Quantum-mechanical approximation to the ground state of cerous magnesium nitrate

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In this paper we perform a complete quantum-mechanical calculation of the ground-state energy of a system of spins 1/2 that are coupled by dipole-dipole forces. The only hypothesis used is the assumption that the ground state has two times the periodicity of the underlying magnetic lattice. This paper is the application to a specific crystal of results derived in a preceding paper. The Hamiltonian is decomposed in eight invariant pieces each with its own coupling constant. The basis wave functions are decomposed according to the eight one-dimensional representations of the permutation group that leaves the cluster invariant. The results are given in the form of tables applicable to any compound that has the spins situated on a Bravais lattice. The calculation is applied to cerous magnesium nitrate and we show that the results for the lowest state of each representation are leading to a spectrum that is different from the results obtained with the classical or Hartree method. Although the lowest state is still the same antiferromagnetic configuration, it turns out now that this state lies barely below the ferromagnetic state; the order in which the ferromagnetic and antiferromagnetic levels appear is different from the order obtained in a classical calculation.

I. INTRODUCTION

This paper is an explicit quantum-mechanical calculation of the ground state of cerous magnesium nitrate (CMN), a salt which has, as far as is known, a pure dipole-dipole coupling between the spins of the magnetic cerium ions. Because of the apparent absence of any trace of exchange interaction, we deal with a case where the interaction law, although complicated, is quantitatively known. The long range of the dipole-dipole interaction makes it more difficult to obtain the energy of the ground state. All previous calculations were based amongst others on the assumption that the expectation values of the spins in the ground state could be considered independently, similar to the product assumption of the wave functions in the Hartree method. We do not make this assumption in the present paper.

In 1946 Luttinger and Tisza[1] calculated the ground state of a system of spins coupled by dipole forces. In order to overcome the difficulties encountered by the long, i.e., infinite range of these forces, they introduced a mathematical lattice with a period twice the primitive translation, in each of the three directions in space. Although this assumption leads to certain restrictions, we have found[2] that the result obtained for the ground state of CMN seems to be independent of the period chosen and thus exact as a classical approximation. That is, calculations with periods 3, 4, ..., 8 give rise to either the same value of the ground-state energy, or give answers that did not satisfy the conditions of the calculation, as specified in Ref. 2.

In their method Luttinger and Tisza used a special condition in order to overcome the obstacles encountered in the diagonalization of the Hamiltonian. This restriction is called the weak constraint. It is a technique, which is known as "sphericalization" in statistical mechanics, applied not to the spin system as a whole, but to the spins in the elementary cell of the superlattice. Niemeijer[3] has shown that this artificial condition is really equivalent to using Hartree wave functions. It is the goal of this paper to apply the ideas of Ref. 4 to a specific salt, to take correctly into account the correlations in the unit cell, so as to give a correct quantum-mechanical calculation of the problem at hand. Although this calculation is laborious, it is worth doing for several reasons: (a) Our calculation is quite general, since the tables of the matrix elements can be applied to any dipolar crystal, with spins $\frac{1}{2}$ and one ion per unit cell. (b) The low-temperature behavior of dipolar systems plays an important role in ultralow-temperature physics. (c) In calculations on the critical behavior of dipolar systems the nature of the ordering of the ground state, i.e., ferromagnetic[5] or antiferromagnetic,[6] enters implicitly into the theory through the assumed form of the propagator.

It is, morevoer, possible that many crystals containing rare-earth ions that are supposedly coupled via exchange and dipole-dipole interaction, may turn out to have actually pure dipolar interactions if only compared with more accurate calculations. The introduction of the exchange parameters[7] to explain experimental measurements, could have been solely due to the lack of a good dipolar theory.

The correct quantum-mechanical theory of the dipolar spin system has only one restriction: It is based on the *ansatz* that dipolar spin systems have a wave function that has no more than twice the lattice periodicity. We have proved in a separate paper[4] that under these circumstances the system can have a ferromagnetic or one of several antiferromagnetic states and, since observation shows that dipolar spin systems have always one of these ground states, we use this argument to support the hypothesis above. As is clear, the hypothesis is sufficient, but not necessary.

The effective Hamiltonian of the problem is described in the Sec. II. It has certain symmetry properties which help greatly to reduce the amount of numerical work. No use has been made of crystal symmetries in this paper in order to keep the calculation as general as possible. Crystal symmetries may serve a purpose, i.e., they can be used to check certain features of the results obtained.

II. HAMILTONIAN

The Hamiltonian of the system is given by

$$\mathcal{H}=\frac{1}{2}\sum_{\alpha,\beta}\mu_i^\alpha D_{ij}^{\alpha\beta}\mu_j^\beta \quad , \tag{1}$$

where D_{ij} is the dipole-dipole tensor:

$$D_{ij}^{\alpha\beta}=\delta_{\alpha\beta}r_{ij}^{-3}-3r_{ij}^\alpha r_{ij}^\beta r_{ij}^{-5} \quad . \tag{2}$$

Following Daniels[8] we assume that every ion carries a magnetic moment

$$\mu_i^\alpha=\mu_B g_i^{\alpha\beta}S_i^\beta \quad (i=1,\ldots,N) \quad , \tag{3}$$

where μ_B is the Bohr magneton, $g^{\alpha\beta}$ are the components of the g tensor, and S are the spin operators. We have assumed summations over all Greek superscripts. The ground level of the Ce ions of CMN have an effective spin $\frac{1}{2}$, hence the operators S are equal to the Pauli matrices multiplied by $\frac{1}{2}$. Substitution from (3) and (2) into (1) leads to

$$\mathcal{H}=\tfrac{1}{2}\mu_B^2\sum_{i,j}S^\alpha J_{ij}^{\alpha\beta}S^\beta$$
$$=\tfrac{1}{8}\mu_B^2\sum_{i,j}\sigma_i^\alpha J_{ij}^{\alpha\beta}\sigma_j^\beta \quad , \tag{4}$$

where J is given in Ref. 3 with $v=0$. The distances r_{ij} refer to distances from one lattice site i, to another lattice site j. Both are characterized by multiples of the three primitive translation vectors, since we are dealing with a Bravais lattice. Let us call the group of translations Γ. We ignore the small deviation found by the x-ray work of Zalkin *et al.*[9]: The different layers in the c direction are not exactly equidistant giving rise to two atoms per unit cell.

The expectation value of the energy per spin, is given by:

$$E=\frac{1}{N}\sum_{i<j}\sum_{\alpha,\beta}J_{ij}^{\alpha\beta}\langle\Psi|S_i^\alpha S_j^\beta|\Psi\rangle$$
$$=\frac{1}{16}\sum_{i\neq j=1}^{8}{}'\sum_{\alpha\beta}\langle\chi|S_i^\alpha S_j^\beta|\chi\rangle\sum_{l\in\{j\}}J_{il}^{\alpha\beta}$$
$$+\frac{1}{8}\sum_{i=1}^{8}{}'\sum_{\alpha,\beta}\langle\chi|S_i^\alpha|\chi\rangle\langle\chi|S_i^\beta|\chi\rangle\sum_{\substack{l\in\{i\}\\ l\neq i}}J_{il}^{\alpha\beta}. \tag{5}$$

In this equation Ψ refers to the wave function of the total spin system of N spins. We consider this function as a product of identical functions χ, representing the wave function of a cluster of eight neighboring spins, which we will call the basic cell. The prime on the summation sign means that the sum is taken over the sites of the basic cell. If we call Γ^2 the subgroup of the translation group Γ, consisting of all translations over the double primitive lattice vectors, then $\{i\}$ denotes the superlattice of sites generated by Γ^2 from the ith site of the basic cell. The separation of the sum into $i\neq j$ and $i=j$ is quite useful. The main problem is to solve for the eigenvalues of the first summation in (5). The second sum, which we will refer to as the "self-energy" term,[4] is a correction that has to be applied afterwards. Moreover, this term has a very simple structure, namely, it is the sum over eight equal terms. At this moment we have left out another correction needed only in the ferromagnetic case, viz., the demagnetization factor, which takes surface effects into account.

The lattice sums necessary to obtain the values of J_{ij} have been evaluated using the lattice constants of Schiferl,[10] they were used in an earlier publication by the same authors. We give the numerical values in Table I.

In order to treat the matrix constituted by the effective Hamiltonian in (5), i.e., (6), it is convenient to use the operators S^+ and S^-. In terms of these operators the Hamiltonian is

$$\mathcal{H}=\frac{1}{8}\sum_{i\,j=1}^{8}{}'\sum_{\alpha=1}^{6}J_{ij}^\alpha\,\mathcal{O}_{ij}^\alpha \quad , \tag{6}$$

where

$$\mathcal{O}_{ij}^1\equiv\mathcal{O}_{ij}^{zz}=\sigma_i^z\sigma_j^z \quad ,$$
$$\mathcal{O}_{ij}^{2,6}\equiv\mathcal{O}_{ij}^{z\pm}=\sigma_i^z\sigma_j^\pm+\sigma_j^z\sigma_i^\pm \quad ,$$
$$\mathcal{O}_{ij}^3\equiv\mathcal{O}_{ij}^{+-}=\sigma_i^+\sigma_j^-+\sigma_j^+\sigma_i^- \quad ,$$
$$\mathcal{O}_{ij}^{4,5}\equiv\mathcal{O}_{ij}^{\pm\pm}=\sigma_i^\pm\sigma_j^\pm \quad ,$$

and

$$J^1=J^{zz};\ J^{2,6}=\tfrac{1}{2}(J^{xz}\pm iJ^{yz}) \quad ,$$
$$J^3=\tfrac{1}{2}(J^{xx}+J^{yy});\ J^{4,5}=\tfrac{1}{4}(J^{xx}-J^{yy}\pm 2iJ^{xy}) \quad .$$

The matrices $S^\pm$ are given by $S^\pm=\frac{1}{2}(S^x\pm iS^y)$. The

TABLE I. Lattice sums in units $1/a^3$, where a is the distance between the ions in the plane. "Lattice" stands for the superlattice generated by Γ^2.

Lattice	$xx=1$	$yy=2$	$zz=3$	$yz=4$	$xz=5$	$xy=6$
000	0.2834	0.2834	−0.0002	0	0	0
100	−3.6317	7.8210	−0.0013	−0.1719	−0.2978	−9.9193
010	−3.6317	7.8210	−0.0013	−0.1719	0.2978	9.9193
110	−8.1669	5.9427	0.0007	−0.0604	0	0
001	13.5485	−9.3592	−0.0013	0.3439	0	0
101	2.4158	−4.6391	0.0007	0.0302	−0.0523	−6.1094
011	2.4158	−4.6391	0.0007	0.0302	0.0523	6.1094
111	−0.9193	−0.9193	0.0006	0	0	0

Hamiltonian is invariant under the eight permutations given by Table I in Ref. 2. Upon inspection one can see that the Hamiltonian can be separated in eight parts, each invariant under the transformations of the permutation group. It is convenient to separate the Hamiltonian in this form. We notice that the 8×8 matrix J_{ij} has only eight different elements and if we group all spin operators that are multiplied with the same J_{ij} together we obtain these eight invariant parts. It is convenient to label the eight different J – sums with the same labels as we use for the permutation: We thus introduce the operators

$$\mathcal{O}_P^{\alpha\beta}=\sum_i \sigma_i^\alpha \sigma_{P(i)}^\beta \ , \tag{7}$$

and the Hamiltonian can now be written as:

$$\mathcal{H}=\frac{1}{8}\sum_{\gamma=1}^{6}\sum_{P=1}^{8} J_P \mathcal{O}_P^\gamma \ . \tag{8}$$

Now comes the laborious task of determining the matrix elements of $\mathcal{O}_P$ for $\gamma=1,2,3$, and 4 (5 and 6 follow from 2 and 4 since they are each other's Hermitian conjugate). Before doing this, we first have to make a choice of the wave functions we are going to use as a basis in the calculations.

III. CHOICE OF BASIS WAVE FUNCTIONS

There are $(2S+1)^N$ wave functions. Since the effective spin is equal to $\frac{1}{2}$ and since the basic cluster contains eight spins, this amounts to 256 basis functions.

The basis wave functions are the products of eight spin-$\frac{1}{2}$ wave functions quantized along the z direction. In order to avoid writing sequences of "eight plus and minus one's" we used zero for spin up and one for spin down. Each sequence can then be interpreted as a binary number, which is very convenient to use as a label, hence

$$L=\sum_{i=1}^{8} n_i 2^{i-1} \quad (n_i=0,1;\ L=0,1,\ldots,255)\ ,$$

e.g.,

$$(-1)(+1)(+1)(-1)(-1)(-1)(+1)(-1)\rightarrow L=157\ ,$$

and will use these in the tables that follow.

These basis wave functions are not invariant under the permutation group. Starting with a certain wave function we can generate the seven other wave functions that belong to the same representation. The result is given in Table II. The wave functions are grouped according to the value of the total z component of the spin. This grouping is done solely for traditional reasons. Actually the total z component is *not* a good quantum number, and the spin component in any particular direction is not conserved. As can be seen from the table, certain functions will reproduce themselves one or more times; we purposely left those in the table since it simplifies the considerations about the various irreducible representations formed with the help of this table.

To construct the wave functions that transform according to a given irreducible representation, we proceed as follows. To find the basis functions that transform according to the first irreducible representation of the permutation group, Γ_1, we take the sum of all wave functions generated by the permutations. In certain cases the wave function that is generated by one permutation is the same as by another. This duplication may be ignored, since we eventually normalize the wave functions according to the number of different wave functions occurring in a certain representation. The basic vectors, thus formed, we call X. As can be seen in Table II they can be considered as eight-dimensional vectors $X=X_i$, just as the $q(k)$ vectors of Ref. 3. This can be used to obtain the basis vectors $q(k)X$ of the representation Γ_k by the definition

$$q(k)X=\sum_{l=1}^{8} q_i(k)X_i^l \quad (k=1,\ldots\ldots,8)\ . \tag{9}$$

We want to show now that we can formulate the matrix elements of any of the $\mathcal{O}$ operators in such a way that they can be used for all different representations with the help of the components of the vectors $q(k)$. For Γ_1 we have, e.g.,

TABLE II. Linear combinations of basis functions as generated by the permutation group. The labels of the basis functions are the decimal expression of a binary label, as explained in the text. The labels of the linear combinations are arbitrary.

Label	$q_1(k)$	$q_2(k)$	$q_3(k)$	$q_4(k)$	$q_5(k)$	$q_6(k)$	$q_7(k)$	$q_8(k)$
1	0	0	0	0	0	0	0	0
2	1	2	4	8	16	32	64	128
3	3	3	12	12	48	48	192	192
4	5	10	5	10	80	160	80	160
5	6	9	9	6	96	144	144	96
6	17	34	68	136	17	34	68	136
7	18	33	72	132	33	18	132	72
8	20	40	65	130	65	130	20	40
9	24	36	66	129	129	66	36	24
10	7	11	13	14	112	176	208	224
11	19	35	76	140	49	50	196	200
12	21	42	69	138	81	162	84	168
13	22	41	73	134	97	146	148	104
14	25	38	70	137	145	98	100	152
15	26	37	74	133	161	82	164	88
16	28	44	67	131	193	194	52	56
17	15	15	15	15	240	240	240	240
18	60	60	195	195	195	195	60	60
19	51	51	204	204	51	51	204	204
20	105	150	150	105	150	105	105	150
21	85	170	85	170	85	170	85	170
22	102	153	153	102	102	153	153	102
23	90	165	90	165	165	90	165	90
24	23	43	77	142	113	178	212	232
25	27	39	78	141	177	114	228	216
26	29	46	71	139	209	226	116	184
27	45	30	135	75	210	225	120	180
28	53	58	197	202	83	163	92	172
29	54	57	201	198	99	147	156	108
30	86	169	89	166	101	154	149	106
31	227	211	188	124	62	61	203	199
32	229	218	181	122	94	173	91	167
33	230	217	185	118	110	157	155	103
34	233	214	182	121	158	109	107	151
35	234	213	186	117	174	93	171	87
36	236	220	179	115	206	205	59	55
37	248	244	242	241	143	79	47	31
38	231	219	189	126	126	189	219	231
39	235	215	190	125	190	125	235	215
40	237	222	183	123	222	237	123	183
41	238	221	187	119	238	221	187	119
42	249	246	246	249	159	111	111	159
43	250	245	250	245	175	95	175	95
44	252	252	243	243	207	207	63	63
45	254	253	251	247	239	223	191	127
46	255	255	255	255	255	255	255	255

$$\mathcal{O}X_i = \sum C_{ij} X_j = \sum C_{ij}\, q X_j \quad , \tag{10}$$

since all the components of $q(1)$ are one.

We generate the other representations by introducing $q(k)X$,

$$\mathcal{O}q(k)X_i = \sum C'_{ij}\, q(k) X_j \quad , \tag{11}$$

and we will show that:

Theorem: The matrix elements C'_{ij} can be written as C_{ij} times a linear combination (with coefficients one) of the column vectors P of Table I, Ref. 3.

To prove this theorem let us start with a set of X belonging to Γ_1. The basic vectors of the other irreducible representations are, we claim, then given by $q(k)X$ $(k=2,\ldots,8)$.

Let us consider now a certain matrix element

$$\langle X_i | \mathcal{O} | X_j \rangle = C_{ij} \quad .$$

We write each irreducible basis wave function explicitly as a linear combination of eight functions x, where x are the eight-spin-product wave functions: $X_i = \sum_l x_i^{(l)}$. In this manner we can write the above-mentioned matrix element in a more general way:

$$\frac{1}{64}\left\langle \sum_{l'} P_{l'}(k)\, x_j^{l'} \middle| \mathcal{O} \middle| \sum_{l} P_l(k)\, x_j^{(l)} \right\rangle = C_{ij}^{(k)} \quad , \tag{12}$$

since we have incorporated all possible representations by utilizing the label k for irreducible representations. We can take these factors outside and use the fact that in an Abelian group all structure factors are either one or zero. That is, the product of two classes labeled by l and l' can always be written as a third class l''. Hence we have

$$C_{ij}^{(k)} = \frac{1}{8} \sum_{l''(l,l')} P_{l''} \langle x_j^{(l')} | \mathcal{O} | x_i^{(l)} \rangle \quad .$$

This proves that all matrix elements can be written as a linear function of the P's. Hence it is possible to present *one* table (and to use *one* computation program) for all eight representations.

IV. GENERATORS

One of the eight parts of the operators $\mathcal{O}_P$ is trivial. This part, to which we will refer as the self-part, P_1, stems from the lattice sums between like points on the superlattice. The remaining seven operators (for each component) have the interesting property that six can be generated from the seventh. For the sake of notation we choose number 2 as being known and will show that numbers $3,\ldots,8$ can be found from this operator. In this section we will drop all superscripts and write

$$\mathcal{O}_P = \sum_{i=1}^{8} \sigma_i\, \sigma_{P(i)} \quad , \tag{13}$$

where the label P is both a permutation and the label of the lattice sum J_P this operator refers to.

If we consider a second operator labeled by P': $O_{P'}$, then we can relate it to the first, labeled by P, using a conjugation with the permutation operator $Q_{PP'}$ as follows:

$$P'_j = Q_{PP'}\, P_j\, Q'_{PP'} \quad . \tag{14}$$

These Q permutations do not of course, belong to the group of permutations that leave the cluster invariant. To construct the permutations $Q_{PP'}$ we write the permutations P and P' in cycle notation. The permutations $Q_{PP'}$ are not unambigously defined. One can make, however, a choice, such that the transformation induced in the basis wave functions reproduces complete sets of basis wave functions. Let us describe the permutations that create $Q_{PP'}$ $(P'=3, \ldots, 8)$ by

$$Q_{2P'} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ i_1 & i_2 & i_3 & i_4 & i_5 & i_6 & i_7 & i_8 \end{pmatrix} , \qquad (15)$$

where $i_1, i_2, i_3, i_4, i_5, i_6, i_7, i_8,$ are given in Table III. This choice of permutation leaves the largest number of elements in each row on their places.

Let us give an example. If we determine that $\langle 24 | \mathcal{O}_2^4 | 8 \rangle = 1$ then we find from the above mentioned permutations that

$$\begin{aligned} \langle 26 | \mathcal{O}_3^4 | 9 \rangle &= \langle 25 | \mathcal{O}_4^4 | 7 \rangle \\ &= \langle 28 | \mathcal{O}_5^4 | 9 \rangle = \langle 25 | \mathcal{O}_6^4 | 5 \rangle \qquad (16) \\ &= \langle 24 | \mathcal{O}_7^4 | 3 \rangle = \langle 27 | \mathcal{O}_8^4 | 5 \rangle = 1 \ . \end{aligned}$$

This result was obtained by letting the permutations $Q_{PP'}$ operate on the linear combinations of the basis functions:

$$\begin{aligned} \langle Q_{PP}^{-1} M' | \mathcal{O}_P | Q_{PP'} M \rangle &= \langle M' | Q_{PP}^{-1} \mathcal{O}_P Q_{PP'} | M \rangle \qquad (17) \\ &= \langle M' | \mathcal{O}_P | M \rangle \ , \end{aligned}$$

where M is the label of the various functions belonging to a certain irreducible basis. This result holds for each of the irreducible representations.

V. MATRIX ELEMENTS

In Tables IV–VII we collected the results of the application of the operators $\mathcal{O}_1, \mathcal{O}_2, \mathcal{O}_3,$ and $\mathcal{O}_4$ to the basic functions given in Table II. As explained, above, the various values of the representatives of each matrix element can be found by substituting the appropriate values for the P's. The elements contain either one, two, or four P's with the exception of the elements for $\mathcal{O}^{+z}$ and $\mathcal{O}^{++}$ in the lower corner, which give rise to matrix elements that are nonzero for $\Gamma = 1$ and zero for all other representations. We used the symbol P_9 for these elements.

There are certain elements that are repeated in the $\mathcal{O}^{+-}$ operators. Finally we would like to state that all unlisted matrix elements are zero. The tables also provide us with the necessary information to calculate the self-terms. In order to calculate the $S^\pm$ in each representation, as given by

TABLE III. Permutations associated with the generators.

P'	i_1	i_2	i_3	i_4	i_5	i_6	i_7	i_8
3	1	3	2	4	5	7	6	8
4	1	4	3	2	5	8	7	6
5	1	5	3	7	2	6	4	8
6	1	6	3	8	5	2	7	4
7	1	7	3	5	4	6	2	8
8	1	8	3	6	5	4	7	2

TABLE IV. Results of the application of the operator $\mathcal{O}_1$ on the basis vectors of *all eight irreducible representations*.

$\mathcal{O}^{zz} | 1 \rangle = 4(J_2 + J_3 + J_4 + J_5 + J_6 + J_7 + J_8) P_9 | 1 \rangle$

$\mathcal{O}^{zz} | 2 \rangle = 2(J_2 + J_3 + J_4 + J_5 + J_6 + J_7 + J_8) P_1 | 2 \rangle$

$\mathcal{O}^{zz} | 3 \rangle = 2J_2 (P_1 + P_2) | 3 \rangle$

$\mathcal{O}^{zz} | 4 \rangle = 2J_3 (P_1 + P_3) | 4 \rangle$

$\mathcal{O}^{zz} | 5 \rangle = 2J_4 (P_1 + P_4) | 5 \rangle$

$\mathcal{O}^{zz} | 6 \rangle = 2J_5 (P_1 + P_5) | 6 \rangle$

$\mathcal{O}^{zz} | 7 \rangle = 2J_6 (P_1 + P_6) | 7 \rangle$

$\mathcal{O}^{zz} | 8 \rangle = 2J_7 (P_1 + P_7) | 8 \rangle$

$\mathcal{O}^{zz} | 9 \rangle = 2J_8 (P_1 + P_8) | 9 \rangle$

$\mathcal{O}^{zz} | 10 \rangle = 2(+J_2 + J_3 + J_4 - J_5 - J_6 - J_7 - J_8) P_1 | 10 \rangle$

$\mathcal{O}^{zz} | 11 \rangle = 2(+J_2 - J_3 - J_4 + J_5 + J_6 - J_7 - J_8) P_1 | 11 \rangle$

$\mathcal{O}^{zz} | 12 \rangle = 2(-J_2 + J_3 - J_4 + J_5 - J_6 + J_7 - J_8) P_1 | 12 \rangle$

$\mathcal{O}^{zz} | 13 \rangle = 2(-J_2 - J_3 + J_4 - J_5 + J_6 + J_7 - J_8) P_1 | 13 \rangle$

$\mathcal{O}^{zz} | 14 \rangle = 2(-J_2 - J_3 + J_4 + J_5 - J_6 - J_7 + J_8) P_1 | 14 \rangle$

$\mathcal{O}^{zz} | 15 \rangle = 2(-J_2 + J_3 - J_4 - J_5 + J_6 - J_7 + J_8) P_1 | 15 \rangle$

$\mathcal{O}^{zz} | 16 \rangle = 2(+J_2 - J_3 - J_4 - J_5 - J_6 + J_7 + J_8) P_1 | 16 \rangle$

$\mathcal{O}^{zz} | 17 \rangle = (+J_2 + J_3 + J_4 - J_5 - J_6 - J_7 - J_8)(P_1 + P_2 + P_3 + P_4) | 17 \rangle$

$\mathcal{O}^{zz} | 18 \rangle = (+J_2 - J_3 - J_4 - J_5 - J_6 + J_7 + J_8)(P_1 + P_2 + P_7 + P_8) | 18 \rangle$

$\mathcal{O}^{zz} | 19 \rangle = (+J_2 - J_3 - J_4 + J_5 + J_6 - J_7 - J_8)(P_1 + P_2 + P_5 + P_6) | 19 \rangle$

$\mathcal{O}^{zz} | 20 \rangle = (-J_2 - J_3 + J_4 - J_5 + J_6 + J_7 - J_8)(P_1 + P_4 + P_6 + P_7) | 20 \rangle$

$\mathcal{O}^{zz} | 21 \rangle = (-J_2 + J_3 - J_4 + J_5 - J_6 + J_7 - J_8)(P_1 + P_3 + P_5 + P_7) | 21 \rangle$

$\mathcal{O}^{zz} | 22 \rangle = (-J_2 - J_3 + J_4 + J_5 - J_6 - J_7 + J_8)(P_1 + P_4 + P_5 + P_8) | 22 \rangle$

$\mathcal{O}^{zz} | 23 \rangle = (-J_2 + J_3 - J_4 - J_5 + J_6 - J_7 + J_8)(P_1 + P_3 + P_6 + P_8) | 23 \rangle$

$\mathcal{O}^{zz} | 24 \rangle = -4 J_8 P_1 | 24 \rangle$

$\mathcal{O}^{zz} | 25 \rangle = -4 J_7 P_1 | 25 \rangle$

$\mathcal{O}^{zz} | 26 \rangle = -4 J_6 P_1 | 26 \rangle$

$\mathcal{O}^{zz} | 27 \rangle = -4 J_5 P_1 | 27 \rangle$

$\mathcal{O}^{zz} | 28 \rangle = -4 J_4 P_1 | 28 \rangle$

$\mathcal{O}^{zz} | 29 \rangle = -4 J_3 P_1 | 29 \rangle$

$\mathcal{O}^{zz} | 30 \rangle = -4 J_2 P_1 | 30 \rangle$

$\mathcal{O}^{zz} | 31 \rangle = 2(+J_2 - J_3 - J_4 - J_5 - J_6 + J_7 + J_8) P_1 | 31 \rangle$

$\mathcal{O}^{zz} | 32 \rangle = 2(-J_2 + J_3 - J_4 - J_5 + J_6 - J_7 + J_8) P_1 | 32 \rangle$

$\mathcal{O}^{zz} | 33 \rangle = 2(-J_2 - J_3 + J_4 + J_5 - J_6 - J_7 + J_8) P_1 | 33 \rangle$

$\mathcal{O}^{zz} | 34 \rangle = 2(-J_2 - J_3 + J_4 - J_5 + J_6 + J_7 - J_8) P_1 | 34 \rangle$

$\mathcal{O}^{zz} | 35 \rangle = 2(-J_2 + J_3 - J_4 + J_5 - J_6 + J_7 - J_8) P_1 | 35 \rangle$

$\mathcal{O}^{zz} | 36 \rangle = 2(+J_2 - J_3 - J_4 + J_5 + J_6 - J_7 - J_8) P_1 | 36 \rangle$

$\mathcal{O}^{zz} | 37 \rangle = 2(+J_2 + J_3 + J_4 - J_5 - J_6 - J_7 - J_8) P_1 | 37 \rangle$

$\mathcal{O}^{zz} | 38 \rangle = 2J_8 (P_1 + P_8) | 38 \rangle$

$\mathcal{O}^{zz} | 39 \rangle = 2J_7 (P_1 + P_7) | 39 \rangle$

$\mathcal{O}^{zz} | 40 \rangle = 2J_6 (P_1 + P_6) | 40 \rangle$

$\mathcal{O}^{zz} | 41 \rangle = 2J_5 (P_1 + P_5) | 41 \rangle$

TABLE IV. *(Continued)*

$$\mathcal{O}^{zz}|42\rangle = 2J_4(P_1+P_4)|42\rangle$$

$$\mathcal{O}^{zz}|43\rangle = 2J_3(P_1+P_3)|43\rangle$$

$$\mathcal{O}^{zz}|44\rangle = 2J_2(P_1+P_2)|44\rangle$$

$$\mathcal{O}^{zz}|45\rangle = 2(J_2+J_3+J_4+J_5+J_6+J_7+J_8)P_1|45\rangle$$

$$\mathcal{O}^{zz}|46\rangle = 4(J_2+J_3+J_4+J_5+J_6+J_7+J_8)P_9|46\rangle$$

$$S^{\pm} = \sum_{i=1}^{8} S_i^{\pm} , \qquad (18)$$

we simply used the absolute value of the $\mathcal{O}^{+z}$ matrix elements.

VI. PROPERTIES OF CMN

The properties of CMN that enter into the calculations, are the g factors and the lattice constants. The g factor in the perpendicular direction is 1.829. For the g factor parallel to the z axis we took 0.032; there seems to be general

TABLE V. Results of the application of the operator $\mathcal{O}_2$ on the basis vectors of *all eight irreducible representations*.

$$\mathcal{O}^{+z}|1\rangle = 0$$

$$\mathcal{O}^{+z}|2\rangle = 8^{1/2}(J_2+J_3+J_4+J_5+J_6+J_7+J_8)P_9|1\rangle$$

$$\mathcal{O}^{+z}|3\rangle = 2^{-1/2}(-J_2+J_3+J_4+J_5+J_6+J_7+J_8)(P_1+P_2)|2\rangle$$

$$\mathcal{O}^{+z}|4\rangle = 2^{-1/2}(J_2-J_3+J_4+J_5+J_6+J_7+J_8)(P_1+P_3)|2\rangle$$

$$\mathcal{O}^{+z}|5\rangle = 2^{-1/2}(J_2+J_3-J_4+J_5+J_6+J_7+J_8)(P_2+P_3)|2\rangle$$

$$\mathcal{O}^{+z}|6\rangle = 2^{-1/2}(J_2+J_3+J_4-J_5+J_6+J_7+J_8)(P_1+P_5)|2\rangle$$

$$\mathcal{O}^{+z}|7\rangle = 2^{-1/2}(J_2+J_3+J_4+J_5-J_6+J_7+J_8)(P_2+P_5)|2\rangle$$

$$\mathcal{O}^{+z}|8\rangle = 2^{-1/2}(J_2+J_3+J_4+J_5+J_6-J_7+J_8)(P_3+P_5)|2\rangle$$

$$\mathcal{O}^{+z}|9\rangle = 2^{-1/2}(J_2+J_3+J_4+J_5+J_6+J_7-J_8)(P_4+P_5)|2\rangle$$

$$\mathcal{O}^{+z}|10\rangle = 2^{-1/2}(J_2-J_3-J_4+J_5+J_6+J_7+J_8)(P_1+P_2)|3\rangle + (-J_2+J_3-J_4+J_5+J_6+J_7+J_8)(P_1+P_3)|4\rangle + (-J_2-J_3+J_4+J_5+J_6+J_7+J_8)(P_1+P_4)|5\rangle$$

$$\mathcal{O}^{+z}|11\rangle = 2^{-1/2}(J_2+J_3+J_4-J_5-J_6+J_7+J_8)(P_1+P_2)|3\rangle + (-J_2+J_3+J_4+J_5-J_6+J_7+J_8)(P_1+P_5)|6\rangle + (-J_2+J_3+J_4-J_5+J_6+J_7+J_8)(P_1+P_6)|7\rangle$$

$$\mathcal{O}^{+z}|12\rangle = 2^{-1/2}(J_2+J_3+J_4-J_5+J_6-J_7+J_8)(P_1+P_3)|4\rangle + (J_2-J_3+J_4+J_5+J_6-J_7+J_8)(P_1+P_5)|6\rangle + (J_2-J_3+J_4-J_5+J_6+J_7+J_8)(P_1+P_7)|8\rangle$$

$$\mathcal{O}^{+z}|13\rangle = 2^{-1/2}(J_2+J_3+J_4+J_5-J_6-J_7+J_8)(P_1+P_4)|5\rangle + (J_2+J_3-J_4+J_5+J_6-J_7+J_8)(P_1+P_6)|7\rangle + (J_2+J_3-J_4+J_5-J_6+J_7+J_8)(P_1+P_7)|8\rangle$$

$$\mathcal{O}^{+z}|14\rangle = 2^{-1/2}(J_2+J_3+J_4-J_5+J_6+J_7-J_8)(P_2+P_3)|5\rangle + (J_2+J_3-J_4+J_5+J_6+J_7-J_8)(P_1+P_5)|6\rangle + (J_2+J_3-J_4-J_5+J_6+J_7+J_8)(P_1+P_8)|9\rangle$$

$$\mathcal{O}^{+z}|15\rangle = 2^{-1/2}(J_2+J_3+J_4+J_5-J_6+J_7-J_8)(P_2+P_4)|4\rangle + (J_2-J_3+J_4+J_5+J_6+J_7-J_8)(P_1+P_6)|7\rangle + (J_2-J_3+J_4+J_5-J_6+J_7+J_8)(P_1+P_8)|9\rangle$$

$$\mathcal{O}^{+z}|16\rangle = 2^{-1/2}(J_2+J_3+J_4+J_5+J_6-J_7-J_8)(P_3+P_4)|3\rangle + (-J_2+J_3+J_4+J_5+J_6+J_7-J_8)(P_1+P_7)|8\rangle + (-J_2+J_3+J_4+J_5+J_6-J_7+J_8)(P_1+P_8)|9\rangle$$

$$\mathcal{O}^{+z}|17\rangle = \tfrac{1}{2}(-J_2-J_3-J_4+J_5+J_6+J_7+J_8)(P_1+P_2+P_3+P_4)|10\rangle$$

$$\mathcal{O}^{+z}|18\rangle = \tfrac{1}{2}(-J_2+J_3+J_4+J_5+J_6-J_7-J_8)(P_1+P_2+P_7+P_8)|16\rangle$$

$$\mathcal{O}^{+z}|19\rangle = \tfrac{1}{2}(-J_2+J_3+J_4-J_5-J_6+J_7+J_8)(P_1+P_2+P_5+P_6)|11\rangle$$

$$\mathcal{O}^{+z}|20\rangle = \tfrac{1}{2}(+J_2+J_3-J_4+J_5-J_6-J_7+J_8)(P_2+P_3+P_5+P_8)|13\rangle$$

$$\mathcal{O}^{+z}|21\rangle = \tfrac{1}{2}(+J_2-J_3+J_4-J_5+J_6-J_7+J_8)(P_1+P_3+P_5+P_7)|12\rangle$$

$$\mathcal{O}^{+z}|22\rangle = \tfrac{1}{2}(+J_2+J_3-J_4-J_5+J_6+J_7-J_8)(P_2+P_3+P_6+P_7)|14\rangle$$

$$\mathcal{O}^{+z}|23\rangle = \tfrac{1}{2}(+J_2-J_3+J_4+J_5-J_6+J_7-J_8)(P_1+P_3+P_6+P_8)|15\rangle$$

$$\mathcal{O}^{+z}|24\rangle = (+J_2+J_3+J_4-J_5-J_6-J_7+J_8)P_1|10\rangle + (+J_2-J_3-J_4+J_5+J_6-J_7+J_8)P_1|11\rangle + (-J_2+J_3-J_4+J_5-J_6+J_7+J_8)P_1|12\rangle + (-J_2-J_3+J_4-J_5+J_6+J_7+J_8)P_1|13\rangle$$

$$\mathcal{O}^{+z}|25\rangle = (+J_2+J_3+J_4-J_5-J_6+J_7-J_8)P_2|10\rangle + (+J_2-J_3-J_4+J_5+J_6+J_7-J_8)P_1|11\rangle + (-J_2-J_3+J_4+J_5-J_6+J_7+J_8)P_1|14\rangle + (-J_2+J_3-J_4-J_5+J_6+J_7+J_8)P_1|15\rangle$$

$$\mathcal{O}^{+z}|26\rangle = (+J_2+J_3+J_4-J_5+J_6-J_7-J_8)P_3|10\rangle + (-J_2+J_3-J_4+J_5+J_6+J_7-J_8)P_1|12\rangle$$

TABLE V. (*Continued*).

$$+(-J_2-J_3+J_4+J_5+J_6-J_7+J_8)P_1\,|14\rangle+(+J_2-J_3-J_4-J_5+J_6+J_7+J_8)P_1\,|16\rangle$$

$$\mathcal{O}^{+z}|27\rangle=(+J_2+J_3+J_4+J_5-J_6-J_7-J_8)P_3\,|10\rangle+(-J_2-J_3+J_4+J_5+J_6+J_7-J_8)P_2\,|13\rangle+(-J_2+J_3-J_4+J_5+J_6-J_7+J_8)P_2\,|15\rangle+(+J_2-J_3-J_4+J_5-J_6+J_7+J_8)P_2\,|16\rangle$$

$$\mathcal{O}^{+z}|28\rangle=(+J_2-J_3+J_4+J_5+J_6-J_7-J_8)P_5\,|11\rangle+(-J_2+J_3+J_4+J_5-J_6+J_7-J_8)P_1\,|12\rangle+(-J_2+J_3+J_4-J_5+J_6-J_7+J_8)P_2\,|15\rangle+(+J_2-J_3+J_4-J_5-J_6+J_7+J_8)P_7\,|16\rangle$$

$$\mathcal{O}^{+z}|29\rangle=(+J_2+J_3-J_4+J_5+J_6-J_7-J_8)P_6\,|11\rangle+(-J_2+J_3+J_4-J_5+J_6+J_7-J_8)P_1\,|13\rangle+(-J_2+J_3+J_4+J_5-J_6-J_7+J_8)P_2\,|14\rangle+(+J_2+J_3-J_4-J_5-J_6+J_7+J_8)P_7\,|16\rangle$$

$$\mathcal{O}^{+z}|30\rangle=(+J_2+J_3-J_4+J_5-J_6+J_7-J_8)P_7\,|12\rangle+(+J_2-J_3+J_4-J_5+J_6+J_7-J_8)P_1\,|13\rangle+(+J_2-J_3+J_4+J_5-J_6-J_7+J_8)P_3\,|14\rangle+(+J_2+J_3-J_4-J_5-J_6+J_7+J_8)P_6\,|15\rangle$$

$$\mathcal{O}^{+z}|31\rangle=(-J_2+J_3+J_4+J_5-J_6-J_7-J_8)P_6\,|26\rangle+(-J_2+J_3+J_4-J_5+J_6-J_7-J_8)P_6\,|27\rangle+(-J_2+J_3-J_4+J_5+J_6-J_7-J_8)P_6\,|28\rangle+(-J_2-J_3+J_4+J_5+J_6-J_7-J_8)P_5\,|29\rangle+\tfrac{1}{2}(+J_2-J_3-J_4-J_5-J_6+J_7+J_8)(P_3+P_4+P_5+P_6)\,|18\rangle$$

$$\mathcal{O}^{+z}|32\rangle=(+J_2-J_3+J_4+J_5-J_6-J_7-J_8)P_7\,|25\rangle+(+J_2-J_3+J_4-J_5-J_6+J_7-J_8)P_6\,|27\rangle+(+J_2-J_3-J_4+J_5-J_6+J_7-J_8)P_3\,|28\rangle+(-J_2-J_3+J_4+J_5-J_6+J_7-J_8)P_5\,|30\rangle+\tfrac{1}{2}(-J_2+J_3-J_4-J_5+J_6-J_7+J_8)(P_2+P_4+P_5+P_7)\,|23\rangle$$

$$\mathcal{O}^{+z}|33\rangle=(+J_2+J_3-J_4-J_5+J_6-J_7-J_8)P_7\,|25\rangle+(+J_2+J_3-J_4-J_5-J_6+J_7-J_8)P_6\,|26\rangle+(+J_2-J_3-J_4-J_5+J_6+J_7-J_8)P_4\,|29\rangle+(-J_2+J_3-J_4-J_5+J_6+J_7-J_8)P_4\,|30\rangle+\tfrac{1}{2}(-J_2-J_3+J_4+J_5-J_6-J_7+J_8)(P_1+P_4+P_5+P_8)\,|22\rangle$$

$$\mathcal{O}^{+z}|34\rangle=(+J_2+J_3-J_4+J_5-J_6-J_7-J_8)P_8\,|24\rangle+(+J_2+J_3-J_4-J_5-J_6-J_7+J_8)P_6\,|27\rangle+(+J_2-J_3-J_4+J_5-J_6-J_7+J_8)P_3\,|29\rangle+(-J_2+J_3-J_4+J_5-J_6-J_7+J_8)P_2\,|30\rangle+\tfrac{1}{2}(-J_2-J_3+J_4-J_5+J_6+J_7-J_8)(P_1+P_4+P_6+P_7)\,|20\rangle$$

$$\mathcal{O}^{+z}|35\rangle=(+J_2-J_3+J_4-J_5+J_6-J_7-J_8)P_8\,|24\rangle+(+J_2-J_3+J_4-J_5-J_6-J_7+J_8)P_6\,|26\rangle+(+J_2-J_3-J_4-J_5+J_6-J_7+J_8)P_4\,|28\rangle+(-J_2-J_3+J_4-J_5+J_6-J_7+J_8)P_8\,|30\rangle+\tfrac{1}{2}(-J_2+J_3-J_4+J_5-J_6+J_7-J_8)(P_2+P_4+P_6+P_8)\,|21\rangle$$

$$\mathcal{O}^{+z}|36\rangle=(-J_2+J_3+J_4-J_5-J_6+J_7-J_8)P_8\,|24\rangle+(-J_2+J_3+J_4-J_5-J_6-J_7+J_8)P_7\,|25\rangle+(-J_2+J_3-J_4-J_5-J_6+J_7+J_8)P_8\,|28\rangle+(-J_2-J_3+J_4-J_5-J_6+J_7+J_8)P_8\,|29\rangle+\tfrac{1}{2}(+J_2-J_3-J_4+J_5+J_6-J_7-J_8)(P_3+P_4+P_7+P_8)\,|19\rangle$$

$$\mathcal{O}^{+z}|37\rangle=(-J_2-J_3-J_4+J_5+J_6+J_7-J_8)P_8\,|24\rangle+(-J_2-J_3-J_4+J_5+J_6-J_7+J_8)P_8\,|25\rangle+(-J_2-J_3-J_4+J_5-J_6+J_7+J_8)P_8\,|26\rangle+(-J_2-J_3-J_4-J_5+J_6+J_7+J_8)P_7\,|27\rangle+\tfrac{1}{2}(+J_2+J_3+J_4-J_5-J_6-J_7-J_8)(P_5+P_6+P_7+P_8)\,|17\rangle$$

$$\mathcal{O}^{+z}|38\rangle=2^{-1/2}[(+J_2-J_3-J_4-J_5-J_6+J_7-J_8)(P_1+P_8)|31\rangle+(-J_2+J_3-J_4-J_5+J_6-J_7-J_8)(P_1+P_8)\,|32\rangle+(-J_2-J_3+J_4+J_5-J_6-J_7-J_8)(P_1+P_8)\,|33\rangle]$$

$$\mathcal{O}^{+z}|39\rangle=2^{-1/2}[(+J_2-J_3-J_4+J_5-J_6-J_7+J_8)(P_1+P_7)\,|31\rangle+(-J_2-J_3+J_4-J_5+J_6-J_7-J_8)(P_1+P_7)\,|34\rangle+(-J_2+J_3-J_4+J_5-J_6-J_7-J_8)(P_1+P_7)\,|35\rangle]$$

$$\mathcal{O}^{+z}|40\rangle=2^{-1/2}[(-J_2+J_3-J_4-J_5-J_6-J_7+J_8)(P_1+P_6)\,|32\rangle+(-J_2-J_3+J_4-J_5-J_6+J_7-J_8)(P_1+P_6)\,|34\rangle+(+J_2-J_3-J_4+J_5-J_6-J_7-J_8)(P_1+P_6)\,|36\rangle]$$

$$\mathcal{O}^{+z}|41\rangle=2^{-1/2}[(-J_2-J_3+J_4-J_5-J_6-J_7+J_8)(P_1+P_5)\,|33\rangle+(-J_2+J_3-J_4-J_5-J_6+J_7-J_8)(P_1+P_5)\,|35\rangle+(+J_2-J_3-J_4-J_5+J_6-J_7-J_8)(P_1+P_5)\,|36\rangle]$$

$$\mathcal{O}^{+z}|42\rangle=2^{-1/2}[(-J_2-J_3-J_4+J_5-J_6-J_7+J_8)(P_2+P_3)\,|33\rangle+(-J_2-J_3-J_4-J_5+J_6+J_7-J_8)(P_1+P_4)\,|34\rangle+(+J_2+J_3-J_4-J_5-J_6-J_7-J_8)(P_1+P_4)\,|37\rangle]$$

$$\mathcal{O}^{+z}|43\rangle=2^{-1/2}[(-J_2-J_3-J_4-J_5+J_6-J_7+J_8)(P_2+P_4)\,|32\rangle+(-J_2-J_3-J_4+J_5-J_6+J_7-J_8)(P_1+P_3)\,|35\rangle+(+J_2-J_3+J_4-J_5-J_6-J_7-J_8)(P_1+P_3)\,|37\rangle]$$

$$\mathcal{O}^{+z}|44\rangle=2^{-1/2}[(-J_2-J_3-J_4-J_5-J_6+J_7+J_8)(P_3+P_4)\,|31\rangle+(-J_2-J_3-J_4+J_5+J_6-J_7-J_8)(P_1+P_2)\,|36\rangle+(-J_2+J_3+J_4-J_5-J_6-J_7-J_8)(P_1+P_2)\,|37\rangle]$$

$$\mathcal{O}^{+z}|45\rangle=2^{-1/2}[(-J_2-J_3-J_4-J_5-J_6-J_7+J_8)(P_4+P_5)\,|38\rangle+(-J_2-J_3-J_4-J_5-J_6+J_7-J_8)(P_3+P_5)\,|39\rangle+(-J_2-J_3-J_4-J_5+J_6-J_7-J_8)(P_2+P_5)\,|40\rangle+(-J_2-J_3-J_4+J_5-J_6-J_7-J_8)(P_1+P_5)\,|41\rangle+(-J_2-J_3+J_4-J_5-J_6-J_7-J_8)(P_2+P_3)\,|42\rangle+(-J_2+J_3-J_4-J_5-J_6-J_7-J_8)(P_1+P_3)\,|43\rangle+(+J_2-J_3-J_4-J_5-J_6-J_7-J_8)(P_1+P_2)\,|44\rangle]$$

$$\mathcal{O}^{+z}|46\rangle=-8^{1/2}[(J_2+J_3+J_4+J_5+J_6+J_7+J_8)P_9\,|45\rangle]$$

agreement that it is too small to be measured. We have found in earlier work[2] that this small value has no influence on the results.

The lattice parameters are taken from the paper of Schifferl[10]: $a=10.9857$ Å and $c=17.034$ Å at 4.2 K. The calculations are performed on units a, hence

TABLE VI. Results of the application of the operator $\mathcal{O}_3$ on the basis vectors of *all eight irreducible representations*.

$$\mathcal{O}^{+-}|1\rangle=0$$

$$\mathcal{O}^{+-}|2\rangle=(J_2P_2+J_3P_3+J_4P_4+J_5P_5+J_6P_6+J_7P_7+J_8P_8)|2\rangle$$

$$\mathcal{O}^{+-}|3\rangle=\tfrac{1}{2}[J_3(P_1+P_2+P_3+P_4)|5\rangle+J_4(P_1+P_2+P_3+P_4)|4\rangle+J_5(P_1+P_2+P_5+P_6)|7\rangle+J_6(P_1+P_2+P_5+P_6)|6\rangle +J_7(P_3+P_4+P_5+P_6)|9\rangle+J_8(P_3+P_4+P_5+P_6)|8\rangle]$$

$$\mathcal{O}^{+-}|4\rangle=\tfrac{1}{2}[J_2(P_1+P_2+P_3+P_4)|5\rangle+J_4(P_1+P_2+P_3+P_4)|3\rangle+J_5(P_1+P_3+P_5+P_7)|8\rangle+J_6(P_2+P_4+P_5+P_7)|9\rangle +J_7(P_1+P_3+P_5+P_7)|6\rangle+J_8(P_2+P_4+P_5+P_7)|7\rangle]$$

$$\mathcal{O}^{+-}|5\rangle=\tfrac{1}{2}[J_2(P_1+P_2+P_3+P_4)|4\rangle+J_3(P_1+P_2+P_3+P_4)|3\rangle+J_5(P_2+P_3+P_6+P_7)|9\rangle+J_6(P_1+P_4+P_6+P_7)|8\rangle +J_7(P_1+P_4+P_6+P_7)|7\rangle+J_8(P_2+P_3+P_6+P_7)|6\rangle]$$

$$\mathcal{O}^{+-}|6\rangle=\tfrac{1}{2}[J_2(P_1+P_2+P_5+P_6)|7\rangle+J_3(P_1+P_3+P_5+P_7)|8\rangle+J_4(P_1+P_4+P_5+P_8)|9\rangle+J_6(P_1+P_2+P_5+P_6)|3\rangle +J_7(P_1+P_3+P_5+P_7)|4\rangle+J_8(P_2+P_3+P_6+P_7)|5\rangle]$$

$$\mathcal{O}^{+-}|7\rangle=\tfrac{1}{2}[J_2(P_1+P_2+P_5+P_6)|6\rangle+J_5(P_1+P_3+P_6+P_8)|9\rangle+J_4(P_1+P_4+P_6+P_7)|8\rangle+J_5(P_1+P_2+P_5+P_6)|3\rangle +J_7(P_1+P_4+P_6+P_7)|5\rangle+J_8(P_2+P_4+P_5+P_7)|4\rangle]$$

$$\mathcal{O}^{+-}|8\rangle=\tfrac{1}{2}[J_2(P_1+P_2+P_7+P_8)|9\rangle+J_3(P_1+P_3+P_5+P_7)|6\rangle+J_4(P_1+P_4+P_6+P_7)|7\rangle+J_5(P_1+P_3+P_5+P_7)|4\rangle +J_6(P_1+P_4+P_6+P_7)|5\rangle+J_8(P_3+P_4+P_5+P_6)|3\rangle]$$

$$\mathcal{O}^{+-}|9\rangle=\tfrac{1}{2}[J_2(P_1+P_2+P_7+P_8)|8\rangle+J_3(P_1+P_3+P_6+P_8)|7\rangle+J_4(P_1+P_4+P_5+P_8)|6\rangle+J_5(P_2+P_3+P_6+P_7)|5\rangle +J_6(P_2+P_4+P_5+P_7)|4\rangle+J_7(P_3+P_4+P_5+P_6)|3\rangle]$$

$$\mathcal{O}^{+-}|10\rangle=(J_2P_2+J_3P_3+J_4P_4)|10\rangle+(J_7P_1+J_8P_2)|11\rangle+(J_6P_1+J_8P_3)|12\rangle+(J_5P_1+J_8P_4)|13\rangle +(J_6P_2+J_7P_3)|14\rangle+(J_5P_2+J_7P_4)|15\rangle+(J_5P_3+J_6P_4)|16\rangle$$

$$\mathcal{O}^{+-}|11\rangle=(J_2P_2+J_5P_5+J_6P_6)|11\rangle+(J_7P_1+J_8P_2)|10\rangle+(J_4P_1+J_8P_5)|12\rangle+(J_3P_1+J_8P_6)|13\rangle +(J_3P_1+J_7P_5)|14\rangle+(J_4P_1+J_7P_6)|15\rangle+(J_3P_3+J_4P_4)|16\rangle$$

$$\mathcal{O}^{+-}|12\rangle=(J_3P_3+J_5P_5+J_7P_7)|12\rangle+(J_6P_1+J_8P_3)|10\rangle+(J_4P_1+J_8P_5)|11\rangle+(J_2P_1+J_8P_7)|13\rangle +(J_2P_1+J_6P_5)|14\rangle+(J_2P_2+J_4P_4)|15\rangle+(J_4P_1+J_6P_7)|16\rangle$$

$$\mathcal{O}^{+-}|13\rangle=(J_4P_4+J_6P_6+J_7P_7)|13\rangle+(J_5P_1+J_8P_4)|10\rangle+(J_3P_1+J_8P_6)|11\rangle+(J_2P_1+J_8P_7)|12\rangle +(J_2P_2+J_3P_3)|14\rangle+(J_2P_1+J_5P_6)|15\rangle+(J_3P_1+J_5P_7)|16\rangle$$

$$\mathcal{O}^{+-}|14\rangle=(J_4P_4+J_5P_5+J_8P_8)|14\rangle+(J_6P_2+J_7P_3)|10\rangle+(J_3P_1+J_7P_5)|11\rangle+(J_2P_1+J_6P_5)|12\rangle +(J_2P_2+J_3P_3)|13\rangle+(J_2P_1+J_7P_8)|15\rangle+(J_3P_1+J_6P_8)|16\rangle$$

$$\mathcal{O}^{+-}|15\rangle=(J_3P_3+J_6P_6+J_8P_8)|15\rangle+(J_5P_2+J_7P_4)|10\rangle+(J_4P_1+J_7P_6)|11\rangle+(J_2P_2+J_4P_4)|12\rangle +(J_2P_1+J_5P_6)|13\rangle+(J_2P_1+J_7P_8)|14\rangle+(J_4P_1+J_5P_8)|16\rangle$$

$$\mathcal{O}^{+-}|16\rangle=(J_2P_2+J_7P_7+J_8P_8)|16\rangle+(J_5P_3+J_6P_4)|10\rangle+(J_3P_3+J_4P_4)|11\rangle+(J_4P_1+J_6P_7)|12\rangle +(J_3P_1+J_5P_7)|13\rangle+(J_3P_1+J_6P_8)|14\rangle+(J_4P_1+J_5P_8)|15\rangle$$

$$\mathcal{O}^{+-}|17\rangle=\tfrac{1}{2}[(P_1+P_2+P_3+P_4)(J_5|27\rangle+J_6|26\rangle+J_7|25\rangle+J_8|24\rangle)]$$

$$\mathcal{O}^{+-}|18\rangle=\tfrac{1}{2}[(P_1+P_2+P_7+P_8)(J_3|29\rangle+J_4|28\rangle+J_5|27\rangle+J_6|26\rangle)]$$

$$\mathcal{O}^{+-}|19\rangle=\tfrac{1}{2}[(P_1+P_2+P_5+P_6)(J_3|29\rangle+J_4|28\rangle+J_7|25\rangle+J_8|24\rangle)]$$

$$\mathcal{O}^{+-}|20\rangle=\tfrac{1}{2}[(P_2+P_3+P_5+P_8)(J_2|30\rangle+J_3|29\rangle+J_8|24\rangle)+(P_1+P_4+P_7+P_6)J_5|27\rangle]$$

$$\mathcal{O}^{+-}|21\rangle=\tfrac{1}{2}[(P_1+P_3+P_5+P_7)(J_2|30\rangle+J_4|28\rangle+J_6|26\rangle+J_8|24\rangle)]$$

$$\mathcal{O}^{+-}|22\rangle=\tfrac{1}{2}[(P_1+P_4+P_5+P_8)(J_2|30\rangle+J_3|29\rangle)+(P_2+P_3+P_6+P_7)(J_6|26\rangle+J_7|25\rangle)]$$

$$\mathcal{O}^{+-}|23\rangle=\tfrac{1}{2}[(P_1+P_3+P_6+P_8)(J_2|30\rangle+J_7|25\rangle)+(P_2+P_4+P_5+P_7)(J_4|28\rangle+J_5|27\rangle)]$$

$$\mathcal{O}^{+-}|24\rangle=J_2(P_1+P_2)|25\rangle+J_3(P_1+P_3)|26\rangle+J_4(P_2+P_3)|27\rangle+J_5(P_1+P_5)|28\rangle+J_6(P_1+P_6)|29\rangle+J_7(P_1+P_7)|30\rangle +\tfrac{1}{2}J_8[(P_2+P_3+P_5+P_8)|20\rangle+(P_1+P_3+P_5+P_7)|21\rangle+(P_1+P_2+P_5+P_6)|19\rangle+(P_1+P_2+P_3+P_4)|17\rangle]$$

$$\mathcal{O}^{+-}|25\rangle=J_2(P_1+P_2)|24\rangle+J_3(P_2+P_4)|27\rangle+J_4(P_1+P_4)|26\rangle+J_5(P_2+P_6)|29\rangle+J_6(P_2+P_5)|28\rangle+J_8(P_3+P_6)|30\rangle +\tfrac{1}{2}J_7[(P_1+P_3+P_6+P_8)|23\rangle+(P_2+P_3+P_6+P_7)|22\rangle+(P_1+P_2+P_3+P_4)|17\rangle+(P_1+P_2+P_5+P_6)|19\rangle]$$

$$\mathcal{O}^{+-}|26\rangle=J_2(P_1+P_2)|27\rangle+J_3(P_1+P_3)|24\rangle+J_4(P_1+P_4)|25\rangle+J_5(P_3+P_7)|30\rangle+J_7(P_1+P_7)|28\rangle+J_8(P_2+P_7)|29\rangle +\tfrac{1}{2}J_6[(P_1+P_2+P_7+P_8)|18\rangle+(P_1+P_2+P_3+P_4)|17\rangle+(P_1+P_3+P_5+P_7)|21\rangle+(P_2+P_3+P_6+P_7)|22\rangle]$$

$$\mathcal{O}^{+-}|27\rangle=J_2(P_1+P_2)|26\rangle+J_3(P_2+P_4)|25\rangle+J_4(P_2+P_3)|24\rangle+J_6(P_2+P_5)|30\rangle+J_7(P_2+P_8)|29\rangle+J_8(P_1+P_8)|28\rangle +\tfrac{1}{2}J_5[(P_1+P_2+P_7+P_8)|18\rangle+(P_1+P_2+P_3+P_4)|17\rangle+(P_1+P_4+P_6+P_7)|20\rangle+(P_2+P_4+P_5+P_7)|23\rangle]$$

$$\mathcal{O}^{+-}|28\rangle=J_2(P_1+P_2)|29\rangle+J_3(P_5+P_7)|30\rangle+J_5(P_1+P_5)|24\rangle+J_6(P_2+P_5)|25\rangle+J_7(P_1+P_7)|26\rangle+J_8(P_1+P_8)|27\rangle +\tfrac{1}{2}J_4[(P_1+P_2+P_7+P_8)|18\rangle+(P_1+P_2+P_5+P_6)|19\rangle+(P_2+P_4+P_5+P_7)|23\rangle+(P_1+P_3+P_5+P_7)|21\rangle]$$

$$\mathcal{O}^{+-}|29\rangle=J_2(P_1+P_2)|28\rangle+J_4(P_1+P_4)|30\rangle+J_5(P_2+P_7)|25\rangle+J_6(P_1+P_6)|24\rangle+J_7(P_2+P_8)|27\rangle+J_8(P_2+P_7)|26\rangle +\tfrac{1}{2}J_3[(P_1+P_2+P_5+P_6)|19\rangle+(P_1+P_2+P_7+P_8)|18\rangle+(P_1+P_4+P_5+P_8)|22\rangle+(P_2+P_3+P_5+P_8)|20\rangle]$$

TABLE VI. (*Continued*)

$$\mathcal{O}^{+-}|30\rangle = J_3(P_5+P_7)|28\rangle + J_4(P_1+P_4)|29\rangle + J_5(P_3+P_7)|26\rangle + J_6(P_2+P_5)|27\rangle + J_7(P_1+P_7)|24\rangle + J_8(P_3+P_6)|25\rangle + \tfrac{1}{2}J_2[(P_1+P_3+P_5+P_7)|21\rangle + (P_1+P_3+P_6+P_8)|23\rangle + (P_1+P_4+P_5+P_8)|22\rangle + (P_2+P_3+P_5+P_8)|20\rangle]$$

$$\mathcal{O}^{+-}|31\rangle = (J_2P_2+J_7P_7+J_8P_8)|31\rangle + (J_4P_1+J_5P_8)|32\rangle + (J_3P_1+J_6P_8)|33\rangle + (J_3P_1+J_5P_7)|34\rangle + (J_4P_1+J_6P_7)|35\rangle + (J_3P_3+J_4P_4)|36\rangle + (J_5P_3+J_6P_4)|37\rangle$$

$$\mathcal{O}^{+-}|32\rangle = (J_3P_3+J_6P_6+J_8P_8)|32\rangle + (J_4P_1+J_5P_8)|31\rangle + (J_2P_1+J_7P_8)|33\rangle + (J_2P_1+J_5P_6)|34\rangle + (J_2P_2+J_4P_4)|35\rangle + (J_4P_1+J_7P_6)|36\rangle + (J_5P_2+J_7P_4)|37\rangle$$

$$\mathcal{O}^{+-}|33\rangle = (J_4P_4+J_5P_5+J_8P_8)|33\rangle + (J_3P_1+J_6P_8)|31\rangle + (J_2P_1+J_7P_8)|32\rangle + (J_2P_2+J_3P_3)|34\rangle + (J_2P_1+J_6P_5)|35\rangle + (J_3P_1+J_7P_5)|36\rangle + (J_6P_2+J_7P_3)|37\rangle$$

$$\mathcal{O}^{+-}|34\rangle = (J_4P_4+J_6P_6+J_7P_7)|34\rangle + (J_3P_1+J_5P_7)|31\rangle + (J_2P_1+J_5P_6)|32\rangle + (J_2P_2+J_3P_3)|33\rangle + (J_2P_1+J_8P_7)|35\rangle + (J_3P_1+J_8P_6)|36\rangle + (J_5P_1+J_8P_4)|37\rangle$$

$$\mathcal{O}^{+-}|35\rangle = (J_3P_3+J_5P_5+J_7P_7)|35\rangle + (J_4P_1+J_6P_7)|31\rangle + (J_2P_2+J_4P_4)|32\rangle + (J_2P_1+J_6P_5)|33\rangle + (J_2P_1+J_8P_7)|34\rangle + (J_4P_1+J_8P_5)|36\rangle + (J_6P_1+J_8P_3)|37\rangle$$

$$\mathcal{O}^{+-}|36\rangle = (J_2P_2+J_5P_5+J_6P_6)|36\rangle + (J_3P_3+P_4P_4)|31\rangle + (J_4P_1+J_7P_6)|32\rangle + (J_3P_1+J_7P_5)|33\rangle + (J_3P_1+J_8P_6)|34\rangle + (J_4P_1+J_8P_5)|55\rangle + (J_7P_1+J_8P_2)|37\rangle$$

$$\mathcal{O}^{+-}|37\rangle = (J_2P_2+J_3P_3+J_4P_4)|37\rangle + (J_5P_3+J_6P_4)|31\rangle + (J_5P_2+J_7P_4)|32\rangle + (J_6P_2+J_7P_3)|33\rangle + (J_5P_1+J_8P_4)|34\rangle + (J_6P_1+J_8P_3)|35\rangle + (J_7P_1+J_8P_2)|36\rangle$$

$$\mathcal{O}^{+-}|38\rangle = \tfrac{1}{2}[J_2(P_1+P_2+P_7+P_8)|39\rangle + J_3(P_1+P_3+P_6+P_8)|40\rangle + J_4(P_1+P_4+P_5+P_8)|41\rangle + J_5(P_2+P_3+P_6+P_7)|42\rangle + J_6(P_2+P_4+P_5+P_7)|43\rangle + J_7(P_3+P_4+P_5+P_6)|44\rangle]$$

$$\mathcal{O}^{+-}|39\rangle = \tfrac{1}{2}[J_2(P_1+P_2+P_7+P_8)|38\rangle + J_3(P_1+P_3+P_5+P_7)|41\rangle + J_4(P_1+P_4+P_6+P_7)|40\rangle + J_5(P_1+P_3+P_5+P_7)|43\rangle + J_6(P_1+P_4+P_6+P_7)|42\rangle + J_8(P_3+P_4+P_5+P_6)|44\rangle]$$

$$\mathcal{O}^{+-}|40\rangle = \tfrac{1}{2}[J_2(P_1+P_2+P_5+P_6)|41\rangle + J_3(P_1+P_3+P_6+P_8)|38\rangle + J_4(P_1+P_4+P_6+P_7)|39\rangle + J_5(P_1+P_2+P_5+P_6)|44\rangle + J_7(P_1+P_4+P_6+P_7)|42\rangle + J_8(P_2+P_4+P_5+P_7)|43\rangle]$$

$$\mathcal{O}^{+-}|41\rangle = \tfrac{1}{2}[J_2(P_1+P_2+P_5+P_6)|40\rangle + J_3(P_1+P_3+P_5+P_7)|39\rangle + J_4(P_1+P_4+P_5+P_8)|38\rangle + J_6(P_1+P_2+P_5+P_6)|44\rangle + J_7(P_1+P_3+P_5+P_7)|43\rangle + J_8(P_2+P_3+P_6+P_7)|42\rangle]$$

$$\mathcal{O}^{+-}|42\rangle = \tfrac{1}{2}[(P_1+P_2+P_3+P_4)(J_2|43\rangle + J_3|44\rangle) + (P_2+P_3+P_6+P_7)(J_5|38\rangle + J_8|41\rangle) + (P_1+P_4+P_6+P_7)(J_6|39\rangle + J_7|40\rangle)]$$

$$\mathcal{O}^{+-}|43\rangle = \tfrac{1}{2}[(P_1+P_2+P_3+P_4)(J_2|42\rangle + J_4|44\rangle) + (P_1+P_3+P_5+P_7)(J_5|39\rangle + J_7|41\rangle) + (P_2+P_4+P_5+P_7)(J_6|38\rangle + J_8|40\rangle)]$$

$$\mathcal{O}^{+-}|44\rangle = \tfrac{1}{2}[(P_1+P_2+P_3+P_4)(J_3|42\rangle + J_4|43\rangle) + (P_1+P_2+P_5+P_6)(J_5|40\rangle + J_6|41\rangle) + (P_3+P_4+P_5+P_6)(J_7|38\rangle + J_8|39\rangle)]$$

$$\mathcal{O}^{+-}|45\rangle = (J_2P_2+J_3J_3+J_4P_4+J_5P_5+J_6P_6+J_7P_7+J_8P_8)|45\rangle$$

$$\mathcal{O}^{+-}|46\rangle = 0$$

the only lattice parameter that enters the lattice sums is $c/a = 1.5506$. We took a unit cell (Bravais lattice) ignoring the slight displacement of every other layer of spins in the c direction. The values in Table I are the lattice sums multiplied by the appropriate g factors. The lattice sums are

$$J_{IJ}^{\alpha\beta} = \sum_{ij} J_{ij}^{\alpha\beta} \quad , \tag{19}$$

where $I = i\,\mathrm{mod}(8)$ and $J = j\,\mathrm{mod}(8)$. The labels α and β are replaced by $\gamma = 1, \ldots, 6$ in the Voight-notation since the matrix is symmetrical. The labels I and J are replaced by the eight labels that give the relative values of I and J as described in Ref. 2.

VII. COMPUTATIONS AND RESULTS

In order to introduce the matrix elements in the diagonalization program we used the un-normalized values. In this manner the values of each matrix element is a rational fraction, both integers having only one digit. One has to specify: both labels, an indicator giving the $\mathcal{O}$ operator involved, the value of the (common) numerator, and subsequently for as many J values as were involved, the numerator including its sign, the label of the J value involved and the sequence of P's that were playing a role in this particular matrix element. The last set occurred from one to seven times. After this information was read in, the program would compute the value of this particular matrix element in three steps: (i) Sum the values of the P's, as given by the representation chosen. (ii) Multiply by the lattice sums belonging to the indicator value of the operator $\mathcal{O}$ for each for the values of J_i ($i = 2, \ldots, 8$) for both the real and imaginary part. In this step the matrix element is also divided by the square root out of the norm of the bra and of the ket. (iii) Arranging the matrix elements labeled n, m in the Hermitian matrix in a real symmetric matrix of double dimension, such that they form a vector. This is done

TABLE VII. Results of the application of the operator $\mathcal{O}_4$ on the basis vectors of ***all eight irreducible representations***.

$$\mathcal{O}^{++}|1\rangle=0$$

$$\mathcal{O}^{++}|2\rangle=0$$

$$\mathcal{O}^{++}|3\rangle=2J_2P_9|1\rangle$$

$$\mathcal{O}^{++}|4\rangle=2J_3P_9|1\rangle$$

$$\mathcal{O}^{++}|5\rangle=2J_4P_9|1\rangle$$

$$\mathcal{O}^{++}|6\rangle=2J_5P_9|1\rangle$$

$$\mathcal{O}^{++}|7\rangle=2J_6P_9|1\rangle$$

$$\mathcal{O}^{++}|8\rangle=2J_7P_9|1\rangle$$

$$\mathcal{O}^{++}|9\rangle=2J_8P_9|1\rangle$$

$$\mathcal{O}^{++}|10\rangle=(J_2P_3+J_3P_2+J_4P_1)|2\rangle$$

$$\mathcal{O}^{++}|11\rangle=(J_2P_5+J_5P_2+J_6P_1)|2\rangle$$

$$\mathcal{O}^{++}|12\rangle=(J_3P_5+J_5P_3+J_7P_1)|2\rangle$$

$$\mathcal{O}^{++}|13\rangle=(J_4P_5+J_6P_3+J_7P_2)|2\rangle$$

$$\mathcal{O}^{++}|14\rangle=(J_4P_5+J_5P_4+J_8P_1)|2\rangle$$

$$\mathcal{O}^{++}|15\rangle=(J_3P_5+J_6P_4+J_8P_2)|2\rangle$$

$$\mathcal{O}^{++}|16\rangle=(J_2P_5+J_7P_4+J_8P_3)|2\rangle$$

$$\mathcal{O}^{++}|17\rangle=2^{-3/2}[J_2(P_1+P_2+P_3+P_4)|3\rangle+J_3(P_1+P_2+P_3+P_4)|4\rangle+J_4(P_1+P_2+P_3+P_4)|5\rangle]$$

$$\mathcal{O}^{++}|18\rangle=2^{-3/2}[J_2(P_3+P_4+P_5+P_6)|3\rangle+J_7(P_1+P_2+P_7+P_8)|8\rangle+J_8(P_1+P_2+P_7+P_8)|9\rangle]$$

$$\mathcal{O}^{++}|19\rangle=2^{-3/2}[J_2(P_1+P_2+P_5+P_6)|3\rangle+J_5(P_1+P_2+P_5+P_6)|6\rangle+J_6(P_1+P_2+P_5+P_6)|7\rangle]$$

$$\mathcal{O}^{++}|20\rangle=2^{-3/2}[J_4(P_2+P_3+P_5+P_8)|5\rangle+J_6(P_2+P_3+P_5+P_8)|7\rangle+J_7(P_2+P_3+P_5+P_8)|8\rangle]$$

$$\mathcal{O}^{++}|21\rangle=2^{-3/2}[J_3(P_1+P_3+P_5+P_7)|4\rangle+J_5(P_1+P_3+P_5+P_7)|6\rangle+J_7(P_1+P_3+P_5+P_7)|8\rangle]$$

$$\mathcal{O}^{++}|22\rangle=2^{-3/2}[J_4(P_1+P_4+P_5+P_8)|5\rangle+J_5(P_2+P_3+P_6+P_7)|6\rangle+J_8(P_2+P_3+P_6+P_7)|9\rangle]$$

$$\mathcal{O}^{++}|23\rangle=2^{-3/2}[J_3(P_2+P_4+P_5+P_7)|4\rangle+J_6(P_1+P_3+P_6+P_8)|7\rangle+J_8(P_1+P_3+P_6+P_8)|9\rangle]$$

$$\mathcal{O}^{++}|24\rangle=2^{-1/2}[J_2(P_1+P_7)|8\rangle+J_3(P_1+P_6)|7\rangle+J_4(P_1+P_5)|6\rangle+J_5(P_1+P_4)|5\rangle+J_6(P_1+P_3)|4\rangle+J_7(P_1+P_2)|3\rangle]$$

$$\mathcal{O}^{++}|25\rangle=2^{-1/2}[J_2(P_1+P_8)|9\rangle+J_3(P_1+P_5)|6\rangle+J_4(P_1+P_6)|7\rangle+J_5(P_2+P_4)|4\rangle+J_6(P_2+P_3)|5\rangle+J_8(P_1+P_2)|3\rangle]$$

$$\mathcal{O}^{++}|26\rangle=2^{-1/2}[J_2(P_1+P_5)|6\rangle+J_3(P_1+P_8)|9\rangle+J_4(P_1+P_7)|8\rangle+J_5(P_3+P_4)|3\rangle+J_7(P_2+P_3)|5\rangle+J_8(P_1+P_3)|4\rangle]$$

$$\mathcal{O}^{++}|27\rangle=2^{-1/2}[J_2(P_2+P_5)|7\rangle+J_3(P_2+P_8)|8\rangle+J_4(P_2+P_7)|9\rangle+J_6(P_3+P_4)|3\rangle+J_7(P_1+P_3)|4\rangle+J_8(P_2+P_3)|5\rangle]$$

$$\mathcal{O}^{++}|28\rangle=2^{-1/2}[J_2(P_1+P_3)|4\rangle+J_3(P_5+P_6)|3\rangle+J_5(P_2+P_7)|9\rangle+J_6(P_1+P_7)|8\rangle+J_7(P_2+P_5)|7\rangle+J_8(P_1+P_5)|6\rangle]$$

$$\mathcal{O}^{++}|29\rangle=2^{-1/2}[J_2(P_1+P_4)|5\rangle+J_4(P_5+P_6)|3\rangle+J_5(P_1+P_7)|8\rangle+J_6(P_2+P_7)|9\rangle+J_7(P_2+P_6)|6\rangle+J_8(P_1+P_6)|7\rangle]$$

$$\mathcal{O}^{++}|30\rangle=2^{-1/2}[J_3(P_1+P_4)|5\rangle+J_4(P_5+P_7)|4\rangle+J_5(P_1+P_6)|7\rangle+J_6(P_3+P_7)|6\rangle+J_7(P_3+P_6)|9\rangle+J_8(P_1+P_7)|8\rangle]$$

$$\mathcal{O}^{++}|31\rangle=(J_3P_3+J_4P_4+J_5P_5+J_6P_6)|16\rangle+J_2(P_8|10\rangle+P_2|11\rangle)+J_7(P_6|12\rangle+P_5|13\rangle)+J_8(P_7|14\rangle+P_5|15\rangle)$$

$$\mathcal{O}^{++}|32\rangle=(J_2P_2+J_4P_4+J_5P_5+J_7P_7)|15\rangle+J_3(P_8|10\rangle+P_3|12\rangle)+J_6(P_7|11\rangle+P_5|13\rangle)+J_8(P_7|14\rangle+P_5|16\rangle)$$

$$\mathcal{O}^{++}|33\rangle=(J_2P_2+J_3P_3+J_6P_6+J_7P_7)|14\rangle+J_4(P_8|10\rangle+P_4|13\rangle)+J_5(P_7|11\rangle+P_6|12\rangle)+J_8(P_7|15\rangle+P_6|16\rangle)$$

$$\mathcal{O}^{++}|34\rangle=(J_2P_2+J_3P_3+J_5P_5+J_8P_8)|13\rangle+J_4(P_8|10\rangle+P_4|14\rangle)+J_6(P_8|11\rangle+P_5|15\rangle)+J_7(P_8|12\rangle+P_5|16\rangle)$$

$$\mathcal{O}^{++}|35\rangle+(J_2P_2+J_4P_4+J_6P_6+J_8P_8|12\rangle+J_3(P_8|10\rangle+P_3|15\rangle)+J_5(P_8|11\rangle+P_6|14\rangle)+J_7(P_8|13\rangle+P_6|16\rangle)$$

$$\mathcal{O}^{++}|36\rangle=(J_3P_3+J_4P_4+J_7P_7+J_8P_8|11\rangle+J_2(P_8|10\rangle+P_2|16\rangle)+J_5(P_8|12\rangle+P_7|14\rangle)+J_6(P_8|13\rangle+P_7|15\rangle)$$

$$\mathcal{O}^{++}|37\rangle=(J_5P_5+J_6P_6+J_7P_7+J_8P_8)|10\rangle+J_2(P_8|11\rangle+P_8|16\rangle)+J_3(P_8|12\rangle+P_8|15\rangle)+J_4(P_8|13\rangle+P_8|14\rangle)$$

$$\mathcal{O}^{++}|38\rangle=2^{-1/2}[J_2(P_2+P_7)|25\rangle+J_3(P_3+P_6)|26\rangle+J_4(P_3+P_6)|27\rangle+J_5(P_3+P_6)|28\rangle+J_6(P_4+P_5)|29\rangle+J_7(P_4+P_5)|30\rangle]$$
$$+2^{-3/2}J_8[(P_1+P_4+P_5+P_8)|22\rangle+(P_2+P_4+P_5+P_7)|23\rangle+(P_3+P_4+P_5+P_6)|18\rangle]$$

$$\mathcal{O}^{++}|39\rangle=2^{-1/2}[J_2(P_2+P_8)|24\rangle+J_3(P_4+P_6)|27\rangle+J_4(P_4+P_6)|26\rangle+J_5(P_3+P_5)|29\rangle+J_6(P_4+P_6)|28\rangle+J_8(P_2+P_8)|30\rangle]$$
$$+2^{-3/2}J_7[(P_2+P_4+P_6+P_8)|21\rangle+(P_3+P_4+P_5+P_6)|18\rangle+(P_1+P_4+P_6+P_7)|20\rangle]$$

$$\mathcal{O}^{++}|40\rangle=2^{-1/2}[J_2(P_1+P_6)|27\rangle+J_3(P_3+P_8)|24\rangle+J_4(P_4+P_7)|25\rangle+J_5(P_2+P_5)|30\rangle+J_7(P_3+P_8)|28\rangle+J_8(P_3+P_8)|29\rangle]$$
$$+2^{-3/2}J_6[(P_1+P_4+P_6+P_7)|20\rangle+(P_2+P_4+P_5+P_7)|23\rangle+(P_3+P_4+P_7+P_8)|19\rangle]$$

TABLE VII. (*Continued*)

$\mathcal{O}^{++}|41\rangle = 2^{-1/2}[J_2(P_2+P_6)|26\rangle + J_3(P_3+P_7)|25\rangle + J_4(P_4+P_8)|24\rangle + J_6(P_4+P_8)|30\rangle + J_7(P_4+P_8)|29\rangle + J_8(P_4+P_8)|28\rangle]$
$+2^{-3/2} J_5[(P_1+P_4+P_5+P_8)|22\rangle + (P_3+P_4+P_7+P_8)|19\rangle + (P_2+P_4+P_6+P_8)|21\rangle]$

$\mathcal{O}^{++}|42\rangle = 2^{-1/2}[J_2(P_2+P_3)|29\rangle + J_3(P_2+P_3)|30\rangle + J_5(P_5+P_8)|24\rangle + J_6(P_5+P_8)|25\rangle + J_7(P_5+P_8)|26\rangle + J_8(P_6+P_7)|27\rangle]$
$+2^{-3/2} J_4[(P_5+P_6+P_7+P_8)|17\rangle + (P_2+P_3+P_6+P_7)|22\rangle + (P_1+P_4+P_6+P_7)|20\rangle]$

$\mathcal{O}^{++}|43\rangle = 2^{-1/2}[J_2(P_2+P_4)|28\rangle + J_4(P_6+P_8)|30\rangle + J_5(P_6+P_8)|25\rangle + J_6(P_6+P_8)|24\rangle + J_7(P_5+P_7)|27\rangle + J_8(P_6+P_8)|26\rangle]$
$+2^{-3/2} J_3[(P_2+P_4+P_6+P_8)|21\rangle + (P_5+P_6+P_7+P_8)|17\rangle + (P_1+P_3+P_6+P_8)|23\rangle]$

$\mathcal{O}^{++}|44\rangle = 2^{-1/2}[J_3(P_7+P_8)|28\rangle + J_4(P_7+P_8)|29\rangle + J_5(P_7+P_8)|26\rangle + J_6(P_7+P_8)|27\rangle + J_7(P_7+P_8)|24\rangle + J_8(P_7+P_8)|25\rangle]$
$+2^{-3/2} J_2[(P_1+P_2+P_7+P_8)|18\rangle + (P_5+P_6+P_7+P_8)|17\rangle + (P_3+P_4+P_7+P_8)|19\rangle]$

$\mathcal{O}^{++}|45\rangle = (J_2P_5+J_7P_4+J_8P_3)|31\rangle + (J_3P_5+J_6P_4+J_8P_2)|32\rangle + (J_4P_5+J_5P_4+J_8P_1)|33\rangle + (J_4P_5+J_6P_3+J_7P_2)|34\rangle$
$+ (J_3P_5+J_5P_3+J_7P_1)|35\rangle + (J_2P_5+J_5P_2+J_6P_1)|36\rangle + (J_2P_3+J_3P_2+J_4P_1)|37\rangle$

$\mathcal{O}^{++}|46\rangle = 2[(J_2|44\rangle + J_3|43\rangle + J_4|42\rangle + J_5|41\rangle + J_6|40\rangle + J_7|39\rangle + J_8|38\rangle)P_9]$

by introducing the following four labels:

$$i_1 = 2n^2 - 3n + 2m \quad (n \geq m) \ ,$$
$$i_3 = (2n-1)n + 2m \ , \tag{20}$$
$$i_2 = i_3 - 1; \quad i_4 = i_1 + 1 \quad \text{(except where } n = m) \ .$$

Now the diagonalization is performed by calling the appropriate subroutine. This program is a Jacobi method with successive iterations, designed by Corbato.[11] It took usually about seven sweeps through all elements to obtain off-diagonal elements less than 10^{-9}, in double precision. In the case of $\Gamma = 1$ we obtain 92 eigenvalues, each doubly degenerate, i.e., we have 46 eigenvalues corresponding to the Hermitian matrix. We are only interested in the lowest eigenvalue. The eigenvalues are arranged in declining order, hence this is the last eigenvalue. For the representations 2, ..., 8 we have 30 eigenvalues. In the procedure we used here we have 46 of which 16 are exactly zero. Since the eigenvalues are ordered these zero eigenvalues show up in the middle of the sequence.

The results of the computation (using the lattice sums of Table II) are given in Table VIII. All energy values are normalized by the Boltzmann constant and expressed in mK. In the first column we give the lowest eigenvalue of the 46 or 30-dimensional matrix. In the next column we give the result after the correction for the self-term has been made. This correction affects in general only the third significant figure. In the third column we give the demagnetization correction, which enters only in the ferromagnetic case ($\Gamma = 1$). The last two columns are the results obtained by the classical method (Luttinger and Tisza method). These results are based on exactly the same lattice sums. The labels of the representations are the labels used in Ref. 2.

The conclusion seems to be that the difference between one of the antiferromagnetic states and the ferromagnetic state is considerably less, since the first state lies much higher and the second state came down. The demagnetization factor is quite small since the ferromagnetic state lies in the z direction. This effect is probably due to the small value of $g_\parallel$. The difference is actually so small that it is hard to draw a formal conclusion. The other five states are still higher, and can thus be

TABLE VIII. Energy values for the ground states in mK. For comparison we give the classical results (Luttinger-Tisza method). Each horizontal line is the same representation.

	Quantum-mechanical results			Classical results (Luttinger-Tisza)	
	Lowest state of 46 or 30 states				Lowest state of
Rep.	Matrix	Plus Self-Term	Demagnetization	Rep.	three states
$P=1$	−0.9413	−0.94099	1.8	000	0
2	−0.7556	−0.75470	0	111	−0.4943
3	−0.9420	−0.9411	0	010	−1.9154
4	same	same	0	100	same
5	same	same	0	001	same
6	−0.7859	−0.7850	0	110	−0.61359
7	same	same	0	011	same
8	same	same	0	101	same

ruled out. The influence of small variations in the g factor of the c/a ratios will be investigated in the future.

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$$\langle 1, r_1 | S^{\alpha}_{q'} | q, r_2\rangle = \delta_{q,q'} C^{\alpha}_{r_1,r_2,q}, \quad \alpha = x, y, z. \tag{17}$$

In the same way, Eq. (23) should be replaced by

$$\langle 1, r_1 | S^{\alpha}_{q'} | q, r_2\rangle = \delta_{q,q'} D^{\alpha}_{r_1,r_2,q}, \quad \alpha = x, y, z. \tag{23}$$

The rest remains unaltered. One of the authors (Th. N.) would like to thank Professor J. D. van der Waals for pointing out the mistake and Professor B. S. Blaisse for the correction of the proof.

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