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MAGNETIC CONFIGURATIONS DUE TO THE ORBITAL ANGULAR MOMENTUM

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Magnetic configurations arising in substances with small crystal fields, i.e., with an unquenched orbital angular momentum, are investigated. It is shown that the presence of several magnetic sublattices may result in deformation of the crystal (formation of new crystallographic periods).

1. INTRODUCTION

WE consider in the present paper the possible magnetic configurations of dielectric compounds, connected with the existence of a free (unquenched) orbital angular momentum. Such a situation may possibly be realized in compounds of transition or rare-earth elements, in which the crystal fields are weak.

It is usually assumed that the magnetic properties of dielectrics are connected with the system of localized electron spins. Depending on the magnitude and sign of the exchange interaction of the spins, substances can be either ferro- or antiferromagnetic, or else possess a more complicated magnetic structure (some type of helical configuration). It is known (see, for example,[1]), that in dielectrics the spin interaction consists of ordinary and effective exchange. The latter is connected with the virtual transitions of the localized electrons at the nearest sites. Such a system of localized electrons can be sufficiently well described by the Hubbard model Hamiltonian[2]

$$H = v\sum_{\mathbf{r},\mathbf{a},\sigma} c^{+}_{\mathbf{r},\sigma} c_{\mathbf{r}+\mathbf{a},\sigma} + U\sum_{\mathbf{r}} n_{\mathbf{r},\uparrow} n_{\mathbf{r},\downarrow}. \tag{1}$$

Here $c^{+}_{\mathbf{r},\sigma}(c_{\mathbf{r},\sigma})$ are the usual operators for the creation (annihilation) of an electron with spin projection σ at the site $\mathbf{r}$. The sum with respect to $\mathbf{a}$ denotes summation over nearest neighbors. If $v/U \ll 1$ and the number of localized electrons coincides with the number of magnetic sites (the typical dielectric situation), second-order perturbation theory in the kinetic energy yields the effective Hamiltonian

$$H_{\text{eff}} = \frac{4v^2}{U}\sum_{\mathbf{r},\mathbf{a}} \mathbf{S}_{\mathbf{r}}\mathbf{S}_{\mathbf{r}+\mathbf{a}}. \tag{2}$$

We note that the constant in the spin Hamiltonian (2) is always positive, and that the magnitude of this constant frequently turns out to be larger (at least in oxides), than the usual exchange energy[1].

However, the Hubbard model possesses a significant shortcoming, namely, a localized s-electron is considered, whereas the magnetism is due to either d- or f-electrons. In the preceding paper[3], we attempted to improve the Hubbard model so as to be able to use it in the case of a localized electron having an orbital angular momentum. The Hamiltonian (1) was written in the form

$$H = v\sum_{\mathbf{r},\mathbf{a},m,\sigma} c^{+}_{\mathbf{r},m,\sigma} c_{\mathbf{r}+\mathbf{a},m,\sigma} + U\sum_{\mathbf{r}} \frac{N_{\mathbf{r}}(N_{\mathbf{r}}-1)}{2}. \tag{3}$$

We have added here the summation with respect to the projection of the orbital angular momentum (m) and

$$N_{\mathbf{r}} = \sum_{m,\sigma} c^{+}_{\mathbf{r},m,\sigma} c_{\mathbf{r},m,\sigma}.$$

We note that in dielectric compounds, where the interaction of the magnetic atoms is indirect, the Hamiltonian (3) describes quite well a system of weakly-interacting localized electrons.

If the crystal fields are strong, i.e., the orbital angular momentum in the crystal is quenched, then (3) reduces to an effective Hamiltonian of approximately the same form as (2).

On the other hand, if the crystal fields are weak, as in certain transition-metal compounds and in most rare-earth-element compounds[4], then the orbital angular momentum is weakly coupled to the lattice. Therefore a good quantum number for the localized electron is not only the spin, but also the orbital angular momentum. In this case, when determining the magnetic properties of a substance, we cannot confine ourselves to one (ferromagnetism) or two (antiferromagnetism) magnetic sublattices. The presence of a free orbital angular momentum leads to the appearance of several magnetic sublattices.

2. DERIVATION OF THE EFFECTIVE HAMILTONIAN

We shall consider henceforth the simplest case, when the number of electrons coincides with the number of sites N. The problem consists of determining the energy and the wave function of the ground state of such a system, described by the Hamiltonian (3).

We put $v = 0$ in the zeroth approximation. Then any state in which one electron is localized on each site has an energy equal to zero. This is the minimum possible energy. The ground state in the approximation under consideration is strongly degenerate (the degree of degeneracy is p^N, where p is the number of different localized states of the electron on one site). Turning on the "jump-over" interaction $(v \neq 0)$ lifts the degeneracy almost completely. At small values of v, the ground state can be represented as a superposition of the ground states of the unperturbed Hamiltonian H_0, i.e., states with one electron per site. Let λ denote the number of the state of the electrons at the site $(\lambda = 1, 2, \ldots, p)$. The states with one electron on each site form a subspace Λ of the vectors $(\lambda_1, \lambda_2, \ldots, \lambda_N)$.

It is useful to express the eigenvalues of the Hamiltonian H in the representation of the quantum numbers λ_n. We confine ourselves to the second order of perturbation theory in v. The effective Hamiltonian is

$$H_{\text{eff}} = \frac{2v^2}{U} \sum_{\mathbf{r},\mathbf{a},\lambda,\lambda'} \overset{+}{c}_{\mathbf{r},\lambda} c_{\mathbf{r},\lambda'} \overset{+}{c}_{\mathbf{r}+\mathbf{a},\lambda'} c_{\mathbf{r}+\mathbf{a},\lambda}. \tag{4}$$

We recall once more that H_{eff} acts only in the subspace Λ. Use was made of the fact that in Λ we have for the operator

$$\sum_{\lambda} c^{(+)}_{\mathbf{r},\lambda} c_{\mathbf{r},\lambda} = 1.$$

It can be verified that the operator

$$\sum_{\lambda,\lambda'} \overset{+}{c}_{\mathbf{r},\lambda} c_{\mathbf{r},\lambda'} \overset{+}{c}_{\mathbf{r}',\lambda'} c_{\mathbf{r}',\lambda}$$

is none other than the permutation operator $P_{\mathbf{r},\mathbf{r}'}$, which interchanges the quantum numbers λ on the sites $\mathbf{r}$ and $\mathbf{r}'$. The final form of H_{eff} is

$$H_{\text{eff}} = g \sum_{\mathbf{r},\mathbf{a}} P_{\mathbf{r},\mathbf{r}+\mathbf{a}}. \tag{5}$$

Formula (4) remains valid also when an integer number of electrons, larger than one, is located at each site, but expression (5) does not hold, owing to Hund's rule.

3. MAGNETIC CONFIGURATIONS

The simplest approximation customarily employed in the theory of magnetism, the Hartree approximation, yields for the Hamiltonian (5) an obvious result, namely, the lowest energy, equal to zero, is possessed by all states in which the quantum numbers λ of the nearest neighbors are different. Thus, in the Hartree approximation, the ground state is multiply degenerate (with the exception of the cases $p = 1$ and $p = 2$, corresponding to ferro- and antiferromagnetism, respectively). On the other hand, in the one-dimensional case with $p = 3$, the problem was solved exactly by one of the authors[5]. The exact solution shows that the ground state is not degenerate and that the numbers of electrons are the same for all three values of λ. From the nondegeneracy of the ground state it follows that in the one-dimensional case there are no sublattices filled with different states λ. A similar situation also arises in an ordinary antiferromagnetic chain. In the three-dimensional case, however, there arise antiferromagnetic sublattices that disintegrate in the one-dimensional case as a result of the large fluctuations. It is natural to expect in the present model, too, that a regular order with several sublattices will occur in the three-dimensional case.

Let us show how to find the most convenient sublattice. For simplicity we consider first a planar quadratic lattice and $p = 4$[1]. We seek the ground state in the class of regular lattices, on which the following limitations are imposed: 1) the neighboring sites are occupied by different states; 2) each state corresponds to an area equal to four; 3) the individual states form regular sublattices.

In the case under consideration, three types of such sublattices are possible, which we shall designate A, B, and C (Fig. 1).

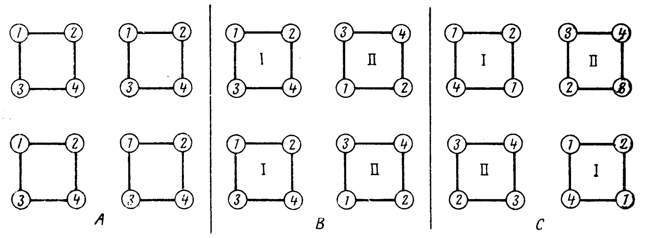


FIG. 1. Possible regular configurations in a planar lattice ($p = 4$).

We have already shown that the Hartree approximation does not suffice for the determination of the energy and the wave function of the ground state. It is necessary to go outside the scope of the usual Hartree approximation. We proceed in the following manner. We break up the lattice into squares as shown in Fig. 1, and seek the wave functions of the corresponding configurations in the form

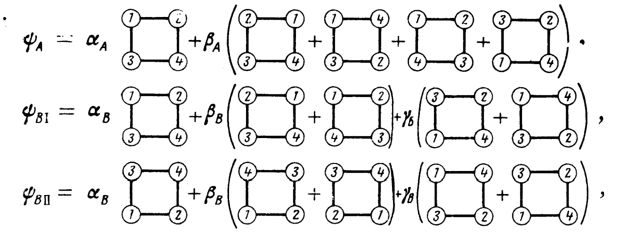
$$\Psi = \prod_j \psi_j, \tag{6}$$

where ψ_j is the wave function of the elementary square. We start from a certain square configuration which we shall call regular (Fig. 1). The state ψ_j contains, besides the regular configuration, also certain irregular ones. The simplest irregular configurations are obtained from the regular one by permuting neighboring sites (see formulas (7)--(9)) in the same or in different squares.

Our approximation is none other than the Hartree method, but no longer for sites, but for squares. Such an approach is reasonable if it is recalled that even the eigenfunctions of an ordinary antiferromagnet contain, besides the regular configuration, also spoiled configurations[2].

Getting ahead of ourselves, we note that, as shown by calculation, the fraction of irregular states due to permutations between squares is small (of the order of 1--3%). In the zeroth approximation, such states can be disregarded.

The simplest of the three is configuration A, in which all squares are the same. Lattices B and C are made up of squares of two different types (I and II). Using the symmetry properties of the obtained lattices, we seek the functions ψ_j in the form



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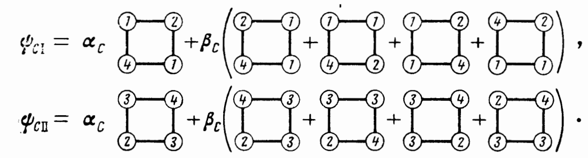
[1] A situation with $p = 4$ is perfectly realistic. It corresponds to large crystal fields but to a small spin-orbit interaction. In this case there remains a twofold degeneracy of the levels with respect to the projection of the orbital angular momentum.

[2] In principle, the lattice can be subdivided into squares of larger dimension. The results become asymptotically exact if the dimension of the square is allowed to tend to infinity. Our method of calculation is the first step in such a process. One can expect, however, that it will give better results than the usual Hartree method. For an ordinary antiferromagnet, the energy of the ground state, calculated by the Hartree method, yields $\epsilon = 0$, our method yields $\epsilon = -0.17$, and the spin-wave method yields $\epsilon = -0.31$.



$$\psi_{CI}=\alpha_C\begin{matrix}1&2\\4&1\end{matrix}+\beta_C\left(\begin{matrix}2&1\\4&1\end{matrix}+\begin{matrix}1&1\\4&2\end{matrix}+\begin{matrix}1&2\\1&4\end{matrix}+\begin{matrix}4&2\\1&1\end{matrix}\right),$$
$$\psi_{CII}=\alpha_C\begin{matrix}3&4\\2&3\end{matrix}+\beta_C\left(\begin{matrix}4&3\\2&3\end{matrix}+\begin{matrix}3&3\\2&4\end{matrix}+\begin{matrix}3&4\\3&2\end{matrix}+\begin{matrix}2&4\\3&3\end{matrix}\right).\qquad(7)$$

The corresponding energies are expressed in terms of the coefficients α, β, and γ as follows:

$$\begin{aligned}E_A&={}^1/_4N(8\alpha_A\beta_A+8\alpha_A{}^2\beta_A{}^2+16\beta_A{}^4),\\E_B&={}^1/_4N(4\alpha_B\beta_B+4\alpha_B\gamma_B+4\gamma_B{}^2-4\gamma_B{}^4),\\E_C&={}^1/_4N(8\alpha_C\beta_C+8\beta_C{}^2-8\beta_C{}^4)\end{aligned}\qquad(8)$$

with the additional conditions

$$\begin{aligned}\alpha_A{}^2+4\beta_A{}^2&=1,\\\alpha_B{}^2+2\beta_B{}^2+2\gamma_B{}^2&=1,\\\alpha_C{}^2+4\beta_C{}^2&=1.\end{aligned}\qquad(9)$$

Table I shows the results of the calculation for configurations A, B, and C.

We carried out the calculations analogously in the case of a simple cubic lattice with p = 4. The energywise most favored lattice turned out to be made up of the small cubes shown in Fig. 2 (type A). Table II lists the results of the calculation for two configurations (see Fig. 2).

A calculation of the coefficients of the irregular configurations connected with the permutation of the sites between squares can readily be carried out by perturbation theory. The results yield in all cases a limit of 3% for the fraction of such states.

Our calculation shows that the energywise favored configurations are those in which atoms of one type are as far from one another as possible. The reason for this is simple. If we let the Hamiltonian (5) act on the state with regular configuration, in which identical atoms are close to one another but are not neighbors, then we obtain irregular configurations with identical neighboring sites. Such configurations make a positive contribution to the ordinary Hartree energy. Thus, for the configurations shown in Fig. 1, any permutation in A and C gives two pairs of nearest neighbors of one type, and in the case B one permutation gives on the average one such pair.

We shall henceforth assume that our hypothesis with respect to the location of the identical atoms is satisfied, and we shall construct the magnetic configurations for sufficiently complicated lattices.

4. MAGNETIC CONFIGURATIONS WITH ALLOWANCE FOR THE SPIN EXCHANGE INTERACTION

So far we have considered to some degree a model situation for dielectrics. In addition to the "effective" exchange connected with the jumps of electrons to neighboring sights, there exists also the usual spin exchange interaction. The Hamiltonian (5) with allowance for this interaction takes the form

$$H=\sum_{\mathbf{r},\mathbf{a}}\left\{\frac{2v^2}{U}P_{\mathbf{r},\mathbf{r}+\mathbf{a}}-\mathcal{J}\mathbf{S}_{\mathbf{r}}\mathbf{S}_{\mathbf{r}+\mathbf{a}}\right\}.\qquad(10)$$

We consider the most interesting case $\mathcal{J}>0$.

We should expect transition-metal compounds to be described by a Hamiltonian similar to (10), with both terms of (10) of the same order. Such an estimate follows from the fact that v is proportional to the overlap of the Wannier functions of neighboring sites, while $\mathcal{J}$ is proportional to the square of this overlap.

Let us see which magnetic configurations will be convenient in this case. The first term in (10) has a tendency to form the maximum possible number of sublattices, which in our situation is equal to 10, while the second tends to align all the spins in parallel. Since the quantities v^2/U and $\mathcal{J}$ are of the same order, the problem of the type of magnetic state is quite complicated. One should expect the energy gain following the addition of an extra state to decrease with increasing number of competing states. Thus, in the one-dimensional case, in accordance with[5], for p = 2 the energy per atom is approximately −0.4, for p = 3 we have $\epsilon\approx-0.7$, and finally for $p\to\infty$ we get $\epsilon\to-1$. The energy gain relative to the energy itself becomes small already at p = 4. This causes the spins at the magnetic-lattice sites to become aligned in parallel, and the orbital angular momenta should form five sublattices. The formation of a new, sixth sublattice, in accordance with the foregoing, gives an energy gain on the order of a small fraction of v^2/U, and a loss on the order of $\mathcal{J}$.

The magnetic configurations constructed in accordance with our hypothesis concerning the arrangement of the magnetic ions with identical λ are shown in Fig.

Table I

	E_{min}	α^2	β^2	γ^2
A	−1.34	0.66	0.09	—
B	−1.72	0.55	0.18	0.04
C	−1.28	0.70	0.08	—

Table II

	E_{min}	α^2
A	−2.65	0.62
B	−1.80	0.77

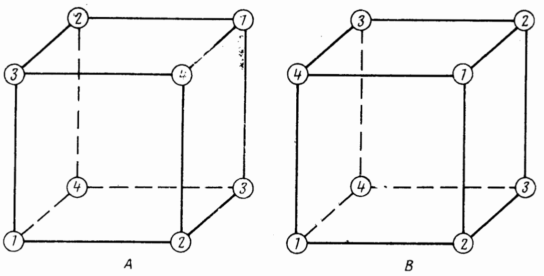


FIG. 2. Elementary cubes used to construct the lattice (p = 4).

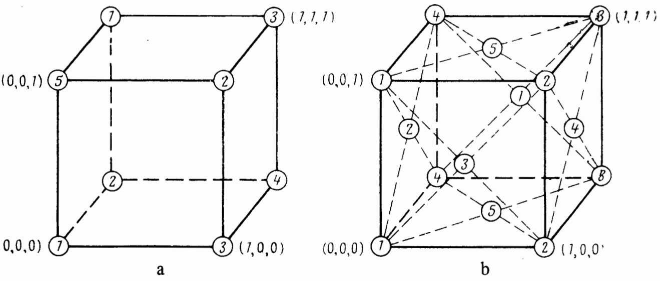


FIG. 3. Magnetic configurations at p = 5. The basis vectors of the sublattices are (2, 1, 0), (−1, 2, 0), (0, 1, 1) (a) and (3/2, 1/2, 0), (−1/2, 3/2, 0), (1/2, 1, 1/2) (b).

3 for the cases of primitive cubic (PC) and face-centered cubic (FCC) lattices.

5. MAGNETIC CONFIGURATIONS WITH ALLOWANCE FOR THE JJ INTERACTION

In rare-earth elements the spin-orbit interaction is no longer small. Therefore such elements or their ions are characterized not only by a spin S and an orbital angular momentum L, but also by a total angular momentum J (see[6]). Thus, in our case of one localized f-electron, we have $S = \frac{1}{2}$, $L = 3$, and $J = \frac{5}{2}$.

The exchange interaction is described by the product of the total angular momenta of the neighboring sites. Instead of the Hamiltonian (10) it is necessary to consider

$$H = \sum_{\mathbf{r},\mathbf{a}} \left\{ \frac{2v^2}{U} P_{\mathbf{r},\mathbf{r}+\mathbf{a}} - I\mathbf{J}_{\mathbf{r}}\mathbf{J}_{\mathbf{r}+\mathbf{a}} \right\}. \tag{11}$$

We shall consider only the case $v^2/U \gg I$. In the reverse situation $I \gg v^2/U$ we obtain ferromagnetic $(I > 0)$ or antiferromagnetic $(I < 0)$ ordering.

The intermediate case $I \sim v^2/U$ is more complicated. The following can be stated concerning the magnetic properties of matter in this region of energy parameters: The subdivision with respect to magnetic sublattices remains in force, but their number is less than six.

Since $v^2/U \gg I$ and $p = 6$ (the number of different projections of the total angular momentum), six magnetic sublattices should be produced. Were we to consider the Hamiltonian (5), we would obtain a state that is degenerate with respect to the permutations of the sublattices. In other words, we can arbitrarily ascribe a total-angular-momentum projection to each sublattice. The second term in (11) lifts this degeneracy partly, and a correlation appears in the distribution of the projections of the total angular momentum over the sublattices. Before we proceed to complicated lattices, let us consider the effect of the JJ interaction in the one-dimensional case. We shall henceforth take this interaction into account in first order of perturbation theory.

The contribution made to the energy by the second term of (11) is

$$E_{JJ} = -I\frac{N}{6}\sum_{i=1}^{6} J_i^z J_{i+1}^z.$$

The energywise favored configurations are those shown in Fig. 4.

Let us consider now a realistic three-dimensional problem. Figure 5 shows the arrangement of the equivalent magnetic ions in an FCC lattice. The contribution of the JJ interaction of site 1 with the nearest neighbors is

$$-IJ_1^z\{3(J_3^z + J_5^z) + 2(J_2^z + J_4^z + J_6^z)\}$$

and the total energy increment is

$$E_{JJ} = -I\frac{N}{12}\Big\{2\Big(\sum_{i=1}^{6} J_i^z\Big)^2 - (J_1^z - J_3^z)^2 - (J_3^z - J_5^z)^2 - (J_5^z - J_1^z)^2 - (J_2^z - J_4^z)^2 - (J_4^z - J_6^z)^2 - (J_6^z - J_2^z)^2\Big\}. \tag{12}$$

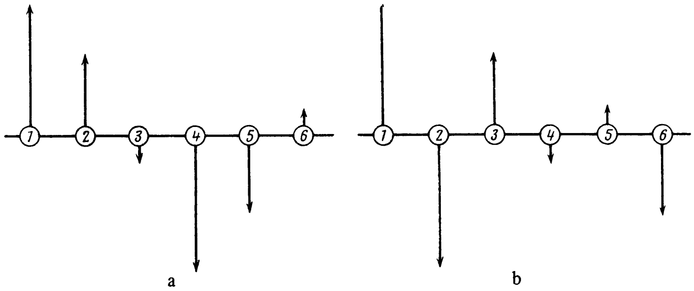


FIG. 4. Distribution over the sublattices in the one-dimensional case (p = 6). The projections of the total angular momentum at sites (1, 2, . . . , 6) are respectively equal to (5/2, 3/2, −1/2, −5/2, −3/2, 1/2) for I > 0 (a) and (5/2, −5/2, 3/2, −1/2, −3/2) for I < 0 (b).

Minimizing the quadratic form (12) (it must be recalled that the J_i are not equal to one another and assume half-integer values from $-\frac{5}{2}$ to $+\frac{5}{2}$), we obtain for $I > 0$

$$E_{JJ} = IN.$$

For $I < 0$, we obtain

$$E_{JJ} = -{}^{13}/_{3}|I|N.$$

The calculated correlations in the arrangement of the sites are demonstrated in Fig. 5.

So far we have considered a localized electron. For a localized f-hole we have $J = \frac{7}{2}$, and under the assumptions made above concerning the energy parameters, eight magnetic sublattices should be produced. The energy increment due to the JJ exchange is

$$E_{JJ} = -IN\Big\{\Big(\sum_{i=1}^{8} J_i^z\Big)^2 - (J_1^z + J_8^z)^2 - (J_2^z + J_3^z)^2 - (J_4^z + J_6^z)^2 - (J_5^z + J_7^z)^2\Big\} \tag{13}$$

and takes on values $E_{JJ} = 0$ $(I > 0)$ and $E_{JJ} = -10|I|N$ $(I < 0)$. The correlations in the arrangement of the projection of the total angular momentum over the sublattices are indicated in Fig. 6.

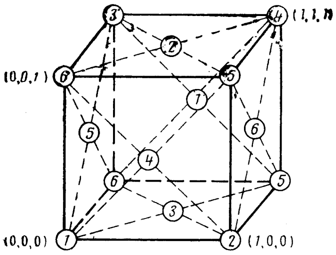


FIG. 5

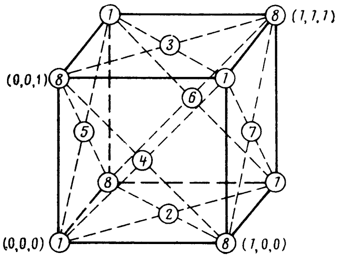


FIG. 6

FIG. 5. Distribution over the sublattices in FCC lattice (p = 6). The projections of the total angular momentum at the sites (1, 2, . . . , 6) are equal to (5/2, −3/2, 3/2, −5/2, 1/2, −1/2) for I > 0 and (5/2; 1/2, −1/2, −3/2, −5/2, 3/2) for I < 0. The basis vectors of the sublattices are (2, 0, 0), (−1/2, 3/2, 0), (1/2, 1, 1/2).

FIG. 6. Distribution over the sublattices in FCC lattice (p = 8). The projections of the total angular momentum at the sites (1, 2, . . . , 8) are (7/2, 5/2, −5/2, 3/2, 1/2, −3/2, 1/2, −7/2) for I > 0 and (7/2, −7/2, −5/2, 3/2, −3/2, 1/2, −1/2, 5/2) for I < 0. The basis vectors of the sublattices are (1, 1, 0), (−1, 1, 0), (0, 1, 1).

6. SHIFT OF MAGNETIC SUBLATTICES IN CRYSTAL

The formation of several sublattices can lead in the case of rare-earth compounds to a shift of the sublattices relative to one another. Let us demonstrate this using as an example a simple one-dimensional chain with $J = 5/2$, described by the Hamiltonian (11). The energywise favored arrangements of the total-angular-momentum projections over the lattice are shown in Fig. 4. But the exchange integral I depends on the distance between the sites. It is therefore clear that the distance between 1 and 2 (see Fig. 4a) decreases (with $|I|$ increasing), and the distance between 2 and 3 increases. This effect leads to the appearance of a new crystallographic period. The new period is equal to three for $I > 0$ and six for $I < 0$.

We note that in the case of ordinary ferromagnetism or antiferromagnetism, there can be no such shift of the magnetic ions, since all the ions are in identical positions.

We present a detailed analysis for the three-dimensional lattices considered above and determine the displacements of the sites from the equilibrium positions. In the nearest-neighbor approximation, the exchange energy I is proportional to $\exp\{-|\mathbf{r}_1 - \mathbf{r}_2|/d\}$ (d is the radius of the magnetic ion). The expansion of the exchange energy in terms of the displacements of two neighboring sites $\delta\mathbf{r}_1$ and $\delta\mathbf{r}_2$ takes the form

$$I(|\delta\mathbf{r}_2 - \delta\mathbf{r}_1 + \mathbf{r}_0|) = I(r_0) + r_0 \left.\frac{dI}{dr}\right|_{r=r_0} \frac{\mathbf{r}_0(\delta\mathbf{r}_2 - \delta\mathbf{r}_1)}{r_0^2} \qquad (14)$$

($\mathbf{r}_0$ is the "equilibrium" distance between sites 1 and 2). In the nearest-neighbor-approximation, it is obvious that $d|I|/dr < 0$ and $r_0 dI/dr_{r=r_0} \equiv \tilde{I}$ is of the order of Ir_0/d.

Let us examine the contribution made to the energy by the displacement of the magnetic sites. From symmetry considerations it is clear that the sites belonging to one sublattice shift in identical manner. This means that each sublattice shifts as a whole. Taking (14) into account, we obtain in the case of a localized electron

$$\Delta E = -{}^1/_3\tilde{I}N\{(z_1+y_1)J_1^z(J_6^z - J_4^z) + (z_2+y_2)J_2^z(J_5^z - J_3^z) + (z_3+y_3)J_3^z(J_2^z - J_6^z) + (z_4+y_4)J_4^z(J_1^z - J_5^z) + (z_5+y_5)J_5^z(J_4^z - J_2^z) + (z_6+y_6)J_6^z(J_3^z - J_1^z)\} + \varepsilon\frac{N}{6}\sum_{i=1}^{6}(x_i^2 + y_i^2 + z_i^2). \qquad (15)$$

The last term in (15) represents the elastic energy (we confine ourselves to the simplest form of elastic energy for crystals of cubic symmetry), and the quantities x_i, y_i, and z_i are the relative displacements of the site in sublattice "i" from the equilibrium position. Upon minimization of ΔE we obtain both a shift of the magnetic ions and a further lifting of the degeneracy due to the distribution of the projections of the total angular momentum over the sublattices. The shift of the magnetic sites, determined from (15), is given in Table III.

Table III. Relative shift of sublattice sites (in units of $|\tilde{I}|/2\varepsilon$)

	$y_1 = z_1$	$y_2 = z_2$	$y_3 = z_3$	$y_4 = z_4$	$y_5 = z_5$	$y_6 = z_6$
$I > 0$	−10	−3	3	10	1	−1
$I < 0$	15	−2	1	−15	10	−9

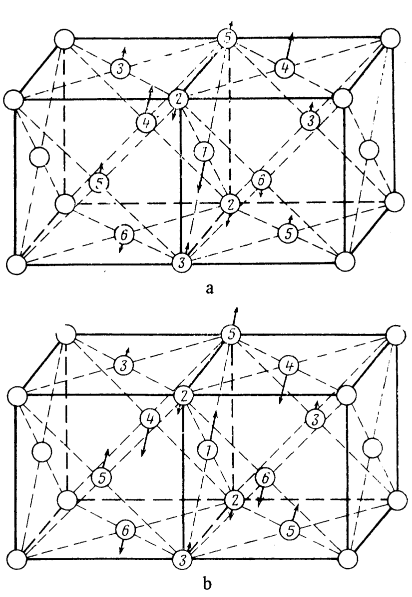


FIG. 7. Shift of magnetic sublattices (p = 6): a–I > 0, b–I < 0.

Each sublattice in Fig. 5 forms a set of planes. Each plane is made up of a grid of equilateral triangles and is perpendicular to the principal diagonal of the cube [1–11]. The shift of the magnetic ions occurs precisely in these planes (see Figs. 7a and 7b).

It should be noted that in transition-element compounds, such an effect can hardly be realized, since in such elements the spins are ferromagnetically ordered and the contribution made to the Hamiltonian by the expansion of the exchange energy begins with terms quadratic in the displacements of the sites. The same can be stated also with respect to a rare-earth compound with a localized f-hole. In this case the arrangement of the magnetic sites has a sufficiently high symmetry and the terms that are linear in the displacements of the atoms are cancelled out.

7. CONCLUSION

All effects connected with the formation of several magnetic sublattices in the crystal can be observed in those compounds of transition or rare-earth elements in which the crystal fields are weak. Several sublattices can be observed experimentally with the aid of neutron-diffraction investigations of the substances.

In the present paper we have considered only one localized electron (hole). If the number of such electrons is a multiple of the number of sites but not equal to it, then Hund's rule comes into effect, and greatly complicates the calculation. Apparently, several magnetic sublattices are produced again, but their number and structure can hardly be determined by such simple rules as in the case of a single electron (hole).

As to the effects of the shift of the magnetic sites, they are observable in principle, since the magnitude of the relative shift of the site $\Delta r/r_0 \sim \tilde{I}/\epsilon$ can be of the order of several percent.

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