{F}(\vec{r})$ for $r \gg 1$ is preserved, as one knows it is, or will the $\tilde{q}_0 \approx 1$ for $r \approx 1$ misleadingly suggest numerically that strong scaling has been violated?

A second question that the work of this paper raises is whether we can safely identify the Λ_0 and θ_0 of the critical isochore with Λ and θ, respectively. The physical significance of θ discussed in Ref. 7 suggests the identification, despite the fact that we cannot safely identify q with q_0. If we do equate θ and θ_0, we have from (9) and our earlier equations that

$$q_0 = q(1 - \alpha)/2\beta \ . \tag{10}$$

Taking $\alpha = 1/8$, $\beta = 5/16$, and using the values $q = 3/50$ and $q = 1/12$, which probably represent two extreme possibilities,[1] we find $q_0 = 21/250$ and $q_0 = 7/60$, respectively. These values are consistent with the $1/7 \pm 1/14$ from Ref. 2. Nevertheless, it would clearly be valuable to have some more-or-less direct numerical assessment of q that eliminates the necessity of our going through (10) in order to make contact with the rest of our scaling relations.

I am indebted to D. Jasnow and M. A. Moore for helpful conversations and correspondence.

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*Work supported in part by the Research Foundation of State University of New York, Albany, N. Y.

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[5]In the spherical model, the argument used in Ref. 1 to obtain Eq. (2) for the Ising model is not applicable. Nevertheless $\hat{F} - \hat{F}_c \approx f_2(\vec{r})M^2$ as $r \to 1$, with $f_2(\vec{r})$ depending on r like r^0. Setting $q \approx 0$ for $r \gg 1$, we find the $f(x)$ of Eq. (1) for the spherical model to be $x^{2/\epsilon}$, and (7a) follows with q still given by (4), although strictly speaking some orientational dependence of $\tilde{q}$ on r must be expected for $r \approx 1$.

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PHYSICAL REVIEW B VOLUME 2, NUMBER 7 1 OCTOBER 1970

Mean g Values of Rare-Earth Ions: Extension to Monoclinic Symmetries

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(Received 14 May 1970)

A previous calculation of the mathematical properties of a Kramers doublet for extrema of the mean g value is extended to monoclinic symmetries. The theory is applied to the paramagnetic resonance data for $LaF_3:Yb^{3+}$. These data are shown to be consistent with a Yb^{3+} site of C_{2v} point symmetry.

In a recent paper,[1] some mathematical properties of an isolated Kramers doublet were derived for the condition that the mean g value was an extremum. The doublet wave functions were expressed as linear combinations of free-ion states associated with a single value of J; i.e.,

$$\begin{aligned} |\alpha\rangle &= \sum_M a_M |J, M\rangle \ , \\ |\beta\rangle &= \sum_M (-1)^{(J-M)} a_M^* |J, -M\rangle \ , \end{aligned} \tag{1}$$

with

$$\sum_M |a_M|^2 = 1 \quad , \tag{2}$$

where a_M^* is the complex conjugate of a_M, and the values of M in the summations depend on the point symmetry of the magnetic ion.

The crystalline potential may be expanded in tesseral harmonics Z_{nm}^c and Z_{nm}^s.[2] The most general application of the theory of Ref. 1 is to systems with rotational symmetries no higher than twofold. Such systems may be classified as orthorhombic or monoclinic.[3] In both classes, a suitable choice of axes limits the tesseral harmonics of even n to those with even m.[4] The two classes may be distinguished as follows: (i) Orthorhombic Symmetries (C_{2v}, D_2, D_{2h})[3]: only harmonics of the type Z_{nm}^c (with n, m even) are considered[4]; the phases of the off-diagonal matrix elements, and hence those of the coefficients a_M,[5] differ by an integral multiple of π; (ii) Monoclinic Symmetries (C_s, C_2, C_{2h})[3]: harmonics of both types Z_{nm}^c and Z_{nm}^s (with n, m even) are considered[4]; no simple phase relationships necessarily exist between the coefficients a_M. The calculation of Ref. 1 is applicable to case (i), since there is no loss of generality if the a_M are treated as real. In this note, a corresponding procedure is outlined for case (ii).[6]

The principal g values are defined as follows[7]:

$$g_z \equiv 2\Lambda \langle \alpha | J_z | \alpha \rangle, \quad g_x \pm g_y \equiv 2\Lambda \langle \alpha | J \pm | \beta \rangle \quad , \tag{3}$$

where Λ is the Landé splitting factor. Substitution of the wave functions of Eq. (1), with a_M expressed as $|a_M| \exp(i\phi_M)$, gives

$$g_z = 2\Lambda \sum_M |a_M|^2 M \quad , \tag{4a}$$

$$g_x + g_y = 2\Lambda \sum_M |a_M| \, |a_{M'}| \exp(i\phi_M')[(J+M)(J+M')]^{1/2} + \Lambda |a_{1/2}|^2 \exp(i\phi_{1/2}') \quad , \tag{4b}$$

$$g_x - g_y = 2\Lambda \sum_M |a_M| \, |a_{M''}| \exp(i\phi_M'')[(J-M)(J-M'')]^{1/2} \quad , \tag{4c}$$

where

$$M' = -M+1 \quad , \quad M'' = -M-1 \quad , \tag{5}$$

and

$$\phi_M' = (J-M)\pi - (\phi_M + \phi_{M'}) \quad ,$$

$$\phi_{1/2}' = (J-\tfrac{1}{2})\pi - 2\phi_{1/2} \quad , \tag{6}$$

$$\phi_M'' = (J-M)\pi - (\phi_M + \phi_{M''}) \quad .$$

An arbitrary phase angle $\pm\delta$ associated with the matrix elements of $J\pm$ has been omitted from Eq. (6).[8]

The sense of the Larmor precession of the magnetic moment has been shown to depend on the sign of the product $g_x g_y g_z$.[9,10] However, according to Eq. (4), the function $g_x g_y g_z$ may be complex and we replace it by the following function:

$$P \equiv \tfrac{1}{2}(g_x^* g_y + g_y^* g_x) g_z$$

$$= \tfrac{1}{4}[(g_x+g_y)^*(g_x+g_y) - (g_x-g_y)^*(g_x-g_y)] g_z \quad . \tag{7}$$

The sign of P thus depends on the sign of g_z and on the relative magnitudes of g_x+g_y and g_x-g_y.

The mean g value is defined experimentally by the equation

$$3\,\bar{g}(\text{expt}) = |g_z| + |g_x| + |g_y| \quad , \tag{8}$$

where $|g_x|$, $|g_y|$, and $|g_z|$ are the principal g values of the paramagnetic resonance spectrum. In order to calculate the maxima of this function, we look for the maxima and minima of the following functions:

$$3\,\bar{g}_1 = g_z \pm |g_x + g_y| \quad , \tag{9a}$$

$$3\bar{g}_2 = g_z \pm |g_x - g_y| \quad . \tag{9b}$$

Equation (2) restricts the magnitudes $|a_M|$ but not the phases ϕ_M. Therefore, for a given set of $|a_M|$, the function g_x+g_y has its maximum magnitude when each term on the right-hand side of Eq. (4b) has the same phase. In calculating the extrema of $\bar{g}_1$, the extreme value of g_x+g_y with respect to phase is substituted into Eq. (9a); i.e., Eq. (4b) is replaced by

$$(g_x+g_y)_e = \{2\Lambda \sum_M |a_M| \, |a_{M'}| \, [(J+M)(J+M')]^{1/2} + \Lambda |a_{1/2}|^2 (2J+1)\} \exp(i\Phi') \quad , \tag{10a}$$

where Φ' is independent of M. Similarly, in calculating the extrema of $\bar{g}_2$, Eq. (4c) is replaced by

$$(g_x-g_y)_e = 2\Lambda \sum_M |a_M| \, |a_{M''}| \times [(J-M)(J-M'')]^{1/2} \exp(i\Phi'') \quad , \tag{10b}$$

where Φ'' is independent of M. The extreme values of $\bar{g}_1$ and $\bar{g}_2$ [Eq. (9)], the sign of P [Eq. (7)], and the relationships between the magnitudes of the coefficients a_M at these extrema may now be derived using the procedures given in Ref. 1. The

results which are shown in Table I are the same as those obtained in Ref. 1, except that no phase relationships between coefficients are obtained.

The paramagnetic resonance spectrum of Yb^{3+} ($4f^{13}$, $J=\frac{7}{2}$, $\Lambda=\frac{8}{7}$) in LaF_3[11] has an experimental mean g value near a maximum $\frac{2}{3}\Lambda(J+1)$, and was treated in Ref. 1 by a procedure valid for a Yb^{3+} site of orthorhombic point symmetry. Recent crystallographic investigations,[12] however, favor the lower symmetry C_2 for the La^{3+} site. In this case, the wave function $|\alpha\rangle$ of Eq. (1) may be written

$$|\alpha\rangle = a\exp(i\phi_1)\left|\tfrac{5}{2}\right\rangle + b\exp(i\phi_2)\left|\tfrac{1}{2}\right\rangle + c\exp(i\phi_3)\left|-\tfrac{3}{2}\right\rangle + d\exp(i\phi_4)\left|-\tfrac{7}{2}\right\rangle , \quad (11)$$

where the quantum number $J=\frac{7}{2}$ is omitted and the parameters a, b, c, d are real and positive. Equations (2) and (4) give

$$a^2+b^2+c^2+d^2=1 , \quad (12)$$

$$g_z=\Lambda'(5a^2+b^2-3c^2-7d^2) , \quad (13)$$

$$g_x+g_y=-8\Lambda'\{\sqrt{(3)}\,ac\exp[-i(\phi_1+\phi_3)] + b^2\exp(-2i\phi_2)\} , \quad (14)$$

$$g_x-g_y=-4\Lambda'\{\sqrt{(7)}\,ad\exp[-i(\phi_1+\phi_4)] + \sqrt{(15)}\,bc\exp[-i(\phi_2+\phi_3)]\} , \quad (15)$$

where Λ' is an effective Landé factor. The value $\Lambda'=1.13$ is found by equating $\bar{g}$ (expt) of Eq. (8) to $\frac{2}{3}\Lambda'(J+1)$,[1] using the 14 °K experimental results[11]

$$|g_z|=5.20\pm0.01, \quad |g_x|=1.210\pm0.005, \quad |g_y|=3.76\pm0.03 . \quad (16)$$

As pointed out in Ref. 1, the only physically acceptable solution occurs when $|g_x-g_y|$ is maximized, so that, by Eq. (10),

$$g_x-g_y=(g_x-g_y)_e=4\Lambda'[\sqrt{(7)}\;ad+\sqrt{(15)}\,bc]\exp(i\Phi'') . \quad (17)$$

The solution is one in which $\bar{g}_2$ of Eq. (9b) is minimized, so that by the lower part of Table I,

$$c=(\tfrac{5}{3})^{1/2}b , \quad d=\sqrt{(7)}\,a . \quad (18)$$

This solution requires that g_x and g_y differ in phase by π, so that the experimental values to be substituted into Eqs. (14) and (15) are

TABLE I. Relationships at the extrema.

$\bar{g}_1$	$\lvert a_{M'}\rvert / \lvert a_M\rvert$	Sign of P
$\frac{2}{3}\Lambda(J+1)$	$[(J+M')/(J+M)]^{1/2}$	+
$-\frac{2}{3}\Lambda J$	$[(J+M)/(J+M')]^{1/2}$	−
$\bar{g}_2$	$\lvert a_{M''}\rvert / \lvert a_M\rvert$	Sign of P
$\frac{2}{3}\Lambda J$	$[(J-M)/(J-M'')]^{1/2}$	−
$-\frac{2}{3}\Lambda(J+1)$	$[(J-M'')/(J-M)]^{1/2}$	+

$$|g_x+g_y|_{\text{expt}}=|g_y|-|g_x|=2.55\pm0.04 , \quad (19)$$

$$|g_x-g_y|_{\text{expt}}=|g_y|+|g_x|=4.97\pm0.04 .$$

Solving Eqs. (12), (18), and either (13) or (15) with the experimental g value of Eq. (16) or (20) substituted, we obtain

$$a=0.311, \quad b=0.290, \quad c=0.375, \quad d=0.824 . \quad (21)$$

So far, the calculation has been essentially that of Ref. 1, except that as yet the relative phases are undetermined. The essential difference in the present calculation is in the interpretation of Eq. (14). By substituting the values of Eq. (21) into Eq. (14), we deduce that

$$1.07 \leq |g_x+g_y| \leq 2.59. \quad (22)$$

A comparison of Eqs. (19) and (22) shows that, to within the experimental error, $|g_x+g_y|$ is also a maximum with respect to phase; thus, Eq. (14) reduces to

$$(g_x+g_y)=(g_x+g_y)_e=8\Lambda'(\sqrt{3}\,ac+b^2)\exp(i\phi') . \quad (23)$$

The relative phases in Eq. (11) may be found by comparing Eqs. (15) and (17) and Eqs. (14) and (23); i.e.,

$$\phi_4-\phi_3=\phi_3-\phi_2=\phi_2-\phi_1 . \quad (24)$$

Thus, the wave function $|\alpha\rangle$ of Eq. (11) may be simplified to

$$|\alpha\rangle = a\left|\tfrac{5}{2}\right\rangle + b\exp(i\phi)\left|\tfrac{1}{2}\right\rangle + c\exp(2i\phi)\left|-\tfrac{3}{2}\right\rangle + d\exp(3i\phi)\left|-\tfrac{5}{2}\right\rangle , \quad (25)$$

where ϕ is an arbitrary phase angle. [An arbitrary phase-factor $\exp(i\phi_1)$ modulus, which is common to each term on the right-hand side, has been omitted.] The factor $\exp(i\phi)$ has no physical significance since it may be considered as an arbitrary phase factor associated with the matrix elements of the operator J_-^2.[7] [The two sets of relative signs obtained in Eq. (19) of Ref. 1 are for the special cases $\phi=n\pi$, with n an integer.] The physical aspects of

the problem are not affected by setting $\phi = 0$; hence, the potential leading to Eq. (25) is one that may be described by Z^c_{nm} terms only (with n, m even). Bauman and Porto[12] point out that a model for LaF_3 involving small distortions from a structure of higher symmetry can be used to explain the experimental results. This model requires that the point symmetry of the La^{3+} site be C_2, but that the distortion from C_{2v} be small. The wave function of Eq. (25) is consistent with a Yb^{3+} site of point symmetry C_{2v}. In comparing this result to the model of Bauman and Porto, [12] we note that the point symmetry of the impurity Yb^{3+} may differ from that of the La^{3+} host. [11] Also, the effect of a small deviation from C_{2v} symmetry on the g values could be masked by the experimental errors [cf. Eqs. (19) and (22)] or by approximations used in the theory, [1] such as the assumption of an isotropic effective Landé factor Λ'.

Calculations of the type given here may be simplified by setting two of the phase factors in Eq. (1) equal to unity. No physically significant results are affected, since one factor is related to an arbitrary phase common to each term in the wave function and the other factor to an arbitrary phase associated with the matrix elements of the operator J_-. Thus, in the $Laf_3:Yb^{3+}$ problem, two of the phase angles in Eq. (11) could have been equated to zero initially.

The author would like to thank Dr. T. D. Black for informative discussions and Mrs. Patricia Rubins for help in preparing the manuscript.

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[5]It is assumed here that the phase factors associated with the angular momentum operators are set equal to unity, as is common practice (see Ref. 8).

[6]The procedures given here also extend the applicability of Ref. 1 to the symmetries S_4, C_4, C_{4h}, C_3, C_{3i}, D_3, D_{3d}, C_{3h}, C_6, and C_{6h} – all of which contain Z^s_{nm} terms of even n (see Ref. 4).

[7]The convention used to remove ambiguities is the same as that given in Ref. 1 [following Eq. (4)], except that $|\alpha\rangle$ is chosen so that g_x and g_y have the same phase, if the z axis has threefold or higher symmetry.

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