which is consistent with an energy separation of 0.047 Mev between the $J=0$ and $J=1$ states, the latter state being the lower. Using this wave function which has its major contribution from the term representing the $(\pi h_{9/2})(\nu i_{11/2})$ configuration, Newby and Konopinski have evaluated the nuclear moment to be $\mu=-0.75$ nm. This value is not in good agreement with the experimentally determined value of $|\mu|=0.0442$ nm although it is possible that minor variation of the coefficients in Eq. (16) may improve the agreement.

Blin-Stoyle gives an expression for the quadrupole moment of an odd-odd nucleus on the single-particle model.[31] Assuming the configuration $(\pi h_{9/2})(\nu h_{9/2})$, we have evaluated this expression for Bi^{210} and find

$$Q(Bi^{210})=0.08 \text{ barn}. \quad (17)$$

If the positive sign of this quadrupole moment is taken to be correct, the sign of the magnetic moment of Bi^{210} is negative. We feel that no great faith should be put in this argument.

[31] R. J. Blin-Stoyle, *Theories of Nuclear Moments* (Oxford University Press, London, 1957), p. 69.

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Nuclear Level Splitting Caused by a Combined Electric Quadrupole and Magnetic Dipole Interaction*†

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The interaction of a static electric field gradient and a static magnetic field with the electromagnetic moments of a nucleus is considered in detail. The eigenvectors and eigenvalues of the interaction Hamiltonian are computed as a function of the angle β between the electric field gradient and magnetic field directions, and as a function of the electric and magnetic interaction parameters ω_E and ω_H. Numerical calculations of the eigenvectors and eigenvalues have been performed for nuclear spin values $I=1$, $\frac{3}{2}$, 2, $\frac{5}{2}$, 3, $\frac{7}{2}$, 4, and $\frac{9}{2}$ and for a wide range of the parameters β, ω_E, and ω_H. The accuracy of the results is 0.001%. Representative numerical results are presented.

I. INTRODUCTION

THE ability to measure the nuclear level splitting with the aid of the Mössbauer effect has greatly increased the need for numerical calculations of the eigenvalues of the interaction Hamiltonian in the case of a combination of an electric quadrupole and a magnetic dipole interaction of comparable strength. At present, the Mössbauer technique is the most powerful tool for investigations of internal fields in solids, a fact which has been demonstrated in a number of recent experiments.[1–3] The level splitting for a nuclear spin $I=1$ and $I=\frac{3}{2}$ has been calculated by Parker[4] as a function of the ratio of the magnetic and the electric interaction strength and for various orientations of the electric field gradient with respect to the direction of the magnetic field. For higher spin values no calculations of this kind are available. However, in both nuclear spectroscopy and solid-state physics there are many problems of interest which require resonance scattering measurements with transitions arising from nuclear states with spin values different from $I=1$ or $I=\frac{3}{2}$. Another field, where the eigenvalues and eigenvectors of the interaction Hamiltonian are of greatest interest, is the theory of the influence of perturbing fields on angular correlations. The calculation of the attenuation factors for an angular correlation which is influenced by a combined electric and magnetic interaction, requires the knowledge of the eigenvalues and eigenvectors of the interaction Hamiltonian. As we are

* Preliminary results of these calculations have been presented at the conference of the Swedish National Committee of Physics at Lund, Sweden, June, 1961.

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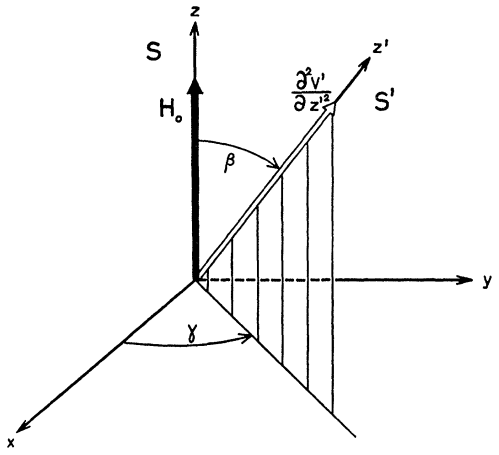

FIG. 1. Extranuclear fields in *one* microcrystal.

engaged in such calculations concerning the general case of randomly oriented electric field gradients in combination with an external magnetic field of a certain direction, we obtain the eigenvalues and eigenvectors as a by-product.[5] They are computed as a function of the ratio of the magnetic and the electric interaction strength for all spin values $I=1, \frac{3}{2}, 2, \cdots, \frac{9}{2}$. The calculations have been carried out for various angles β between the directions of the electric field gradient and the magnetic field.

For the derivation of the interaction Hamiltonian, only electric quadrupole and magnetic dipole interaction terms have been taken into account. Furthermore, the electric field gradient is assumed to have axial symmetry properties. The eigenvalues and eigenvectors have been obtained by diagonalization using a modified type of the Jacobi method (for a detailed discussion see, e.g., reference 6). Because of the tremendous bulk of numerical results it is not possible to publish a complete list of all the data at this place. Only for the nuclear spin values $I=2$ and $I=\frac{5}{2}$ is a complete table of the calculated eigenvalues presented. In addition, typical curves are shown for spin $I=2$ and $I=\frac{7}{2}$ for three different angles β.

II. DESCRIPTION OF THE INTERACTION OF NUCLEAR MOMENTS

The direction of the external magnetic field is chosen parallel to the z axis of a fixed coordinate system S (see Fig. 1). The electrostatic field gradient is assumed to possess axial symmetry with respect to the z' axis of the coordinate system S' fixed to the microcrystal. Thus the components of the electrostatic field gradient are completely determined by $\partial^2 V'/\partial z'^2$. Furthermore, it is assumed that the presence of a magnetic field does not influence the electric field gradient. The total interaction Hamiltonian is then represented by

$$H_{\text{int}}=H_{\text{magn}}+H_{\text{el}}. \tag{1}$$

1. Magnetic Interaction

The magnetic interaction Hamiltonian is given by

$$H_{\text{magn}}=-\mathfrak{y}\cdot\mathbf{H}=-\mu_z H_0, \tag{2}$$

where $\mathfrak{y}=\gamma\mathbf{I}$ is the magnetic dipole moment operator. The energy matrix elements are

$$(Im|H_{\text{magn}}|Im')=-H_0(Im|\mu_z|Im'). \tag{3}$$

Since $\mu_z=\gamma I_z$, the energy matrix is diagonal:

$$\begin{aligned}(Im|H_{\text{magn}}|Im)&=-H_0(Im|\mu_z|Im)\\&=-H_0(-1)^{I-m}\begin{pmatrix}I & 1 & I\\ -m & 0 & m\end{pmatrix}(I\|\mathfrak{y}\|I)\\&=-H_0\frac{m}{[(2I+1)(I+1)I]^{\frac{1}{2}}}(I\|\mathfrak{y}\|I).\end{aligned} \tag{4}$$

Conventionally the "magnetic moment" is defined as

$$\mu=(II|\mu_z|II)=\frac{I}{[(2I+1)(I+1)I]^{\frac{1}{2}}}(I\|\mathfrak{y}\|I). \tag{5}$$

The energy eigenvalues then become

$$(Im|H_{\text{magn}}|Im)=-H_0\mu m/I.$$

With $\omega_H=(H_0/\hbar I)\mu=gH_0\mu_N/\hbar$, one gets finally

$$(Im|H_{\text{magn}}|Im')=-\omega_H\hbar m\delta_{mm'}. \tag{6}$$

2. Electric Interaction

The Hamiltonian for static electric interactions is

$$H_{\text{el}}=\sum_{e,p}\frac{e_p e_e}{|\mathbf{r}_p-\mathbf{r}_e|}, \tag{7}$$

where $\mathbf{r}_p$ is the position vector of the charges in the nucleus, and $\mathbf{r}_e$ denotes the position vector of the charged ions in the crystal (see Fig. 2). Expansion of $1/|\mathbf{r}_p-\mathbf{r}_e|$ for $\mathbf{r}_e>\mathbf{r}_p$ gives

$$\frac{1}{|\mathbf{r}_p-\mathbf{r}_e|}=\sum_{k=0}^{k=\infty}\frac{r_p{}^k}{r_e{}^{k+1}}P_k(\cos(\mathbf{r}_p,\mathbf{r}_e)). \tag{8}$$

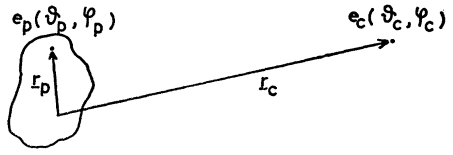

FIG. 2. Definition of the position vectors r_p and r_e.

[5] K. Alder, E. Matthias, W. Schneider, and R. M. Steffen (to be published).

[6] J. Greenstadt, *Mathematical Methods for Digital Computers*, edited by A. Ralston and H. S. Wilf (John Wiley & Sons, Inc., New York, 1960), Part II, Chap. 7.

Application of the addition theorem of spherical harmonics yields[7]:

$$H_{\rm el}=4\pi\sum_{k=0}^{k=\infty}(2k+1)^{-1}\sum_q(-1)^q\sum_p e_p r_p{}^k Y_{k,q}(\vartheta_p,\varphi_p)\times\sum_c\frac{e_c}{r_c{}^{k+1}}Y_{k,-q}(\vartheta_c,\varphi_c). \quad (9)$$

This can be written more compactly by introducing the tensor operators of the nuclear moments, $T^{(k)}$, and those of the field, $V^{(k)}$ (k=rank of the operator=multipole order)

$$T_q{}^{(k)}=\sum_p e_p r_p{}^k Y_{k,q}(\vartheta_p,\varphi_p), \quad (10)$$

$$V_q{}^{(k)}=\sum_c e_c\frac{1}{r_c{}^{k+1}}Y_{k,q}(\vartheta_c,\varphi_c). \quad (11)$$

With the definition of the scalar product of two tensor operators,[7]

$$T^{(k)}\cdot V^{(k)}=\sum_{q=-k}^{q=+k}(-1)^q T_q{}^{(k)}V_{-q}{}^{(k)}, \quad (12)$$

Eq. (9) becomes

$$H_{\rm el}=\sum_{k=0}^{k=\infty}\frac{4\pi}{2k+1}T^{(k)}\cdot V^{(k)}. \quad (13)$$

The Hamiltonian is now expressed as a product of two factors, a nuclear factor and an external field factor. Written in more detail, Eq. (13) becomes

$$H_{\rm el}=4\pi\Big(Ze_p\frac{1}{4\pi}V(0)+\frac{1}{3}\sum_{q=-1}^{q=+1}(-1)^q T_q{}^{(1)}V_{-q}{}^{(1)}+\frac{1}{5}\sum_{q=-2}^{q=+2}(-1)^q T_q{}^{(2)}V_{-q}{}^{(2)}+\frac{1}{7}\sum_{q=-3}^{q=+3}(-1)^q T_q{}^{(3)}V_{-q}{}^{(3)}+\cdots\Big), \quad (14)$$

$V(0)$ in Eq. (14) is the ordinary Coulomb potential. In the following only the electric quadrupole moment $T^{(2)}$ will be considered. The electric dipole moment $T^{(1)}$ and the electric octopole moment $T^{(3)}$ vanish because of the conservation of parity. The effects of the electric hexadecapole moment $T^{(4)}$ are too small to be of interest here. Therefore the electric interaction Hamiltonian $H_{\rm el}$ in Eq. (13) reduces to

$$H_{\rm el}=\tfrac{4}{5}\pi T^{(2)}\cdot V^{(2)}=\tfrac{4}{5}\pi\sum_q(-1)^q T_q{}^{(2)}V_{-q}{}^{(2)}. \quad (15)$$

The quadrupole interaction matrix elements with respect to system S are then given by

$$(Im|H_{\rm el}|Im')=\tfrac{4}{5}\pi\sum_q(-1)^q(Im|T_q{}^{(2)}|Im')V_{-q}{}^{(2)}. \quad (16)$$

[7] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, 1957).

Equation (16) is obtained under the assumption, that the classical treatment of the electrical field is a good approximation.

Application of the Wigner-Eckart theorem[7] yields

$$(Im|H_{\rm el}|Im')=\tfrac{4}{5}\pi\sum_q(-1)^{I-m+q}\begin{pmatrix}I & 2 & I\\ -m & q & m'\end{pmatrix}\times(I\|T^{(2)}\|I)V_{-q}{}^{(2)}. \quad (17)$$

Since $-m+q+m'=0$, there exists only one q for given values m and m', which implies that the sum over q can be dropped,

$$(Im|H_{\rm el}|Im')=\tfrac{4}{5}\pi(-1)^{I-m'}\begin{pmatrix}I & 2 & I\\ -m & q & m'\end{pmatrix}\times(I\|T^{(2)}\|I)V_{-q}{}^{(2)}. \quad (18)$$

The electrostatic field of the crystal is known in the coordinate system S'. Therefore $V_{-q}{}^{(2)}$ in Eq. (18) has to be expanded in terms of the $V_{-\mu}{}'^{(2)}$ in system S'

$$V_{-q}{}^{(2)}=\sum_{\mu=-2}^{\mu=+2}V_\mu{}'^{(2)}D_{\mu,-q}{}^{(2)}(\omega), \quad (19)$$

where ω represents the Euler angles (here: γ, β, and 0).

From the axial symmetry of the crystal field gradient with respect to the z' axis of system S', it follows directly that

$$V_{\pm1}{}'^{(2)}=V_{\pm2}{}'^{(2)}=0 \quad\text{and}\quad V_0{}'^{(2)}\neq0. \quad (20)$$

From the general expression for the $V_q{}^{(k)}$—defined in system S—the expression for the $V_\mu{}'^{(k)}$ in system S' can easily be seen to be [see Eq. (11)]

$$V_\mu{}'^{(k)}=\sum_c e_c\frac{1}{r_c{}'^{k+1}}Y_{k,\mu}(\vartheta_c{}',\varphi_c{}')$$

and

$$V_0{}'^{(2)}=\sum_c\frac{e_c}{r_c{}'^3}Y_{2,0}(\vartheta_c{}',\varphi_c{}')=\sum_c\frac{1}{4}\Big(\frac{5}{\pi}\Big)^{\frac{1}{2}}\frac{e_c}{r_c{}'^3}(3\cos^2\vartheta_c{}'-1).$$

The ordinary Coulomb potential due to the charged ions in the crystal is given by

$$V_{\rm el}{}'(r_c{}')=\sum_c e_c/r_c{}'$$

and thus

$$V_0{}'^{(2)}=\tfrac{1}{4}(5/\pi)^{\frac{1}{2}}\partial^2V_{\rm el}{}'/\partial z'^2. \quad (21)$$

Equation (19) may now be written:

$$V_{-q}{}^{(2)}=V_0{}'^{(2)}D_{0,-q}{}^{(2)}(\omega)=V_0{}'^{(2)}(\tfrac{4}{5}\pi)^{\frac{1}{2}}Y_{2,-q}(\beta,\gamma), \quad (22)$$

or

$$V_{-q}{}^{(2)}=\tfrac{1}{2}(\partial^2V_{\rm el}{}'/\partial z'^2)Y_{2,-q}(\beta,\gamma). \quad (23)$$

TABLE I. Eigenvalues of the interaction Hamiltonian for $I=2$.

cosβ	E_1	E_2	E_3	E_4	E_5
			$y=0.00$		
any	6.000000	−3.000000	−6.000000	−3.000000	6.000000
			$y=0.05$		
1.0	5.900000	−3.050000	−6.000000	−2.950000	6.100000
0.9	5.910053	−3.044812	−6.000474	−2.954818	6.090052
0.8	5.920100	−3.039647	−6.000899	−2.959653	6.080099
0.7	5.930142	−3.034503	−6.001274	−2.964505	6.070141
0.6	5.940178	−3.029381	−6.001599	−2.969374	6.060176
0.5	5.950208	−3.024281	−6.001873	−2.974261	6.050207
0.4	5.960233	−3.019205	−6.002097	−2.979163	6.040232
0.3	5.970252	−3.014153	−6.002273	−2.984078	6.030251
0.2	5.980266	−3.009135	−6.002397	−2.988999	6.020265
0.1	5.990275	−3.004187	−6.002472	−2.993889	6.010274
0.0	6.000277	−3.000278	−6.002498	−2.997780	6.000278
			$y=0.10$		
1.0	5.800000	−3.100000	−6.000000	−2.900000	6.200000
0.9	5.820213	−3.089239	−6.001900	−2.909282	6.180208
0.8	5.840403	−3.078576	−6.003597	−2.918624	6.160396
0.7	5.860570	−3.068010	−6.005094	−2.928027	6.140562
0.6	5.880715	−3.057542	−6.006389	−2.937490	6.120706
0.5	5.900837	−3.047173	−6.007484	−2.947008	6.100828
0.4	5.920937	−3.036910	−6.008379	−2.956575	6.080928
0.3	5.941014	−3.026773	−6.009075	−2.966173	6.061007
0.2	5.961068	−3.016816	−6.009571	−2.975744	6.041036
0.1	5.981101	−3.007302	−6.009869	−2.985027	6.021098
0.0	6.001111	−3.001111	−6.009969	−2.991142	6.001111
			$y=0.15$		
1.0	5.700000	−3.150000	−6.000000	−2.850000	6.300000
0.9	5.730482	−3.133263	−6.004277	−2.863408	6.270468
0.8	5.760912	−3.116772	−6.008092	−2.876935	6.240887
0.7	5.791289	−3.100522	−6.011448	−2.890579	6.211260
0.6	5.821616	−3.084513	−6.014349	−2.904337	6.181583
0.5	5.851890	−3.068752	−6.016798	−2.918199	6.151859
0.4	5.882113	−3.053261	−6.018798	−2.932139	6.122085
0.3	5.912286	−3.038097	−6.020352	−2.946099	6.092263
0.2	5.942408	−3.023437	−6.021460	−2.959901	6.062391
0.1	5.972478	−3.010009	−6.022125	−2.972815	6.032470
0.0	6.002499	−3.002499	−6.022347	−2.980153	6.002500
			$y=0.20$		
1.0	5.600000	−3.200000	−6.000000	−2.800000	6.400000
0.9	5.640861	−3.176869	−6.007609	−2.817210	6.360827
0.8	5.681628	−3.154219	−6.014377	−2.834603	6.321571
0.7	5.722302	−3.132040	−6.020317	−2.852176	6.282231
0.6	5.762882	−3.110331	−6.025441	−2.869916	6.242806
0.5	5.803370	−3.089102	−6.029761	−2.887802	6.203296
0.4	5.843766	−3.068404	−6.033284	−2.905777	6.163700
0.3	5.884071	−3.048363	−6.036017	−2.923708	6.124017
0.2	5.924285	−3.029349	−6.037965	−2.941218	6.084247
0.1	5.964409	−3.012725	−6.039133	−2.956940	6.044390
0.0	6.004442	−3.004442	−6.039523	−2.964924	6.004447
			$y=0.30$		
1.0	5.400000	−3.300000	−6.000000	−2.700000	6.600000
0.9	5.461958	−3.262752	−6.017147	−2.723903	6.541844
0.8	5.523698	−3.226817	−6.032285	−2.748101	6.483506
0.7	5.585222	−3.192137	−6.045487	−2.772581	6.424983
0.6	5.646531	−3.158688	−6.056813	−2.797304	6.366275
0.5	5.707627	−3.126488	−6.066319	−2.822197	6.307377
0.4	5.768514	−3.095673	−6.074042	−2.847088	6.248289
0.3	5.829192	−3.066586	−6.080016	−2.871600	6.189010
0.2	5.889665	−3.040153	−6.084266	−2.894783	6.129537
0.1	5.949934	−3.019027	−6.086809	−2.913965	6.069868
0.0	6.009989	−3.009989	−6.087656	−2.922357	6.010014
			$y=0.50$		
1.0	5.000000	−3.500000	−6.000000	−2.500000	7.000000
0.9	5.105556	−3.428711	−6.047861	−2.534009	6.905026
0.8	5.210466	−3.362579	−6.089120	−2.568342	6.809575
0.7	5.314743	−3.301043	−6.124414	−2.602923	6.713637
0.6	5.418396	−3.243771	−6.154228	−2.637603	6.617207
0.5	5.521435	−3.190682	−6.178931	−2.672096	6.520274
0.4	5.623872	−3.142038	−6.198804	−2.705861	6.422832
0.3	5.725716	−3.098677	−6.214060	−2.737849	6.324870
0.2	5.826976	−3.062487	−6.224853	−2.766018	6.226382
0.1	5.927664	−3.037110	−6.231288	−2.786623	6.127357
0.0	6.027692	−3.027693	−6.233427	−2.794457	6.027884
			$y=0.75$		
1.0	4.500000	−3.750000	−6.000000	−2.250000	7.500000
0.9	4.662841	−3.623806	−6.108603	−2.291478	7.361047
0.8	4.824118	−3.514414	−6.198043	−2.332758	7.221097
0.7	4.983871	−3.418268	−6.272087	−2.373643	7.080126
0.6	5.142137	−3.333323	−6.333136	−2.413788	6.938110
0.5	5.298954	−3.258553	−6.382807	−2.452615	6.795022
0.4	5.454359	−3.193790	−6.422228	−2.489177	6.650836
0.3	5.608387	−3.139747	−6.452187	−2.521978	6.505525
0.2	5.761073	−3.098101	−6.473231	−2.548802	6.359061
0.1	5.912451	−3.071360	−6.485722	−2.566782	6.211414
0.0	6.062072	−3.062072	−6.489864	−2.573174	6.063038
			$y=1.00$		
1.0	4.000000	−4.000000	−6.000000	−2.000000	8.000000
0.9	4.223469	−3.803267	−6.195007	−2.044389	7.819194
0.8	4.443946	−3.647245	−6.345988	−2.087457	7.636745
0.7	4.661526	−3.518721	−6.466455	−2.128952	7.452601
0.6	4.876308	−3.411162	−6.563410	−2.168444	7.266708
0.5	5.088384	−3.321120	−6.640995	−2.205279	7.079011
0.4	5.297846	−3.246929	−6.701848	−2.238519	6.889449
0.3	5.504783	−3.188125	−6.747712	−2.266908	6.697962
0.2	5.709270	−3.145092	−6.779747	−2.288926	6.504486
0.1	5.911417	−3.118691	−6.798693	−2.302987	6.308954
0.0	6.109772	−3.109772	−6.804965	−2.307836	6.112801
			$y=1.50$		
1.0	3.000000	−4.500000	−6.000000	−1.500000	9.000000
0.9	3.355981	−4.110021	−6.446825	−1.540446	8.741312
0.8	3.704164	−3.865433	−6.741765	−1.576416	8.479450
0.7	4.044909	−3.688881	−6.962050	−1.608247	8.214269
0.6	4.378571	−3.555107	−7.132993	−1.636092	7.945621
0.5	4.705505	−3.452174	−7.266704	−1.659970	7.673342
0.4	5.026056	−3.373506	−7.370004	−1.679807	7.397260
0.3	5.340555	−3.315208	−7.447067	−1.695471	7.117190
0.2	5.649315	−3.274918	−7.500525	−1.706809	6.832937
0.1	5.952612	−3.251234	−7.532010	−1.713678	6.544309
0.0	6.243416	−3.243417	−7.542410	−1.715980	6.258390
			$y=2.00$		
1.0	2.000000	−5.000000	−6.000000	−1.000000	10.000000
0.9	2.506039	−4.348310	−6.799871	−1.028245	9.670387
0.8	2.996108	−4.041972	−7.240479	−1.049587	9.335929
0.7	3.471004	−3.845065	−7.556228	−1.066069	8.996359
0.6	3.931618	−3.707557	−7.796529	−1.078915	8.651383
0.5	4.378903	−3.608320	−7.982365	−1.088902	8.300683
0.4	4.813806	−3.536284	−8.124886	−1.096547	7.943911
0.3	5.237229	−3.485033	−8.230688	−1.102197	7.580689
0.2	5.649988	−3.450678	−8.303847	−1.106086	7.210623
0.1	6.052696	−3.430893	−8.346847	−1.108364	6.833408
0.0	6.424429	−3.424429	−8.361038	−1.109114	6.470153
			$y=4.00$		
1.0	1.000000	−6.000000	−7.000000	−2.000000	14.000000
0.9	1.067855	−4.971140	−8.891806	−0.646104	13.441195
0.8	1.323461	−4.752786	−9.790278	0.347577	12.872025
0.7	2.063286	−4.656370	−10.414467	0.715784	12.291766
0.6	2.980717	−4.603373	−10.881012	0.804039	11.699628
0.5	3.877188	−4.570876	−11.237466	0.836369	11.094785
0.4	4.729789	−4.549833	−11.508515	0.852107	10.476415
0.3	5.539532	−4.536015	−11.708514	0.860824	9.844173
0.2	6.308622	−4.527246	−11.846231	0.865808	9.199046
0.1	7.029146	−4.522365	−11.926962	0.868419	8.551763
0.0	7.520797	−4.520797	−11.953573	0.869235	8.084338

The quadrupole interaction matrix elements are then [see Eq. (18)]

$$(Im|H_{\rm el}|Im')=\tfrac{2}{5}\pi(-1)^{I-m'}\begin{pmatrix} I & 2 & I \\ -m & q & m' \end{pmatrix} \times(I\|T^{(2)}\|I)\frac{\partial^2 V_{\rm el}'}{\partial z'^2}Y_{2,-q}(\beta,\gamma). \quad (24)$$

Using the conventional definition of the electric quadrupole moment of the nucleus, the reduced matrix element $(I\|T^{(2)}\|I)$ in Eq. (24) can be eliminated:

$$\begin{aligned} eQ&=(II|\textstyle\sum_p e_p(3z_p^2-r_p^2)|II),\\ T_0^{(2)}&=\textstyle\sum_p e_p r_p^2 Y_{2,0}(\vartheta_p,\varphi_p)\\ &=\textstyle\sum_p e_p r_p^2\times\frac{1}{4}(5/\pi)^{\frac{1}{2}}(3\cos^2\vartheta_p-1)\\ &=\textstyle\sum_p \frac{1}{4}(5/\pi)^{\frac{1}{2}}e_p(3z_p^2-r_p^2), \end{aligned} \quad (25)$$

$$eQ=4(\pi/5)^{\frac{1}{2}}(II|T_0^{(2)}|II). \quad (25a)$$

Application of the Wigner-Eckart theorem on (25a)

yields

$$eQ=4(\pi/5)^{\frac{1}{2}}\begin{pmatrix} I & 2 & I \\ -I & 0 & I \end{pmatrix}(I\|T^{(2)}\|I)$$

or

$$eQ=4(\pi/5)^{\frac{1}{2}}\frac{2I(2I-1)}{[(2I+3)(2I+2)(2I+1)(2I)(2I-1)]^{\frac{1}{2}}}\times(I\|T^{(2)}\|I). \quad (26)$$

Using Eqs. (24) and (26), the matrix elements of the electric quadrupole interaction (in system S) become

$$(Im|H_{\mathrm{el}}|Im')=\frac{1}{2}\left(\frac{\pi}{5}\right)^{\frac{1}{2}}eQ\frac{\partial^2 V_{\mathrm{el}}'}{\partial z'^2}(-1)^{I-m'}\times\frac{\begin{pmatrix} I & 2 & I \\ -m & q & m' \end{pmatrix}}{\begin{pmatrix} I & 2 & I \\ -I & 0 & I \end{pmatrix}}Y_{2,-q}(\beta,\gamma). \quad (27)$$

3. Combined Electric and Magnetic Interaction

Combining Eqs. (6) and (27), the following expression is obtained for the matrix element $H_{m,m'}$ of the total interaction in system S:

$$H_{m,m'}=-\hbar\omega_H m\delta_{mm'}+\hbar\omega_E(-1)^{I-m'}(\pi/5)^{\frac{1}{2}}\times\begin{pmatrix} I & 2 & I \\ -m & m-m' & m' \end{pmatrix}Y_{2,m'-m}(\beta,\gamma)\times[(2I+3)(2I+2)(2I+1)(2I)(2I-1)]^{\frac{1}{2}}, \quad (28)$$

where ω_E is defined as

$$\omega_E=\frac{1}{2}\frac{eQ}{\hbar}\frac{\partial^2 V_{\mathrm{el}}'}{\partial z'^2}\frac{1}{2I(2I-1)}. \quad (29)$$

The eigenvalues E_n and the corresponding eigenvectors u_{Mn} of the matrix H are functions of the angles β and γ. Since the electrostatic field gradient was assumed to possess axial symmetry, the angle γ occurs in $H_{m,m'}$ in the form $e^{i\gamma(m'-m)}$. The diagonalization can therefore be simplified in the following way. It can easily be seen that $H(\beta,0)$ and $H(\beta,\gamma)$ are connected through an unitary transformation $A(\gamma)$:

$$H(\beta,0)=A(\gamma)H(\beta,\gamma)A^{-1}(\gamma),$$

where

$$A(\gamma)=\begin{pmatrix} e^{iI\gamma} & & & & \\ & \ddots & & 0 & \\ & & e^{iM\gamma} & & \\ & 0 & & \ddots & \\ & & & & e^{-iI\gamma} \end{pmatrix}.$$

This implies that the eigenvalues of $H(\beta,\gamma)$ are independent of γ, i.e.,

$$E(\beta,\gamma)=E(\beta,0).$$

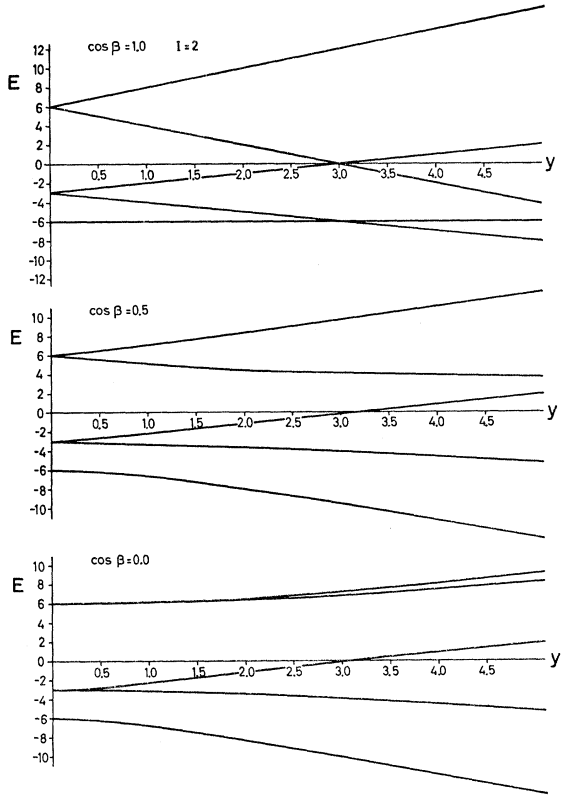

FIG. 3. The eigenvalues of the interaction Hamiltonian for $I=2$ as a function of the interaction parameter y for 3 values of β.

The unitary matrix $U(\beta,\gamma)$ which diagonalizes $H(\beta,\gamma)$ is then given by

$$U(\beta,\gamma)=U(\beta,0)A(\gamma).$$

Thus it is sufficient to compute the eigenvalues and eigenvectors of $H(\beta,0)$ from

$$U(\beta,0)H(\beta,0)U^{-1}(\beta,0)=E(\beta,0)=E(\beta).$$

In order to simplify the diagonalization procedure further, the matrix K with the elements,

$$K_{m,m'}=\frac{1}{\hbar\omega_E}H_{m,m'}(\beta,0),$$

is introduced. The matrix elements $K_{m,m'}$ are then functions of the ratio, $y=\omega_H/\omega_E$, only. Explicitly written, the only nonvanishing matrix elements, $K_{m,m}$, $K_{m,m-1}$, $K_{m,m-2}$, have the form:

$$\begin{aligned} K_{m,m}&=-ym+\tfrac{1}{2}(3\cos^2\beta-1)[3m^2-I(I+1)], \\ K_{m,m-1}&=-\tfrac{3}{2}\cos\beta\sin\beta(1-2m)[(I-m+1)(I+m)]^{\frac{1}{2}}, \\ K_{m,m-2}&=\tfrac{3}{4}\sin^2\beta[(I+m-1)(I+m)\times(I-m+1)(I-m+2)]^{\frac{1}{2}}. \end{aligned} \quad (30)$$

TABLE II. Eigenvalues of the interaction Hamiltonian for $I=\frac{5}{2}$.

$\cos\beta$	E_1	E_2	E_3	E_4	E_5	E_6
			$y=0.00$			
any	10.000000	−2.000000	−8.000000	−8.000000	−2.000000	10.000000
			$y=0.05$			
1.0	9.875000	−2.075000	−8.025000	−7.975000	−1.925000	10.125000
0.9	9.887548	−2.067390	−8.039843	−7.960471	−1.932392	10.112548
0.8	9.900093	−2.059792	−8.049541	−7.951056	−1.939795	10.100091
0.7	9.912631	−2.052205	−8.056767	−7.944079	−1.947209	10.087630
0.6	9.925165	−2.044630	−8.062374	−7.938690	−1.954635	10.075164
0.5	9.937694	−2.037067	−8.066760	−7.934486	−1.962072	10.062692
0.4	9.950217	−2.029516	−8.070153	−7.931244	−1.969520	10.050216
0.3	9.962736	−2.021971	−8.072686	−7.928829	−1.976982	10.037732
0.2	9.975248	−2.014448	−8.074442	−7.927153	−1.984451	10.025248
0.1	9.987756	−2.006932	−8.075479	−7.926168	−1.991933	10.012756
0.0	10.000259	−1.999437	−8.075822	−7.925843	−1.999417	10.000259
			$y=0.10$			
1.0	9.750000	−2.150000	−8.050000	−7.950000	−1.850000	10.250000
0.9	9.775198	−2.134556	−8.080004	−7.921260	−1.864572	10.225195
0.8	9.800376	−2.119161	−8.099677	−7.902720	−1.879188	10.200371
0.7	9.825533	−2.103814	−8.114369	−7.889027	−1.893847	10.175526
0.6	9.850668	−2.088514	−8.125789	−7.878475	−1.908551	10.150661
0.5	9.875782	−2.073262	−8.134737	−7.870261	−1.923298	10.125776
0.4	9.900876	−2.058058	−8.141662	−7.863936	−1.938090	10.100870
0.3	9.925984	−2.042902	−8.146836	−7.859228	−1.952926	10.075944
0.2	9.951000	−2.027790	−8.150430	−7.855967	−1.967808	10.050996
0.1	9.976030	−2.012726	−8.152548	−7.854049	−1.982735	10.026028
0.0	10.001040	−1.997791	−8.153250	−7.853417	−1.997624	10.001040
			$y=0.15$			
1.0	9.625000	−2.225000	−8.075000	−7.925000	−1.775000	10.375000
0.9	9.662949	−2.201492	−8.120482	−7.882367	−1.796546	10.337938
0.8	9.700851	−2.178096	−8.150398	−7.855001	−1.818188	10.300834
0.7	9.738704	−2.154811	−8.172789	−7.834860	−1.839925	10.263683
0.6	9.776509	−2.131636	−8.190218	−7.819383	−1.861758	10.226487
0.5	9.814267	−2.108571	−8.203891	−7.807361	−1.883689	10.189245
0.4	9.851977	−2.085612	−8.214482	−7.798119	−1.905719	10.151956
0.3	9.889639	−2.062761	−8.222401	−7.791251	−1.927848	10.114622
0.2	9.927253	−2.040017	−8.227903	−7.786499	−1.950076	10.077242
0.1	9.964822	−2.017378	−8.231147	−7.783705	−1.972406	10.039815
0.0	10.002343	−1.995121	−8.232222	−7.782783	−1.994560	10.002343
			$y=0.20$			
1.0	9.500000	−2.300000	−8.100000	−7.900000	−1.700000	10.500000
0.9	9.550803	−2.268191	−8.161277	−7.843793	−1.728320	10.450778
0.8	9.601518	−2.236587	−8.201700	−7.807906	−1.756804	10.401478
0.7	9.652148	−2.205184	−8.232011	−7.781598	−1.785453	10.352098
0.6	9.702692	−2.173982	−8.255635	−7.761442	−1.814270	10.302638
0.5	9.753149	−2.142976	−8.274188	−7.745825	−1.843257	10.253096
0.4	9.803522	−2.112165	−8.288569	−7.733844	−1.872417	10.203474
0.3	9.853809	−2.081548	−8.299328	−7.724953	−1.901750	10.153770
0.2	9.904011	−2.051121	−8.306808	−7.718807	−1.931259	10.103984
0.1	9.954130	−2.020885	−8.311218	−7.715197	−1.960945	10.054116
0.0	10.004166	−1.991488	−8.312678	−7.714007	−1.990159	10.004166
			$y=0.30$			
1.0	9.250000	−2.450000	−8.150000	−7.850000	−1.550000	10.750000
0.9	9.326821	−2.400851	−8.243819	−7.767604	−1.591286	10.676740
0.8	9.403442	−2.352186	−8.306016	−7.715628	−1.632919	10.603307
0.7	9.479864	−2.303996	−8.352798	−7.677861	−1.674905	10.529698
0.6	9.556089	−2.256275	−8.389337	−7.649135	−1.717251	10.455909
0.5	9.632118	−2.209016	−8.418076	−7.627003	−1.759965	10.381942
0.4	9.707953	−2.162210	−8.440381	−7.610104	−1.803053	10.307794
0.3	9.783594	−2.115850	−8.457079	−7.597610	−1.846521	10.233466
0.2	9.859043	−2.069932	−8.468693	−7.588996	−1.890375	10.158953
0.1	9.934303	−2.024461	−8.475546	−7.583946	−1.934607	10.084257
0.0	10.009374	−1.981562	−8.477812	−7.582282	−1.977093	10.009374
			$y=0.50$			
1.0	8.750000	−2.750000	−8.250000	−7.750000	−1.250000	11.250000
0.9	8.880140	−2.663002	−8.412746	−7.619127	−1.315031	11.129767
0.8	9.009698	−2.577487	−8.521353	−7.539016	−1.380912	11.009072
0.7	9.138680	−2.493425	−8.603353	−7.482134	−1.447670	10.887903
0.6	9.267094	−2.410789	−8.667555	−7.439680	−1.515330	10.766259

TABLE II (*continued*).

cosβ	E_1	E_2	E_3	E_4	E_5	E_6
			$y=0.50$			
0.5	9.394948	−2.329535	−8.718135	−7.407485	−1.583924	10.644132
0.4	9.522246	−2.249639	−8.757432	−7.383216	−1.653476	10.521516
0.3	9.648999	−2.171069	−8.786874	−7.365453	−1.724007	10.398405
0.2	9.775212	−2.093822	−8.807364	−7.353302	−1.795518	10.274795
0.1	9.900891	−2.018030	−8.819455	−7.346211	−1.867871	10.150675
0.0	10.026041	−1.952587	−8.823455	−7.343881	−1.932166	10.026047
			$y=0.75$			
1.0	8.125000	−3.125000	−8.375000	−7.625000	−0.875000	11.875000
0.9	8.324296	−2.984020	−8.631214	−7.441121	−0.965980	11.698039
0.8	8.522206	−2.846799	−8.802696	−7.334227	−1.058573	11.520088
0.7	8.718755	−2.713289	−8.932320	−7.261424	−1.152852	11.341131
0.6	8.913969	−2.583397	−9.033846	−7.208984	−1.248888	11.161148
0.5	9.107875	−2.457008	−9.113829	−7.170423	−1.346755	10.980120
0.4	9.300495	−2.334011	−9.175959	−7.142043	−1.446509	10.798027
0.3	9.491856	−2.214334	−9.222498	−7.121702	−1.548171	10.614850
0.2	9.681980	−2.098073	−9.254879	−7.107997	−1.651600	10.430569
0.1	9.870891	−1.986272	−9.273984	−7.100080	−1.755716	10.245164
0.0	10.058593	−1.903289	−9.280304	−7.097491	−1.836140	10.058631
			$y=1.00$			
1.0	7.500000	−3.500000	−8.500000	−7.500000	−0.500000	12.500000
0.9	7.771399	−3.296348	−8.858009	−7.272210	−0.613241	12.268410
0.8	8.040191	−3.100232	−9.097076	−7.149174	−0.728867	12.035158
0.7	8.306439	−2.911731	−9.277452	−7.070459	−0.847000	11.800203
0.6	8.570211	−2.730646	−9.418487	−7.016819	−0.967763	11.563505
0.5	8.831568	−2.556664	−9.529431	−6.979233	−1.091261	11.325022
0.4	9.090572	−2.389486	−9.615508	−6.952737	−1.217547	11.084707
0.3	9.347282	−2.228989	−9.679923	−6.934375	−1.346513	10.842517
0.2	9.601757	−2.075679	−9.724708	−6.922327	−1.477450	10.598407
0.1	9.854054	−1.933357	−9.751122	−6.915491	−1.606410	10.352325
0.0	10.104147	−1.844293	−9.759854	−6.913277	−1.691030	10.104306
			$y=1.50$			
1.0	6.250000	−4.250000	−8.750000	−7.250000	0.250000	13.750000
0.9	6.675202	−3.886892	−9.337645	−6.967326	0.101633	13.415030
0.8	7.093838	−3.546435	−9.723127	−6.850755	−0.050238	13.076718
0.7	7.506154	−3.230809	−10.011139	−6.793397	−0.205757	12.734947
0.6	7.912394	−2.938458	−10.234798	−6.763716	−0.365017	12.389597
0.5	8.312789	−2.667142	−10.409851	−6.748360	−0.527974	12.040539
0.4	8.707567	−2.415089	−10.545154	−6.740719	−0.694242	11.687639
0.3	9.096942	−2.181855	−10.646125	−6.737213	−0.862502	11.330756
0.2	9.481122	−1.970309	−10.716189	−6.735814	−1.028552	10.969742
0.1	9.860306	−1.794847	−10.757457	−6.735368	−1.177074	10.604440
0.0	10.234093	−1.713001	−10.771093	−6.735281	−1.250000	10.235281
			$y=2.00$			
1.0	5.000000	−5.000000	−9.000000	−7.000000	1.000000	15.000000
0.9	5.593252	−4.408163	−9.853854	−6.726831	−0.826751	14.568847
0.8	6.173446	−3.881440	−10.396040	−6.678215	0.649865	14.132385
0.7	6.741224	−3.424036	−10.795478	−6.681504	0.469415	13.690380
0.6	7.297213	−3.022374	−11.103039	−6.700052	0.285671	13.242581
0.5	7.842019	−2.665655	−11.342382	−6.722050	0.099348	12.788720
0.4	8.376223	−2.347448	−11.526632	−6.742779	−0.087876	12.328511
0.3	8.900380	−2.066095	−11.663736	−6.760098	−0.272093	11.861643
0.2	9.415015	−1.827256	−11.758686	−6.772960	−0.443902	11.387790
0.1	9.920620	−1.651425	−11.814544	−6.780840	−0.580406	10.906595
0.0	10.415224	−1.582237	−11.832988	−6.783492	−0.636629	10.420121
			$y=4.00$			
1.0	4.000000	−6.000000	−10.000000	−8.000000	0.000000	20.000000
0.9	3.792472	−4.787622	−12.310361	−7.396562	1.458523	19.243550
0.8	3.601667	−3.861439	−13.486465	−7.549406	2.822011	18.473631
0.7	4.171499	−3.184919	−14.309787	−7.716668	3.350578	17.689298
0.6	5.385280	−2.657587	−14.927549	−7.860829	3.171192	16.889491
0.5	6.547949	−2.233058	−15.400689	−7.978963	2.991740	16.073020
0.4	7.657873	−1.890222	−15.761065	−8.072516	2.827396	15.238535
0.3	8.720997	−1.620945	−16.027284	−8.143317	2.686034	14.384515
0.2	9.742864	−1.424488	−16.210744	−8.192851	2.575939	13.509282
0.1	10.727704	−1.303989	−16.318344	−8.222166	2.505451	12.611346
0.0	11.617086	−1.263266	−16.353819	−8.231872	2.481114	11.750758

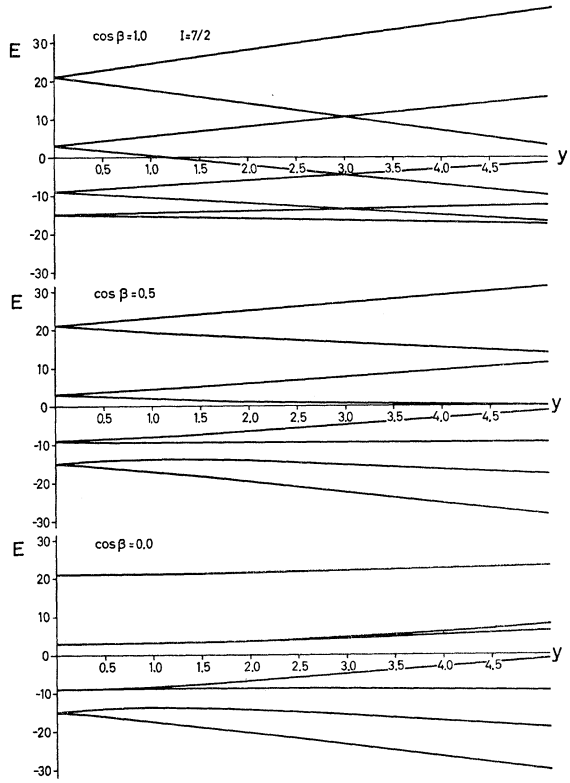

FIG. 4. The eigenvalues of the interaction Hamiltonian for $I=\frac{7}{2}$ as a function of the interaction parameter y for 3 values of β.

In the following the eigenvalues of the matrix K are denoted by E_n (see, e.g., Tables I and II).

III. RESULTS

The numerical calculations have been performed on the IBM-704 of MURA in Madison (Wisconsin). In addition, some of the results for $I=1$ and $I=\frac{3}{2}$ were computed on an IBM-7090 in New York. The calculations were performed for the following values of the nuclear spin: $I=1$, $\frac{3}{2}$, 2, $\frac{5}{2}$, 3, $\frac{7}{2}$, 4, and $\frac{9}{2}$. For $I=1$, $\frac{3}{2}$, and 2 the computation was made for 20 values of y between $y=0$ and $y=20$, and for $\cos\beta$ in intervals of $\Delta\cos\beta=0.05$. For $I=\frac{5}{2}, \cdots, \frac{9}{2}$, the calculations were performed for 12 values of y between $y=0$ and $y=4$, and for $\cos\beta$ in intervals of $\Delta\cos\beta=0.1$.

Typical curves for $I=2$ and $I=\frac{7}{2}$ are shown in Fig. 3 and Fig. 4. for three different values of β. Lists of the numerical results for $I=2$ and $I=\frac{5}{2}$ are presented in Table I and Table II.

The results for the different parameter series mentioned above will be published as a special report.[8] The program is written in FORTRAN II and allows the computation of the eigenvalues and eigenvectors for any value of I, y, and $\cos\beta$. Copies and details are available on request.

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