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Technical Memorandum 33-446

Energy Levels and Transition Matrix Elements of Paramagnetic Crystals for Maser Applications

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JET PROPULSION LABORATORY
CALIFORNIA INSTITUTE OF TECHNOLOGY
PASADENA, CALIFORNIA

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16. Abstract

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Preface

The work described in this report was performed by the Telecommunications Division of the Jet Propulsion Laboratory. The subroutine which diagonalizes the Hermitian matrix was kindly furnished by R. J. Hanson of the Computation and Analysis Section.

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Contents

Figures

Abstract

Computer programs on the Univac 1108 have been developed at the Jet Propulsion Laboratory to give the energy levels and transition probabilities for ruby, emerald, iron-doped rutile, iron-doped zinc tungstate, and chromium-doped rutile. These programs also generate SC-4020 plots of energy levels vs an external dc magnetic field which is at any orientation with respect to the crystal magnetic axes.

Energy Levels and Transition Matrix Elements of Paramagnetic Crystals for Maser Applications

I. Introduction

Investigation of maser performance of paramagnetic crystals is a continuing program in the Microwave Electronics Group at the Jet Propulsion Laboratory (JPL). As the need arises for higher signal frequencies, it is necessary to evaluate the maser qualities of many crystals. Efficient study of maser crystal performance can be achieved by the use of a set of fine structure energy levels and transition probabilities. Such information allows the investigator to determine the optimum orientation of the crystal magnetic axes with respect to the external dc magnetic field and the polarization of the signal and pump frequencies.

To meet this goal, Fortran V language programs for the Univac 1108 computer at JPL have been implemented to diagonalize the spin Hamiltonians of ruby, emerald, iron-doped rutile, iron-doped zinc tungstate, and chromium-doped rutile. For each of these crystals, eigenvalues in GHz, normalized eigenvectors, and transition probabilities are computed, and a plot by the Stromberg-Carlson SC-4020 Plotter is made of eigenvalues vs the external dc magnetic field.

II. Discussion

A. Spin Hamiltonian

The spin Hamiltonian for the case of ruby was derived in detail in Ref. 1. If H_s is the spin Hamiltonian which, because of the physical nature of the problem, is Hermitian then the equation to be solved is

$$H_s|\psi_i\rangle = E_i|\psi_i\rangle \qquad i = 1, \cdots, n = 2S + 1 \tag{1}$$

where eigenvalues E_i are real, and S is the effective total spin of the ion in the crystal, H_s can be diagonalized by a unitary matrix with the result that the eigenvalues occur along the diagonal of the transformed matrix. $|\psi_i\rangle$ is an

n-fold vector representing a linear combination of the n-pure spin states:

$$|\psi_i\rangle = a_i|S\rangle + b_i|S-1\rangle + c_i|S-2\rangle + \cdots + x_i|-S\rangle$$

The $|S\rangle$, etc., are the base states corresponding to the $2S+1$ positions of the spin dipole in a magnetic field.

The diagonalization of H_s by computer methods can be conveniently handled by expanding the $n \times n$ Hermitian matrix into a $2n \times 2n$ real matrix.

Thus, if H_s and $|\psi_i\rangle$ are expressed as $H_s = H_{s1} + iH_{s2}$ and $|\psi_i\rangle = |\psi_i\rangle_1 + i|\psi_i\rangle_2$ then Eq. (1) takes the form

$$\begin{bmatrix} H_{s1} & -H_{s2} \\ H_{s2} & H_{s1} \end{bmatrix} \begin{bmatrix} |\psi_i\rangle_1 \\ |\psi_i\rangle_2 \end{bmatrix} = E_i \begin{bmatrix} |\psi_i\rangle_1 \\ |\psi_i\rangle_2 \end{bmatrix} \qquad (2)$$

B. Transition Probability Matrix Elements

From first order perturbation, the transition probability per unit time of a transition from state ψ_i to state ψ_j is

$$W_{ij} = \frac{1}{4}\gamma^2 G(f)|\langle\psi_i|H'|\psi_j\rangle|^2 \qquad (3)$$

where $\gamma = g\beta\mu_0/h$, H' is the applied perturbation, and $G(f)$ is the density of states as a function of energy. When an RF magnetic field $\mathbf{H}_1 = H_1^0(\phi_1\mathbf{i} + \phi_2\mathbf{j} + \phi_3\mathbf{k})$ is applied to the crystal, the dipole interaction energy is $H' = \boldsymbol{\mu}\cdot\mathbf{H}_1 = g\beta\,\mathbf{S}\cdot\mathbf{H}_1$, where ϕ_1, ϕ_2, and ϕ_3 are the direction cosines of $\mathbf{H}_1$ with respect to the magnetic axes x, y, z of the crystal.

Eq. (3), for $S = 3/2$ becomes

$$\frac{\langle\psi_i|g\mathbf{H}_1\cdot\mathbf{S}|\psi_j\rangle}{H_1^0}$$

$$= [a_i^* b_i^* c_i^* d_i^*]\begin{bmatrix} 3\phi_3 & (3)^{1/2}(\phi_1 - i\phi_2) & 0 & 0 \\ (3)^{1/2}(\phi_1 + i\phi_2) & \phi_3 & 2(\phi_1 - i\phi_2) & 0 \\ 0 & 2(\phi_1 + i\phi_2) & -\phi_3 & (3)^{1/2}(\phi_1 - i\phi_2) \\ 0 & 0 & (3)^{1/2}(\phi_1 + i\phi_2) & -3\phi_3 \end{bmatrix}\begin{bmatrix} a_j \\ b_j \\ c_j \\ d_j \end{bmatrix}$$

$$\equiv \alpha_{ij}\phi_1 + i\beta_{ij}\phi_2 + \gamma_{ij}\phi_3$$

where

$$\alpha_{ij} = (3)^{1/2}(a_i^*b_j + b_i^*a_j + c_i^*d_j + d_i^*c_j) + 2(b_i^*c_j + c_i^*b_j)$$

$$\beta_{ij} = (3)^{1/2}(-a_i^*b_j + b_i^*a_j - c_i^*d_j + d_i^*c_j) + 2(-b_i^*c_j + c_i^*b_j)$$

$$\gamma_{ij} = 3(a_i^*a_j - d_i^*d_j) + b_i^*b_j - c_i^*c_j$$

Similar equations can be derived for the case of $S = 5/2$.

C. Main Programs

1. RUBYCR

a. Purpose

(1) Calculate the eigenvalues of the spin Hamiltonian of chromium (+3) in Al_2O_3 (ruby).

(2) Calculate the transition probability matrix elements.

(3) Plot eigenvalues vs external dc magnetic field, H_{dc}.

b. Input data

THETA ($0\,\text{deg} \leq \theta \leq 90\,\text{deg}$) is the angle between c axis and external dc magnetic field (see Fig. 1).

HMIN, HMAX, DH defines respectively minimum, maximum, and incremental external dc magnetic field for calculations and plots.

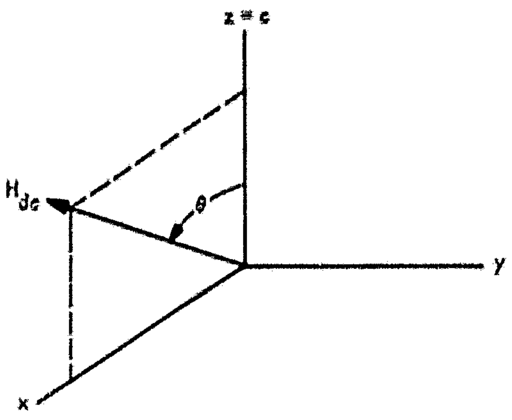

Fig. 1. Orientation of H_{dc} and c axis

c. Spin Hamiltonian (Ref. 2)

$$H_s = g\beta \mathbf{H}_{dc}\cdot \mathbf{S} + D\left[S_z^2 - \frac{1}{3} S(S+1)\right]$$

$$g = 1.99$$

$$D = -5.73 \text{ GHz}$$

$$\mathbf{H}_{dc} = H_0 (\sin\theta \mathbf{i} + \cos\theta \mathbf{j})$$

$$S = \frac{3}{2}$$

d. Spin Hamiltonian matrix

$\frac{3}{2} g\beta H_0 \cos\theta + D$	$\frac{3}{2} g\beta H_0 \sin\theta$	0	0
$\frac{3}{2} g\beta H_0 \sin\theta$	$\frac{1}{2} g\beta H_0 \cos\theta - D$	$g\beta H_0 \sin\theta$	0
0	$g\beta H_0 \sin\theta$	$-\frac{1}{2} g\beta H_0 \cos\theta - D$	$\frac{3}{2} g\beta H_0 \sin\theta$
0	0	$\frac{3}{2} g\beta H_0 \sin\theta$	$-\frac{3}{2} g\beta H_0 \cos\theta + D$

2. *TIO2FE*

a. Purpose

(1) Calculate the eigenvalues of the spin Hamiltonian of Fe(+3) in rutile (TiO_2).

(2) Calculate the transition probability matrix elements.

(3) Plot eigenvalues vs external dc magnetic field, H_{dc}.

b. Input data

THETA, PHI [$0 \text{ deg} \leq (\theta, \phi) \leq 90 \text{ deg}$] are the spherical coordinates of external dc magnetic field with respect to crystal magnetic axes x, y, z (see Fig. 2).

c. Spin Hamiltonian (Ref. 3)

$$H_s = g\beta \mathbf{H}_{dc}\cdot \mathbf{S} + D\left[S_z^2 - \frac{1}{3} s(s+1)\right] + E(S_x^2 - S_y^2)$$

$$+ \frac{a}{6}\left(S_x^4 + S_y^4 + S_z^4 - \frac{707}{16}\right)$$

$$+ \frac{7}{36} F \left(S_z^4 - \frac{75}{14} S_z^2 + \frac{81}{16}\right)$$

$D = 20.35$ GHz $\quad a = 1.1$ GHz

$E = 2.21$ GHz $\quad g = 2.0$

$F = -0.5$ GHz $\quad S = 5/2$

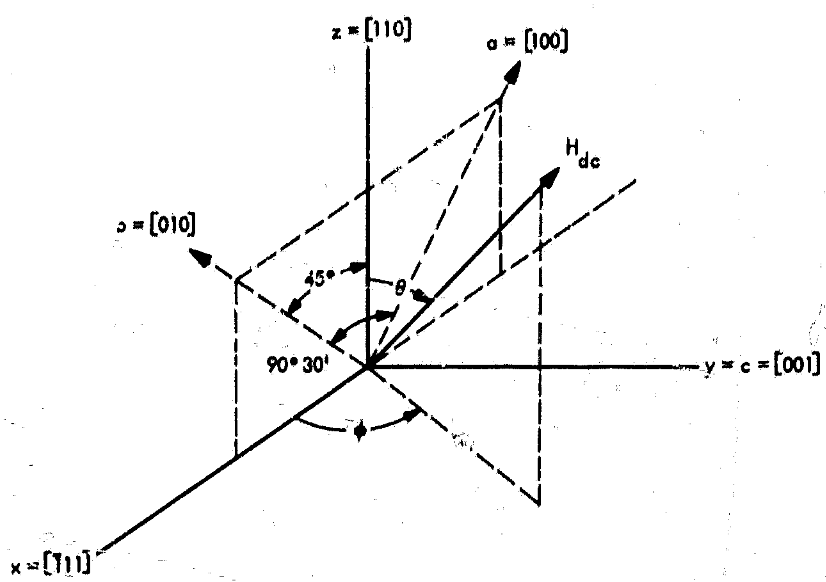

Fig. 2. Orientation of H_{dc} and crystal magnetic axes x, y, z; crystalline axes a, b, c shown with c axis along y direction; a and b axes in x-z plane

d. Spin Hamiltonian matrix

$\frac{5}{2}\frac{g\beta H}{h}\cos\theta + \left(\frac{10}{3}D + \frac{a}{2} + \frac{F}{3}\right)$	$\frac{(5)^{1/2}}{2}\frac{g\beta H}{h}\sin\theta\, e^{i\phi}$	$(10)^{1/2} E$	0	$\frac{(5)^{1/2}}{2} a$	0
$\left(\frac{5}{2}\right)^{1/2}\frac{g\beta H}{h}\sin\theta\, e^{-i\phi}$	$\frac{3}{2}\frac{g\beta H}{h}\cos\theta - \left(\frac{2}{3}D + \frac{3}{2}a + F\right)$	$(2)^{1/2}\frac{g\beta H}{h}\sin\theta\, e^{i\phi}$	$3(2)^{1/2} E$	0	$\frac{(5)^{1/2}}{2} a$
$(10)^{1/2} E$	$(2)^{1/2}\frac{g\beta H}{h}\sin\theta\, e^{-i\phi}$	$\frac{1}{2}\frac{g\beta H}{h}\cos\theta + \left(-\frac{8}{3}D + a + \frac{2}{3}F\right)$	$\frac{3}{2}\frac{g\beta H}{h}\sin\theta\, e^{i\phi}$	$3(2)^{1/2} E$	0
0	$3(2)^{1/2} E$	$\frac{3}{2}\frac{g\beta H}{h}\sin\theta\, e^{-i\phi}$	$-\frac{1}{2}\frac{g\beta H}{h}\cos\theta + \left(-\frac{8}{3}D + a + \frac{2}{3}F\right)$	$(2)^{1/2}\frac{g\beta H}{h}\sin\theta\, e^{i\phi}$	$(10)^{1/2} E$
$\frac{(5)^{1/2}}{2} a$	0	$3(2)^{1/2} E$	$(2)^{1/2}\frac{g\beta H}{h}\sin\theta\, e^{-i\phi}$	$-\frac{3}{2}\frac{g\beta H}{h}\cos\theta - \left(\frac{2}{3}D + \frac{3}{2}a + F\right)$	$\frac{(5)^{1/2}}{2}\frac{g\beta H}{h}\sin\theta\, e^{i\phi}$
0	$\frac{(5)^{1/2}}{2} a$	0	$(10)^{1/2} E$	$\frac{(5)^{1/2}}{2}\frac{g\beta H}{h}\sin\theta\, e^{-i\phi}$	$-\frac{5}{2}\frac{g\beta H}{h}\cos\theta + \left(\frac{10}{3}D + \frac{a}{2} + \frac{F}{3}\right)$

3. EMERCR

a. Purpose

(1) Calculate the eigenvalues of the spin Hamiltonian of chromium (+3) in beryl (emerald: $Be_3Al_2Si_6O_{18}$).

(2) Calculate the transition probability matrix elements.

(3) Plot eigenvalues vs external dc magnetic field, H_{dc}.

b. Input data

THETA ($0\,\text{deg} \leq \theta \leq 90\,\text{deg}$) is the angle between c axis and external dc magnetic field (see Fig. 1).

HMIN, HMAX, DH defines respectively minimum, maximum, and incremental external dc magnetic field for calculations and plots.

c. Spin Hamiltonian (Ref. 4)

$$H_s = g\beta \mathbf{H}_{dc} \cdot \mathbf{S} + D\left[S_z^2 - \frac{1}{3}S(S+1)\right]$$

$$D = -26\ \text{GHz}$$

$$g = 1.97$$

$$S = 3/2$$

The Hamiltonian matrix is the same as that for ruby (see Case 1 in Section C1d).

An example of the computer printout and plot for $\theta = 90$ deg is given in the appendix.

4. ZNWOFE

a. Purpose

(1) Calculate the eigenvalues of the spin Hamiltonian of Fe(+3) in $ZnWO_4$ (zinc tungstate).

(2) Calculate the transition probability matrix elements.

(3) Plot eigenvalues vs external dc magnetic field, H_{dc}.

b. Input data

THETA, PHI [$0\,\text{deg} \leq (\theta, \phi) \leq 90\,\text{deg}$] are the spherical coordinates of external dc magnetic field with respect to crystal magnetic axes x, y, z (see Fig. 3).

HMIN, HMAX, DH defines respectively minimum, maximum, and incremental dc external magnetic field for calculations and plots.

c. Spin Hamiltonian (Ref. 5)

$$\begin{aligned} H_s = {} & \frac{g\beta H}{2}(2S_z \cos\theta + S_+ e^{-i\phi}\sin\theta + S_- e^{i\phi}\sin\theta) \\ & + B_{02}[3S_z^2 - S(S+1)] + \frac{1}{2}B_{22}(S_+^2 + S_-^2) \\ & + B_{04}[35S_z^4 - 30S(S+1)S_z^2 + 25S_z^2 - 6S(S+1) \\ & + 3S^2(S+1)^2] \\ & + \frac{1}{2}B_{24}\{S_+^2[7S_z^2 + 14S_z - S(S+1) + 9] \\ & + S_-^2[7S_z^2 - 14S_z - S(S+1) + 9]\} \\ & + \frac{1}{2}B_{44}(S_+^4 + S_-^4) \end{aligned}$$

$B_{02} = -6.987$ GHz $S_\pm = S_x \pm iS_y$

$B_{22} = 4.935$ GHz

$B_{04} = 0.00326$ GHz $g = 2.0019$

$B_{24} = -0.00178$ GHz

$B_{44} = -0.0173$ GHz $S = 5/2$

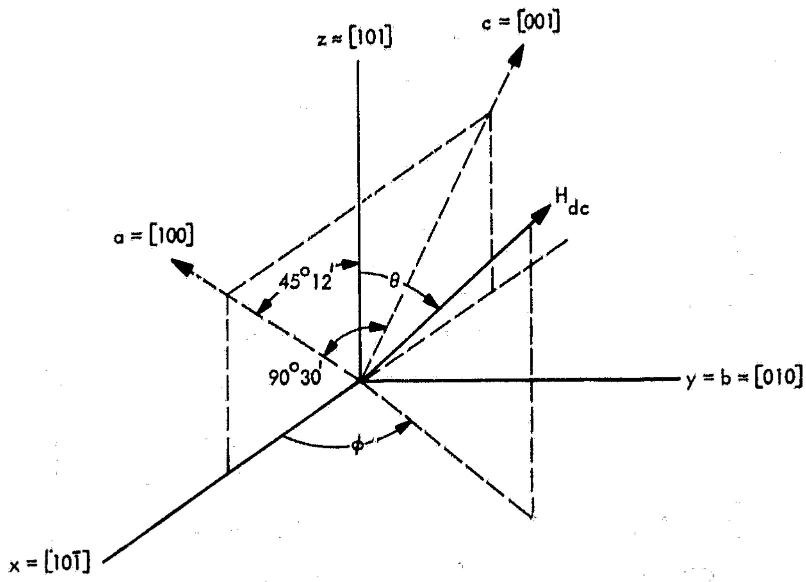

Fig. 3. Orientation of H_{dc} and crystal magnetic axes x, y, z; a, b, c crystalline axes with a and c axes in x-z plane

d. Spin Hamiltonian matrix

$10B_{02} + 60B_{04} + \frac{5}{2} g\beta H_0 \cos\theta$	$\frac{(5)^{1/2}}{2} g\beta H_0 \sin\theta\, e^{i\phi}$	$(10)^{1/2}(B_{22} + 9B_{24})$	0	$12(5)^{1/2} B_{44}$	0
$\frac{(5)^{1/2}}{2} g\beta H_0 \sin\theta\, e^{-i\phi}$	$-2B_{02} - 180B_{04} + \frac{3}{2} g\beta H_0 \cos\theta$	$(2)^{1/2} g\beta H_0 \sin\theta\, e^{i\phi}$	$3(2)^{1/2}(B_{22} - 5B_{24})$	0	$12(5)^{1/2} B_{44}$
$(10)^{1/2}(B_{22} + 9B_{24})$	$(2)^{1/2} g\beta H_0 \sin\theta\, e^{-i\phi}$	$-8B_{02} + 120B_{04} + \frac{1}{2} g\beta H_0 \cos\theta$	$\frac{3}{2} g\beta H_0 \sin\theta\, e^{i\phi}$	$3(2)^{1/2}(B_{22} - 5B_{24})$	0
0	$3(2)^{1/2}(B_{22} - 5B_{24})$	$\frac{3}{2} g\beta H_0 \sin\theta\, e^{-i\phi}$	$-8B_{02} + 120B_{04} - \frac{1}{2} g\beta H_0 \cos\theta$	$(2)^{1/2} g\beta H_0 \sin\theta\, e^{i\phi}$	$(10)^{1/2}(B_{22} + 9B_{24})$
$12(5)^{1/2} B_{44}$	0	$3(2)^{1/2}(B_{22} - 5B_{24})$	$(2)^{1/2} g\beta H_0 \sin\theta\, e^{-i\phi}$	$-2B_{02} - 180B_{04} - \frac{3}{2} g\beta H_0 \cos\theta$	$\frac{(5)^{1/2}}{2} g\beta H_0 \sin\theta\, e^{i\phi}$
0	$12(5)^{1/2} B_{44}$	0	$(10)^{1/2}(B_{22} + 9B_{24})$	$\frac{(5)^{1/2}}{2} g\beta H_0 \sin\theta\, e^{-i\phi}$	$10B_{02} + 60B_{04} - \frac{5}{2} g\beta H_0 \cos\theta$

5. TIO2CR

a. Purpose

(1) Calculate the eigenvalues of the spin Hamiltonian of Cr(+3) in rutile (TiO_2).

(2) Calculate the transition probability matrix elements.

(3) Plot eigenvalues vs external dc magnetic field, H_{dc}.

b. Input data

THETA, PHI [0 deg $\leq (\theta, \phi) \leq$ 90 deg] are the spherical coordinates of external dc magnetic field with respect to crystal magnetic axes x, y, z (see Fig. 2).

HMIN, HMAX, DH defines minimum, maximum, and incremental dc external magnetic field for calculations and plots.

c. Spin Hamiltonian

$$H_s = g\beta \mathbf{H}_{dc} \cdot \mathbf{S} + D\left[S_z^2 - \frac{1}{3} S(S+1)\right] + E(S_x^2 - S_y^2)$$

$D = -20.4$ GHz

$E = -4.2$ GHz

$g = 1.97$

$S = 3/2$

d. Spin Hamiltonian matrix

$\frac{3}{2} g\beta H_0 \cos\theta + D$	$\frac{(3)^{1/2}}{2} g\beta H_0 \sin\theta\, e^{-i\phi}$	$(3)^{1/2} E$	0
$\frac{(3)^{1/2}}{2} g\beta H_0 \sin\theta\, e^{i\phi}$	$\frac{1}{2} g\beta H_0 \cos\theta - D$	$g\beta H_0 \sin\theta\, e^{-i\phi}$	$(3)^{1/2} E$
$(3)^{1/2} E$	$g\beta H_0 \sin\theta\, e^{i\phi}$	$-\frac{1}{2} g\beta H_0 \cos\theta - D$	$\frac{(3)^{1/2}}{2} g\beta H_0 \sin\theta\, e^{-i\phi}$
0	$(3)^{1/2} E$	$\frac{(3)^{1/2}}{2} g\beta H_0 \sin\theta\, e^{i\phi}$	$-\frac{3}{2} g\beta H_0 \cos\theta + D$

Appendix

Energy Levels and Computer Output for the Case of Cr(+3) in Beryl (Emerald) for $\theta = 90$ deg With External dc Magnetic Field as a Parameter

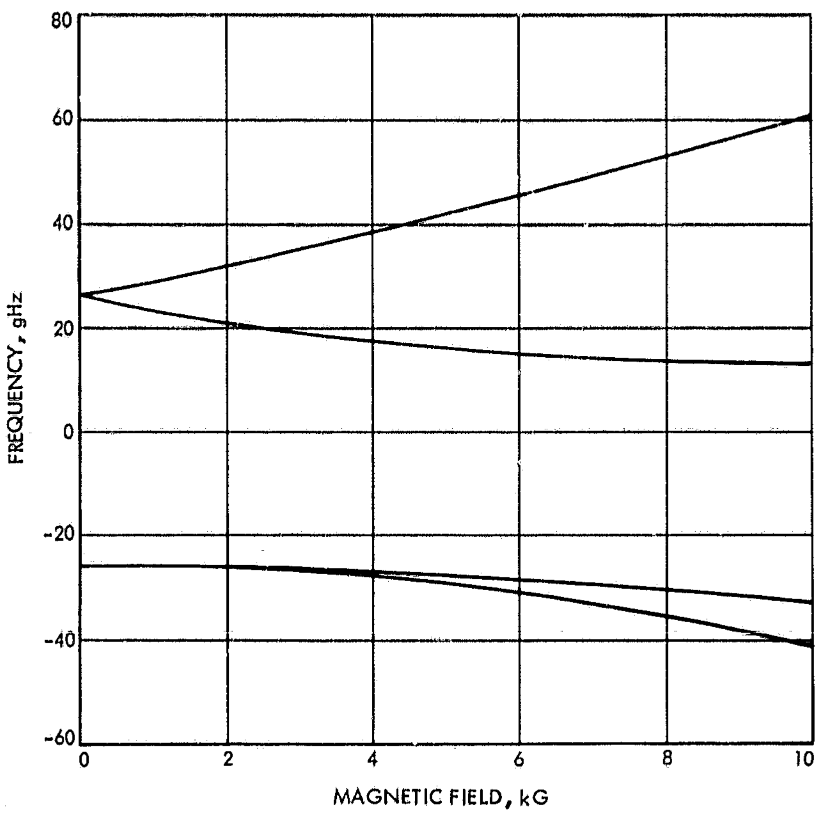

Fig. A-1. Plot of energy levels of Cr(+3) in beryl (emerald) vs external dc magnetic field for $\theta = 90$ deg

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN BERYL(EMERALD)

THETA= 90.000 DEGREES H= .0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 26.00000 GHZ

A(4)	B(4)	C(4)	D(4)
.0000000	.0000000	.0000000	.0000000
.0000000	.0000000	.0000000	.1000000+01

EIGENVECTOR FOR E(3)= 26.00000 GHZ

A(3)	B(3)	C(3)	D(3)
.0000000	.0000000	.1000000+01	.0000000
.0000000	.0000000	.0000000	.0000000

EIGENVECTOR FOR E(2)= -26.00000 GHZ

A(2)	B(2)	C(2)	D(2)
.0000000	.0000000	.0000000	.7828822-00
.0000000	.0000000	.0000000	.6221700-00

EIGENVECTOR FOR E(1)= -26.00000 GHZ

A(1)	B(1)	C(1)	D(1)
.0000000	.0000000	.0000000	.8150723-00
.0000000	.0000000	.0000000	-.5793593-00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
.0000	52.0000	52.0000	52.0000	52.0000	.0000

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L) REAL	ALPHA(K,L) IMAG	ALPHA(K,L) ABS	I*BETA(K,L) REAL	I*BETA(K,L) IMAG	I*BETA(K,L) ABS	GAMMA(K,L) REAL	GAMMA(K,L) IMAG	GAMMA(K,L) ABS
(1,2)	.0000	.0000	.0000	.0000	.0000	.0000	-.8329	-2.8821	3.0000
(1,3)	1.4117	1.0035	1.7321	1.0035	-1.4117	1.7321	.0000	.0000	.0000
(1,4)	.0000	.0000	.0000	.0000	.0000	.0000	1.7381	-2.4452	3.0000
(2,3)	1.3560	-1.0776	1.7321	-1.0776	-1.3560	1.7321	.0000	.0000	.0000
(2,4)	.0000	.0000	.0000	.0000	.0000	.0000	-1.8665	-2.3486	3.0000
(3,4)	.0000	1.7321	1.7321	-1.7321	.0000	1.7321	.0000	.0000	.0000

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	2.2500	.0000
(1,3)	.7500	.7500
(1,4)	2.2500	.0000
(2,3)	.7500	.7500
(2,4)	2.2500	.0000
(3,4)	.7500	.7500

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN BERYL(EMERALD)

THETA= 90.000 DEGREES H= 2000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 31.91875 GHZ

A(4)	B(4)	C(4)	D(4)
.2064018-05	.2499050-04	.2499051-04	.2064018-05
.5820324-01	.7047073-00	.7047073-00	.5820325-01

EIGENVECTOR FOR E(3)= 20.96359 GHZ

A(3)	B(3)	C(3)	D(3)
.6084697-07	.5973690-06	-.5973689-06	-.6084697-07
-.7165393-01	-.7034669-00	.7034669-00	.7165393-01

EIGENVECTOR FOR E(2)= -26.39509 GHZ

A(2)	B(2)	C(2)	D(2)
.2662049-08	-.2198635-09	-.2198705-09	.2662118-08
.7046982-00	-.5820232-01	-.5820417-01	.7047164-00

EIGENVECTOR FOR E(1)= -26.48735 GHZ

A(1)	B(1)	C(1)	D(1)
-.1789021-06	.1822262-07	-.1822224-07	.1788975-06
-.7034759-00	.7165467-01	-.7165319-01	.7034579-00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
10.9552	58.3138	58.4060	47.3587	47.4508	.0922

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L) REAL	ALPHA(K,L) IMAG	ALPHA(K,L) ABS	I*BETA(K,L) REAL	I*BETA(K,L) IMAG	I*BETA(K,L) ABS	GAMMA(K,L) REAL	GAMMA(K,L) IMAG	GAMMA(K,L) ABS
(1,2)	-.0000	-.0000	.0000	.0000	-.0498	.0498	-2.9828	-.0000	2.9828
(1,3)	1.8981	.0000	1.8981	-.0000	.0000	.0000	.0000	.0000	.0000
(1,4)	-.0000	.0000	.0000	-.0001	-1.5298	1.5298	-.1487	.0000	.1487
(2,3)	.0000	.0000	.0000	.0000	-1.8955	1.8955	-.2211	-.0000	.2211
(2,4)	1.5445	-.0001	1.5445	-.0000	-.0000	.0000	-.0000	.0000	.0000
(3,4)	-.0000	.0000	.0000	-.0001	-2.0160	2.0160	-1.0165	.0000	1.0165

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	2.2242	.0006
(1,3)	.9007	.0000
(1,4)	.0052	.5850
(2,3)	.0122	.8982
(2,4)	.5964	.0000
(3,4)	.2583	1.0161

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN BERYL(EMERALD)

THETA= 90.000 DEGREES H= 4000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 38.46715 GHZ

A(4)	B(4)	C(4)	D(4)
.6479976-06	.4366408-05	.4366408-05	.6479977-06
.1038015+00	.6994464-00	.6994464-00	.1038015+00

EIGENVECTOR FOR E(3)= 17.07751 GHZ

A(3)	B(3)	C(3)	D(3)
.3783482-07	.1703549-06	-.1703549-06	-.3783482-07
-.1533087-00	-.6902872-00	.6902872-00	.1533087-00

EIGENVECTOR FOR E(2)= -27.41983 GHZ

A(2)	B(2)	C(2)	D(2)
.7070543-08	-.1049304-08	-.1049314-08	.7070590-08
.6994441-00	-.1038010+00	-.1038020+00	.6994487-00

EIGENVECTOR FOR E(1)= -28.12483 GHZ

A(1)	B(1)	C(1)	D(1)
.1751704-07	-.3890428-08	.3890411-08	-.1751693-07
-.6902895-00	.1533091-00	-.1533084-00	.6902849-00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
21.3896	65.8870	66.5920	44.4973	45.2023	.7050

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L) REAL	ALPHA(K,L) IMAG	ALPHA(K,L) ABS	I*BETA(K,L) REAL	I*BETA(K,L) IMAG	I*BETA(K,L) ABS	GAMMA(K,L) REAL	GAMMA(K,L) IMAG	GAMMA(K,L) ABS
(1,2)	-.0000	.0000	.0000	-.0000	-.1869	.1869	-2.9287	.0000	2.9287
(1,3)	1.9925	.0000	1.9925	-.0000	.0000	.0000	.0000	.0000	.0000
(1,4)	-.0000	.0000	.0000	-.0000	-1.2987	1.2987	-.2155	.0000	.2155
(2,3)	.0000	.0000	.0000	.0000	-2.0143	2.0143	-.5001	-.0000	.5001
(2,4)	1.3670	-.0000	1.3670	-.0008	-.0000	.0000	-.0000	.0000	.0000
(3,4)	-.0000	.0000	.0000	-.0000	-2.0545	2.0545	-1.0611	.0000	1.0611

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	2.1444	.0087
(1,3)	.9925	.0000
(1,4)	.0116	.4217
(2,3)	.0625	1.01[illegible]3
(2,4)	.4672	.0000
(3,4)	.2815	1.0553

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN BERYL(EMERALD)

THETA= 90.000 DEGREES H= 6000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 45.45326 GHZ

A(4)	B(4)	C(4)	D(4)
.5418089-07	.2697673-06	.2697674-06	.5418090-07
.1392370-00	.6932626-00	.6932627-00	.1392370-00

EIGENVECTOR FOR E(3)= 14.51258 GHZ

A(3)	B(3)	C(3)	D(3)
.7813764-08	.2205826-07	-.2205826-07	-.7813765-08
-.2361049-00	-.6665242-00	.6665242-00	.2361049-00

EIGENVECTOR FOR E(2)= -28.88228 GHZ

A(2)	B(2)	C(2)	D(2)
.1985148-06	-.3987028-07	-.3987049-07	.1985154-06
.6932616-00	-.1392366-00	-.1392374-00	.6932636-00

EIGENVECTOR FOR E(1)= -31.08356 GHZ

A(1)	B(1)	C(1)	D(1)
.3057854-07	-.1083192-07	.1083190-07	-.3057844-07
-.6665252-00	.2361051-00	-.2361047-00	.6665232-00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
30.9407	74.3355	76.5368	43.3949	45.5961	2.2013

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	-.0000	.0000	.0000	-.0000	-.3770	.3770	-2.8382	.0000	2.8382
(1,3)	1.9753	-.0000	1.9753	.0000	.0000	.0000	.0000	-.0000	.0000
(1,4)	-.0000	.0008	.0000	-.0000	-1.0598	1.0598	-.2295	.0000	.2295
(2,3)	.0000	.0000	.0000	.0000	-2.0858	2.0858	-.7965	-.0000	.7965
(2,4)	1.2116	-.0000	1.2116	-.0000	-.0000	.0000	-.0000	.0000	.0000
(3,4)	-.0000	.0000	.0000	-.0000	-2.0938	2.0938	-1.1214	.0000	1.1214

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	2.0139	.0355
(1,3)	.9755	.0000
(1,4)	.0132	.2808
(2,3)	.1586	1.0876
(2,4)	.3670	.0000
(3,4)	.3144	1.0960

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN BERYL(EMERALD)

THETA= 90.000 DEGREES H= 8000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 52.74425 GHZ

A(4)	B(4)	C(4)	D(4)
.4980294-07	.2049539-08	.2049540-08	.4980295-07
.1669653-00	.6871118-00	.6871118-00	.1669653-00

EIGENVECTOR FOR E(3)= 13.23668 GHZ

A(3)	B(3)	C(3)	D(3)
.1376967-07	.2823567-07	-.2823567-07	-.1376967-07
-.3099427-00	-.6355592-00	.6355592-00	.3099427-00

EIGENVECTOR FOR E(2)= -30.64961 GHZ

A(2)	B(2)	C(2)	D(2)
.1230419-07	-.2989863-08	-.2989874-08	.1230421-07
.6871112-00	-.1669650-00	-.1669656-00	.6871124-00

EIGENVECTOR FOR E(1)= -35.33132 GHZ

A(1)	B(1)	C(1)	D(1)
.3653815-06	-.1781853-06	.1781851-06	-.3653808-06
-.6355598-00	.3099429-00	-.3099426-00	.6355586-00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
39.5076	83.3939	88.0756	43.8863	48.5680	4.6817

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L)			I*BETA(K,L)			GAMMA(K,L)		
	REAL	IMAG	ABS	REAL	IMAG	ABS	REAL	IMAG	ABS
(1,2)	-.0000	.0000	.0000	-.0000	-.5771	.5771	-2.7237	.0000	2.7237
(1,3)	1.8544	-.0000	1.8544	.0000	.0000	.0000	.0000	-.0000	.0000
(1,4)	-.0000	.0000	.0000	-.0000	-.8402	.8402	-.2108	.0000	.2108
(2,3)	.0000	.0000	.0000	.0000	-2.1165	2.1165	-1.0656	-.0000	1.0656
(2,4)	1.0800	-.0000	1.0800	-.0000	-.0000	.0000	-.0000	.0000	.0000
(3,4)	-.0000	.0000	.0000	-.0000	-2.1169	2.1169	-1.1839	.0000	1.1839

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	1.8546	.0833
(1,3)	.8597	.0000
(1,4)	.0111	.1765
(2,3)	.2839	1.1199
(2,4)	.2916	.0000
(3,4)	.3504	1.1204

ENERGY LEVELS AND TRANSITION PROBABILITY MATRIX ELEMENTS
FOR CR(+3) IN BERYL(EMERALD)

THETA= 90.000 DEGREES H= 10000.0 GAUSS

FIRST ROW OF EIGENVECTOR IS REAL PART, SECOND ROW IS IMAG. PART

EIGENVECTOR FOR E(4)= 60.25101 GHZ

A(4)	B(4)	C(4)	D(4)
-.8310795-07	-.2996948-06	-.2996948-06	-.8310797-07
.1889560-00	.6813924-00	.6813924-00	.1889560-00

EIGENVECTOR FOR E(3)= 13.03661 GHZ

A(3)	B(3)	C(3)	D(3)
-.9280882-06	-.1514725-05	.1514725-05	.9280883-06
-.3694228-00	-.6029318-00	.6029318-00	.3694229-00

EIGENVECTOR FOR E(2)= -32.63271 GHZ

A(2)	B(2)	C(2)	D(2)
-.3679710-07	.1020414-07	.1020417-07	-.3679714-07
.6813920-00	-.1889557-00	-.1889563-00	.6813928-00

EIGENVECTOR FOR E(1)= -40.65491 GHZ

A(1)	B(1)	C(1)	D(1)
-.3223433-07	.1975032-07	-.1975031-07	.3223429-07
-.6029322-00	.3694230-00	-.3699228-00	.6029314-00

E(4)-E(3)	E(4)-E(2)	E(4)-E(1)	E(3)-E(2)	E(3)-E(1)	E(2)-E(1)
47.2144	92.8837	100.9059	45.6693	53.6915	8.0222

TRANSITION PROBABILITY MATRIX ELEMENTS

TR(K,L)	ALPHA(K,L) REAL	ALPHA(K,L) IMAG	ALPHA(K,L) ABS	I*BETA(K,L) REAL	I*BETA(K,L) IMAG	I*BETA(K,L) ABS	GAMMA(K,L) REAL	GAMMA(K,L) IMAG	GAMMA(K,L) ABS
(1,2)	-.0000	-.0000	.0000	.0000	-.7566	.7566	-2.6046	-.0000	2.6046
(1,3)	1.6775	-.0000	1.6775	.0000	.0000	.0000	.0000	-.0000	.0000
(1,4)	-.0000	-.0000	.0000	.0000	-.6581	.6581	-.1801	-.0000	.1801
(2,3)	.0000	-.0000	.0000	-.0000	-2.1207	2.1207	-1.2826	.0000	1.2825
(2,4)	.9697	.0000	.9697	.0000	-.0000	.0000	-.0000	-.0000	.0000
(3,4)	-.0000	-.0000	.0000	.0000	-2.1207	2.1207	-1.2406	-.0000	1.2405

TR(K,L)	.25*(ALPHA**2+GAMMA**2)	.25*(BETA**2)
(1,2)	1.6960	.1431
(1,3)	.7035	.0000
(1,4)	.0081	.1083
(2,3)	.4112	1.1243
(2,4)	.2351	.0000
(3,4)	.3847	1.1243

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