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Quantum-mechanical ground state of crystals with dipole-dipole and exchange interactions*

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The general quantum-mechanical extension of Luttinger and Tisza's approach to the ground state of crystals with dipole-dipole and exchange interactions is given. It is shown that within this approach the ground state can only be ferro- or antiferromagnetic if the unit cell contains only one or two magnetically equivalent atoms or ions.

I. INTRODUCTION

This paper is an extension of the work of Niemeijer[1] and of Niemeijer and Blöte,[2] to be referred to as I and II hereafter; and of Luttinger and Tisza's[3] work on the ground state of regular arrays of classical dipoles. In Ref. 3 the reasonable assumption was made that for classical dipoles on Bravais lattices, with one dipole per unit cell, the ground state would be in the class of states with periodicity of twice that of the lattice. The problem then was reduced to finding the minimum of a 24-dimensional quadratic form with certain additional constraints; hence, the problem is still too difficult to handle in practice. In I it was proved that one could simply look for the lowest eigenvalue of the 24×24 matrix that defined the quadratic form, because the constraints are always automatically fulfilled due to the translational symmetry of the lattice. In II these results were extended to lattices with two ions per unit cell, as was done simultaneously in Ref. 4. It was also shown in II that two equivalent ions per unit cell was the maximum number of ions that could be dealt with generally in the Luttinger-Tisza approach.

In I it was shown that the classical approach was identical to a quantum-mechanical approach when only Hartree wave functions were admitted, i.e., all correlations were neglected. *The present paper is set up completely quantum mechanically*, i.e., *all correlations in the basic cell are correctly taken into account*.

Now for a general value of the spin, the main result is surprisingly the same as that of I and II: if the quantum-mechanical (where the phrase "quantum mechanical" serves as a counterpart to a Hartree wave function) wave function has twice the periodicity of the lattice, it can only be purely ferromagnetic or purely antiferromagnetic, i.e., all canted structures are excluded. As far as the authors are aware, all substances with predominantly dipolar interactions have been found to order ferro- or antiferromagnetically.[5]

II. FORMULATION OF THE PROBLEM

Consider a Bravais lattice with $p(p=1$ or $2)$ magnetically equivalent ions per unit cell. Arbitrary unit cells have been drawn in Fig. 1(a) $(p=1)$ and Fig. 1(b) $(p=2)$. For simplicity, the origin of the coordinate system has been chosen at one of the ions. The position of the second ion in the cell [no. 9 in Fig. 1(b)] is arbitrary. The numbering of the ions in the figures will be used in the text. There are no restrictions on the basis vectors $\vec{a}$, $\vec{b}$, and $\vec{c}$, nor on the angles between them; the whole lattice is invariant under the group Γ of translations $l_1\vec{a}+l_2\vec{b}+l_3\vec{c}$ (l_i integers). (The notation of I is used.)

Every ion carries a magnetic moment $\vec{\mu}$ whose components are

$$\mu^\alpha=\mu_B\sum_\beta g_{\alpha\beta}S^\beta\ ,\quad \alpha,\beta=x,y,z \tag{1}$$

where μ_B is the Bohr magneton and the S's are the spin operators. The total Hamiltonian can be written as

$$H=\sum_{i<j}H_{ij}\ ,\quad H_{ij}=v\Delta_{ij}\vec{S}_i\cdot\vec{S}_j+D_{ij}\ , \tag{2}$$

$$D_{ij}=\frac{1}{r_{ij}^3}\left(\vec{\mu}_i\cdot\vec{\mu}_j-\frac{3(\vec{\mu}_i\cdot\vec{r}_{ij})(\vec{\mu}_j\cdot\vec{r}_{ij})}{r_{ij}^2}\right)\ , \tag{3}$$

where

$$\Delta_{ij}=\begin{cases}1 & \text{if } i \text{ and } j \text{ are nearest neighbors}\\ 0 & \text{otherwise}\end{cases} \tag{4}$$

r_{ij} is the vector that joins ion i to ion j, with components r_{ij}^α; v is the exchange-interaction strength between nearest neighbors; it would be simple to take more-general anisotropic exchange interactions into account. The total Hamiltonian can be written as

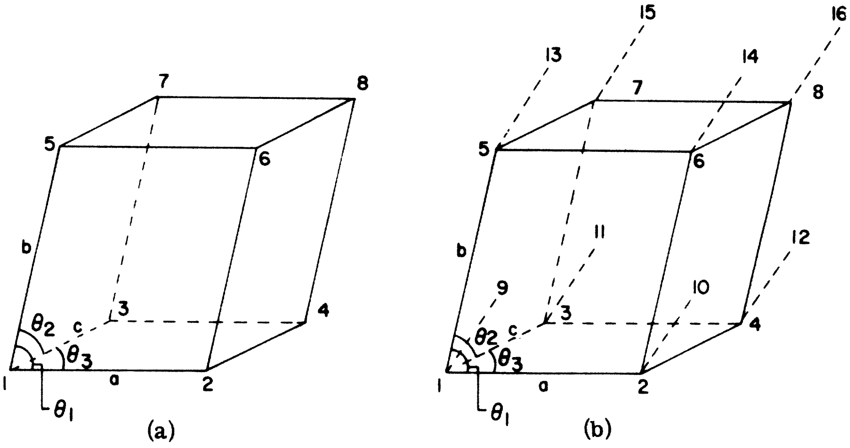

FIG. 1. (a) Basic cell of a lattice with one magnetic ion per unit cell; (b) Basic cell of a lattice with two magnetic ions per unit cell.

$$H=\sum_{i<j}\sum_{\alpha,\beta}J_{ij}^{\alpha\beta}S_i^\alpha S_j^\beta\,, \tag{5}$$

where

$$J_{ij}^{\alpha\beta}=\frac{\mu_B^2}{r_{ij}^3}\Big(\sum_{\nu,\mu}g_{\nu\alpha}g_{\mu\beta}\delta_{\mu\nu}-3g_{\nu\alpha}g_{\mu\beta}\frac{r_{ij}^\nu r_{ij}^\mu}{r_{ij}^2}\Big) + v\Delta_{ij}\delta_{\alpha\beta}\,. \tag{6}$$

We shall now formally construct all wave functions that have twice the periodicity of the unit cell as follows. Let ζ stand for the spin variables of the $8p$ spins of the basic cells of Figs. 1(a) and 1(b), respectively. By Γ^2 we denote the subgroup of Γ consisting of all translations over two lattice sites: $2l_1\vec{a}+2l_2\vec{b}+2l_3\vec{c}$ (l_i integers). Now let $\zeta(\gamma)$ be the set of spin variables of the set of $8p$ spins obtained by applying $\gamma\in\Gamma^2$ to the basic $8p$ spins. For the most general wave function Ψ of the total lattice that has twice the periodicity of the lattice, we can then write

$$\Psi=\prod_{\gamma\in\Gamma^2}\chi[\zeta(\gamma)]\,, \tag{7}$$

where χ is any wave function of the basic set of $8p$ spins.

As noted in I and II, this is the quantum-mechanical analog of Luttinger and Tisza's construction of classical dipolar arrays with twice the periodicity of the lattice. The main point of this paper will be to show that the general class of wave functions as given by Eq. (7) are either purely ferromagnetic or purely antiferromagnetic for $p=1$ or 2. A detailed quantum-mechanical ground-state energy calculation for a specific crystal, viz. cerium magnesium nitrate (CMN), will be given in a sequel to this paper.[6]

Using Eq. (5) we can write for the expectation value of the energy in the state Ψ per particle

$$E=\frac{1}{N}\sum_{i<j}\sum_{\alpha,\beta}J_{ij}^{\alpha\beta}\langle\Psi|S_i^\alpha S_j^\alpha|\Psi\rangle$$

$$=\frac{1}{16p}\sum_{i\neq j=1}^{8p}{}'\sum_{\alpha\beta}\langle\chi|S_i^\alpha S_j^\beta|\chi\rangle\sum_{l\in\{j\}}J_{il}^{\alpha\beta}$$

$$+\frac{1}{8p}\sum_{i=1}^{8p}{}'\sum_{\alpha,\beta}\langle\chi|S_i^\alpha|\chi\rangle\langle\chi|S_i^\alpha|\chi\rangle\sum_{\substack{l\in\{i\}\\ l\neq i}}J_{il}^{\alpha\beta}\,. \tag{8}$$

The prime on the summation sign means that the sum is taken over the sites of the basic cell; it will from now on be omitted; $\{i\}$ denotes the superlattice of sites generated by Γ^2 from the ith site of the basic cell. Here Eq. (7) has been used.

The wave functions χ span a $(2S+1)^{8p}$ dimensional space. In I and II the procedure was to select from this space the Hartree wave functions, so that the correlations disappeared out of Eq. (8), i.e.,

$$\langle\chi|S_i^\alpha S_j^\beta|\chi\rangle\rightarrow\langle\chi_i|S_i^\alpha|\chi_i\rangle\langle\chi_j|S_j^\beta|\chi_j\rangle\,. \tag{9}$$

This step turns the problem into a classical one, since now the expectation values of the spin operators can be separately used as variables and treated as the components of classical vectors, independent of the magnitude of the spins.

We shall not do this now, and the problem will be set up completely quantum mechanically. Introducing the abbreviations

$$A_{ij}^{\alpha\beta}(p)=\frac{1}{16p}\sum_{l\in\{i\}}J_{il}^{\alpha\beta}\,,$$
$$A_{ii}^{\alpha\beta}(p)=\frac{1}{8p}\sum_{\substack{l\in\{i\}\\ l\neq i}}J_{il}^{\alpha\beta} \tag{10}$$

(here the sums again run over the selected parts of the entire lattice), Eq. (8) can be rewritten as

$$E=\sum_{i\neq j=1}^{8p}\sum_{\alpha,\beta}A_{ij}^{\alpha\beta}(p)\langle\chi|S_i^\alpha S_j^\beta|\chi\rangle$$
$$+\sum_{i=1}^{8p}\sum_{\alpha\beta}A_{ii}^{\alpha\beta}\langle\chi|S^\alpha|\chi\rangle\langle\chi|S^\beta|\chi\rangle$$
$$=\langle\chi|H_0^{(p)}|\chi\rangle+E_s(\chi)\,. \tag{11}$$

Equation (11) can be considered as the expectation value of a Hamiltonian

$$H_0^{(p)} = \sum_{i\neq j=1}^{8p} \sum_{\alpha,\beta} A_{ij}^{\alpha\beta}(p) S_i^\alpha S_j^\beta \tag{12}$$

describing the interaction between $8p$ spins, the energy of every eigenstate χ being corrected by a "self-energy" $E_s(\chi)$, which for each dipolar system is predetermined for every eigenstate χ of $H_0^{(p)}$.

All the properties of the eigenstates of $H_0^{(p)}$, such as their being ferro- or antiferromagnetic or their having a canted structure, [except for the energy, which has to be corrected by a factor $E_s(\chi)$] are completely determined by the Hamiltonian $H_0^{(p)}$. If the ground state of $H_0^{(p)}$ turns out to be ferromagnetic, a correction for the energy due to demagnetizing effects also has to be made, but this will be a problem in actual calculations only.

Here we shall only be concerned with the properties of the Hamiltonian $H_0^{(p)}$, and shall show on the basis of its symmetry properties that, for $p = 1$ or 2, its eigenstates always fall into two classes, namely the purely ferromagnetic and the several purely antiferromagnetic ones.

III. CASE OF ONE ION PER UNIT CELL: p = 1

The Hamiltonian in this case is

$$H_0^{(1)} = \sum_{i\neq j=1}^{8} \sum_{\alpha,\beta} A_{ij}^{\alpha\beta}(1) S_i^\alpha S_j^\beta . \tag{13}$$

We denote by P_t, $t = 1, \ldots, 8$ the permutations

$$\begin{aligned} &P_1 = I \text{ (identity)},\\ &P_2 = (1,2)(3,4)(5,6)(7,8),\\ &P_3 = (1,3)(2,4)(5,7)(6,8),\\ &P_4 = (1,4)(2,3)(5,8)(6,7),\\ &P_5 = (1,5)(2,6)(3,7)(4,8),\\ &P_6 = (1,6)(2,5)(3,8)(4,7),\\ &P_7 = (1,7)(2,8)(3,5)(4,6),\\ &P_8 = (1,8)(2,7)(3,6)(4,5). \end{aligned} \tag{14}$$

It was shown in I that the matrix $A_{i,j}^{\alpha\beta}(1)$ is invariant under the operations

$$A_{i,j}^{\alpha\beta}(1) = A_{P_t i}^{\alpha\beta}(1)_{P_t j} . \tag{15}$$

The permutations P_t, $t = 1, \ldots, 8$, form a group P_t which is equivalent to the Abelian group $C_2 \otimes C_2 \otimes C_2$, and which correspondingly has eight classes and eight different one-dimensional irreducible representations Γ_q. Its character table is given in Table I.

There are $(2S+1)^8$ basis wave functions. On account of the fact that the Hamiltonian $H_0^{(1)}$ is invariant under the group P_t, it is possible to form linear combinations such that each forms the basis of an irreducible representation Γ_q of the group P_t. Hence q is a good quantum number, and we can label the wave functions as $|q, r\rangle$, where r labels the different eigenfunctions of $H_0^{(1)}$ belonging to the same representation Γ_q.

For a fixed α ($\alpha = x, y, z$) of course, eight linear combinations S_β^α of the operators S_i^α, $i = 1, \ldots, 8$ can also be formed such that they transform as one of the representations Γ_q. If one defines by q_i the ith component of the row vector $\vec{q}$ ($= 1, \ldots, 8$) in Table I, one readily verifies that these operators $\mathcal{S}_q^\alpha$ are given by the expressions

$$\mathcal{S}_q^\alpha = \sum_{i=1}^{8} S_i^\alpha q_i . \tag{16}$$

If we want to calculate the expectation of any $\mathcal{S}_{q'}^\alpha$ in a representation Γ_q, we have, according to Wigner's theorem,

$$\langle P_t(q\,r)|\mathcal{S}_{q'}^\alpha|P_t(q\,r)\rangle = \langle q\,r|P_t^{-1}\mathcal{S}_{q'}^\alpha|qr\rangle \tag{17}$$

and since all elements have cycle 2, we do not have to distinguish between the operator P_t and its inverse; consequently

$$\langle qr|\mathcal{S}_{q'}^\alpha|qr\rangle = \delta_{q,q'} C_r^\alpha , \quad \alpha = x, y, z .$$

Inspecting now Eq. (16) and Table I, we note that all the wave functions in the representation Γ_1 are ferromagnetic, and all wave functions belonging to the representations Γ_q, $q = 2, \ldots, 8$ are antiferromagnetic. In the latter case, the expectation values of the components of the spins on sites $i = 2, \ldots, 8$ (parallel: +1, antiparallel: −1) with respect to the spin on site 1 are given by the q_i:

$$\langle S_i^\alpha \rangle = q_i \langle S_1^\alpha \rangle . \tag{18}$$

The result of the foregoing property is that [whatever the values of $E_s(\chi)$ of the different eigenvalues of the Hamiltonian $H_0^{(1)}$ are] if the quantum-mechanical wave function of a system with one ion per unit cell and dipole-dipole and exchange interactions is invariant under the operations of Γ^2, it can only be purely ferromagnetic or antiferromagnetic. The corresponding possibilities are shown in Fig. 2. Only in the case of *purely accidental* degeneracy of the lowest level of Γ_1 with the lowest of all other Γ_q's, both after correction

TABLE I. Character table of P_t.

Γ_q	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8
$q=1$	1	1	1	1	1	1	1	1
$q=2$	1	−1	−1	1	−1	1	1	−1
$q=3$	1	1	−1	−1	1	1	−1	−1
$q=4$	1	1	1	1	−1	−1	−1	−1
$q=5$	1	−1	1	−1	1	−1	1	−1
$q=6$	1	1	−1	−1	−1	−1	1	1
$q=7$	1	−1	−1	1	1	−1	−1	1
$q=8$	1	−1	1	−1	−1	1	−1	1

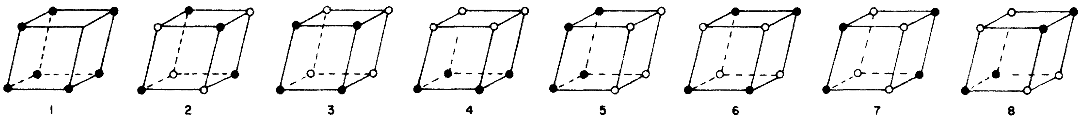

FIG. 2. Possible configurations of the ground state for the basic cell for one ion per unit cell. Spins on open circles are parallel to each other and antiparallel to the ones on the black circles. The number of the configurations corresponds with the number q of the corresponding representation. There is one ferromagnetic, and seven antiferromagnetic configurations.

with $E_s(\chi)$ and the one of Γ_1 also corrected for demagnetizing effects, can the ground state possibly show a canted structure, e.g., one induced by a small symmetry-breaking field.

IV. CASE OF TWO EQUIVALENT IONS PER UNIT CELL: p=2

This case can be treated in essentially the same way as the preceding one (Sec. III). The pertinent Hamiltonian now is

$$H_0^{(2)} = \sum_{i\neq j=1}^{16} A^{\alpha\beta}_{ij}(2) S^\alpha_i S^\beta_j \ . \tag{19}$$

As was shown in II, and also in Ref. 4, the matrix $A^{\alpha\beta}_{ij}(2)$ now is invariant under the operations

$$A^{\alpha\beta}_{i,j}(2) = A^{\alpha\beta}_{P'_t i P'_t j}(2) \ , \tag{20}$$

where now the operations P'_t are the group of permutations

$P'_1 = I$ (identity) ,

$P'_2 = (1, 2)(3, 4)(5, 6)(7, 8)(9, 10)(11, 12)(13, 14)(15, 16)$,

$P'_3 = (1, 3)(2, 4)(5, 7)(6, 8)(9, 11)(10, 12)(13, 15)(14, 16)$,

$P'_4 = (1, 4)(2, 3)(5, 8)(6, 7)(9, 12)(10, 11)(13, 16)(14, 15)$,

$P'_5 = (1, 5)(2, 6)(3, 7)(4, 8)(9, 13)(10, 14)(11, 15)(12, 16)$,

$P'_6 = (1, 6)(2, 5)(3, 8)(4, 7)(9, 14)(10, 13)(11, 16)(12, 15)$,

$P'_7 = (1, 7)(2, 8)(3, 5)(4, 6)(9, 15)(10, 16)(11, 13)(12, 14)$,

$P'_8 = (1, 8)(2, 7)(3, 6)(4, 5)(9, 16)(10, 15)(11, 14)(12, 13)$,

$P'_9 = (1, 9)(2, 10)(3, 11)(4, 12)(5, 13)(6, 14)(7, 15)(8, 16)$,

$P'_{10} = (1, 10)(2, 9)(3, 12)(4, 11)(5, 14)(6, 13)(7, 16)(8, 15)$,

$P'_{11} = (1, 11)(2, 12)(3, 9)(4, 10)(5, 15)(6, 16)(7, 13)(8, 14)$,

$P'_{12} = (1, 12)(2, 11)(3, 10)(4, 9)(5, 16)(6, 15)(7, 14)(8, 13)$,

$P'_{13} = (1, 13)(2, 14)(3, 15)(4, 16)(5, 9)(6, 10)(7, 11)(8, 12)$,

$P'_{14} = (1, 14)(2, 13)(3, 16)(4, 15)(5, 10)(6, 9)(7, 12)(8, 11)$,

$P'_{15} = (1, 15)(2, 16)(3, 13)(4, 14)(5, 11)(6, 12)(7, 9)(8, 10)$,

$P'_{16} = (1, 16)(2, 15)(3, 14)(4, 13)(5, 12)(6, 11)(7, 10)(8, 9)$. (21)

[Note that this is only true when the two ions are equivalent, because the g tensors enter into $A^{\alpha\beta}_{ij}(2)$.]

The group P'_t is equivalent to $C_2 \otimes C_2 \otimes C_2 \otimes I$, where I is the inversion with respect to the point halfway between the line connecting the two ions in the unit cell; consequently it is Abelian, contains 16 different classes, and 16 different irreducible one-dimensional representations Γ_q, $q = 1, \ldots, 16$. Its character table is given in Table II.

The $(2S+1)^{16}$ wave functions can now be grouped together in linear combinations that transform according to one of the irreducible representations Γ_q of the group P'_t. Again q is a good quantum number, and the eigenfunctions of $H_0^{(2)}$ can be labeled as $|q, r\rangle$, where r labels the different eigenfunctions of $H_0^{(2)}$ in one representation Γ_q (from now on q and r refer to the group P'_t rather than P_t).

For a fixed α ($\alpha = x, y, z$), sixteen linear combinations s^α_q of the operators S_i, $i = 1, \ldots, 16$ can be found such that they transform as one of the representations Γ_q. They can be explicitly formed now with the help of the character table II: by defining q_i as the ith component of the row vector $\vec{q}$ $(=1, \ldots, 16)$, it can in the same way be verified that these sixteen operators are given by the expressions

$$s^\alpha_q = \sum_{i=1}^{16} S^\alpha_i q_i , \quad \alpha = x, y, z \ . \tag{22}$$

If we now want to calculate the expectation value of $S^\alpha_{q'}$ in any representation Γ_q, we find according to the same reasoning following Eq. (17) in Sec. III

$$\langle q, r | S^\alpha_{q'} | q, r \rangle = \delta_{q,q'} D^\alpha_r , \quad \alpha = x, y, z \ . \tag{23}$$

Inspecting Eq. (22) and Table II, we come to a conclusion similar to the one in Sec. III: all the wave functions in the representation Γ_1 are ferromagnetic, and all wave functions belonging to the representations Γ_q, $q = 2, \ldots, 16$ are antiferromagnetic. Again, in the latter case, the expectation values of the components of the spins on sites $i = 2, \ldots, 16$ (parallel $= +1$, antiparallel $= -1$) with respect to the spin on site 1 are given by the q_i, respectively. The corresponding possibilities for the basic cell are shown in Fig. 3.

Again the result of the foregoing property is that whatever the values of the $E_s(\chi)$ of the eigenfunctions of the Hamiltonian $H_0^{(2)}$ are, if the quantum-mechanical ground-state wave function of a system

TABLE II. Character table of P_t'.

Γ_q	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	P_9	P_{10}	P_{11}	P_{12}	P_{13}	P_{14}	P_{15}	P_{16}
$q=1$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
$q=2$	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
$q=3$	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	−1	1	1	−1
$q=4$	1	−1	−1	1	−1	1	1	−1	−1	1	1	−1	1	−1	−1	1
$q=5$	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1
$q=6$	1	1	−1	−1	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1
$q=7$	1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
$q=8$	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1
$q=9$	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
$q=10$	1	−1	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1
$q=11$	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1	1	1
$q=12$	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1	1	1	−1	−1
$q=13$	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1
$q=14$	1	−1	−1	1	1	−1	−1	1	−1	1	1	−1	−1	1	1	−1
$q=15$	1	−1	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	−1	1
$q=16$	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1	1	−1	1	−1

with two equivalent magnetic ions per unit cell and dipole-dipole and exchange interactions is invariant under the operations of Γ^2, then it can only be purely ferromagnetic or antiferromagnetic.

The statement about the accidental degeneracy at the end of Sec. III applies here identically.

V. IMPOSSIBILITY OF EXTENDING GENERAL METHOD TO MORE THAN TWO (EQUIVALENT) IONS PER UNIT CELL, OR HIGHER PERIODICITY OF THE GROUND-STATE WAVE FUNCTION

It should first be remarked that the whole structure of the proof of the main result for the case of two ions per unit cell is based on the underlying group P_t'. If the two ions are no longer magnetically equivalent, the matrix $A_{ij}^{\alpha\beta}(2)$ is no longer invariant under the inversion I—hence, under the permutations $P_9', \ldots, P_{16}'$—and as a result the proof breaks down. The invariance under these last permutations gives rise to the fact that the matrix $A(2)$ can formally be written as

$$A(2)=\begin{pmatrix} M & N \\ N & M \end{pmatrix} , \tag{24}$$

where M and N are both 24×24 matrices, although they still have the same invariance group P_t as $A(1)$.

If there were three (even equivalent) ions per unit cell, in order for an analogous proof to go through, as in the two preceding cases, one would need an underlying symmetry group P_t'' of 24 elements, which is a natural extension of P_t and P_t'. This, however, is generally impossible (except when the three ions would occupy very special posi-

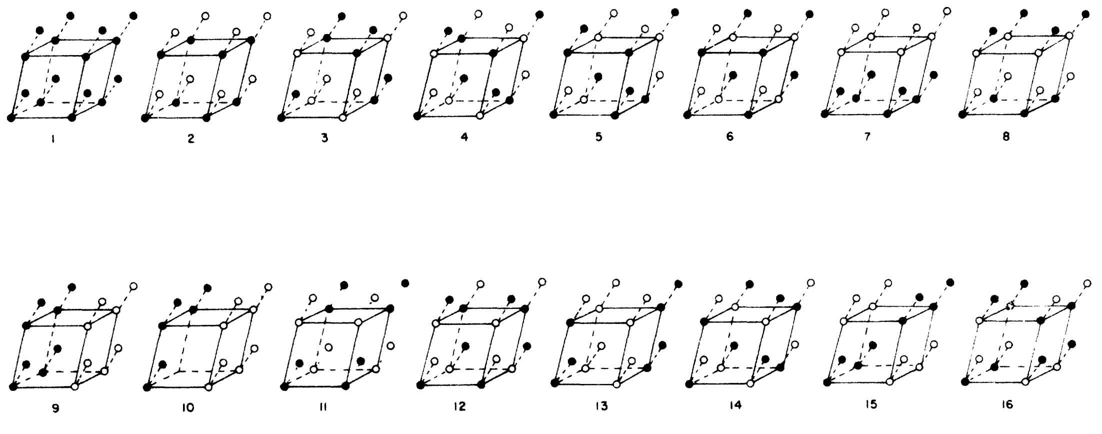

FIG. 3. Possible configurations of the ground state for the basic cell for two ions per unit cell. Spins on open circles are parallel to each other and antiparallel to the ones on the black circles. The number of the configuration corresponds with the number q of the corresponding representation. There is one ferromagnetic and, therefore, fifteen antiferromagnetic configurations.

tions in the unit cell) since, for three ions per unit cell, the matrix $A(3)$ will obviously have the following structure:

$$A(3)=\begin{pmatrix} M & N & O \\ N & M & P \\ O & P & M \end{pmatrix} , \tag{25}$$

where the 24×24 matrices M, N, O, and P still have the same symmetry as $A(1)$, viz., P_t.

The impossibility of extending the method in general to wave functions that have a periodicity of more than twice that of the unit cell has been discussed at length in II, and is a result of the fact that the character tables would then always contain complex numbers.

VI. CONCLUSION

It has been shown that the ground-state quantum-mechanical wave function with twice the periodicity of the lattice, for arrays of spins of arbitrary magnitude and one or two equivalent ions per unit cell, with dipole-dipole and exchange interactions, always is purely ferromagnetic or antiferromagnetic. This conclusion can in general not be made for crystals with more than two ions per unit cell, or if the ground-state wave function has a higher periodicity than twice that of the unit cell.

As mentioned before, a detailed calculation of the ground-state energy of a crystal of spins $\frac{1}{2}$, with one ion per unit cell, and almost exclusively dipolar interactions, viz., cerium magnesium nitrate, will appear as a sequel to this paper.[6]

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