Low-temperature properties of spin systems with tensor order parameters

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A generalized Maleev-Dyson transformation is proposed for magnetic systems characterized by tensor interactions—single-ion anisotropy and (or) higher-order exchange interactions—in addition to the spin-spin exchange. As an application, the low-temperature properties of a ferromagnet with easy-plane single-ion anisotropy are studied in a magnetic field perpendicular to the easy plane. The existence of three fundamentally different types of spin structures is predicted, only one of which corresponds to the usual ferromagnetic structure. A detailed study is made of the features of these structures, the spectra of the collective excitations, the low-temperature behavior of the thermodynamic functions, and the possible phase transitions.

1. INTRODUCTION

In this paper a unified approach is developed for the description of magnets having tensor interactions—higher-order exchange interactions and (or) single-ion anisotropy—in addition to the ordinary spin-spin interactions. Systems of this kind have been studied intensively in recent years.[1–19] This is particularly true of ferromagnets with single-ion anisotropy,[3–19] the role of which until quite recently was considered indistinguishable from that of the exchange anisotropy. Recently, however, it has become clear that the use of the standard methods of the theory of magnetism in studying these systems runs up against serious difficulties. In relation to the diagram technique of Vaks, Larkin, and Pikin[20,21] these difficulties were discussed in Refs. 21 and 5 and were linked to the fact that Wick's theorem does not hold for the spin operators when the single-ion anisotropy is included in the zeroth-order Hamiltonian. Two versions of a generalized diagram technique permitting exact allowance for the single-ion anisotropy have been proposed.[3,5] As to the quasiparticle approach based on the introduction of Bose operators with the aid of the Maleev-Dyson (MD) or Holstein-Primakoff (HP) representations, it leads to unphysical results when the ratio of the single-ion anisotropy and exchange constants is not small: The density of quasiparticles and the corrections from the anharmonic terms are not small at $T = 0$.[1)] However, it is hard to agree with the statements that have been made in this regard in several papers (e.g. Ref. 4): that the quasiparticle description itself is invalid at arbitrary relationships between the single-ion anisotropy and exchange constants (i.e., that the weak-nonideality criterion for the Bose gase of quasiparticles is violated in principle at low T), that the zero-point vibrations are extremely large in this case (this view was maintained in Ref. 6), etc.

The point of view developed in the present paper is as follows. The quasiparticle concept is applicable to the same extent as it is in the description of any ordered system, but the quasiparticles should be introduced by a method other than the transformations mentioned above. The first goal of this paper is to construct a transformation from spin to Bose operators that is suitable for spin systems with tensor interactions. The necessity of using a different method of introducing the quasiparticles is due to the possible existence of peculiar spin structures in which there is no magnetization at all or in which the magnetization is very different from the saturation value. In the standard MD and HP transformations there is understood to be complete or almost complete ferromagnetic order in the ground state, since one uses the representation $S^z = S - a^+a$ in a coordinate system with the z axis along the magnetization.

The second objective of this study is the classification and description of the corresponding magnetic structures, their low-temperature properties, and the phase transitions between them. This classification and the formalism developed apply to arbitrary systems with tensor interactions, including, in particular, single-ion anisotropy of arbitrary symmetry and arbitrary order, and briefly consists of the following. Besides the ordinary ferromagnetic structure there are two more structures: a tensor structure in which the order is determined by tensor characteristics and the magnetization is equal to zero, and a tensor-ferromagnetic structure in which the order is characterized by a superposition of vector and tensor variables. In the particular case of second-order single-ion anisotropy these structures can be called quadrupole-ordered (QO) and quadrupole-ferromagnetic (QFM). All of the types of ordering are described by an $(n^2 - 1)$-dimensional $(n = 2S + 1)$ vector order parameter defined in the space of tensor operators O_l^m or rank l $(l = 1,...,2S)$, and the collective excitations in the system at low T correspond to oscillations of this order parameter about an equilibrium position. Accordingly, the transitions between different structures at low T involve the reorientation of the order parameter. The approach developed here enables one to describe the properties of such structures using the standard scheme of regular allowance for both the leading (at low T) spin-wave contributions and the anharmonic terms with the aid of the usual diagram technique[22] for Bose systems, for example.

Concrete calculations are done for an easy-plane ferromagnet in a field perpendicular to the easy plane. This system is described by the Hamiltonian

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}(\mathbf{S}_i\mathbf{S}_j) + D\sum_i (S_i^z)^2 - h\sum_i S_i^z, \quad D>0. \quad (1)$$

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Even this simplest case, as we shall see, exhibits all the spin structures described above. We emphasize that in the study of easy-plane ferromagnets the external field is usually directed parallel to the easy plane,[3,6,8] simplifying the problem considerably.[2)] This simplification, however, is due to the existence of a single phase in this case: a collinear ferromagnetic structure with magnetization along the field.

We study the ground state, the spectra of the collective excitations in all the phases, the low-temperature behavior of the magnetization, susceptibility, and quadrupole averages, and the transitions between the existing structures; we refine the existence criterion for ferromagnetism at $T=0, h=0$. We estimate the renormalization of the order parameter due to zero-point vibrations and find that it is small at any values of D/J_0. The low density of true quasiparticles allows us to use the spin-wave approximation to describe the leading characteristics of the system at low T. The nonlinear theory for each of the structures will be given separately.

The calculations are done for the case $S=1$. This is the minimum spin value at which single-ion anisotropy exists and, consequently, it is in this case that the quantum effects which give rise to the features discussed above are manifested most clearly. The generalization to arbitrary S is discussed in the Conclusion.

At low T the quasiparticle approach developed here is equivalent to the diagram technique for spin operators.[5] In particular, the results obtained here for the magnetization and susceptibility can be found by the technique of Ref. 5 in the first approximation in $1/r_0^3$, as can be seen by direct calculations.

2. GENERAL FORMALISM

The problem of adequately describing magnets having tensor interactions requires independent allowance for both the vector (magnetic) fields and the tensor fields—the external fields created by the single-ion anisotropy and the internal fields created by the intersite spin-spin interactions of higher orders—and their incorporation into the zeroth-order Hamiltonian. For the system described by (1), the latter is of the form

$$\mathcal{H}_0=(-J_0\langle S^z\rangle+h)\sum_i S_i^z-J_0\langle S^x\rangle\sum_i S_i^x+D\sum_i (S_i^z)^2,$$
$$J_0\equiv\sum_j J_{ij}. \qquad (2)$$

As has been pointed out previously,[11,16] this procedure is equivalent to enlarging the basis of the operators characterizing the state of an individual ion from the three spin operators of the Lie algebra $SU(2)$ in the case of an exchange ferromagnet to (n^2-1) operators of the Lie algebra $SU(n)$ $(n=2S+1)$. For $S=1$ the eight operators O_l^m of the algebra $SU(3)$ include three spin and five quadrupole operators:

$$O_1^0\equiv S^z,\quad O_1^{\pm 1}\equiv S^{\pm},\quad S^{\pm}=\mp\frac{1}{\sqrt{2}}(S^x\pm iS^y),$$
$$O_2^0\equiv O^0=(S^z)^2-{}^2/_3,\quad O_2^{\pm 1}\equiv O^{\pm 1}=-(S^zS^{\pm}+S^{\pm}S^z), \qquad (3)$$
$$O_2^{\pm 2}\equiv O^{\pm 2}=(S^{\pm})^2.$$

Accordingly, it is necessary to replace the standard MD and HP transformations, which reflect the symmetry of the $SU(2)$ algebra and apply to magnets having only spin-spin but no tensor interactions, to the analogous transformations incorporating the symmetry of the algebra $SU(3)$. Such a transformation—a generalized MD transformation—is offered below. As usual, it includes two stages: a conversion to local coordinates rigidly bound to the orientation of the vector order parameter, and, the proper introduction of second-quantization operators when a preferred axis of the local coordinates is chosen as the quantization axis. Each of these stages, however, is done with allowance for the properties of the $SU(3)$ algebra [in the general case $SU(n)$] in a way which is different from the standard method.

A. Conversion to local coordinates

For an exchange ferromagnet the vector order parameter $\boldsymbol{\eta}$ is the magnetization, with three components $\langle S^z\rangle, \langle S^x\rangle, \langle S^y\rangle$, and the conversion to local coordinates is accomplished by rotations in three-dimensional space—the unitary transformations of the group $SU(2)$. In such a coordinate system the zeroth-order Hamiltonian is diagonal, and at $T=0$ one has $\langle\tilde{S}^z\rangle_0=S$; here and below a letter with a tilde refers to the local coordinate system, and the index 0 denotes an average with the zeroth-order Hamiltonian.

In the case under study that state of the system is determined by eight independent averages of the operators (3), and the vector order parameter $\boldsymbol{\eta}$ is defined in an eight-dimensional isotopic space. By analogy with the three-dimensional case, it is expedient to convert to local coordinates in which the preferred axis (the z axis) coincides with the direction of the order parameter, so that all but one of the averages of the operators (3) are equal to zero. Then the value of the only nonzero average determines the degree of order in the system, and the orientation of the preferred axis determines the structure of this order.

However, this transparent picture requires some refinement in connection with the difference from unity of the rank r of the $SU(n)$ algebra in all cases except $n=2$, since $r=n-1$. Because r determines the number of independent commuting operators of the algebra, the minimum number of nonzero averages in the local coordinates is equal to r. For $SU(3)$ $(r=2)$ this is $\sigma=\langle\tilde{S}^z\rangle, \lambda=\langle 3\tilde{O}^0\rangle$. The conversion to the local coordinates is done with the aid of the unitary transformations of the $SU(3)$ group, $\exp\{i\varphi_l O_l^m\}$ $(l=1,2)$, which are described in detail elsewhere.[11] The angles of the unitary transformations, which fix the position of the local coordinates and have the meaning of generalized Euler angles, are determined from the condition that the six averages of the operators in (3), except σ and λ, are equal to zero. In our case, when the y component of the field is absent (for both the external and internal fields), three of these averages are identically zero. Accordingly, we have three equations for the angles φ, K, and L

$$(D/2)\sin 2\varphi\cos K+h\cos\varphi\sin K+(J_0/2)\sigma\sin 2K\cos 2L=0, \qquad (4a)$$

$$(D/2)\cos^2\varphi\sin 2K+h\sin\varphi\cos 2K$$
$$+(J_0/4)\sin 4K(\lambda+\sigma\sin 2L)=0, \qquad (4b)$$

$$\tilde{H}\sin 2L+\tilde{D}_2\cos 2L=0, \tag{4c}$$

$$\tilde{H}=h\cos\varphi\cos K-(D/2)\sin 2\varphi\sin K+J_0\sigma\cos^2 K\cos 2L,$$

$$\tilde{D}_2=-(h/2)\sin\varphi\sin 2K+(D/2)(\cos^2 K\cos^2\varphi-\cos 2\varphi)$$
$$-(J_0/4)\sin^2 2K(\lambda+\sigma\sin 2L)$$

of the three unitary transformations:

$$U_1=\exp\{\varphi(S^+ +S^-)/\sqrt{2}\},\quad U_2=\exp\{iK(O^1+O^{-1})/\sqrt{2}\},$$
$$U_3=\exp\{iL(O^2-O^{-2})\}. \tag{5}$$

In the zeroth approximation, the averages σ and λ appearing in (4) are given by the equations

$$\sigma_0=\frac{e^{-\tilde{d}/\theta}2\,\mathrm{sh}\,(\tilde{h}/\theta)}{1+e^{-\tilde{d}/\theta}2\,\mathrm{ch}\,(\tilde{h}/\theta)},\quad \lambda_0=1-\frac{3}{1+e^{-\tilde{d}/\theta}2\,\mathrm{ch}\,(\tilde{h}/\theta)},$$
$$\theta\equiv kT. \tag{6}$$

In obtaining (6) we used the explicit form of $\tilde{\mathscr{H}}\equiv U_3U_2U_1\mathscr{H}_0U_1^{-1}U_2^{-1}U_3^{-1}$:

$$\tilde{\mathscr{H}}_0=-\tilde{h}\sum\tilde{S}_i^z+\tilde{d}\sum\tilde{O}_i^0, \tag{7}$$

$$\tilde{h}=\tilde{H}\cos 2L-\tilde{D}_2\sin 2L, \tag{7a}$$

$$\tilde{d}=\frac{D}{2}(3\cos^2 K\cos^2\varphi-1)-\frac{3h}{2}\sin\varphi\sin 2K$$
$$-\frac{3J_0}{4}\sin^2 2K(\lambda+\sigma\sin 2L).$$

We notice that for $T=0$, three versions of solutions (6) are possible:

$$\sigma_0=1,\quad \lambda_0=1, \tag{8a}$$

$$\sigma_0=0,\quad \lambda_0=-2, \tag{8b}$$

$$\sigma_0=-1,\quad \lambda_0=1. \tag{8c}$$

Each of these corresponds to different values of the angles determined by expressions (4). This means that three types of local coordinates are possible.[3)] The most transparent is the type corresponding to (8a): Having $\langle\tilde{S}^z\rangle_0=1$ means that in this coordinate system there is a "complete ordering of the spins along the z axis" at $T=0$ (in the zeroth approximation), and at finite T the value of σ will characterize the degree of order in the system. The quotation marks are meant to emphasize that this "ferromagnetic" order is realized only in certain coordinates of the eight-dimensional space; the true structure of the order in real three-dimensional space can be radically different from ferromagnetic. It

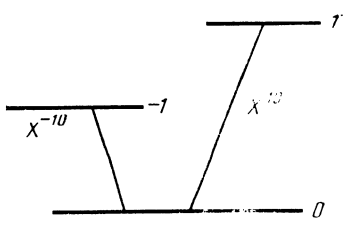

FIG. 1. Level scheme of an ion with $S=1$ in local coordinates of the second type [for which Eq. (8b) holds at $T=0$]. The levels are labeled by the eigenvalues of the operator $\tilde{S}^z$.

is specified by the components

$$\langle S^z\rangle,\ \langle S^x\rangle,\quad Q_0\equiv\langle\sqrt{3}O^0\rangle,\quad Q_2\equiv\langle O^2+O^{-2}\rangle,$$
$$Q_1\equiv\langle O^1-O^{-1}\rangle/\sqrt{2},$$

which determines $\langle\tilde{S}^z\rangle$:

$$\langle\tilde{S}^z\rangle=\alpha_z\langle S^z\rangle+\alpha_x\langle S^x\rangle+\beta_0Q_0+\beta_2Q_2+\beta_1Q_1,$$
$$\alpha_z=\cos 2L\cos K\cos\varphi+{}^1/_2\sin 2L\sin 2K\sin\varphi,$$
$$\alpha_x=\cos 2L\cos K\sin\varphi-{}^1/_2\sin 2L\sin 2K\cos\varphi,$$
$$\beta_0=2^{-1}\sqrt{3}[\cos 2L\sin K\sin 2\varphi-\sin 2L(\cos 2\varphi-\cos^2 K\cos^2\varphi)],$$
$$\beta_2={}^1/_2[-\cos 2L\sin K\sin 2\varphi \tag{9}$$
$$+\sin 2L(\cos 2\varphi-\cos^2 K\cos^2\varphi+2\cos^2 K)],$$
$$\beta_1=[-\cos 2L\sin K\cos 2\varphi-{}^1/_2\sin 2L\sin 2\varphi(1+\sin^2 K)],$$
$$\alpha_z^2+\alpha_x^2+\beta_0^2+\beta_2^2+\beta_1^2=1.$$

The quantities α_p and β_p play the role of the direction cosines determining the orientation of the preferred axis of the local coordinates with respect to the fixed system with basis vectors along $\langle S^z\rangle,\langle S^x\rangle,Q_0,Q_2,Q_1,\ldots$.

It remains for us to introduce the vector order parameter

$$\boldsymbol{\eta}=|\eta|\mathbf{e}, \tag{10}$$

whose direction is determined by the unit vector $\mathbf{e}$ with components α_z, α_x, β_0, β_2, and β_1 (the three remaining components are zero) and whose modulus is the value of $\langle\tilde{S}^z\rangle$ in the local system under study: $|\eta|=\sigma$. Clearly, the direction of $\boldsymbol{\eta}$ characterizes the structure of the order: if all the β_p are zero we have the ordinary ferromagnetic structure, for $\alpha_p=0$ we have the QO structure, and for $\alpha_p\neq 0$, $\beta_p\neq 0$ we have the QFM structure. Regardless of the structure of the order, the degree of ordering, characterized by $|\eta|$, goes to unity for $T\to 0$.

In the general case it is a rather awkward problem to obtain explicit nontrivial solutions for the angles. Substantial simplification of system (4) can be achieved in the case $T=0$ by using local coordinates of the second type. In fact, when (8b) is used, system (4) decomposes into one independent equation for $\sin 2L$ and two coupled equations for $\sin\varphi$ and $\cos 2K$. Therefore, although these coordinates are less transparent, we shall for the sake of uniformity use them to describe all the phases. One can readily see that the subsequent conversion from these coordinates to the physical coordinates of the first type requires one more, trivial rotation specified by the angles $\cos\varphi=\cos 2K=\cos 2L=0$. Hence one can obtain formulas relating the order parameter $\boldsymbol{\eta}$ introduced earlier to the characteristics of this coordinate system, σ and λ, and to the angles φ, K, and L. In particular, the modulus $|\eta|$ and direction cosines of the unit vector $\mathbf{e}$ ($\tilde{\alpha}_p$ and $\tilde{\beta}_p$) of the order parameter are given by

$$|\eta|={}^1/_2(\sigma-\lambda),\quad 2\tilde{\alpha}_p=\alpha_p-\sqrt{3}A_p,\quad 2\tilde{\beta}_p=\beta_p-\sqrt{3}B_p. \tag{11}$$

Here α_p and β_p are determined by formulas (9), and A_p and B_p are determined by formulas (A.1) of the Appendix. The proof of (11) is given in the Appendix.

Let us finally give the formulas relating the original averages with the parameters σ, λ, φ, K, and L:

$$M_l \equiv \langle S^l \rangle = \alpha_l \sigma + A_l \lambda / \sqrt{3}, \quad l = z, x;$$
$$Q_m = \beta_m \sigma + B_m \lambda / \sqrt{3}, \quad m = 0, 1, 2. \tag{12}$$

B. Second-quantization operators

After the conversion to the local coordinates the intersite interaction contains not only spin-spin but also quadrupole-quadrupole and spin-quadrupole exchanges:

$$\tilde{\mathcal{H}} - \tilde{\mathcal{H}}_0 = -\frac{1}{2}\sum_{\substack{ij \\ \alpha\beta}} \tilde{J}_{ij}^{\alpha\beta} \tilde{S}_i^{\alpha} \tilde{S}_j^{\beta} - \frac{1}{2}\sum_{\substack{ij \\ mn}} \tilde{K}_{ij}^{mn} \tilde{O}_i^{m} \tilde{O}_j^{n} - \frac{1}{2}\sum_{\substack{ij \\ \alpha m}} \tilde{P}_{ij}^{\alpha m} \tilde{S}_i^{\alpha} \tilde{O}_j^{m}. \tag{13}$$

The expressions for the "exchange integrals" $\tilde{J}$, $\tilde{K}$, and $\tilde{P}$ in terms of the angles φ, K, L and the constants of the original Hamiltonian are written out in Eqs. (14)–(18) of Ref. 16. The conversion to Bose operators would require the use of a transformation that would take into account the equal status of the spin and quadrupole operators in $SU(3)$.

We propose a representation in which the spin and quadrupole operators in the local coordinates are expressed in terms of the Hubbard operators, the other independent generators[16] of the algebra $SU(n)$:

$$\tilde{S}^z = X^{11} - X^{-1-1}, \quad \tilde{O}^0 = (X^{11} + X^{-1-1}) - {}^2/_3,$$
$$\tilde{S}^+ = -(X^{10} + X^{0-1}), \quad \tilde{O}^1 = X^{10} - X^{0-1}, \quad \tilde{O}^2 = X^{1-1}, \tag{14}$$

and the latter are expressed in terms of the Bose operators according to the formulas

$$X^{10} = b^+(1 - a^+a - b^+b), \quad X^{01} = b,$$
$$X^{-10} = a^+(1 - a^+a - b^+b), \quad X^{0-1} = a, \tag{15}$$
$$X^{1-1} = b^+a, \quad X^{-11} = a^+b, \quad X^{11} = b^+b, \quad X^{-1-1} = a^+a.$$

The choice of this transformation, which is the MD transformation generalized to the $SU(3)$ case, becomes obvious when we consider the level scheme of an individual ion in the local coordinates (Fig. 1); we see from this scheme that the Hubbard operators X^{10} and X^{-10} are the operators for transitions from the ground level to excited levels at a site; at low T these operators, to first approximation, have Bose commutation relations:

$$[X_i^{01}, X_j^{10}] = \delta_{ij}(1 - 2X_i^{11} - X_i^{-1-1}) \approx \delta_{ij},$$
$$[X_i^{0-1}, X_j^{-10}] = \delta_{ij}(1 - 2X_i^{-1-1} - X_i^{11}) \approx \delta_{ij}, \tag{16}$$

whereas the operators X^{1-1} obey

$$[X_i^{1-1}, X_j^{-11}] = \delta_{ij}(X_i^{11} - X_i^{-1-1}) \approx 0. \tag{17}$$

Furthermore, this representation follows from a comparison of the present approach with that of the diagram technique[5]: in the presence of single-ion anisotropy it is precisely for the off-diagonal Hubbard operators in coordinates in which $\tilde{\mathcal{H}}_0$ is diagonal (i.e., in the local coordinates introduced above) that the generalized form of Wick's theorem holds.

By doing all the transformations described above, we obtain an explicit form for the quadratic Hamiltonian in a local coordinate system of the second type:

$$\tilde{\mathcal{H}}_2 = \varepsilon_a \sum_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \varepsilon_b \sum_{\mathbf{k}} b_{\mathbf{k}}^+ b_{\mathbf{k}} + \sum_{\mathbf{k}} \{V_3(\mathbf{k}) a_{\mathbf{k}}^+ a_{\mathbf{k}} - {}^1/_2 V_4(\mathbf{k}) (a_{\mathbf{k}}^+ a_{-\mathbf{k}}^+ + a_{\mathbf{k}} a_{-\mathbf{k}}) + V_1(\mathbf{k}) b_{\mathbf{k}}^+ b_{\mathbf{k}} - {}^1/_2 V_2(\mathbf{k}) (b_{\mathbf{k}}^+ b_{-\mathbf{k}}^+ + b_{\mathbf{k}} b_{-\mathbf{k}}) + v_2(\mathbf{k}) (a_{\mathbf{k}}^+ b_{\mathbf{k}} + b_{\mathbf{k}}^+ a_{\mathbf{k}}) - v_1(\mathbf{k}) (a_{\mathbf{k}}^+ b_{-\mathbf{k}}^+ + b_{\mathbf{k}} a_{-\mathbf{k}})\}. \tag{18}$$

The constants of this Hamiltonian depend on the angles φ, K, and L in the following way:

$$V_1(\mathbf{k}) = -J_{\mathbf{k}}[1 - {}^1/_2 \sin^2 2K(1 + \sin 2L)],$$
$$V_3(\mathbf{k}) = -J_{\mathbf{k}}[1 - {}^1/_2 \sin^2 2K(1 - \sin 2L)],$$
$$V_2(\mathbf{k}) = J_{\mathbf{k}} \cos 2K[\sin 2L \cos^2 K - \sin^2 K],$$
$$V_4(\mathbf{k}) = -J_{\mathbf{k}} \cos 2K[\sin 2L \cos^2 K + \sin^2 K],$$
$$v_1(\mathbf{k}) = J_{\mathbf{k}} \cos^2 K \cos 2K \cos 2L,$$
$$v_2(\mathbf{k}) = 2J_{\mathbf{k}} \cos^2 K \sin^2 K \cos 2L, \tag{19}$$
$$\varepsilon_a = \tilde{h} + \tilde{d}, \quad \varepsilon_b = \tilde{d} - \tilde{h};$$

here $J_{\mathbf{k}}$ is the Fourier transform of the exchange integral.

The general formulas for the terms of higher order in the operators $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ are rather awkward, and we shall not give them here. We note that the condition that the Hamiltonian contain no terms linear in $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$—the condition usually used to determine the equilibrium spin configurations—leads to the same equations (4) for the angles as we obtained earlier.

From here on the analysis is done in the usual way. The quadratic Hamiltonian determines the spectrum of collective excitations in the spin-wave approximation:

$$(\omega_{\mathbf{k}}^{\pm})^2 = {}^1/_2(\varepsilon_b + V_1 + V_2)(\varepsilon_b + V_1 - V_2) + {}^1/_2(\varepsilon_a + V_3 + V_4)(\varepsilon_a + V_3 - V_4) + v_2^2 - v_1^2 \pm \{[{}^1/_2(\varepsilon_b + V_1 + V_2)(\varepsilon_b + V_1 - V_2) - {}^1/_2(\varepsilon_a + V_3 + V_4)(\varepsilon_a + V_3 - V_4)]^2 + [(\varepsilon_b + V_1 + V_2)(v_2 - v_1) + (\varepsilon_a + V_3 - V_4)(v_1 + v_2)] \times [(\varepsilon_b + V_1 - V_2)(v_2 + v_1) + (\varepsilon_a + V_3 + V_4)(v_2 - v_1)]\}^{1/2}. \tag{20}$$

[In Eq. (20) the argument $\mathbf{k}$ has been dropped from the coefficients $V_1, V_2, V_3, V_4, v_1, v_2$.] Using this Hamiltonian, one can determine the corrections to the averages σ and λ by proceeding from the expressions relating the diagonal spin and quadrupole operators to the Bose operators:

$$\sigma=\sigma_0+\Delta\sigma,\quad \lambda=\lambda_0+\Delta\lambda,\quad \sigma_0=0,\quad \lambda_0=-2,$$

$$\Delta\sigma=\frac{1}{N}\sum_{\mathbf{p}}\{N_b(\mathbf{p})-N_a(\mathbf{p})\},\quad \Delta\lambda=\frac{3}{N}\sum_{\mathbf{p}}\{N_b(\mathbf{p})+N_a(\mathbf{p})\},\tag{21}$$

$$N_b(\mathbf{p})\equiv\langle b_{\mathbf{p}}^{+}b_{\mathbf{p}}\rangle,\qquad N_a(\mathbf{p})\equiv\langle a_{\mathbf{p}}^{+}a_{\mathbf{p}}\rangle.$$

Further, on substitution of the renormalized σ and λ into system (4), we obtained the renormalized values of the angles φ, K, and L. Substitution of both into formulas (11) and (12) gives the renormalized values of the order parameter and of the initial averages M_z, M_x, Q_0, Q_2, and Q_1. A study of the influence of the anharmonic terms on the low-temperature dynamics of the system can also be done by the highly developed standard methods for weakly interacting bosons.

3. STRUCTURE OF THE ORDERED PHASES OF AN EASY-PLANE FERROMAGNET

System (4) determines three branches of solutions for the angles φ, K, and L. The first,

$$\cos\varphi=\cos 2K=\cos 2L=0,\tag{22}$$

describes the ordinary ferromagnetic structure, since all the $\tilde{\beta}_p$ in (11) are zero. This is a saturated phase with magnetization parallel to the field: $M_z^{(0)}=1$, $M_x=0$.

The second solution,

$$\sin\varphi=\sin 2K=\sin 2L=0,\tag{23}$$

corresponds at $T=0$ to a nonmagnetic structure in which the order is determined exclusively by the quadrupole component Q_0:

$$|\eta|=-2^{-1}\sqrt{3}Q_0\quad Q_0^{(0)}=-2/\sqrt{3},\qquad M_x=M_z=Q_1=Q_2=0.\tag{24}$$

The quadrupole order is characterized, according to the definition of Q_0, by a spin alignment perpendicular to the z axis ($\langle(S^z)^2\rangle=0$), with an arbitrary alignment in the xy plane. At finite T a nonzero magnetization $M_z\neq 0$ (calculated in the next section) arises along the field. Then $|\eta|=-1/2(\sqrt{3}Q_0+M_z)$. The given solutions exist for any values of h, D, and T.

There is also a nontrivial solution which at $T=0$ is characterized by the angles

$$\cos 2K=\xi(1-H^2),$$

$$\sin\varphi=-H\left\{\left(\frac{1}{\xi}-1+H^2\right)\Big/\left(\frac{1}{\xi}+1-H^2\right)\right\}^{1/2},\tag{25}$$

$$\tan 2L=-\tilde{D}_2/\tilde{H},\quad \xi=D/2J_0,\quad H\equiv h/D.$$

This solution describes the QFM structure, in which the contribution of the vector and tensor components to the order parameters is determined by the values of the coefficients $\tilde{\alpha}_p$ and $\tilde{\beta}_p$ in formulas (11) and (10). This solution exists in the field region $H_{c1}<H<H_{c2}$; it goes over to the QO solution at $H=H_{c1}$ and to the FM solution at $H=H_{c2}$. In the zeroth approximation $H_{c1}^{(0)}=(1-1/\xi)^{1/2}$, $H_{c2}^{(0)}=1$. In the case $\xi<1$ solution (25) exists in the field region $0<H<H_{c2}$. From the standpoint of its ferromagnetic properties the QFM phase is canted (with respect to the external field and easy plane). Here the components of the magnetization are given by

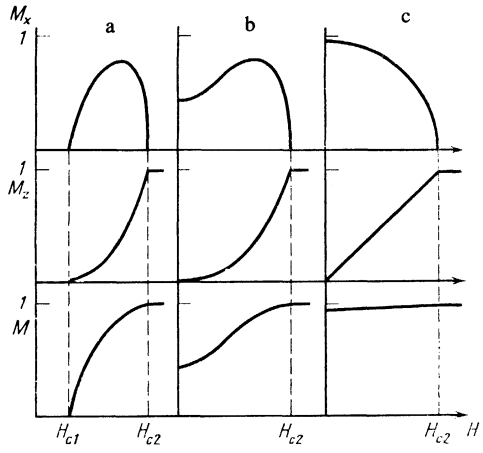

FIG. 2. Field dependence of the total magnetization M and its longitudinal (M_z) and transverse (M_x) components at $T=0$: a) $\xi=D/2J_0>\xi^{cr}$, b) $\xi<\xi^{cr}$, c) $\xi\ll\xi^{cr}$. In the molecular-field approximation $\xi^{cr}=1$, and the renormalized value is given by Eq. (67).

$$M_z^{(0)}=-\sin\varphi\sin 2K,\qquad M_x^{(0)}=\cos\varphi\sin 2K.\tag{26}$$

The features of the low-temperature behavior of this phase are determined, however, not by the canting, but mainly by the contribution of the quadrupole components to the order parameter. At $T=0$ this contribution varies from 1 to 0 as H changes from H_{c1} to H_{c2}, leading to unusual behavior of the total magnetization for a ferromagnet: It increases in a nonlinear manner from 0 at $H=H_{c1}$ to 1 at $H=H_{c2}$:

$$M^{(0)}(T=0)=\sin 2K=[1-\xi^2(1-H^2)^2]^{1/2}.\tag{27}$$

Peculiar behavior is also exhibited by the cooperative component of the magnetization, $M_x^{(0)}$ (see Fig. 2). For $\xi<1$, in which case there is no H_{c1}, the peculiar behavior of M and M_x persists (Fig. 2). It vanishes only for $\xi\ll 1$, when the entire existence region of the QFM phase is effectively the region adjacent to H_{c2}. Let us give the dependence of M, M_z, and M_x on H for $H^2=H_{c1}^2+\Delta H$:

$$M_x^{(0)}=(\Delta H)^{1/2}(2\xi)^{1/2},\qquad M_z^{(0)}=\Delta H[\xi(\xi-1)]^{1/2},$$

$$M^{(0)}=(\Delta H)^{1/2}(2\xi)^{1/2};\tag{28}$$

for $H^2=H_{c2}^2-\Delta H$ we have

$$M_x^{(0)}=(\Delta H)^{1/2}[2(1+2\xi)]^{1/2},\qquad M_z^{(0)}=1-(\Delta H)(2\xi+1),$$

$$M^{(0)}=1-2\xi^2(\Delta H)^2;\tag{29}$$

and, finally, for $H=0+\Delta H$ we have

$$M_x^{(0)}=(1-\xi^2)^{1/2}+(\Delta H)^2\frac{\xi^2+2\xi-1}{2(1-\xi^2)^{1/2}},\qquad M_z^{(0)}=\Delta H(1-\xi),$$

$$M^{(0)}=(1-\xi^2)^{1/2}+\frac{(\Delta H)^2\xi^2}{(1-\xi^2)^{1/2}}.\tag{30}$$

4. SPIN-WAVE SPECTRUM AND THERMODYNAMIC FUNCTIONS

Let us give the explicit calculations of the spectrum and thermodynamic functions, using the explicit form of the Hamiltonian $\tilde{\mathscr{H}}_2$ for each phase.

1. FM phase. The Hamiltonian is

$$\tilde{\mathscr{H}}_2=\sum_{\mathbf{k}}(\varepsilon_a+V_3(\mathbf{k}))a_{\mathbf{k}}^{+}a_{\mathbf{k}}+\varepsilon_b\sum_{\mathbf{k}}b_{\mathbf{k}}^{+}b_{\mathbf{k}}, \tag{31}$$

since $V_1=V_2=V_4=v_1=v_2=0$. Here $V_3=-J_{\mathbf{k}}$, $\varepsilon_a=h-D+J_0$, $\varepsilon_b=2(h+J_0)$. Accordingly, the single branch of excitations, with dispersion relation

$$\omega_{\mathbf{k}}=h-D+J_0-J_{\mathbf{k}}, \tag{32}$$

has the form typical of an ordinary ferromagnet. At small $\mathbf{k}$ we get $\omega_{\mathbf{k}}=\Delta+A\mathbf{k}^2$, and the gap $\Delta=h-D\equiv D(H-H_{c2})$ goes to zero at $H=H_{c2}$, so that at the field value $H=H_{c2}$ the FM phase likewise becomes unstable.

The corrections $\Delta\sigma$ and $\Delta\lambda$ calculated by formulas (21) are zero at $T=0$, i.e., even in the spin-wave approximation we have $\sigma=0$ and $\lambda=-2$ at $T=0$. Accordingly, the ground state in the FM phase is a state of complete FM order along the z axis: $M_z=1, M_x=0$. The absence of zero-point vibrations is due to the relation $[(\Sigma_j S_j^z),\mathscr{H}]=0$. At finite T we have

$$\Delta\sigma(T)=-\frac{1}{N}\sum_{\mathbf{k}}n(\omega_{\mathbf{k}}),$$

$$\Delta\lambda(T)=\frac{3}{N}\sum_{\mathbf{k}}n(\omega_{\mathbf{k}}),\quad n(\omega_{\mathbf{k}})=(e^{\omega_{\mathbf{k}}/\theta}-1)^{-1}, \tag{33}$$

and the magnetization change determined by formula (12) is

$$\Delta M_z(T)\equiv M_z(T)-M_z(0)=\frac{1}{N}\sum_{\mathbf{k}}n(\omega_{\mathbf{k}}), \tag{34}$$

which is also the standard formula for a ferromagnet. Explicit calculations give

$$\Delta M_z(T)=\frac{\Gamma(3/2)}{4\pi^2}\left(\frac{\theta}{A}\right)^{3/2}Z_{3/2}\left(\frac{\Delta}{\theta}\right),\quad Z_p(x)=\sum_{n=1}^{\infty}n^{-p}e^{-nx}, \tag{35}$$

and for the susceptibility

$$\chi_{zz}(T)\equiv\frac{\partial M_z}{\partial h_z}=\frac{\Gamma(3/2)}{4\pi^2\theta}\left(\frac{\theta}{A}\right)^{3/2}Z_{1/2}\left(\frac{\Delta}{\theta}\right). \tag{36}$$

Using the explicit form[23] of $Z_p(x)$ for small x, we obtain expressions for the magnetization and susceptibility under the condition $\Delta\ll\theta$

$$\Delta M_z(T)\approx 0.06\left(\frac{\theta}{A}\right)^{3/2}\left[1-1.36\left(\frac{\Delta}{\theta}\right)^{1/2}\right],\quad \chi_{zz}(T)\propto\frac{\theta}{\sqrt{\Delta}}. \tag{37}$$

The behavior of the magnetic characteristics in the phase under study is thus the same as in an ordinary ferromagnet. Here it is pertinent to note that a formula with a structure exactly like (37) was recently obtained[13] for the magnetization of a ferromagnet with a cubic single-ion anisotropy, and it was pointed out that the magnetization at small Δ/θ contains a term linear in T in addition to the terms $\sim T^{3/2}$. Such a behavior, however, is not peculiar solely to ferromagnets with single-ion anisotropy but is also typical of ferromagnets with $\Delta=h\to 0$ (Ref. 23), ferromagnets with exchange anisotropy near the point of a spin-reorientation phase transition,[24] and uniaxial antiferromagnets near a field-induced phase transition.[23] This behavior can be said to be universal for spin structures in which there is a mode $\omega_{\mathbf{k}}=\Delta+A\mathbf{k}^2$ near a point at which a loss of stability occurs, i.e., for $\Delta\to 0$. For spin-reorientation phase transitions of various types one usually has $\Delta\sim|H-H_c|$, and the universal of $M_{\|}$, the magnetization along the field,

$$\Delta M_{\|}(T)=C_1\Theta^{3/2}+C_2\Theta\Delta^{1/2},\quad \chi_{\|}(T)\propto\theta/\sqrt{\Delta} \tag{38}$$

is a reflection of the universal behavior of the thermodynamic functions near second-order transition points with allowance for Gaussian fluctuations.

2. QO phase. Using formulas (18) and (19) with angle values (23), we obtain a Hamiltonian of the form

$$\tilde{\mathscr{H}}_2=\sum_{\mathbf{k}}(D-h-J_{\mathbf{k}})a_{\mathbf{k}}^{+}a_{\mathbf{k}}+\sum_{\mathbf{k}}(D+h-J_{\mathbf{k}})b_{\mathbf{k}}^{+}b_{\mathbf{k}}-\sum_{\mathbf{k}}J_{\mathbf{k}}(a_{\mathbf{k}}^{+}b_{-\mathbf{k}}^{+}+b_{-\mathbf{k}}a_{\mathbf{k}}). \tag{39}$$

This Hamiltonian is diagonalized with the aid of the U-V transformation:

$$a_{\mathbf{k}}^{+}=U_{\mathbf{k}}\alpha_{\mathbf{k}}^{+}+V_{\mathbf{k}}\beta_{\mathbf{k}},\quad b_{-\mathbf{k}}^{+}=V_{\mathbf{k}}\alpha_{\mathbf{k}}+U_{\mathbf{k}}\beta_{\mathbf{k}}^{+}. \tag{40}$$

The frequencies of the two branches of the spectrum and the functions $U_{\mathbf{k}}$ and $V_{\mathbf{k}}$ are of the form

$$\omega_{\mathbf{k}}^{\pm}=[D(D-2J_{\mathbf{k}})]^{1/2}\pm h, \tag{41}$$

$$U_{\mathbf{k}}^2=\frac{1}{2}\left(\frac{D-J_{\mathbf{k}}}{[D(D-2J_{\mathbf{k}})]^{1/2}}+1\right),$$

$$V_{\mathbf{k}}^2=\frac{1}{2}\left(\frac{D-J_{\mathbf{k}}}{[D(D-2J_{\mathbf{k}})]^{1/2}}-1\right). \tag{42}$$

At $H=0$ the spectrum is twofold degenerate. A field removes the degeneracy, decreasing the frequency of the lower branch (rather than increasing it as in a ferromagnet). At small $\mathbf{k}$ (and finite H_{c1}) the frequencies are of the form

$$\omega_{\mathbf{k}}^{\pm}=\Delta_{\pm}+\frac{A}{H_{c1}}\mathbf{k}^2,\quad \Delta_{\pm}=D(H_{c1}\pm H). \tag{43}$$

Since $\Delta_{-}=0$ at $H=H_{c1}$, this field is a point at which the QO phase suffers a loss of stability. If $H_{c1}=0$, Eq. (41) implies that $\omega_{\mathbf{k}}^{-}\propto\mathbf{k}$.

The correlation functions are

$$N_b(\mathbf{p})=U_{\mathbf{p}}^2n(\omega_{\mathbf{p}}^{+})+V_{\mathbf{p}}^2n(\omega_{\mathbf{p}}^{-})+V_{\mathbf{p}}^2,$$
$$N_a(\mathbf{p})=U_{\mathbf{p}}^2n(\omega_{\mathbf{p}}^{-})+V_{\mathbf{p}}^2n(\omega_{\mathbf{p}}^{+})+V_{\mathbf{p}}^2, \tag{44}$$
$$\mu(\mathbf{p})\equiv\langle b_{\mathbf{p}}^{+}a_{-\mathbf{p}}^{+}\rangle\equiv\langle a_{\mathbf{p}}b_{-\mathbf{p}}\rangle=U_{\mathbf{p}}V_{\mathbf{p}}[1+n(\omega_{\mathbf{p}}^{+})+n(\omega_{\mathbf{p}}^{-})].$$

Accordingly, for $\Delta\sigma$ and $\Delta\lambda$ we obtain from (21)

$$\Delta\sigma=\Delta\sigma(0)+\Delta\sigma(T),\quad \Delta\lambda=\Delta\lambda(0)+\Delta\lambda(T),$$

$$\Delta\sigma(0)=0,\quad \Delta\lambda(0)=\frac{6}{N}\sum_{\mathbf{p}}V_{\mathbf{p}}^{2}$$

$$=\frac{3}{N}\sum_{\mathbf{p}}\left[\left(1-\frac{1}{2\xi}\gamma_{\mathbf{p}}\right)\left(1-\frac{1}{\xi}\gamma_{\mathbf{p}}\right)^{-1/2}-1\right], \tag{45}$$

$$\Delta\sigma(T)=\frac{1}{N}\sum_{\mathbf{p}}\{n(\omega_{\mathbf{p}}^{+})-n(\omega_{\mathbf{p}}^{-})\};$$

$$\Delta\lambda(T)=\frac{3}{N}\sum_{\mathbf{p}}\left[\left(1-\frac{1}{2\xi}\gamma_{\mathbf{p}}\right)\left(1-\frac{1}{\xi}\gamma_{\mathbf{p}}\right)^{-1/2}\right]$$

$$\times[n(\omega_{\mathbf{p}}^{+})+n(\omega_{\mathbf{p}}^{-})],$$

$$\gamma_{\mathbf{p}}\equiv\frac{1}{Z}\sum_{\boldsymbol{\delta}}e^{i\mathbf{p}\boldsymbol{\delta}}, \tag{46}$$

where Z is the number of nearest neighbors and $\boldsymbol{\delta}$ is a vector joining two nearest neighbors. We recall that for the QO phase Eqs. (12) and (11) imply that

$$M_z=\Delta\sigma,\quad Q_0=-2+\Delta\lambda,\quad M_x=Q_1=Q_2=0, \tag{47}$$

and the order parameter is

$$|\eta|=1-(\Delta\lambda-\Delta\sigma)/2. \tag{48}$$

Equations (45) and (48) imply that the ground state remains nonmagnetic in the spin-wave approximation, since $\Delta\sigma(0)=0$. Moreover, we can state that the equation $M_z(T=0)=0$ is satisfied exactly, since

$$\left[\left(\frac{1}{N}\sum_{j}S_j^{z}\right),\mathcal{H}\right]=0,$$

and the order at $T=0$ is determined exclusively by the quadrupole parameter Q_0. Accordingly, $\chi_{zz}(T=0)=0$. Because

$$\left[\left(\frac{1}{N}\sum_{j}O_j^{0}\right),\mathcal{H}\right]\neq 0,$$

the ground state cannot correspond to a state of complete quadrupole order. Let us estimate the correction $\Delta\eta(0)$ to the order parameter ($\eta=1-\Delta\eta$) due to zero-point vibrations; this correction is determined by $\Delta\lambda(0)$ in (45): $\Delta\eta(0)=\Delta\lambda(0)/2$. Its absolute value depends on the parameter ξ, which falls off monotonically in the interval $1<\xi<\infty$, the existence region of the QO phase For $\xi=1$, our Eq. (45) for $\Delta\lambda(0)$ coincides up to a factor of 3 with the formula for the correction to the magnetization at $T=0$ in the transverse xy model; the latter was evaluated in the three-dimensional case for simple cubic (sc) and body-centered cubic (bcc) lattices in Ref. 25. Those vlaues can therefore be used to estimate an upper limit on $\Delta\eta(0)$. Because $\Delta\lambda(0)=0$ at $\xi=\infty$, we see from (45), we have

$$0\leqslant\delta(\xi)\equiv\Delta\eta(0)\leqslant\begin{cases}{}^{3}/_{2}\cdot 0{,}022 & \text{for an sc lattice}\\ {}^{3}/_{2}\cdot 0{,}017 & \text{for a bcc lattice.}\end{cases} \tag{49}$$

We conclude that the renormalization of the ground state due to zero-point vibrations is small at any value of D/J_0 and does not depend on the field. We note that the QO phase under discussion is precisely that phase in which it is believed[4,6] that quantum fluctuations are most highly developed and for which some sort of special higher-order approximations are needed.

For the temperature-dependent corrections $\Delta\sigma(T)$ and $\Delta\lambda(T)$ we have explicitly

$$\Delta\sigma(\theta)=\frac{\Gamma(^{3}/_{2})}{4\pi^{2}}\left(\frac{\theta H_{c1}}{A}\right)^{1/2}\left\{Z_{1/2}\left(\frac{\Delta_+}{\theta}\right)-Z_{1/2}\left(\frac{\Delta_-}{\theta}\right)\right\},$$

$$\Delta\lambda(\theta)=\frac{3\Gamma(^{3}/_{2})}{4\pi^{2}}\frac{1-1/2\xi}{H_{c1}}\left(\frac{\theta H_{c1}}{A}\right)^{1/2} \tag{50}$$

$$\times\left\{Z_{1/2}\left(\frac{\Delta_+}{\theta}\right)+Z_{1/2}\left(\frac{\Delta_-}{\theta}\right)\right\}.$$

Equations (50) and (47) imply that for $T\neq 0$ there is a longitudinal magnetization M_z which depends linearly on the field for smal h and nonlinearly for larger h; in both cases this magnetization is exponentially small because of the small value of $\theta/\Delta_{\pm}$, i.e., θ/D. As H approaches H_{c1} the T dependence takes on a power-law behavior and has the characteristic form in (38).

The form of the temperature dependence of the magnetization, susceptibility, specific heat, and other thermodynamic functions in the spin-wave approximation is determined solely by the form of the spectrum $\omega_{\mathbf{k}}^{\pm}$ and can be obtained not only from (45)–(50) but also from analysis of the form of the free energy of noninteracting bosons

$$\Omega_s=\theta\sum_{j\mathbf{k}}\ln(1-\exp\{-\omega_{j\mathbf{k}}/\theta\}) \tag{51}$$

and the thermodynamic relations. Since the spectrum has exactly the same form as that of a uniaxial antiferromagnet in the low-field phase, the results will be identical. In particular, for the specific heat $C_s=T\partial^{2}\Omega_s/\partial T^{2}$ and the susceptibility $\Delta\chi_{zz}\equiv\chi(T)-\chi(0)=-\partial^{2}\Omega_s/\partial H_z$ we have:

1) in the case of small fields $H\ll H_{c1}$:

$$C_s\approx 0,\quad \Delta\chi_{zz}\approx 0; \tag{52}$$

2) near $H=H_{c1}$, i.e., for $H_{c1}-H\ll\theta/D$:

$$C_s=a_1T^{1/2},\quad a_1=\frac{15(2H_{c1}k)^{1/2}k}{32\pi^{1/2}A^{3}},$$

$$\Delta\chi_{zz}=b_1\frac{T}{(H_{c1}-H)^{1/2}},\quad b_1=2\sqrt{2}\pi^{2}\frac{k(H_{c1})^{1/2}}{A^{3}}; \tag{53}$$

3) for small $H_{c1}\ll\theta/D$:

$$C_s=a_2T^{3},\quad a_2=\frac{4\pi^{2}}{15}k\left(\frac{k}{A}\right)^{3},$$

$$\Delta\chi_{zz}=b_2T^{2},\quad b_2=k^{2}/3A^{3}. \tag{54}$$

In the expressions for $a_{1,2}$ and $b_{1,2}$, k is the Boltzmann constant.

3. QFM phase. At the angle values given by (25), all the constants in (19) are nonzero, and, consequently, the form $\mathcal{H}_2$ for this phase is the same as (18). The formulas for the frequencies over the entire existence region of the QFM phase, $H_{c1}<H<H_{c2}$, are of form (20). The expression for the lower branch simplifies somewhat:

$$(\omega_{\mathbf{k}}^{-})^2 = \frac{\{(\varepsilon_b+V_1+V_2)(\varepsilon_a+V_3+V_4)-(v_1+v_2)^2\}\{(\varepsilon_b+V_1-V_2)(\varepsilon_b+V_3-V_4)-(v_1-v_2)^2\}}{(\varepsilon_b+V_1-V_2)(\varepsilon_b+V_1+V_2)+(\varepsilon_a+V_3-V_4)(\varepsilon_a+V_3+V_4)+2(v_2^2-v_1^2)}. \quad (55)$$

After substituting the explicit expressions for the constants $V_1(\mathbf{k})$, $V_2(\mathbf{k})$, $V_3(\mathbf{k})$, $V_4(\mathbf{k})$, $v_1(\mathbf{k})$, $v_2(\mathbf{k})$, ε_a, and ε_b determined by formulas (19) with the use of (25), we can see that for small $\mathbf{k}$ the dependence on $\mathbf{k}$ is of the form

$$(\omega_{\mathbf{k}}^{-})^2 = J_0^2(1-\gamma_{\mathbf{k}})f(H^2). \quad (56)$$

Because the explicit form of the function $f(H^2)$ is rather awkward we shall not write it out here—it can easily be obtained using the explicit formulas mentioned above; at $H=0$ we have $f(0)=(1+\xi)[1+\xi-\gamma_{\mathbf{k}}(1-\xi)]$, and at small H the function $f(H^2)$ is a power-law function of H^2.

Thus in the entire existence region of the QFM phase there is a Goldstone mode with a linear dispersion relation. This mode arises because a continuous symmetry operation of Hamiltonian (1)—rotation about the z axis—is spontaneously broken in this phase.

Let us give the explicit formulas for small $\mathbf{k}$ in several particular cases:

a) $H=0$:

$$(\omega_{\mathbf{k}}^{-})^2 = J_0^2(1-\gamma_{\mathbf{k}})(1+\xi)2\xi, \quad (57)$$

b) $H^2 = H_{c1}^2 + \Delta H$:

$$(\omega_{\mathbf{k}}^{-})^2 = (J_0/H_{c1})^2(1-\gamma_{\mathbf{k}})(1-\gamma_{\mathbf{k}}+\Delta H), \quad (58)$$

c) $H^2 = H_{c2}^2 - \Delta H$:

$$(\omega_{\mathbf{k}}^{-})^2 = J_0^2(1-\gamma_{\mathbf{k}})(1-\gamma_{\mathbf{k}}+2\Delta H). \quad (59)$$

It follows from (58) and (59) that at the boundaries of the existence region of the QFM phases the spectrum becomes quadratic, coinciding with the spectrum of the QO phase for $H=H_{c1}$ and with the spectrum of the FM phase for $H=H_{c2}$. The sound velocity of the Goldstone mode is zero at the boundaries and increases toward the center of the region (H_{c1}, H_{c2}).

Since for the lower branch we have $\omega_{\mathbf{k}}^{-} \propto \mathbf{k}$, all the temperature corrections to the thermodynamic functions at the lowest values of T will be interger powers of T; in particular,

$$C_s \propto T^3, \quad \chi_{zz}(T) \propto T^4, \quad \Delta M_z(T) \propto T^4, \quad \Delta M_x(T) \propto T^2. \quad (60)$$

The qualitative difference in the behavior of the thermodynamic functions in the QO, QFM, and FM phases leads to a peculiar change in their values and temperature dependences on changes in the external field. For example, the spin specific heat at the lowest values of T exhibits the following characteristic behavior: It has an exponentially small value for $H \ll H_{c1}$, increases with increasing H, and as $H \to H_{c1}$ goes over from an exponential dependence on T to a power-law dependence $C_s \propto T^{3/2}$; at $H=H_{c1}$ the specific heat exhibits a downward jump, and with the change in the structure of the phase there is also a change in the character of the temperature dependence: $C_s \propto T^3$ for $H_{c1} < H < H_{c2}$. Thereafter the changes are the mirror image of the previous changes: At the transition through $H=H_{c2}$ the specific heat exhibits an upward jump and again $C_s \propto T^{3/2}$ at small $H-H_{c2}$; it then falls off with increasing H and reverts to an exponential dependence on T.

The jumps and the mirror-like nature of the behavior of $C_s(H)$ are due to two successive second-order transitions QO→QFM and QFM→FM occurring at the points $H=H_{c1}$ and $H=H_{c2}$, respectively. Actually, at $H=H_{c1}$ and $H=H_{c2}$ formulas (25) for the angles describing the QFM solution go over to the formulas for the QO and FM solutions. The same fields correspond to a softening of the low-lying mode in the spectrum of the QO and FM phases. At these same points the velocity of the Goldstone mode in the QFM phase goes to zero. All these circumstances make up the typical pattern for a second-order transition. The behavior of the susceptibility is also typical—there are jumps in the longitudinal susceptibility χ_{zz} and a divergence of the off-diagonal components of the susceptibility tensor as the transitions are approached from the QFM side (from the phase with broken symmetry): $\chi_{zx} \equiv \partial M_x/\partial H_z \propto H^{-1/2}$, $\Delta H = |H_c - H|$ in the molecular-field approximation, and $\chi_{zz} \propto (\Delta H)^{d/2-2}$ with allowance for the spin waves, i.e., the quantum Gaussian fluctuations [in the $d=3$ case this is Eq. (37)], where d is the dimensionality of the crystal lattice.[4] We note that the latter anomaly in $\chi_{zz}(\Delta H)$ vanishes at $T=0$, and the critical behavior corresponds to the molecular-field approximation. An interesting feature of these transitions, which leads to the mirror-like character of $C_s(\Delta H)$, $\chi_{zz}(\Delta H)$, and the other characteristics, is that the transition from the low-symmetry to the high-symmetry phase occurs on an increase in H at $H=H_{c1}$ and on a decrease in H at $H=H_{c2}$.

5. RENORMALIZATION OF THE CRITICAL FIELDS

The renormalized critical fields can be found, as before, from the condition for the vanishing of the nontrivial QFM solution described by system (4) but with σ and λ given not by the unrenormalized values (8b) but by the spin-wave renormalized values (21). Explicit solutions of system (4) for $\sigma \neq 0$ is difficult, but it will not be necessary.

To obtain the phase boundary $H_{c1}(T)$ we first eliminate from system (4) the trivial QO solution (23). To do this we use (4b) to express $\sin\varphi$ in terms of $\sin K$ and, after substituting into (4a), we cancel out $\sin K$. Then after setting the values of the angles in this question equal to (23), we obtain an equation for the phase boundary $H_{c1}(T)$ at low T:

$$D^2 - h(h+J_0\sigma) + J_0 D\lambda = 0. \quad (61)$$

In this equation σ and λ are determined by general formulas (21) at angles (23) corresponding to the QO solution, i.e., by formulas (45) and (46). In an analogous way we obtain an equation for the phase boundary $H_{c2}(T)$:

$$2J_0 D\sigma + (D-h)[D+h-{}^1/_2 J_0(\lambda+\sigma)] = 0. \quad (62)$$

In this case σ and λ are determined by formulas (33). The corrections $\Delta\sigma(T)$ and $\Delta\lambda(T)$ in both cases depend on H through the special functions $Z_p(x)$, so that Eqs. (61) and (62) have a rather complicated form. Proceeding in the spirit of an iterative scheme, we shall assume that $H = H_{c1}^{(0)}$ and $H = H_{c2}^{(0)}$, respectively, in the corrections $\Delta\sigma(T)$ and $\Delta\lambda(T)$ which figure in (61) and (62) and solve the quadratic equation with respect to H_c. We then get

$$H_{c1}(T) = \frac{1}{2\xi}\frac{\Delta\sigma(T)}{2} + \left\{\left(\frac{1}{2\xi}\frac{\Delta\sigma(T)}{2}\right)^2 + \frac{1}{2\xi}\Delta\lambda(T) + \frac{1}{2\xi}\Delta\lambda(0) + (H_{c1}^{(G)})^2\right\}^{1/2}. \quad (63)$$

At the lowest temperatures, $\theta/D \ll H_{c1}$, we have

$$H_{c1}(T) = H_{c1}^{(0)} + \Delta H_{c1}(0) + \Delta H_{c1}(T),$$

$$H_{c1}^{(0)} = \left(1 - \frac{1}{\xi}\right)^{1/2}, \quad \Delta H_{c1}(0) = -\frac{1}{2\xi}\frac{\delta(\xi)}{H_{c1}^{(0)}}, \quad (64)$$

$$\Delta H_{c1}(T) = \frac{4\xi - 1}{2(\xi-1)}\frac{1}{4\xi}\frac{\Gamma(3/2)\zeta(3/2)}{4\pi^2}\left(\frac{\theta}{A}H_{c1}\right)^{3/2},$$

$$\zeta(p) \equiv Z_p(0),$$

where $\delta(\xi)$ is determined by formulas (49) and (45); formula (49) fixes the boundaries of its numerical values. Equations (64) imply that both corrections $\Delta H_{c1}(0)$ and $\Delta H_{c1}(T)$ are positive and work to increase H_{c1}.

For $H_{c1}(0) \approx 0 (\xi \approx 1)$, or under the condition $H_{c1}(0) \ll \theta/D$, we have

$$\Delta H_{c1}(T) \propto \theta^{3/4}. \quad (65)$$

In an analogous way, for $H_{c2}(T)$ we get from (62) to first order in $\Delta\sigma$ and $\Delta\lambda$

$$H_{c2}(T) = H_{c2}^{(0)} + \Delta H_{c2}(T), \quad H_{c2}^{(0)} = 1, \quad (66)$$

$$\Delta H_{c2}(T) = \frac{2}{1+4\xi}\Delta\sigma(T) = -\frac{2}{1+4\xi}\frac{\Gamma(3/2)\zeta(3/2)}{4\pi^2}\left(\frac{\theta}{A}\right)^{3/2}.$$

Unlike H_{c1}, the second critical field decreases with increasing T. The two tendencies work to narrow the existence region of the low-symmetry phase, as typically happens when fluctuations of the order parameter are taken into account.

Formulas (63) and (64) also permit refinement of the existence criterion for ferromagnetism in the absence of field at $T = 0$: $\xi < \xi^{cr}$. Since the vanishing of the ferromagnetism at the point $H = 0$, $T = 0$ under the opposite $\xi \geqslant \xi^{cr}$ is due to a transition to the QO phase, a refined value of ξ^{cr} can be determined from (64) under the condition $H_{c1}(0) = 0$:

$$\xi^{cr} = 1 - \delta(\xi = 1)/2. \quad (67)$$

According to the estimates of Sec. 4, in the three-dimensional case $\delta(\xi = 1)$ is $(3/2)\cdot 0.022$ and $(3/2)\cdot 0.017$ for simple cubic and bcc lattices, respectively.

6. CONCLUSION

The formalism developed in this paper is a generalization of the MD transformation to the case of systems whose Hamiltonians are constructed on generators of the group $SU(3)$, i.e., on spin and quadrupole operators.

We made a detailed study of the particular case of a ferromagnet with easy-plane single-ion anisotropy in a field perpendicular to the easy plane and showed that, contrary to the existing opinion, the quasiparticle description is valid in concept at any value of the ratio D/J_0. We showed that the deviation of the ground state from a state of ferromagnetic saturation is due not to zero-point vibrations but to an order structure that is other than ferromagnetic. In particular, the structure of the QFM phase is determined by a superposition of two different types of order, ferromagnetic and quadrupole, in analogy with the coexistence of antiferromagnetic and ferromagnetic order in weak ferromagnets. This circumstance is responsible for the peculiar magnetic properties, including those illustrated in Fig. 2. At $H = 0$ the predominance of one type of order or the other is determined by the relationship of the constants D and J_0, while for $H \neq 0$ it is determined by the proximity to the field H_{c1} or H_{c2}: near H_{c1} the quadrupole order dominates; near H_{c2}, the ferromagnetic. For $H < H_{c1}$ there is a spin structure characterized by quadrupole order only. We have shown that in regard to its magnetic properties this structure is in many respects analogous to an easy-plane antiferomagnet in the low field phase. For $H > H_{c2}$ an ordinary ferromagnetic structure is realized. The phase transitions between the three types of structures are spin-reorientation transitions. Here the reorientation occurs in an eight-dimensional isotopic space.

The generalization to the case of an arbitrary form of the Hamiltonian in the framework of $SU(3)$ (i.e., allowance for a more complex symmetry of the second-order single-ion anisotropy, for a field of arbitrary direction, for exchange anisotropy, and for biquadratic exchange) is trivial. The only thing that changes is the system of equations for the angles which fix the position of the local coordinate system. In particular, this system of equations is written out in Ref. 12 for the case of rhombic symmetry and a field of arbitrary direction. The second stage—the conversion to Bose operators—is done using the same formulas (14) and (15). Because the form of the system of equations for the angles is different, the analysis of its solutions, which determine the possible spin structures, should be carried out separately for each geometry of the system. However, the possibility of the existence of three phases and the characteristic behavioral features of the phases are preserved.

Let us now discuss the possibility of generalizing the formalism to the case $S > 1$, i.e., to algebras $SU(n)$ with $n > 3$. In principle the approach remains the same: a conversion to local coordinates and the subsequent introduction of Bose operators. The first stage is done with the aid of the unitary transformations of the group $SU(2S+1)$; the basic description of these transformations is discussed in Ref. 11. If one has found the law describing the behavior of the spin operators under the corresponding transformations, the conversion of the total Hamiltonian to local coordinates (in which the only nonzero averages are $\langle O_1^0\rangle, \langle O_2^0\rangle, \ldots, \langle O_{2S}^0\rangle$ in the notation of Ref. 11) does not present difficulties, but it is

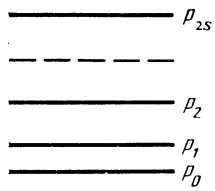

FIG. 3. Level scheme of an ion in the case of arbitrary S.

awkward. The system of equations for the generalized Euler angles is obtained from the condition that the remaining averages of the generators of the group $SU(2S+1)$ be zero. The Hamiltonian of the intersite interaction in the local coordinates in general contains terms of the form

$$\sum_{\substack{ij \\ ll',mm'}} P_{mm'}^{ll'}(ij) O_l^m(i) O_{l'}^{m'}(j),$$

where $l,l' = 1,\ldots,2S$ is the rank of the tensor operator, m, $m' = l, l-1,\ldots,-l+1, -1$ is the index of the spherical component, and i and j are the site indices.

The generalization of the second stage is trivial. Just as for $S=1$, one should first convert from the operators O_l^m to the other generators of $SU(n)$—the Hubbard operators $X^{pp'}$, which are connected by a linear relation which is analogous to (14) and is given for arbitrary S in Ref. 26, for example, and then to the Bose operators by means of formulas analogous to (15). If the level system of an individual ion is denoted as in Fig. 3, these latter formulas are of the form

$$X^{p_l p_0} = a_l^+ \left(1 - \sum_{n=1}^{2S} a_n^+ a_n\right), \quad (X^{p_l p_0})^+ \equiv X^{p_0 p_l} = a_l,$$
$$X^{p_l p_l} = a_l^+ a_l, \quad X^{p_l p_{l'}} = a_l^+ a_{l'}, \quad l, l' = 1,\ldots,2S. \tag{68}$$

One can also use in the second state a symmetrized representation analogous to the Holstein-Primakoff representation:

$$X^{p_l p_0} = a_l^+ \left(1 - \sum_{n=1}^{2S} a_n^+ a_n\right)^{1/2}, \quad X^{p_0 p_l} = \left(1 - \sum_{n=1}^{2S} a_n^+ a_n\right)^{1/2} a_l,$$
$$X^{p_l p_l} = a_l^+ a_l, \quad X^{p_l p_{l'}} = a_l^+ a_{l'}, \quad l, l' = 1,\ldots,2S. \tag{69}$$

For the algebra $SU(2)$ the off-diagonal Hubbard operators are the same as the spin operators, $X^{1/2\,-1/2} \equiv S^+$, $X^{-1/2\,1/2} \equiv S^-$, and the representations in (68) and (69) go over to the ordinary MD and HP representations, respectively.

On the whole, therefore, the approach developed here is universal, like the approach in Ref. 5, although, as was mentioned in that paper, the explicit form of the unitary transformations used in the first stage and the behavior of the spin operators under these transformations becomes increasing complicated as S increases. It should be noted that the idea discussed in Ref. 13 that the technique[3] used in that study is universal with respect to the value of S is actually only true of the second stage, since the Hamiltonian $\mathscr{H}_0$ is assumed to have been diagonalized and the conversion to local coordinates is assumed to have been done. I believe that the first stage, including the classification and the description of the possible spin structures and their existence regions, is the most important part of the study and can be omitted only in two cases. The first of these is for the simplest geometry of the system, when the type of spin structure is obvious and is of the ferromagnetic type, e.g., in the case of easy-axis single-ion anisotropy with the field parallel to the easy axis, i.e., the case considered in Refs. 14 and 15. The second case is for $\Delta = D/J_0 S \ll 1$, when the only possible phases are the FM phase and a QFM phase with a small (of order Δ) quadrupole component. We also note that although the use of the MD and HP representations is incorrect for the description of magnets with single-ion anisotropy in the general case, for $\Delta \ll 1$ they can be used for any direction of the field under the condition that a summation is made of the contributions of all the anharmonic terms in the chosen order in Δ, as is done in Refs. 4, 18, and 19 for small D/J_0 and arbitrary S.

APPENDIX

Since the rank of the algebra $SU(3)$ (i.e., the number of different unitary-nonequivalent operators) is two, the state of the system in the local coordinates is characterized by two averages, e.g., $\sigma = \langle \tilde{S}^z \rangle$ and $\lambda = \langle 3\tilde{O}^0 \rangle$. The relation of the first to the original averages is given by formula (9) and that of the second by the formula

$$\langle 3^{1/2}\tilde{O}^0 \rangle = A_z \langle S^z \rangle + A_x \langle S^x \rangle + B_0 Q_0 + B_2 Q_2 + B_1 Q_1,$$
$$A_z = \frac{3^{1/2}}{2} \sin\varphi \sin 2K, \quad A_x = -\frac{3^{1/2}}{2} \cos\varphi \sin 2K,$$
$$B_0 = \frac{1}{2}(3\cos^2 K \cos^2\varphi - 1), \tag{A.1}$$
$$B_2 = \frac{3^{1/2}}{2}(-1 + 2\cos^2 K - \cos^2 K \cos^2\varphi),$$
$$B_1 = \frac{3^{1/2}}{2} \cos^2 K \sin\varphi,$$
$$A_z^2 + A_x^2 + B_0^2 + B_2^2 + B_1^2 = 1.$$

Accordingly, in these local coordinates there are two preferred axes. The position of the first is characterized by the direction cosines α_p and β_p, and that of the second by the direction cosines A_p and B_p. Thus, one can say that the state of the system is characterized by two vectors: $\langle \tilde{\mathbf{S}}^z \rangle$ and $\langle 3\tilde{\mathbf{O}}^0 \rangle$.

In Sec. 2 we introduced the order parameter $\boldsymbol{\eta}$ as a vector coinciding with the vector $\langle \tilde{\mathbf{S}}^z \rangle$ given in local coordinates of the first type [for which (8a) holds]. The same vector $\boldsymbol{\eta}$ in local coordinates of the second type, to which one can convert using an additional rotation specified by the angles

$$\cos\varphi = \cos 2K = \cos 2L = 0, \tag{A.2}$$

is determined by a superposition of the vectors $\langle \tilde{\mathbf{S}}^z \rangle$ and $\langle 3\tilde{\mathbf{O}}^0 \rangle$. We easily see from (12), (9), (A.1), and (A.2), for example, that the absolute value and direction cosines $\tilde{\alpha}_p$ and $\tilde{\beta}_p$ of this vector are given by formula (11).

[1)]The discussion pertains to all cases except an easy-axis ferromagnet in a field **h** parallel to the easy plane.

[2)]The geometry corresponding to (1) has been considered only in Ref. 4, for $T = 0$ and $D/J_0 \ll 1$, when only structures which differ little from the ferromagnetic structure are possible, and in Ref. 10, for the case of antiferromagnetic exchange, at $T = 0$ and in the molecular-field approximation.

[3)]The number l of different local coordinates is also determined by the rank of the Lie algebra: $l = r + 1$. In the present case of the $SU(3)$ algebra, the number of such coordinates is equal to three, while for the $SU(2)$ algebra, corresponding to an exchange ferromagnet, $l = 2$. The first type of coordinate corresponds to $\langle \tilde{S}^z \rangle_0 = S$, the second to $\langle \tilde{S}^z \rangle_0 = -S$.

[4)]Recall that at the field-induced transition the role of the susceptibility is identical to the role of the specific heat at temperature transitions.

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