# Anharmonic theory of a phase with a spontaneously broken symmetry in ferromagnets exhibiting an easy-plane single-ion anisotropy of arbitrary magnitude

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An investigation is reported of dynamic properties of a phase with a spontaneously broken symmetry of a ferromagnet characterized by a single-ion anisotropy of the easy-plane type. The method used, based on unitary transformations of the Lie groups and the subsequent application of a low-temperature modification of a diagram technique for the Hubbard operators, gives symmetry-correct results satisfying the Goldstone theorem and the Adler principle for the scattering amplitudes and arbitrary ratios of the anisotropy to the exchange  $\xi$ . The following quantities are determined: the spectrum of collective excitations; the scattering amplitudes renormalized allowing for the interaction between quasiparticles; the free energy; the magnetization and the quadrupole averages. A study is made of the critical behavior of the system near the point of an orientational phase transition to a quadrupole-ordered phase. The properties of the system are close to the properties of an exchange ferromagnet of the same symmetry only at low values of  $\xi$ . When  $\xi$  rises, the specific single-ion anisotropy mechanism alters the behavior of the system: the contribution of optical modes becomes important (these are the modes that determine the critical behavior of the anisotropy constant in the vicinity of an orientational phase transition), the attraction between long-wavelength Goldstone quasiparticles changes to repulsion, the velocity of sound of a Goldstone mode begins to rise with temperature at the lowest values of T, etc. It is also shown that the characteristic features of quantum critical behavior of the anisotropy constant of the system in the vicinity of an orientational phase transition are due to the fact that this transition occurs at a multicritical point.

## INTRODUCTION

Our task will be to develop a microscopic theory of a phase with a spontaneously broken symmetry which forms in ferromagnets exhibiting an easy-plane single-ion anisotropy in the case of arbitrary values of the ratio of the anisotropy constant D and the exchange integral  $J_0$ . This phase has been investigated only for the case when  $D/SJ_0 \ll 1$  in Refs. 1-5 (here, S is the site spin). Even in this limiting case such a phase does not behave in a trivial manner: it is found that application of the standard methods from the theory of magnetism gives strange results such as an imaginary unrenormalized spectrum of collective excitations obtained as a result of diagonalization of a quadratic Hamiltonian  $\varkappa_2$  after application of the Holstein-Primakoff transformation.<sup>3,5</sup> Only inclusion of the contribution of  $\mathcal{H}_{int} = \mathcal{H} - \mathcal{H}_2$ , by summation of all the diagrams of lower order in  $D/J_0$ , gives a real spectrum characterized by weak damping (Ref. 5).<sup>1)</sup> This situation is a direct consequence of the fact that a system of this kind exhibits well-defined collective excitations, but these have to be introduced in some other way.

The reason for this situation is readily understood if we adopt the concept of dynamics of systems described at relatively low temperatures by a Hamiltonian which includes not only the spin but also the tensor interactions (the singleion anisotropy is an example of one of the latter interactions).<sup>6</sup> According to this concept, collective excitations excited in such systems at low temperatures T represent small fluctuations of the order-parameter vector relative to the equilibrium position. However, the order parameter is generally not the magnetization vector with three components  $\langle S^{\alpha} \rangle$ , but a vector defined in a  $(n^2 - 1)$ -dimensional space of the SU(n) algebra (n = 2S + 1), the components of which are the magnetizations and the tensor contributions. Consequently, such collective excitations should be introduced in a different way without recourse to the Holstein– Primakoff or Maleev–Dyson transformations or to other methods developed and used in the standard theory of magnetism in the case of systems with a pure spin order parameter, but by special methods acceptable in the case of systems with tensor interactions. These methods include the generalized Holstein–Primakoff and Maleev–Dyson transformations,<sup>6</sup> a diagram technique for the Hubbard operators,<sup>7</sup> and a generalized diagram technique for spin operators.<sup>8</sup>

It is clear from the above discussion that special features of the systems with the single-ion anisotropy are manifested to an increasing degree on increase in the relative contribution of the tensor components of the order parameter (if  $D/J_0 \ll 1$  this contribution is small because of the smallness of  $D/J_0$ ). However, investigations of magnetic materials with a single-ion anisotropy of arbitrary magnitude have been made only for those structures with the order parameter governed exclusively by the ferromagnetic components, such a collinear ferromagnetic structures in which the magnetization reaches saturation already at T = 0 (Refs. 9 and 10); this applies to nonlinear theories. We have recently investigated also the opposite limiting case of nonmagnetic structures with the order parameter governed entirely by the tensor (specifically, quadrupole) components: these are quadrupole-ordered structures or, in other words, structures of a spin nonmagnetic material.<sup>11</sup>

A phase with a spontaneously broken ferromagnetic symmetry considered in the present paper and described by a model Hamiltonian

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

can be observed in the range of parameters  $0 < \xi < \xi_{cr}$  $(\xi \equiv D/2J_0)$  when H = 0 (see Fig. 1). This phase is interesting for two reasons. Firstly, the contribution of the tensor components to the order parameter of this phase varies continuously with  $\xi$  ranging from zero for  $\xi = 0$  to unity for  $\xi = \xi_{cr}$ , which makes it possible to study changes in the properties from those typical of a "pure" ferromagnet to the properties of a "pure" spin nonmagnetic material. Secondly, the phase in question belongs to structures with a degenerate ground state which are generally of considerable interest. On the other hand, these two circumstances impose stringent conditions on the results: they must agree with the known anharmonic results for an isotropic ferromagnet when  $\xi = 0$ and for a quadrupole-ordered structure when  $\xi = \xi_{cr}$ ; moreover, the Goldstone theorem for the spectrum and the Adler principle for the scattering amplitudes must be satisfied for any value of  $\xi$ . In this connection it should be mentioned that in the only treatment<sup>7</sup> of an easy-plane phase with an arbitrary value of  $D/J_0$  the calculated scattering amplitudes of acoustic excitations satisfy the Adler principle just for D = 0(other harmonic quantities were not calculated).

We shall consider the case when S = 1, which is the minimum value of a site spin for which the single-ion anisotropy can exist and, consequently, the effects associated with this anisotropy are manifested most strongly. We shall use the Born approximation to find the spectrum of collective excitations, the scattering amplitudes, the free energy, the magnetization and the quadrupole averages at low T. We shall analyze the characteristic features of quantum critical behavior of the system (i.e., of the critical behavior at



We shall tackle our task employing a low-temperature modification<sup>11</sup> of a diagram technique for the Hubbard operators.<sup>7</sup>

# 1. HAMILTONIAN IN LOCAL COORDINATES. SYMMETRY OPERATIONS

The use of a diagram technique for the Hubbard operators implies that local coordinates are adopted first and the zeroth-order Hamiltonian is diagonal in these coordinates (because otherwise the Wick theorem is not satisfied by the Hubbard operators). These local coordinates are obtained by unitary transformations of the SU(3) group described in Ref. 14, when the generators are spin operators  $S^{\alpha}$  and quadrupole operators  $O_2^m$ , which in turn form the SU(3) algebra. The unitary transformation applicable to a ferromagnetic phase with a spontaneously broken symmetry (FM <sub><</sub>) corresponding to Eq. (1) is given by

$$V = \exp[L(O_2^2 - O_2^{-2})] \exp[K(O_2^4 + O_2^{-4})/2^{\frac{1}{2}}]$$
  
× exp[\phi(S^+ + S^-)/2^{\frac{1}{2}}], (2)

where the angles  $\varphi$ , K, and L are described by the system of equations (4) in Ref. 6. The quadrupole operators occurring in Eq. (2) are defined by

$$O_2^{0} = (S^{z})^2 - \frac{1}{3}S(S+1), \quad O_2^{\pm 1} = -(S^{z}S^{\pm} + S^{\pm}S^{z}), \quad O_2^{\pm 2} = (S^{\pm})^2.$$
(3)

In the zeroth approximation, which is the self-consistent field approximation when H = 0 and T = 0, the solution obtained in Ref. 6 is

$$\sin \varphi = \cos 2L = 0, \quad \cos 2K = \xi, \quad \xi = D/2J_0, \quad J_0 = \sum_j J_{ij}.$$
(4)



FIG. 1. *D*-*H* phase diagram at T = 0. Here, FM<sub><</sub> is the phase with a spontaneously broken symmetry for rotation about the *z* axis; the spin order in the phase has ferromagnetic components  $M_z = S^z$  and  $M_x = S^x$  and quadrupole components  $\langle O_2^0 \rangle$ ,  $\langle O_2^2 + O_2^{-2} \rangle$ , and  $\langle O_2^1 \pm O_2^{-1} \rangle$  [see Eq. (3)]. The ferromagnetic (FM<sub>1</sub>) and the quadrupole-ordered (QO) phases retain the indicated symmetry: at T = 0 in the case of the FM<sub>1</sub>, phase we have  $M_z = 1$  and  $M_x = 0$ , whereas in the case of the QO phase we have  $M_z = M_x = 0$ . In the present treatment we are dealing only with the FM<sub><</sub> phase only along the H = 0 line, where it is of the easy-plane type and is characterized by the averages described by Eq. (10). More detailed information on this phase diagram and on the properties of QO and FM<sub>11</sub> phases can be found in Refs. 11 and 12.



FIG. 2. Three-dimensional T-D-H phase diagram represented by sections in the D = const planes corresponding to different values of D. The continuous curves represent second-order phase transitions.

In general, if H = 0, we have

$$\sin \varphi = \cos 2L = 0, \quad \cos 2K = \eta = -2\xi/(\lambda + \sigma), \tag{5}$$

where  $\sigma = \langle \tilde{S}^z \rangle$  and  $\lambda = \langle 3\tilde{O}_2^0 \rangle$  are the averages of these operators in terms of local coordinates with the total Hamiltonian valid at an arbitrary temperature T (the equations for these quantities will be given later).

We can write down the Hamiltonian of Eq. (1) in terms of local coordinates if we know the relationship between the initial spin and quadrupole operators  $S^{\alpha}$ ,  $O_2^{m}$  and the spin and quadrupole operators  $\tilde{S}^{\alpha}$ ,  $\tilde{O}_2^{m}$  in terms of local coordinates. For arbitrary values of  $\varphi$ , K, and L this relationship is easily obtained from the expressions given in Ref. 14. Adopting then the Hubbard operators, which are related linearly to the operators  $\tilde{S}^{\alpha}$  and  $\tilde{O}_2^{m}$  [described by the system of equations (14) in Ref. 6], we obtain

$$S^{z} = -2^{-\frac{1}{h}} [(1-\eta)^{\frac{1}{h}} (X^{-10} + X^{0-1}) + (1+\eta)^{\frac{1}{h}} (X^{1-1} + X^{-11})],$$

$$S^{+} + S^{-} \equiv -2^{\frac{1}{h}} i S^{y} = (1+\eta)^{\frac{1}{h}} (X^{-10} - X^{0-1}) + (1-\eta)^{\frac{1}{h}} (X^{1-1} - X^{-11}),$$

$$S^{+} - S^{-} \equiv -2^{\frac{1}{h}} S^{z} = 2^{-\frac{1}{h}} [(1-\eta^{2})^{\frac{1}{h}} (\tilde{S}^{z} + 3\tilde{O}^{0}) - 2\eta (X^{10} + X^{01})].$$
(6)

[The expressions for the quadrupole operators given by Eq. (3) are readily obtained from the system (6) using the following rule for multiplication of the Hubbard operators:  $X_i^{pq}X_i^{rs} = \delta_{qr}X_i^{ps}$ ]. Here and later the operators without a tilde are defined in the original space, whereas the operators with the tilde are defined in the space of local coordinates; we shall omit the tilde above the Hubbard operators because they are defined only in terms of local coordinates in which the levels of an ion given by the zeroth-order Hamiltonian  $\mathcal{H}_0$  are labeled by the spin projections along the z axis. The distribution of levels in terms of local coordinates and the effect of the Hubbard operators are shown schematically in Fig. 3.

We find thus that the original Hamiltonian expressed in local coordinates becomes

$$\begin{aligned} \widetilde{\mathscr{H}}_{0} = E_{v} + \widetilde{\mathscr{H}}_{0} + (\widetilde{\mathscr{H}} - \widetilde{\mathscr{H}}_{0}), \quad E_{v} = -J_{v}(1 - \eta^{2})/2 + D(1 - \eta)/2, \\ \widetilde{\mathscr{H}}_{0} = J_{v}y_{a}\sum_{i} X_{i}^{-i-i} + J_{0}y_{b}\sum_{i} X_{i}^{ii}, \\ \widetilde{\mathscr{H}} - \widetilde{\mathscr{H}}_{v} = \sum_{ij} \{ [-J_{ij}X_{i}^{-i0}X_{j}^{0-i} + 1/2J_{ij}\eta(X_{i}^{-i0}X_{j}^{-i0} + X_{i}^{0-i}X_{j}^{0-i})] \\ + [-J_{ij}X_{i}^{1-i}X_{j}^{-ii} - 1/2J_{ij}\eta(X_{i}^{1-i}X_{j}^{1-i} + X_{i}^{-1i}X_{j}^{-ii})] - J_{ij}(1 - \eta^{2})^{*b} \end{aligned}$$

$$\times [X_{i}^{0-1}X_{j}^{i-1} + X_{i}^{-10}X_{j}^{-11}] - \frac{i}{2}J_{ij}[\eta(X_{i}^{01} + X_{i}^{10}) - (1 - \eta^{2})^{\frac{1}{2}}(2X_{i}^{11} + X_{i}^{-1-1})]$$

$$\times [\eta(X_{j}^{01} + X_{j}^{10}) - (1 - \eta^{2})^{\frac{1}{2}}(2X_{j}^{11} + X_{j}^{-1-1})] \}.$$

(7)

 $y_{b} = \frac{y_{c}}{y_{a}} - \frac{x^{1-t}}{x^{-10}} = 0$ 

FIG. 3. Schematic representation of levels of an uncorrelated ion described by  $\tilde{\mathscr{H}}_0$  in terms of local coordinates.

This form of the Hamiltonian corresponds to inclusion of the self-consistent field in the zeroth Hamiltonian  $\mathcal{H}_0$ , which is a starting point in the diagram technique for the Hubbard operators, as well as in the Vaks–Larkin–Pikin technique.<sup>15</sup> The dimensionless local fields (including the single-ion anisotropy and the self-consistent fields) are given by

$$y_{a} = -(1+\eta) (\lambda+\sigma)/2, \quad y_{b} = -(\lambda+\sigma), \quad y_{c} = -(1-\eta) (\lambda+\sigma)/2.$$
(8)

The averages  $\sigma = \langle \tilde{S}^z \rangle$  and  $\lambda = \langle 3\tilde{O}^0 \rangle$  obtained in the zeroth approximation are given by the equations

$$\sigma^{(0)} = \frac{e^{-\nu_{b}/\theta} - e^{-\nu_{a}/\theta}}{1 + e^{-\nu_{b}/\theta} + e^{-\nu_{a}/\theta}}, \quad \lambda^{(0)} = 1 - \frac{3}{1 + e^{-\nu_{b}/\theta} + e^{-\nu_{a}/\theta}},$$
$$\theta = k_{B} T/J_{0}, \qquad (9)$$

from which we find that  $\sigma^{(0)} = 0$ ,  $\lambda^{(0)} = -2$  at T = 0.

Before we include the corrections to the self-consistent field approximation, we note that Eqs. (4) and (5) for the angles describe the structure of a spin-ordered system generally determined by which of the eight independent Hermitian averages  $\langle S^z \rangle$ ,  $\langle S^+ - S^- \rangle$ ,  $i\langle S^+ + S^- \rangle$ ,  $\langle O_2^0 \rangle$ ,  $\langle O_2^2 + O_2^{-2} \rangle$ ,  $i\langle O_2^2 - O_2^{-2} \rangle$ ,  $\langle O_2^1 - O_2^{-1} \rangle$ ,  $i\langle O_2^1 + O_2^{-1} \rangle$  of the *SU*(3) algebra differs from zero. In particular, it follows from Eq. (4) that in the case of an easy-plane phase of the kind discussed here we have

$$M_{x} \equiv \langle S^{x} \rangle \equiv -(1-\eta^{2})^{\frac{1}{2}} (\lambda+\sigma)/2,$$

$$Q_{0} \equiv \langle 3O_{2}^{0} \rangle \equiv \lambda - 3(1-\eta) (\lambda+\sigma)/4,$$

$$Q_{2} \equiv \langle O_{2}^{2} + O_{2}^{-2} \rangle \equiv \sigma - (1-\eta) (\lambda+\sigma)/4,$$

$$\langle S^{t} \rangle \equiv \langle S^{y} \rangle \equiv \langle O_{2}^{1} \pm O_{2}^{-1} \rangle \equiv \langle O_{2}^{2} - O_{2}^{-2} \rangle \equiv 0.$$
(10)

If  $\eta = 1$  (or  $\xi = \xi_{cr}$  at T = 0), which corresponds to an orientational phase transition to a quadrupole-ordered phase, we find that  $M_x$  and  $Q_2$  vanish (the latter follows from  $y_a = y_b$  and, consequently, from  $\sigma = 0$  and  $\eta = 1$ ) and then we find that  $M_x = 0$  and  $Q_2 = 0$  remain valid for a quadrupole-ordered phase in which the spin order is characterized by just one parameter  $Q_0$  (Ref. 11). The existence of nonzero value of  $M_x$  and  $Q_2$  in an easy-plane phase is related to spontaneous symmetry breaking as a result of a phase transition from a quadrupole-ordered phase.

An analysis of the symmetry of the operations of the Hamiltonian (1) defined by the SU(3) group shows that after transition to the easy-plane phase there are two independent symmetry operations which are now spontaneously

broken. This is a continuous symmetry operation  $\exp(i\psi S^z)$ (rotation by an arbitrary angle  $\psi$  about the z axis) and a discrete operation

$$\exp(i\pi S^{\nu}) = \exp\left[\pi \left(O_{2}^{i} - O_{2}^{-i}\right)\right], \qquad (11)$$

at which the operators are transformed as follows:

$$S^{z} \to -S^{z}, S^{x} \to -S^{x}, O_{2}^{z} - O_{2}^{-2} \to -(O_{2}^{z} - O_{2}^{-2}),$$
$$O_{2}^{i} + O_{2}^{-i} \to -(O_{2}^{i} + O_{2}^{-i})$$

(the other operators are unaffected).

Before analyzing the influence of the term  $\tilde{\mathcal{H}} - \tilde{\mathcal{H}}_0$  on the dynamics of such a system by a diagram technique, we shall conclude this section with some simple considerations which make it possible to determine the spectrum of noninteracting collective excitations and which in our opinion make subsequent treatment somewhat clearer. We obtain such an unrenormalized spectrum employing the linear part of the transformation of the off-diagonal Hubbard operators to the Bose operators<sup>6</sup>:

$$X_{i}^{-10} = a_{i}^{+}, \quad X_{i}^{0-1} = a_{i},$$
  
$$X_{i}^{10} = b_{i}^{+}, \quad X_{i}^{01} = b_{i} \quad (X_{i}^{11} = b_{i}^{+}b_{i}, \quad X_{i}^{-1-1} = a_{i}^{+}a_{i}), \quad (12)$$

and also employing the low-temperature limit for  $\sigma^{(0)}$  and  $\lambda^{(0)}$  which gives  $\eta^{(0)} = \xi$ . Substituting Eq. (12) into Eq. (7), going over to the space of quasimomenta **k**, and diagonalizing the quadratic Hamiltonian, we obtain a spectrum  $E_k^{\mu} = J_0 \varepsilon_k^{\mu}$ , where

$$\varepsilon_{\mathbf{k}}^{a} = (1 - \gamma_{\mathbf{k}})^{\nu_{b}} (1 + \xi)^{\nu_{b}} [1 - \gamma_{\mathbf{k}} + \xi (1 + \gamma_{\mathbf{k}})]^{\nu_{b}},$$
  

$$\varepsilon_{\mathbf{k}}^{b} = 2(1 - \xi^{2} \gamma_{\mathbf{k}})^{\nu_{b}}, \quad \gamma_{\mathbf{k}} = J_{\mathbf{k}}/J_{0}.$$
(13)

Excitations of the c type, associated with transitions between the levels 1 $\rangle$  and  $|-1\rangle$ , remain localized in the quadratic approximation:

$$\varepsilon_{\mathbf{k}}^{c} = y_{c} = 1 - \xi. \tag{14}$$

#### 2. GREEN FUNCTIONS AND THE ZEROTH-APPROXIMATION SPECTRUM FOR LARKIN-IRREDUCIBLE PARTS OF DIAGRAMS

We shall define a matrix causal Green function

$$\hat{G}(l, \tau; l', \tau') = \langle T\mathbf{A}_{l}(\tau) \mathbf{A}_{l'}(\tau') \rangle$$
(15)

using vector operators  $\mathbf{A}(\tau)$  and  $\mathbf{A}(\tau')$ , where  $\mathbf{A}^+ = [(X^a)^+, X^a, (X^c)^+, X^c, (X^b)^+, X^b]$ ; A is a column of Hermitian operators;  $X^a \equiv X^{0-1}, X^b \equiv X^{01}, X^c \equiv X^{-11}$ ; *l* is the site index;  $\tau$  is the imaginary time.

In the self-consistent field approximation the Green function  $\hat{G}(\mathbf{k},\omega_n)$ , which is a Fourier transform of the Green function of Eq. (15) (**k** is the quasimomentum and  $\omega_n$  is a discrete frequency), is diagonal and its components are

$$G_{\mu\mu^{\dagger}}^{(0)}(\mathbf{k},\omega_{n}) = b_{\mu}K_{\mu\mu^{\dagger}}^{(0)}(\omega_{n})$$

where  $b_{\mu}$  are the characteristics of blocks given by

$$b_{a} = \langle X^{00} - X^{-1-1} \rangle_{0}, \quad b_{b} = \langle X^{00} - X^{11} \rangle_{0}, \quad b_{c} = \langle X^{-1-1} - X^{11} \rangle_{0},$$
(16)

and the Green functions  $K_{\mu\mu+}^{(1)}(\omega_n)$  are described by

$$K_{\mu\mu^{+}}^{(0)}(\omega_{n}) = 1/[\beta(y_{\mu} - i\omega_{n})].$$
(17)

The frequencies  $y_{\mu}$  are described by the system of equations (8) and the equations for  $b_{\mu}$  at finite temperatures T are given by the system (9) because

$$b_a = -(\lambda^{(0)} - \sigma^{(0)})/2, \quad b_b = -(\lambda^{(0)} + \sigma^{(0)})/2, \quad b_c = -\sigma^{(0)}.$$
(18)

We can obtain higher approximations for  $\widehat{G}(\mathbf{k},\omega_n)$  employing a scheme developed specifically for a diagramatic Vaks-Larkin-Pikin technique<sup>15</sup> described in detail in Ref. 16, which utilizes the concept of Larkin-irreducible parts of diagrams, i.e., of diagrams which are not cut along one interaction line. In such a scheme the relationship between the Green functions and the total irreducible part  $\widehat{\Sigma}$  is given by the Larkin equation, which retains the same form also in the diagram technique for the Hubbard operators. Its solution is

$$\hat{G}(\mathbf{k},\,\omega_n) = [\hat{I} - \hat{\Sigma}(\mathbf{k},\,\omega_n)\,\hat{\mathcal{V}}_{\mathbf{k}}]^{-1} \hat{\Sigma}(\mathbf{k},\,\omega_n)\,, \qquad (19)$$

where  $\hat{I}$  is a unit matrix and the interaction matrix  $\hat{V}_k$  is easily obtained from Eq. (7) if we represent the off-diagonal part of  $\tilde{\mathcal{H}} - \tilde{\mathcal{H}}_0$  in the form

$$\tilde{\mathscr{H}} - \tilde{\mathscr{H}}_{0} = \sum_{\mu\nu} \sum_{\mathbf{k}} V_{\mathbf{k}}^{\mu\nu} X_{\mathbf{k}}^{\mu} (X_{\mathbf{k}}^{\nu})^{+}, \quad \mu, \nu = a, b, c.$$
(20)

It is important to note that the matrix  $\hat{V}_k$  is of the blockdiagonal form

$$\widehat{\mathcal{V}}_{\mathbf{k}} = \begin{pmatrix} \widehat{\mathcal{V}}_{\mathbf{k}}^{(ac)} & \widehat{\mathbf{0}} \\ \widehat{\mathbf{0}} & \widehat{\mathcal{V}}_{\mathbf{k}}^{(b)} \end{pmatrix} \mathbf{0}$$
(21)

where the components of the  $4 \times 4 \hat{V}_k$  block relate the operators  $X^a$ ,  $(X^a)^+$ ,  $X^c$ , and  $(X^c)^+$ , whereas the components of the  $\hat{V}_k^{(b)}$  block relate the operators  $X^b$  and  $(X^b)^+$ . Since this determines the analogous structure of the matrix  $\hat{G}(\mathbf{k},\omega_n)$ , collective excitations represent superposition of excitations of the *a* and *c* types, as well as independent excitations of the *b* type.

In the lowest approximation the matrix  $\widehat{\Sigma}(\mathbf{k},\omega_n)$  is diagonal and its components are

$$\Sigma_{\mu\mu^*}^{(0)}(\mathbf{k},\omega_n) = b_{\mu} K_{\mu\mu^*}^{(0)}(\omega_n).$$

The Green function deduced by the substitution of the above Eq. (19) is known as the zeroth-approximation Green function for  $\hat{\Sigma}$  and in the limit of low temperatures *T* it is identical with the Green function of noninteracting quasiparticles. This function will be used later in the unrenormalized form when we shall allow for the interaction between quasiparticles; more precisely, we shall use the Green function  $\hat{K}(\mathbf{k}, \omega_n)$  related to  $\hat{G}(\mathbf{k}, \omega_n)$  by

$$\hat{G} = K\hat{b}, \quad \hat{b} = \begin{pmatrix} b_{a}\hat{I} & \hat{0} & \hat{0} \\ \hat{0} & b_{c}\hat{I} & \hat{0} \\ \hat{0} & \hat{0} & b_{b}\hat{I} \end{pmatrix}, \quad (22)$$

because in the low-temperature modification of the diagram

technique for the Hubbard operators<sup>11</sup> used by us the graph rows are written down for the Green functions found without the  $b_{\mu}$  multipliers [ $\hat{I}$  in Eq. (22) is a unit 2×2 matrix].

Explicit calculations in the limit of low temperatures T, when  $b_c = 0$  and  $b_a = b_b = 1$ , yield the following expressions for the components of  $\tilde{K}_{\mu\nu}(\mathbf{k},\omega_n)$ :

$$\beta K_{aa^*}(\mathbf{k}, \omega_n) = \beta K_{a^*}(\mathbf{k}, -\omega_n)$$
$$= (u_{\mathbf{k}}^a)^2 / (\varepsilon_{\mathbf{k}}^a - i\omega_n) + (v_{\mathbf{k}}^a)^2 / (\varepsilon_{\mathbf{k}}^a + i\omega_n), \quad (23)$$

$$\beta K_{aa}(\mathbf{k}, \omega_{n}) = \beta K_{a^{*}a^{*}}(\mathbf{k}, -\omega_{n})$$

$$= u_{\mathbf{k}}^{a} \upsilon_{\mathbf{k}}^{a} [1/(\varepsilon_{\mathbf{k}}^{a} - i\omega_{n}) + 1/(\varepsilon_{\mathbf{k}}^{a} + i\omega_{n})],$$

$$\beta K_{ac^{*}}(\mathbf{k}, \omega_{n}) = \beta K_{a^{*}c}(\mathbf{k}, -\omega_{n})$$

$$= \gamma_{\mathbf{k}} (1 - \xi^{2})^{\frac{1}{2}} \{ [(u_{\mathbf{k}}^{a})^{2}/(y_{c} - \varepsilon_{\mathbf{k}}^{a})] [1/(\varepsilon_{\mathbf{k}}^{a} - i\omega_{n}) - 1/(y_{c} - i\omega_{n})] + [(\upsilon_{\mathbf{k}}^{a})^{2}/(y_{c} + \varepsilon_{\mathbf{k}}^{a})] [1/(\varepsilon_{\mathbf{k}}^{a} + i\omega_{n}) + 1/(y_{c} - i\omega_{n})] \},$$

$$(24)$$

$$= \gamma_{\mathbf{k}} (1 - \xi^{2})^{\frac{y_{i}}{2}} u_{\mathbf{k}}^{a} v_{\mathbf{k}}^{a} \{ [1/(y_{c} - \varepsilon_{\mathbf{k}}^{a})] [1/(\varepsilon_{\mathbf{k}}^{a} - i\omega_{n}) - 1/(y_{c} - i\omega_{n})] + [1/(y_{c} + \varepsilon_{\mathbf{k}}^{a})] [1/(\varepsilon_{\mathbf{k}}^{a} + i\omega_{n}) + 1/(y_{c} - i\omega_{n})] \},$$
  
$$\beta K_{cc^{*}}(\mathbf{k}, \omega_{n}) = \beta K_{c^{*}c}(\mathbf{k}, -\omega_{n}) = 1/(y_{c} - i\omega_{n}), \qquad (25)$$

 $\beta K_{a^*c^*}(\mathbf{k}, \omega_n) = \beta K_{ac}(\mathbf{k}, -\omega_n)$ 

$$K_{ca} = K_{ca^*} = K_{cc} = K_{c^*c^*} = K_{c^*a^*} = K_{c^*a^*} = 0, \qquad (26)$$

$$\beta K_{bb^*}(\mathbf{k}, \omega_n) = \beta K_{b^*b}(\mathbf{k}, -\omega_n)$$
$$= (u_{\mathbf{k}}^{b})^2 / (\varepsilon_{\mathbf{k}}^{b} - i\omega_n) + (v_{\mathbf{k}}^{b})^2 / (\varepsilon_{\mathbf{k}}^{b} + i\omega_n), (27)$$
$$\beta K_{bb}(\mathbf{k}, \omega_n) = \beta K_{b^*b^*}(\mathbf{k}, -\omega_n)$$

$$= u_{\mathbf{k}}^{b} v_{\mathbf{k}}^{b} \left[ \frac{1}{(\varepsilon_{\mathbf{k}}^{b} - i\omega_{n})} + \frac{1}{(\varepsilon_{\mathbf{k}}^{b} + i\omega_{n})} \right]$$

All the other components of the matrix  $\hat{K}$  vanish, owing to the block-diagonal form of Eq. (21) for the  $\hat{V}_k$  matrix. The functions  $u_k^{\mu}$  and  $v_k^{\mu}$  in Eqs. (23)–(27) are identical with the functions of the *u*-*v* transformation that diagonalizes the quadratic form of the Bose operators of Eq. (12), and are given by

$$(u_{\mathbf{k}^{\mu}})^{2} = \frac{1}{2} \left( \frac{A_{\mathbf{k}^{\mu}}}{\varepsilon_{\mathbf{k}^{\mu}}} + 1 \right), \quad (v_{\mathbf{k}^{\mu}})^{2} = \frac{1}{2} \left( \frac{A_{\mathbf{k}^{\mu}}}{\varepsilon_{\mathbf{k}^{\mu}}} - 1 \right),$$

$$u_{\mathbf{k}^{\mu}}v_{\mathbf{k}^{\mu}} = -\frac{1}{2} \frac{B_{\mathbf{k}^{\mu}}}{\varepsilon_{\mathbf{k}^{\mu}}}, \quad \mu = a, b,$$
(28)

where

$$A_{\mathbf{k}}^{a} = 1 + \xi - \gamma_{\mathbf{k}}, \quad B_{\mathbf{k}}^{a} = \xi \gamma_{\mathbf{k}}, \quad A_{\mathbf{k}}^{b} = 2 - \xi^{2} \gamma_{\mathbf{k}}, \quad B_{\mathbf{k}}^{b} = -\xi^{2} \gamma_{\mathbf{k}},$$

$$(29)$$

and the expressions for the frequencies

 $\varepsilon_{\mathbf{k}}^{\mu} = \{ (A_{\mathbf{k}}^{\mu})^{2} - (B_{\mathbf{k}}^{\mu})^{2} \}^{\frac{1}{2}}$ 

are identical with those given by Eq. (13). In Eqs. (23)–(29) we allowed, in accordance with the definition, for all the averages of the operators occurring in the unrenormalized Green functions and these averages were used in the zeroth approximation corresponding to Eq. (9), including the averages defining the angle K in Eq. (5). In the limit of low temperatures T the "zeroth" value of the angle corresponds to  $\eta^{(0)} = \xi$ .

We shall use also the explicit form of the following correlation functions, which are related to the Green functions  $K_{\mu\nu}(\mathbf{k},\omega_n)$ :

$$n_{\mathbf{k}}^{r} = \lim_{\tau \to 0^{-}} \sum_{\omega_{n}} K_{rr} \cdot (\mathbf{k}, \omega_{n}) e^{i\omega_{n}\tau},$$

$$\mu_{\mathbf{k}}^{r} = \lim_{\tau \to 0^{-}} \sum_{\omega_{n}} K_{rr} (\mathbf{k}, \omega_{n}) e^{i\omega_{n}\tau}, \quad r=a, b, \qquad (30)$$

$$v_{\mathbf{k}} = \lim_{\tau \to 0^-} \sum_{\mathbf{e}_n} K_{ac^+}(\mathbf{k}, \omega_n) e^{i\mathbf{e}_n \tau}, \quad \eta_{\mathbf{k}} = \lim_{\tau \to 0^-} \sum_{\mathbf{e}_n} K_{ac}(\mathbf{k}, \omega_n) e^{i\mathbf{e}_n \tau},$$

which are given by

$$n_{\mathbf{k}}^{r} = [(u_{\mathbf{k}}^{r})^{2} + (v_{\mathbf{k}}^{r})^{2}]n(\varepsilon_{\mathbf{k}}^{r}) + (v_{\mathbf{k}}^{r})^{2},$$

$$v_{\mathbf{k}} = \gamma_{\mathbf{k}}(1 - \xi^{2})^{\frac{y_{2}}{2}} \left\{ (u_{\mathbf{k}}^{a})^{2} \frac{n(\varepsilon_{\mathbf{k}}^{a}) - n(y_{c})}{y_{c} - \varepsilon_{\mathbf{k}}^{a}} \right.$$

$$\mu_{\mathbf{k}}^{r} = u_{\mathbf{k}}^{r} v_{\mathbf{k}}^{r} [2n(\varepsilon_{\mathbf{k}}^{r}) + 1],$$

$$+ (v_{\mathbf{k}}^{a})^{2} \frac{1 + n(\varepsilon_{\mathbf{k}}^{a}) + n(y_{c})}{y_{c} + \varepsilon_{\mathbf{k}}^{a}} \right\}, \qquad (31)$$

$$\eta_{\mathbf{k}} = \gamma_{\mathbf{k}} (1 - \xi^2)^{\frac{1}{2}} u_{\mathbf{k}}^{a} v_{\mathbf{k}}^{a} \left\{ \frac{n(\varepsilon_{\mathbf{k}}^{a}) - n(y_{c})}{y_{c} - \varepsilon_{\mathbf{k}}^{a}} + \frac{1 + n(\varepsilon_{\mathbf{k}}^{a}) + n(y_{c})}{y_{c} + \varepsilon_{\mathbf{k}}^{a}} \right\},$$
$$n(x) = [\exp(\beta x) - 1]^{-1}.$$

An analysis of these results shows the following. The unrenormalized Green functions  $G_{ac^+}$ ,  $G_{a^+c^+}$ ,  $G_{cc^+}$  vanish at T = 0, since they are proportional to the factor  $b_c$ . These and not the functions  $K_{\mu\nu}$  are the true Green functions [for a definition see Eq. (15)] and it would seem that introduction of the Green functions  $K_{\mu\nu}$  with indices  $\mu$  or  $\nu$  equal to c and  $c^+$  is unnecessary. However, this is not true: it is the inclusion of these Green functions that will ensure, in the later stages of developing an anharmonic theory, that the results are symmetry-correct and satisfy both the Goldstone theorem and the Adler principle. This is associated with the special characteristic of the diagram technique for the Hubbard operators (and also of the Vaks-Larkin-Pikin technique) for which at the vertices of the third, fourth, and higher orders there are Green functions of the  $K_{\mu\nu}$  type, defined without the multipliers  $b_{\mu}$ , whereas  $b_{\mu}$  are characteristic of the block as a whole; the index  $\mu$  is determined by the nature of the Green function used in the subsequent pairing. For this reason the Green functions of Eqs. (24) and (25) may occur in graphs as intermediate elements and, therefore, the processes involving participation of a mode  $\varepsilon_{\mathbf{k}}^{c}$ , which are not excited in reality at low temperatures T, can contribute to the anharmonic results.

We shall analyze the characteristic features of the unrenormalized spectrum by beginning with the formulas for arbitrary temperatures T (i.e., without satisfying the condition  $b_c = 0$ ). The secular equation  $\det[\hat{I} - \hat{\Sigma}^{(0)}\hat{V}] = 0$  is factorizable. In the case of *b*-type collective excitations, defined by the 2×2 block of the matrix  $\hat{\Sigma}^{(0)}\hat{V}$ , we obtain

$$(\tilde{\boldsymbol{\varepsilon}}_{\mathbf{k}}^{b})^{2} = 4b_{b}^{2}(1 - \eta^{2} \boldsymbol{\gamma}_{\mathbf{k}}).$$
(32)

In the case of excitations defined by the  $4 \times 4$  block of the same matrix, we obtain

$$(\tilde{\varepsilon}_{\mathbf{k}}^{a^{\gamma}})^{2} = [(\tilde{\varepsilon}_{\mathbf{k}}^{a})^{2} + (\tilde{\varepsilon}_{\mathbf{k}}^{c})^{2}]/2 + b_{a}b_{c}(V_{\mathbf{k}}^{ac})^{2} \pm \{[(\tilde{\varepsilon}_{\mathbf{k}}^{a})^{2} - (\tilde{\varepsilon}_{\mathbf{k}}^{c})^{2}]^{2}/4 + b_{a}b_{c}(V_{\mathbf{k}}^{ac})^{2}R_{\mathbf{k}}\}^{\gamma_{2}}, \qquad (33)$$

where

$$V_{\mathbf{k}}^{ac} = \gamma_{\mathbf{k}} (1-\eta^{2})^{t_{b}}, \quad R_{\mathbf{k}} = (\tilde{A}_{\mathbf{k}}^{a} + \tilde{A}_{\mathbf{k}}^{c})^{2} - (\tilde{B}_{\mathbf{k}}^{a} + \tilde{B}_{\mathbf{k}}^{c})^{2}, (\tilde{\varepsilon}_{\mathbf{k}}^{\mu})^{2} = (\tilde{A}_{\mathbf{k}}^{\mu})^{2} - (\tilde{B}_{\mathbf{k}}^{\mu})^{2}, \quad \mu = a, b, \tilde{A}_{\mathbf{k}}^{a} - \tilde{B}_{\mathbf{k}}^{a} = (1+\eta) [b_{c} + (1-\gamma_{\mathbf{k}})b_{a}], \\\tilde{A}_{\mathbf{k}}^{a} + \tilde{B}_{\mathbf{k}}^{a} = (1+\eta) b_{b} - (1-\eta) \gamma_{\mathbf{k}} b_{a}, \\\tilde{A}_{\mathbf{k}}^{c} - \tilde{B}_{\mathbf{k}}^{c} = (1-\eta) [b_{a} + (1-\gamma_{\mathbf{k}}) b_{c}], \\\tilde{A}_{\mathbf{k}}^{c} + \tilde{B}_{\mathbf{k}}^{c} = (1-\eta) b_{b} - (1+\eta) \gamma_{\mathbf{k}} b_{c}.$$
(34)

We can now see that, in contrast to the T = 0 ( $b_c = 0$ ) case when there are independent *a*- and *c*-type modes of frequencies  $\varepsilon_k^a$  and  $\varepsilon_k^c$  defined by Eqs. (13) and (14), at a finite (no matter how low) temperature these modes become mixed and in the quasimomentum range  $k \sim k_0$  ( $\mathbf{k}_0$  is the quasimomentum corresponding to the point of intersection of spinwave modes) we can expect "repulsion" and a gap in the spectrum. The magnitude of the gap is proportional to  $b_c$ , i.e., it is small because the temperatures *T* are low. One of these modes (of the Goldstone type) has a linear spectrum at low values of  $k(\varepsilon_k^a \propto k)$ , but exhibits a very weak dispersion in the range  $k > k_0$  (Fig. 4).

The position of the point  $k_0$ , governed by the condition

$$\varepsilon_{\mathbf{k}_0} = y_c = 1 - \xi, \tag{35}$$

and the magnitude of the gap  $\Delta$  depend on the value of  $\xi$ . If  $\xi = 0$ , we find that  $k_0$  is governed by the equality  $\gamma_{k_0} = 0$ . As  $\xi$  increases the absolute value of  $k_0$  decreases and at  $\xi = 1$  we have  $k_0 = 0$ .

If, as expected, we have  $\xi = 0$ , there is no mixing: the interaction  $V_{\mathbf{k}}^{ac}$  in Eq. (33) vanishes at the point of intersection of the renormalized modes, because  $\gamma_{\mathbf{k}_0} = 0$  and we have one Goldstone mode characterized by  $\tilde{\epsilon}\epsilon_{\mathbf{k}}^a = b_b (1 - \gamma_{\mathbf{k}})$  (if  $\xi = 0$ , we find that  $b_b = \langle S^x \rangle_0$ ), corresponding to spin excitations, and two dispersion-free modes  $\tilde{\epsilon}_{\mathbf{k}}^b = 2b_b$ ,  $\tilde{\epsilon}_{\mathbf{k}}^\gamma = b_b$ , corresponding to localized quadrupole excitations.

A second special point at which mixing is absent is the boundary of the range of existence of the investigated phase, which is the point where  $\xi = \xi_{cr}(T)$  (or  $\eta = 1$ ). At this point we have

$$\tilde{\varepsilon}_{\mathbf{k}}^{\alpha} = \tilde{\varepsilon}_{\mathbf{k}}^{c} = 0, \quad \tilde{\varepsilon}_{\mathbf{k}}^{\gamma} = \tilde{\varepsilon}_{\mathbf{k}}^{\alpha} = 2b_{b}(1-\gamma_{\mathbf{k}})^{\frac{1}{2}}$$

(we are assuming here that if  $\eta = 1$ , we have  $b_c = 0$  and  $b_a = b_b$ ), i.e., a Goldstone mode vanishes identically, whereas

FIG. 4. Dispersion laws for three branches of selective excitations  $\varepsilon_k^a$ ,  $\varepsilon_k^b$ , and  $\varepsilon_k^{\gamma}$ . The 1 and 2 lines are the spin-wave spectra  $\varepsilon_k^a$  and  $\gamma_k^c$ . The repulsion between the modes in the region of intersection of the spin-wave spectra  $k \sim k_0$  is due to the temperature factor in the case of unrenormalized spectra or the anharmonic interaction factor in the case of collective excitations. The gap  $\Delta$  is small because temperatures are low so that  $\Delta^2$  $\propto r_0^{-3}$  at T = 0. The results plotted in this figure correspond to some value of  $\xi$  in the range  $0 < \xi < \xi_{cr}$ .

two optical modes soften and become degenerate.

For all other values of  $\xi$  we have a situation shown in Fig. 4 and in the range of energies  $\sim 1 - \xi$  there is a gap in the spectrum. It should be noted that this is true of the system as a whole and not only at finite temperatures T; in particular, when T = 0 the same situation applies if we allow for the anharmonic effects (see Sec. 4). Mixing of the a- and c-type modes is due to the fact that because of the interaction  $V^{ac}$  in the Hamiltonian of Eq. (20) the 4×4 block of the matrix of the Green functions  $\hat{K}^{(ac)}$  does not factorize into  $2 \times 2$  blocks associated with the *a* and *c* excitations. Independence of the spin-wave frequencies is the effect of the approximation adopted here and it is associated with the triangular form of the 4×4 matrix at  $b_c = 0$  also in the absence of the anharmonic effects. It should be stressed that mixing involves a mode corresponding to transitions between excited modes, which makes the effect nontrivial.

The transformation of the spectra due to variation of  $\xi$ is as follows. In the case of a Goldstone mode an increase in  $\xi$ alters the range of quasimomenta where this mode is characterized by an approximately linear dispersion law:  $\tilde{\varepsilon}_{\mathbf{k}}^{\alpha} \propto (1 - \gamma_{\mathbf{k}})^{1/2}$ . In the case of optical modes and finite values of  $\xi$  we can expect dispersion which grows on increase in  $\xi$ , whereas a gap at  $\mathbf{k} = 0$  decreases and at the orientational phase transition point characterized by  $\xi = \xi_{cr}$  the modes become softer and we have  $\tilde{\varepsilon}_{\mathbf{k}}^{\gamma} = \tilde{\varepsilon}_{\mathbf{k}}^{b} \sim k$ . The separation between the modes  $\tilde{\varepsilon}_{\mathbf{k}}^{\alpha}$  and  $\tilde{\varepsilon}_{\mathbf{k}}^{\gamma}$  in the region of the maximum approach is greater at some point within the interval  $(0, \xi_{cr})$ and it decreases on approach to the edges of this interval. It should also be mentioned that at the point  $\xi = \xi_{cr}$  the spectra  $\tilde{\varepsilon}_{\mathbf{k}}^{\alpha}$  and  $\tilde{\varepsilon}_{\mathbf{k}}^{\gamma}$  become nonanalytic at k = 0; the velocity of sound  $c_k^{\alpha,\gamma} = \partial \varepsilon_k^{\alpha,\gamma} / \partial k$  depends on the order of the transition to the limit  $\Delta \xi = \xi_{cr} - \xi \rightarrow 0, k \rightarrow 0$ . In particular, in the case of a  $\gamma$  mode, we have

$$c_{k}^{\gamma} = \begin{cases} 0, & k \to 0, & \Delta \xi \to 0 \\ \text{const.} & \Delta \xi \to 0, & k \to 0, \end{cases}$$

which is in agreement with an analogous result obtained on investigation of the spectrum on the side of the quadrupoleordered phase<sup>11</sup>; similarly, in the case of the  $\alpha$  mode, we have

$$c_{k}^{\alpha} = \begin{cases} \text{const,} & k \to 0, \quad \Delta \xi \to 0 \\ 0, & \Delta \xi \to 0, \quad k \to 0 \end{cases}$$

This picture can be understood if we turn to the expressions relating the spin and quadrupole operators to the Hubbard operators [see Eq. (6)]. It is clear from these relationships that, for example, a Goldstone mode associated with the breaking of the continuous symmetry of rotations about the z axis, i.e., a mode generated by  $S_k^z$ , is a superposition of oscillations of the a and c types generated by the operators  $X_{\mathbf{k}}^{0-1} + X_{-\mathbf{k}}^{-10}$  and  $X_{\mathbf{k}}^{-11} + X_{-\mathbf{k}}^{1-1}$ . As  $\xi$  increases, the width of the region where  $\tilde{\varepsilon}_{\mathbf{k}}^{\alpha} (1 - \gamma_{\mathbf{k}})^{1/2}$  is valid decreases because of a corresponding reduction in the contribution of the operator  $X_{k}^{0-1} + X_{-k}^{-10}$  to  $S_{k}^{z}$  and the spectrum of this operator is  $\tilde{\varepsilon}^{\alpha}_{\mathbf{k}}$ . The behavior of the  $\tilde{\varepsilon}^{b}_{\mathbf{k}}$  mode generated by the  $X_{\mathbf{k}}^{01} + X_{-\mathbf{k}}^{10}$  operator is as follows. If  $\xi \neq 0$ , such operators represent superpositions of spin and quadrupole operators, and the dispersion of the mode is proportional to the contribution of the spin operators (because in the initial Hamiltonian we allowed only for the spin-spin interaction and not for the biquadratic exchange interaction). If  $\xi = 0$  this contribution vanishes and there is no dispersion. This is also true of the second optical mode  $\varepsilon_{\mathbf{k}}^{\gamma}$ .

It is interesting to note also that two soft modes with a linear dispersion law,  $\tilde{\varepsilon}_{\mathbf{k}}^{b}$  and  $\tilde{\varepsilon}_{\mathbf{k}}^{\gamma}$ , exist at the phase transition point. This is a special feature of an orientational phase transition at a multicritical point A (Fig. 1) and it differs from the behavior at any other point on the line 1 where there is a soft mode characterized by the dispersion law  $\varepsilon_k \propto k^2$  (Ref. 11). The following comments can be made when considering a phase transition between quadrupole-ordered and FM configurations in a field H. In the case of the quadrupoleordered phase there are two collective excitation modes.<sup>11</sup> One of them is critical at an orientational phase transition which occurs in the upper part of the line 1 and the other is critical in the lower part of this line. At the point A, where the two parts of the lines converge, we can expect simultaneous softening of both modes so that their dependence on the quasimomentum changes to  $\varepsilon_k \propto k$ . (This is a self-evident consequence of the  $1/k^2$  Bogolyubov theorem, <sup>17</sup> but we shall not consider this in any detail.)

The characteristic features of the behavior of the spectrum at the point A can be explained also by a different approach involving an analysis of the symmetry operations of the Hamiltonian when the symmetry is broken spontaneously as a result of a phase transition from a quadrupole-ordered to an easy-plane phase. As pointed out in Sec. 1, this represents one continuous symmetry operation and two identical discrete operations. Consequently, a phase transition from a quadrupole-ordered to an easy-plane phase creates a Goldstone mode and two modes which are soft only at the phase transition point. [It should be noted that if  $H \neq 0$ , the unitary transformations of Eq. (11) are not symmetry operations of the Hamiltonian, so that there is only one soft mode, identical with the Goldstone mode, at the phase transition point.]

#### 3. POLARIZATION OPERATOR IN THE BORN APPROXIMATION

An allowance for the interaction of collective excitations yields a renormalized Green function  $\tilde{K}(\mathbf{k},\omega_n)$ , which is defined—in the low-temperature variant of the diagram technique for the Hubbard operators—by the Dyson equation

$$\hat{K} = \hat{K} + \hat{K} \hat{\Pi} \hat{K}, \qquad (36)$$

where  $\hat{K}$  is the matrix of the unperturbed Green functions of Eqs. (23)–(27) and  $\hat{\Pi}$  is the matrix polarization operator with the components  $\Pi_{\mu\nu}$  usually represented by a set of graphs which are not cut along one Green function line and which have an ingoing vertex of the  $\mu$  type and an outgoing vertex of the  $\nu$  type. In the Born approximation these graphs have the topologically standard form in the Vaks–Larkin–Pikin and Hubbard operator diagram techniques (see, for example, Fig. 29 in Ref. 16 and Fig. 1 in Ref. 11). In view of the large number of graphs of topologically identical form, we shall not give them explicity; we shall simply point out that they differ from those shown in Fig. 1 of Ref. 11 by additional components described by Eq. (24). The analytic form of the results of the *a*- and *c*-type components are as follows:

$$\Pi_{aa^{*}}(\mathbf{k}) = \Pi_{a^{*}a}(\mathbf{k}) = -\frac{\beta}{N} \sum_{\mathbf{p}} \left\{ \left[ \left[ 2(\gamma_{\mathbf{k}} + \gamma_{\mathbf{p}}) - (1 - \xi^{2}) (1 + \gamma_{\mathbf{k}-\mathbf{p}}) \right] n_{\mathbf{p}}^{a} - 2\xi\gamma_{\mathbf{p}}\mu_{\mathbf{p}}^{a} + (1 - \xi^{2}) ''_{2} (1 + \gamma_{\mathbf{k}-\mathbf{p}}) \eta_{\mathbf{p}} \right] + \left[ \xi^{2}\gamma_{\mathbf{p}} (\mu_{\mathbf{p}}^{b} + n_{\mathbf{p}}^{b}) - \left[ \gamma_{\mathbf{k}-\mathbf{p}} - \gamma_{\mathbf{k}} + 2(1 - \xi^{2}) \right] n_{\mathbf{p}}^{b} \right] \right\},$$

$$\Pi_{aa}(\mathbf{k}) = \Pi_{a^{*}a^{*}}(\mathbf{k}) = -\frac{\beta}{N} \sum_{\mathbf{p}} \left\{ \left[ \left[ 2\gamma_{\mathbf{p}} - (1 - \xi^{2}) \gamma_{\mathbf{k}-\mathbf{p}} \right] \mu_{\mathbf{p}}^{a} - 2\xi(\gamma_{\mathbf{k}} + \gamma_{\mathbf{p}}) n_{\mathbf{p}}^{a} - \xi(1 - \xi^{2}) ''_{2} \gamma_{\mathbf{k}-\mathbf{p}} \nu_{\mathbf{p}} \right] - \left[ \xi\gamma_{\mathbf{k}-\mathbf{p}} \mu_{\mathbf{p}}^{b} + \xi\gamma_{\mathbf{k}} n_{\mathbf{p}}^{b} \right] \right\},$$

$$\Pi_{ca^{*}}(\mathbf{k}) = \Pi_{c^{*}a}(\mathbf{k}) = -\frac{\beta}{N} \sum_{\mathbf{p}} \left\{ \left[ \xi(1 - \xi^{2}) ''_{2} \gamma_{\mathbf{k}-\mathbf{p}} \mu_{\mathbf{p}}^{a} - 3(37) \right] \right\}$$

$$-(1-\xi^2)^{1/2}(\gamma_k+\gamma_p)n_p^{a}$$

$$+(\xi^2\gamma_{\mathbf{k}-\mathbf{p}}-\gamma_{\mathbf{p}})\nu_{\mathbf{p}}+\xi(\gamma_{\mathbf{k}}+\gamma_{\mathbf{p}})\eta_{\mathbf{p}}]+[(1-\xi^2)^{\frac{1}{2}}(\gamma_{\mathbf{k}-\mathbf{p}}+\gamma_{\mathbf{k}})n_{\mathbf{p}}^{b}]\},$$

$$\Pi_{ca}(\mathbf{k}) = \Pi_{c^*a^*}(\mathbf{k}) = -\frac{\beta}{N} \sum_{\mathbf{p}} \{ [-(1-\xi^2)^{\frac{1}{2}} \gamma_{\mathbf{p}} \mu_{\mathbf{p}}^{a} + \xi (1-\xi^2)^{\frac{1}{2}} (1+\gamma_{\mathbf{k}-\mathbf{p}}) n_{\mathbf{p}}^{a} \}$$

+
$$(1+\gamma_{\mathbf{k}-\mathbf{p}})\xi^2\eta_{\mathbf{p}}$$
]+ $[\xi(1-\xi^2)^{\frac{1}{2}}\gamma_{\mathbf{p}}(n_{\mathbf{p}}^{b}+\mu_{\mathbf{p}}^{b})+2\xi(1-\xi^2)^{\frac{1}{2}}n_{\mathbf{p}}^{b}]$ },

$$\Pi_{c^{*}c}(\mathbf{k}) = \Pi_{cc^{*}}(\mathbf{k}) = -\frac{\beta}{N} \sum_{\mathbf{p}} \{ [(\gamma_{\mathbf{p}} - \xi^{2} \gamma_{\mathbf{k}-\mathbf{p}}) n_{\mathbf{p}}^{a} - \xi \gamma_{\mathbf{p}} \mu_{\mathbf{p}}^{a}] + [(\xi^{2} \gamma_{\mathbf{p}} - \gamma_{\mathbf{k}-\mathbf{p}}) n_{\mathbf{p}}^{b} + \xi^{2} \gamma_{\mathbf{p}} \mu_{\mathbf{p}}^{b}] \},$$

whereas the b-type components are described analytically by

$$\Pi_{bb^*}(\mathbf{k}) = \Pi_{b^*b}(\mathbf{k}) = -\frac{\beta}{N} \sum_{\mathbf{p}} \left\{ \left[ \left[ 2\xi^2 (\gamma_{\mathbf{k}} + \gamma_{\mathbf{p}}) -4(1 - \xi^2) (1 + \gamma_{\mathbf{k} - \mathbf{p}}) \right] n_{\mathbf{p}}^b \right] \right\}$$

 $+2\xi^{2}\gamma_{p}\mu_{p}{}^{b}]+[[\gamma_{p}+\xi^{2}\gamma_{k}-\gamma_{k-p}-2(1-\xi^{2})]n_{p}{}^{a}$ 

$$-\xi \gamma_{p} \mu_{p}^{a} + (1 - \xi^{2})^{\frac{1}{2}} (\gamma_{p} + \gamma_{k-p}) \nu_{p} + \xi (1 - \xi^{2})^{\frac{1}{2}} (2 + \gamma_{k}) \eta_{p}] \}, \qquad (38)$$

$$\Pi_{bb}(\mathbf{k}) = \Pi_{b^{*}b^{*}}(\mathbf{k}) = -\frac{\beta}{N} \sum_{p} \{ [2\xi^{2} (\gamma_{k} + \gamma_{p}) n_{p}^{b} + [2\xi^{2} \gamma_{p} - 4(1 - \xi^{2}) \gamma_{k-p}] \mu_{p}^{b} \} \}$$

+[
$$\xi^2 \gamma_k n_p^a - \xi \gamma_{k-p} \mu_p^a + \xi (1-\xi^2)^{\prime a} \gamma_k \eta_p$$
]}.

The other components of  $\Pi_{\mu\nu}$  vanish. The above expressions are obtained allowing for the following equalities valid at low temperatures:  $b_a = b_b = 1$ ,  $b_c = 0$  and also using the zeroth approximation for the angle:  $\eta = \eta^{(0)} = \xi$ . The expressions given for  $\Pi_{\mu\nu}$  are quantities of the first order in  $r_0^{-3}$ ( $r_0$  is the radius of the exchange interaction) and the validity of the Born approximation is in this case related to the long interaction radius; the higher approximations contain higher powers of  $r_0^{-3}$ , as well as terms allowing for the corrections  $\Delta\eta$  to  $\eta^{(0)}$ .

#### 4. RENORMALIZATION OF THE SPECTRUM

The renormalized frequencies of collective excitations are governed by poles of the Green function  $\hat{K}(\mathbf{k}, \omega_n)$ . According to the Dyson equation [Eq. (36)], these poles can be found from

$$\det[\hat{I} - \hat{K}\hat{\Pi}] = 0. \tag{39}$$

Since the matrixes  $\hat{K}$  and  $\hat{\Pi}$  are block-diagonal, the secular equation (39) is factorizable. In the case of the  $2 \times 2$   $\tilde{K}^{(b)}$  block, which governs the renormalized frequencies  $\hat{\tilde{\epsilon}}_{k}^{k}$ , this equation becomes

$$(i\omega_n)^2 = (\tilde{\tilde{\varepsilon}}_{\mathbf{k}}^{\,b})^2 = (\varepsilon_{\mathbf{k}}^{\,b})^2 - 2(A_{\mathbf{k}}^{\,b}\Pi_{bb} - B_{\mathbf{k}}^{\,b}\Pi_{bb}). \tag{40}$$

The solution of the secular equation for the  $4 \times 4 \hat{K}^{(ac)}$  block is

$$\begin{split} (\tilde{\tilde{\mathbf{e}}}_{\mathbf{k}}^{a,\mathbf{\gamma}})^{2} &= [(\tilde{\tilde{\mathbf{e}}}_{\mathbf{k}}^{a})^{2} + (\tilde{\tilde{\mathbf{e}}}_{\mathbf{k}}^{c})^{2}]/2 + V_{\mathbf{k}}^{ac} \Pi_{ca^{+}} \pm \{ [(\tilde{\tilde{\mathbf{e}}}_{\mathbf{k}}^{a})^{2} - (\tilde{\tilde{\mathbf{e}}}_{\mathbf{k}}^{c})^{2}]^{2}/4 \\ &+ V_{\mathbf{k}}^{ac} [[(\tilde{\mathbf{e}}_{\mathbf{k}}^{a})^{2} + y_{c}^{2}] \Pi_{ca^{+}} + 2y_{o} (A_{\mathbf{k}}^{a} \Pi_{ca^{+}} - B_{\mathbf{k}}^{a} \Pi_{ca})] \}^{1/2}, \end{split}$$

$$(41)$$

$$(\tilde{\tilde{\mathbf{e}}}_{\mathbf{k}}^{a})^{2} = (\tilde{\mathbf{e}}_{\mathbf{k}}^{a})^{2} - 2(A_{\mathbf{k}}^{a} \Pi_{aa^{+}} - B_{\mathbf{k}}^{a} \Pi_{aa}), \qquad (41)$$

$$(\tilde{\tilde{\mathbf{e}}}_{\mathbf{k}}^{c})^{2} = y_{c}^{2} - 2y_{c} \Pi_{cc^{+}}, V_{\mathbf{k}}^{ac} = \gamma_{\mathbf{k}} (1 - \xi^{2})^{\frac{1}{2}}. \end{split}$$

It is clear from these expressions that the anharmonic effects, like the temperature factor in the case of the unrenormalized spectra, mix the a and c modes, i.e., they produce an effect similar to that discussed in Sec. 2; see also Fig. 4. As in the case of the unrenormalized spectra (and mathematically

for the same reason), there is no mixing if  $\xi = 0$  and  $\xi = 1$ . In the case of an arbitrary value of  $\xi$  the graph  $\Delta$  between the  $\hat{\varepsilon}_{\mathbf{k}}^{\alpha}, \hat{\varepsilon}_{\mathbf{k}}^{\gamma}$  spectra in the region of the maximum approach  $k \sim k_0$  is a small quantity:  $\Delta^2 \approx r_0^{-3}$  at T = 0. The coefficient depends on  $\xi$  and its maximum value occurs at some point within the interval  $(0, \xi_{\rm cr})$  and decreases toward the edges. If  $\xi \ll 1$ , we find that the gap obeys  $\Delta^2 \approx \xi^{5/2}$ .

We can readily show that the Born correction of Eq. (41) maintains the Goldstone nature of the  $\tilde{\tilde{e}}_{k}^{\alpha}$  mode. In fact, it follows from Eq. (1) that the gap is absent at k = 0 ( $\tilde{\tilde{e}}_{k=0}^{\alpha} = 0$ ) if

$$\Pi_{aa} - \Pi_{aa}|_{k=0} = -[(1+\xi)/(1-\xi)]^{\frac{1}{2}}(\Pi_{ca} - \Pi_{ca})|_{k=0},$$

which is satisfied for all values of  $\xi$ , as can readily be deduced from Eq. (37).

The nature of the spectrum (41) simplifies if the anharmonic corrections are small compared with  $|(\varepsilon_k^{\alpha})^2 - y_c^2|$ :

$$\Pi_{\mu\nu}(\mathbf{k}) \ll |(\varepsilon_{\mathbf{k}}^{a})^{2} - y_{c}^{2}|,$$

i.e., far from the point  $k = k_0$ . When this is ensured by the inequality  $k \ll k_0$ , we find that the Goldstone mode is described by

$$\Delta \omega_{\mathbf{k}}^{\alpha} \equiv (\varepsilon_{\mathbf{k}}^{\alpha})^{2} - (\varepsilon_{\mathbf{k}}^{\alpha})^{2} \equiv -2 (A_{\mathbf{k}''} \Pi_{\alpha \alpha} - B_{\mathbf{k}''} \Pi_{\alpha \alpha}),$$

$$\Pi_{\alpha \alpha}^{*} = \Pi_{aa}^{*} + [(1+\xi)/(1-\xi)]^{\frac{1}{2}} \Pi_{ca}^{*}, \qquad (41a)$$

$$\Pi_{\alpha \alpha}^{*} = \Pi_{aa}^{*} + [(1+\xi)/(1-\xi)]^{\frac{1}{2}} \Pi_{ca}^{*}$$

whereas in the case of a  $\tilde{\tilde{\varepsilon}}_{\mathbf{k}}^{\gamma}$  mode, we have

$$\Delta \omega_{\mathbf{k}}^{T} = (\tilde{\epsilon}_{\mathbf{k}}^{T})^{2} - y_{c}^{2} = -2y_{c}\Pi_{TT^{*}},$$

$$\Pi_{TT^{*}} = \Pi_{cc^{*}} - \{[(1+\xi)/(1-\xi)]^{\frac{1}{2}}/(1-\xi)\}\Pi_{ca^{*}}$$

$$- \{[(1+\xi)/(1-\xi)]^{\frac{1}{2}}\xi/(1-\xi)\}\Pi_{ca}.$$
(41b)

Thus, all the modes can be described by

$$\widetilde{\widetilde{k}}_{\mathbf{k}}^{\mu} = \{ (\widetilde{A}_{\mathbf{k}}^{\mu})^{2} - (\widetilde{B}_{\mathbf{k}}^{\mu})^{2} \}^{\nu_{b}}, \ \mu = \alpha, \ \gamma, \ b,$$

$$\widetilde{\mathcal{A}}_{\mathbf{k}}^{\mu} = \mathcal{A}_{\mathbf{k}}^{\mu} - \Pi \qquad \widetilde{\mathcal{B}}_{\mathbf{k}}^{\mu} - \mathcal{B}_{\mathbf{k}}^{\mu} - \Pi$$

$$(42)$$

where

$$A_{\mathbf{k}}^{\alpha} = A_{\mathbf{k}}^{a}, \ B_{\mathbf{k}}^{\alpha} = B_{\mathbf{k}}^{a}, \ A_{\mathbf{k}}^{\gamma} = y_{c}, \ B_{\mathbf{k}}^{\gamma} = 0.$$

[Beginning from Eq. (40), we have to substitute  $\Pi_{\mu\nu} \equiv \Pi_{\mu\nu} (\mathbf{k}) / \beta$  in the above expressions.]

Using the explicit expressions for  $II_{\mu\nu}$ , we can write down the dispersion law for a Goldstone mode at low values of k:

$$(\tilde{\varepsilon}_{\mathbf{k}}^{\alpha})^{2} = (1 - \gamma_{\mathbf{k}}) [c^{2} + \Delta c_{\mathbf{k}}(0) + \Delta c_{\mathbf{k}}(T)], c^{2} = 2\xi (1 + \xi).$$
(43)

The dimensionless correction to the square of the velocity of sound at T = 0 is

$$\Delta c_{\mathbf{k}}(0) = -(2/N) \sum_{\mathbf{p}} \{\xi(1+\xi) [[(v_{\mathbf{p}}^{a})^{2}+u_{\mathbf{p}}^{a}v_{\mathbf{p}}^{a}](1+\gamma_{\mathbf{p}})(1-\xi) + [(v_{\mathbf{p}}^{a})^{2}-u_{\mathbf{p}}^{a}v_{\mathbf{p}}^{a}](1-\gamma_{\mathbf{p}})] - \xi(1+\xi) \frac{\gamma_{\mathbf{p}}}{(1-\xi)+\varepsilon_{\mathbf{p}}^{a}} [[(v_{\mathbf{p}}^{a})^{2}+u_{\mathbf{p}}^{a}v_{\mathbf{p}}^{a}] + (1-\xi)(1-\xi) + \xi[(v_{\mathbf{p}}^{a})^{2}-u_{\mathbf{p}}^{a}v_{\mathbf{p}}^{a}](1-\gamma_{\mathbf{p}}) + (v_{\mathbf{p}}^{a})^{2}(1+\xi)(1-\gamma_{\mathbf{p}})] - \xi[\xi^{2}\gamma_{\mathbf{p}}[(v_{\mathbf{p}}^{b})^{2}+u_{\mathbf{p}}^{b}v_{\mathbf{p}}^{b}] + 2\xi(1+\xi)(v_{\mathbf{p}}^{b})^{2} - (1+\xi)(1-\gamma_{\mathbf{p}})(v_{\mathbf{p}}^{b})^{2}]\}, \quad k \ll k_{0},$$

for the functions  $u_k^{\mu}$  and  $v_k^{\mu}$  given by the expressions in Eq. (28). The correction for finite temperatures T is

$$\Delta c_{\mathbf{k}}(T) = -\frac{2f_{\mathbf{i}}(\xi)}{N} \sum_{\mathbf{p}} [(1-\gamma_{\mathbf{p}})/\varepsilon_{\mathbf{p}}{}^{a}]n(\varepsilon_{\mathbf{p}}{}^{a})$$
$$= -\theta^{4}2f_{\mathbf{i}}(\xi) [2\xi(1+\xi)\rho]^{-s/\mathbf{i}}$$
$$\times \Gamma(4)\xi(4)/4\pi^{2}, \quad k \ll k_{0}, \quad \theta \ll 1-\xi, \quad \theta \ll \xi,$$
(45)

$$f_{i}(\xi) = \xi (2 - 3\xi - 11\xi^{2}) (1 + \xi) / (1 - \xi).$$
(46)

The following notation is used in Eq. (45):

$$\rho = (1-\gamma_k)/k^2, \quad \zeta(s) = \sum_{n=1}^{\infty} n^{-s}.$$

In the derivation of Eq. (45) we allowed for the fact that because of the kinematic relationships, we have

$$\sum_{\mathbf{p}} \mu_{\mathbf{p}^{a}} = \sum_{\mathbf{p}} v_{\mathbf{p}} = 0.$$

The temperature correction was calculated only for the limiting case defined by

$$\theta \ll 1-\xi, \ \theta \ll \xi.$$
 (47)

With the exception of the regions adjoining the limits of the interval  $(0, \xi_{cr})$  and requiring a separate discussion, these relationships apply also in the limit of low temperatures T irrespective of the low value of  $\xi$ . The first inequality in Eq. (47) makes it possible to use the substitution  $1/(y_c \pm \varepsilon_p^{\alpha}) \rightarrow 1/y_c$  when expressions for the correlation functions  $v_p$  and  $\eta_e$  are integrated with respect to **p** and this also makes it possible to ignore the contributions of  $n_p^b$  and  $\mu_p^b$  because they are exponentially small. The second inequality in Eq. (47) makes it possible to limit the integration with respect to **p** to the terms linear in **p** in the unrenormalized dispersion law of Eq. (13).

In the same limit we find that the temperature correction to  $(\varepsilon_k^b)^2$  corresponding to  $k \rightarrow 0$  is

$$\Delta \omega_{\mathbf{k}^{b}}(T) = (\tilde{e}_{\mathbf{k}^{b}})^{2} - (e_{\mathbf{k}^{b}})^{2} = \frac{2f_{2}(\xi)}{N} \sum_{\mathbf{p}} [(1 - \gamma_{\mathbf{p}})/e_{\mathbf{p}^{a}}]n(e_{\mathbf{p}^{a}})$$
$$= \theta^{4} 2f_{2}(\xi) [2\xi(1 + \xi)\rho]^{-s/2} \Gamma(4) \zeta(4)/4\pi^{2}, \quad \theta \ll 1 - \xi, \quad \theta \ll \xi,$$

$$f_2(\xi) = 2\xi^2 [\xi + (1+\xi) (2-\xi^2)].$$
(49)

We shall not write down the explicit form of  $\Delta \omega_{\mathbf{k}}^{b}(0)$  because it is too cumbersome. We can readily obtain the relevant expression by direct substitution of Eqs. (38) and (31) into Eq. (40).

We shall now consider the behavior of the anharmonic corrections near the boundaries of the range of existence of the easy-plane phase.

Left-hand boundary. If  $\xi = 0$ , when  $\varepsilon_{\mathbf{k}}^{\alpha} = 1 - \gamma_{\mathbf{k}}$ , we find that Eqs. (41) or (41a) yield

$$\tilde{\varepsilon}_{\mathbf{k}}^{\alpha} = \varepsilon_{\mathbf{k}}^{\alpha} - (1 - \gamma_{\mathbf{k}}) \frac{1}{N} \sum_{\mathbf{p}} (1 - \gamma_{\mathbf{p}}) n(\varepsilon_{\mathbf{p}}^{\alpha})$$

representing the familiar Born result for an isotropic ferromagnet. If  $\xi \ll 1$ , the condition of low temperatures T is compatible with two inequalities setting the limits:  $\theta \ll \xi$  and  $\theta \gg \xi$ . We consequently obtain

$$\Delta c_{\mathbf{k}}(T) = -\theta^{4} \xi (2\xi\rho)^{-s/2} \Gamma(4) \zeta(4) / \pi^{2}, \ \theta \ll \xi \ll 1,$$
  
$$\Delta c_{\mathbf{k}}(T) = -\theta^{3/2} \xi\rho^{-\frac{s}{2}} \Gamma(^{3}/_{2}) \zeta(^{3}/_{2}) / \pi^{2}, \ 1 \gg \theta \gg \xi.$$

The first of the above expressions follows from Eq. (45) in a lower order in  $\xi$ , whereas the second follows from the last equality in Eq. (45) if we integrate using the unrenormalized dispersion law  $\varepsilon_{\mathbf{p}}^{\alpha} = 1 - \gamma_{\mathbf{p}}$ . Both expressions are identical with the results obtained in Refs. 1, 2, and 5 in the limit  $\xi \leq 1$ .

Right-hand boundary. If  $\xi = 1$ , when there are two  $\varepsilon_{\mathbf{k}}^{b}$  and  $\varepsilon_{\mathbf{k}}^{\gamma} = \varepsilon_{\mathbf{k}}^{a}$ , modes with the unrenormalized dispersion laws

$$\varepsilon_{\mathbf{k}}^{b} = \varepsilon_{\mathbf{k}}^{a} = 2(1-\gamma_{\mathbf{k}})^{\frac{1}{2}}$$

where

$$v_{p} = \eta_{p} = \prod_{ca^{*}} = 0, \ n_{p}{}^{a} = n_{p}{}^{b}, \ \mu_{p}{}^{a} = -\mu_{p}{}^{b},$$

and we find from Eqs. (40) and (41) that

$$\Delta \omega_{k}^{b} = \Delta \omega_{k}^{\gamma} = (2/N) \sum_{p} \{ (1 - \gamma_{k})^{2} \gamma_{p} (n_{p}^{b} + \mu_{p}^{b}) + [6 \gamma_{k} n_{p}^{b} + 5 \gamma_{p}^{\dagger} (n_{p}^{b} + \mu_{p}^{b}) - \gamma_{k-p} (n_{p}^{b} - \mu_{p}^{b}) ] \}$$

is an expression identical with the results obtained for a quadrupole-ordered phase in Ref. 11 provided we substitute  $\xi = 1$  and H = 0 and bear in mind that the correlation functions  $n_p$ ,  $N_p$ , and  $\mu_p$  are related when  $\xi = 1$  to the correlation functions used in the present study by the expressions  $n_p = n_p^a$ ,  $N_p = n_p^b$ ,  $\mu_p = \mu_p^b$ . Near the right-hand boundary the condition of low temperatures T is compatible with the following two limiting inequalities:

$$\theta \ll 1 - \xi$$
 and  $\theta \gg \xi_{\rm cr}(T) - \xi$ ;

the latter inequality is analogous to the condition  $\theta \ge \xi$  near the left-hand boundary.<sup>2)</sup> If  $\theta \le 1 - \xi$ , then Eqs. (45) and (48) are valid. If  $\theta \ge \xi_{cr}(T) - \xi$ , we obtain

$$\Delta c_{\mathbf{k}}(T) = -\theta^{2} \rho^{-\gamma_{c}} \xi(2) / 8\pi^{2},$$
  

$$\Delta \omega_{\mathbf{k}}{}^{b}(T) = \Delta \omega_{\mathbf{k}}{}^{\dagger}(T)$$
  

$$= \theta^{2} [2 - \frac{3}{4} (1 - \gamma_{\mathbf{k}})] \xi(2) / 4\pi^{2}, \xi_{cr}(T) - \xi \ll \theta.$$
(50)

The result given by the system (50) for the  $\varepsilon_k^b$  and  $\varepsilon_k^{\gamma}$  modes, which exist on opposite sides of a phase transition, is identical with the corresponding result for the spectrum of a quadrupole-ordered phase near the phase transition point, obtained in Ref. 11 [it is understood that the expressions in the system (50) are valid outside the scaling region].

Summarizing, we should mention the following features of the anharmonic corrections to the spectrum of a Goldstone mode. These are, firstly, the change in the temperature dependence of the velocity of sound of a Goldstone mode when  $\xi$  is varied: according to Eq. (45), the behavior usual of ordered magnetic systems, which is a fall of the velocity of sound on increase in *T* observed at low values of  $\xi$ ( $\xi < \xi_0$ ), changes to an increase at sufficiently high values of  $\xi$ , i.e., in the region where the quadrupole ordering predominates. The quantity  $\xi_0$  is found from  $f_1(\xi) = 0$  and its value is  $\xi_0 \approx 0.31$ . This behavior occurs at the lowest temperatures *T*. At higher values of *T* the velocity of sound begins to decrease even at high values of  $\xi$ , as demonstrated by Eq. (50). Secondly, there is an interesting change in the nature of the power laws

$$\Delta c_{\mathbf{k}} (T) \propto T^{\frac{3}{2}}, T^{4}, T^{6}, T^{4}, T^{2}.$$

The  $T^{3/2}$  and  $T^2$  laws are observed, respectively, near the left- and right-hand boundaries of existence of the easyplane phase, whereas the  $T^6$  law occurs when  $|\xi - \xi_0| \ll \theta$  and the  $T^4$  law applies for all other values of  $\xi$  [the  $T^6$  law is obtained if the expression for  $\Delta c_k$  (T) includes higher powers in the momentum than those in Eq. (45)].

#### 5. FREE ENERGY. SCATTERING AMPLITUDES

The complete expression for the free energy is

$$F = F_0 + F^{fr} + \Delta F^{int},$$

where  $F_0$  is the free energy in the self-consistent field approximation, which in the limit of low values of T is identical with  $E_0$  of Eq. (7);

$$F^{\rm fr} = \frac{J_0}{\beta} \sum_{\mathbf{k}\mathbf{\mu}} \left[ \ln\left(1 - e^{-\beta \varepsilon_{\mathbf{k}}\mathbf{\mu}}\right) \right]$$

is the contribution associated with noninteracting collective excitations characterized by dispersion laws  $\varepsilon_k^{\mu}$ ;  $\Delta F^{\text{int}}$  is the contribution due to the interaction between such excitations, which in the Born approximation is governed by standard diagrams (see, for example, Fig. 3 in Ref. 11). Calculation of the last contribution gives

$$\beta \Delta F^{int} = -\frac{J_o}{N} \sum_{\mathbf{k}} \{ \Pi_{aa} \cdot n_{\mathbf{k}}^a + \Pi_{aa} \mu_{\mathbf{k}}^a + \Pi_{ca} \cdot v_{\mathbf{k}} + \Pi_{ca} \eta_{\mathbf{k}} + \Pi_{bb} \cdot n_{\mathbf{k}}^b + \Pi_{bb} \mu_{\mathbf{k}}^b \} = \Delta F_1(0) + \Delta F_2(T) + \Delta F_3(T), \quad \Pi_{\mu\nu} \equiv \Pi_{\mu\nu}(\mathbf{k}).$$
(51)

The expression for the *T*-independent correction  $\Delta F_1(0)$ 

which follows from Eq. (51) is in fact the correction to the energy of the ground state due to the interaction of the zeropoint vibrations. Its explicit form for an arbitrary  $\xi$  is found by direct substitution of Eqs. (31), (37), and (38) into Eq. (51). We can easily show that the value of  $\Delta F_1$  (0) rises on increase in  $\xi$  [this is due to an increase in  $(v_k^{\mu})^2$  and  $u_k^{\mu}v_k^{\mu}$ ]. The maximum value obtained for  $\xi = 1$  is

$$\Delta F_{i}(0) = \Delta E_{0}^{ini} = \frac{2J_{0}}{N^{2}} \sum_{\mathbf{k}\mathbf{p}} \{ [3(\gamma_{\mathbf{k}} + \gamma_{\mathbf{p}}) - \gamma_{\mathbf{k}-\mathbf{p}}] v_{\mathbf{k}}^{2} v_{\mathbf{p}}^{2} + (2\gamma_{\mathbf{p}} + \gamma_{\mathbf{k}-\mathbf{p}}) \}$$

 $\times u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{p}}v_{\mathbf{p}}+2u_{\mathbf{k}}v_{\mathbf{k}}v_{\mathbf{p}}^{2}(3\gamma_{\mathbf{k}}+\gamma_{\mathbf{p}})\}\approx 0.034J_{0}, \quad \xi=1,$ 

where  $u_{\mathbf{k}} \equiv u_{\mathbf{k}}^{b}$  ( $\xi = 1$ ),  $v_{\mathbf{k}} \equiv v_{\mathbf{k}}^{b}$  ( $\xi = 1$ ). This applies to a simple cubic lattice. The correction to the ground-state energy due to the noninteracting collective excitations has the following value for  $\xi = 1$ :

$$\Delta E_{0}^{\text{fr}} = -\frac{1}{2} \sum_{\mu=a,b} (A_{k}^{\mu} - \varepsilon_{k}^{\mu}) \approx -0.054 J_{0}, \quad \xi = 1.$$

The T-dependent corrections are

$$\Delta F_{2}(T) = \frac{J_{0}}{N} \sum_{\mathbf{k}\mu} \Delta \varepsilon_{\mathbf{k}}^{\mu}(0) n(\varepsilon_{\mathbf{k}}^{\mu}), \quad \Delta \varepsilon_{\mathbf{k}}^{\mu} \equiv \tilde{\varepsilon}_{\mathbf{k}}^{\mu} - \varepsilon_{\mathbf{k}}^{\mu},$$
$$\Delta F_{3}(T) = -\frac{J_{0}}{(\beta N^{2})} \sum_{\mathbf{k}p,\mu\nu} \Gamma^{\mu\nu}(\mathbf{k}p, \mathbf{p}\mathbf{k}) n(\varepsilon_{\mathbf{k}}^{\mu}) n(\varepsilon_{p}^{\nu}),$$

 $\mu, \nu = \alpha, \gamma, b,$ 

where  $\Gamma^{\mu\nu}(\mathbf{kp}, \mathbf{pk})$  are the forward scattering amplitudes of quasiparticles of types  $\mu$  and  $\nu$ . The explicit expressions for these amplitudes obtained for arbitrary values of  $\mathbf{k}$  and  $\mathbf{p}$  will not be given because they are too cumbersome; however, they can be readily deduced from Eq. (51). We shall simply write down the amplitudes for the scattering involving Goldstone particles and valid in the long-wavelength limit.

The amplitude of the scattering involving two Goldstone quasiparticles and two quasiparticles of type b is

$$\Gamma^{ab}(\mathbf{kp},\mathbf{pk}) = \Gamma^{ab}(\mathbf{kp},\mathbf{pk}) = -\frac{1-\gamma_{\mathbf{k}}}{\varepsilon_{\mathbf{k}}{}^{a}\varepsilon_{\mathbf{p}}{}^{b}} f_{2}(\xi)\beta, \quad k \ll k_{0}, \quad ap \ll 1;$$
(52)

The amplitude of the scattering involving four Goldstone particles is

$$\Gamma^{\alpha\alpha}(\mathbf{kp},\mathbf{pk}) = \Gamma^{\alpha\alpha}(\mathbf{kp},\mathbf{pk}) = \frac{(1-\gamma_{\mathbf{k}})(1-\gamma_{\mathbf{p}})}{\varepsilon_{\mathbf{k}}{}^{\alpha}\varepsilon_{\mathbf{p}}{}^{\alpha}} f_{1}(\xi)\beta,$$
  
$$k \ll k_{0}, \quad p \ll p_{0}.$$
(53)

The quantities  $f_1(\xi)$  and  $f_2(\xi)$  in Eqs. (52) and (53) are given by Eqs. (46) and (49). In the derivation of Eqs. (52) and (53) we are assuming that  $q \leqslant q_0$  (q = p, k) allows us to use the approximation  $1/(y_c \pm \varepsilon_q^a) \rightarrow 1/y_c$  in calculating the correlation functions of Eq. (31). We can easily see that the amplitude of Eq. (53) changes sign as a result of variation of  $\xi$ , showing that in the case of low values of  $\xi$  the amplitude corresponds to attraction between quasiparticles (in agreement with the well-known behavior in the range  $\xi \ll 1$ ), whereas at high values of  $\xi$  the amplitude corresponds to repulsion. If  $\xi = 0$ , the amplitude of Eq. (53) vanishes and in the next order in k and p, we obtain the familiar results for an isotropic ferromagnet.

The amplitudes of Eqs. (52) and (53) tend to zero as the quasimomentum of a Goldstone quasiparticle approaches zero, i.e., they satisfy the Adler principle for systems with degenerate vacuum.<sup>18,19</sup> The nature of the dependences on the quasimomenta corresponds to the symmetry of the system and has the usual form for easy-plane ferromagnets.<sup>19,20</sup>

The specific properties are, firstly, the repulsive nature of the interaction of Goldstone quasiparticles, realized for high values of  $\xi$ ; secondly, on approach to the point  $\xi = 0$ Eqs. (52) and (53) remain valid for a decreasing range of quasimomenta characterized by  $aq \ll \Delta \xi$  (q = k, p). At the phase transition point itself these equations retain their original form only if k = p = 0:

$$\Gamma^{aa}(\mathbf{kp, pk}) = \Gamma^{aa}(\mathbf{kp, pk}) = 0, \quad k = p = 0, \quad \Delta \xi = 1 - \xi \rightarrow 0.$$
(54)

It is interesting to note that the results given by Eq. (54) correspond to a specific sequence on approach to the limit in the calculation of  $\Gamma^{aa}(\mathbf{kp}, \mathbf{pk})$ : we first have  $k, p \rightarrow 0$ , and then  $\Delta \xi \rightarrow 0$ . For the opposite sequence when  $\Pi_{ca} = \Pi_{ca} = 0$ , we obtain from Eq. (51)

$$\frac{1}{\beta}\Gamma^{\alpha\alpha}(\mathbf{kp},\mathbf{pk}) = -4\xi/\varepsilon_{\mathbf{k}}^{\alpha}\varepsilon_{\mathbf{p}}^{\alpha}, \quad \Delta\xi = 0, \ k, \ p \to 0.$$
(55)

For this sequence of going to the limit we have  $\varepsilon_{\mathbf{k}}^{a} = \varepsilon_{\mathbf{k}}^{\gamma}$  (see Sec. 2), so that  $\Gamma^{aa} = \Phi^{\gamma\gamma}$ , and the amplitude given by Eq. (55) no longer applies to Goldstone quasiparticles, i.e., the Adler principle is no longer obeyed. The same form of Eq. (55) at low values of k, p, and  $\xi = 1$  is exhibited by the scattering amplitudes  $\Gamma^{bb}$  and  $\Gamma^{ab}$ . This result is identical with the result for the scattering amplitudes in the case of a quadrupole-ordered phase.<sup>11</sup>

We shall finally write down the explicit form of the temperature Born corrections  $\Delta F_2(T)$  and  $\Delta F_3(T)$ . In the limiting case described by Eq. (57), they are given by

$$\Delta F_{2}(T) = \theta^{4} J_{0} \Delta c_{0}(0) \left[ 2\xi (1+\xi) \right]^{-5/2} \rho^{-2} \Gamma(4) \xi(4) / 8\pi^{2},$$
  

$$\Delta F_{3}(T) = -\theta^{8} J_{0} \left[ 2\xi (1+\xi) \rho \right]^{-5} \rho^{5/4} f_{1}(\xi) (\Gamma(4) \xi(4) / 4\pi^{2})^{2},$$
(56)

with the exception of the range  $|\xi - \xi_0| \ll \theta$  where the terms proportional to  $\theta^{10}$  make the dominant contribution to  $\Delta F_3(T)$  [the numerical value of  $\Delta c_0(0)$  in Eq. (56) is given by Eq. (54)]. If  $\xi = 0$ , we obtain

$$\Delta F_2(T) = 0, \quad \Delta F_3(T) = -J_0 \theta^5 \zeta^2 (5/2) 3 \pi^{-3} 4^{-5},$$

i.e., the result is identical with the familiar Born expression for an isotropic ferromagnet. From the system (56) we readily obtain the required expressions for various thermodynamic quantities if we use thermodynamic relationships.

### 6. MAGNETIZATION AND QUADRUPOLE AVERAGES

The expressions for the free energy readily yield also the expression for the quadrupole average  $Q_0 = 3\partial F / \partial D - 2$ ,

but we cannot calculate the magnetization  $M_x = -\partial F / \partial H^x$ , because F(T) in Eq. (56) is defined at  $H^x = 0$ . Therefore, we shall calculate the averages of the spin and quadrupole operators independently using the renormalized Green function  $\hat{K} = (\hat{K}^{-1} - \Pi)^{-1}$ , the relationship between the averages of the diagonal Hubbard operators and the components of the Green function

$$\langle X_{i}^{11} \rangle \equiv \langle X_{i}^{10} X_{i}^{01} \rangle = K_{bb^{*}}(i\tau, j\tau') |_{i=j, \tau=\tau'},$$

$$\langle X_{i}^{-1-1} \rangle \equiv \langle X_{i}^{-10} X_{i}^{0-1} \rangle = K_{aa^{*}}(i\tau, j\tau') |_{i=j, \tau=\tau'},$$
(57)

and the relationship (10) between the spin and quadrupole averages and the averages  $\sigma = \langle X^{11} - X^{-1-1} \rangle$ ,  $\lambda = 3 \langle X^{11} + X^{-1-1} \rangle - 2$ . If in Eq. (57) we use the unrenormalized Green functions of Eqs. (23) and (27), we obtain the spin-wave result for  $\langle X^{\mu\mu} \rangle$ :

$$\langle X^{\mu\mu} \rangle = r^{\mu}(T) + \varphi^{\mu},$$
  

$$r^{\mu}(T) = \frac{1}{N} \sum_{\mathbf{k}} [(u_{\mathbf{k}}^{\mu})^{2} + (v_{\mathbf{k}}^{\mu})^{2}] n(\varepsilon_{\mathbf{k}}^{\mu}),$$
  

$$\varphi^{\mu} = \frac{1}{N} \sum_{\mathbf{k}} (v_{\mathbf{k}}^{\mu})^{2}, \quad \mu = a, b$$
(58)

(we recall that  $X^{aa} \equiv X^{-1-1}, X^{bb} \equiv X^{11}$ ) or explicitly

$$r^{a}(T) = c\theta^{2}, c = \xi \left[ 2\xi \left( 1+\xi \right) \rho \right]^{-\frac{1}{2}} \Gamma(2) \xi(2) / 4\pi^{2}, \theta \ll \xi, \theta \ll 1-\xi; r^{a}(T) = d\theta^{\frac{1}{2}}, d = \rho^{-\frac{1}{2}} \Gamma(\frac{3}{2}) \xi(\frac{3}{2}) / 4\pi^{2}, \xi \ll \theta; r^{a}(T) = r^{b}(T) = e\theta^{2}, e = 2^{-3} \rho^{-\frac{1}{2}} \Gamma(2) \xi(2) / 4\pi^{2}, \xi_{c}(T) - \xi \ll \theta$$

 $[r^{b}(T)$  is exponentially small in the first two cases].

The corrections due to the interaction of collective excitations, obtained using the renormalized Green function  $\hat{K}(\mathbf{k}, \omega_n)$ , are

$$\Delta \langle X^{\mu\mu} \rangle = \Delta \varphi^{\mu} + \Delta r^{\mu}(T) + P^{\mu}(T),$$
  

$$\Delta \varphi^{\mu} = \frac{1}{N} \sum_{\mathbf{k}} \Delta (v_{\mathbf{k}}^{\mu})^{2},$$
  

$$\Delta r^{\mu}(T) = \frac{1}{N} \sum_{\mathbf{k}} \{2(v_{\mathbf{k}}^{\mu})^{2}n(\varepsilon_{\mathbf{k}}^{\mu}) - \beta \Delta \varepsilon_{\mathbf{k}}^{\mu}(0)$$
  

$$\times (A_{\mathbf{k}}^{\mu} / \varepsilon_{\mathbf{k}}^{\mu}) n(\varepsilon_{\mathbf{k}}^{\mu}) [1 + n(\varepsilon_{\mathbf{k}}^{\mu})]\},$$
  

$$P^{\mu}(T) = \frac{1}{N^{2}} \sum_{\mathbf{k}, \mathbf{k}} \{(A_{\mathbf{k}}^{\mu} / \varepsilon_{\mathbf{k}}^{\mu}) [\Gamma^{\mu\mu}(\mathbf{k}\mathbf{p}, \mathbf{p}\mathbf{k}) n(\varepsilon_{\mathbf{p}}^{\mu})$$
  
(60)

$$\times n(\varepsilon_{\mathbf{k}^{\mu}})[1+n(\varepsilon_{\mathbf{k}^{\mu}})]\}.$$

 $+\Gamma^{\mu\nu}(\mathbf{kp},\mathbf{pk})n(\varepsilon_{\mathbf{p}}^{\nu})]$ 

Here,

$$\Delta \varepsilon_{\mathbf{k}}^{\mu} = \varepsilon_{\mathbf{k}}^{\mu} - \widetilde{\widetilde{\varepsilon}}_{\mathbf{k}}^{\mu}, \ \Delta (v_{\mathbf{k}}^{\mu})^2 = (v_{\mathbf{k}}^{\mu})^2 - (v_{\mathbf{k}}^{\mu})^2,$$
  
$$\Delta (u_{\mathbf{k}}^{\mu})^2 = (\widetilde{u_{\mathbf{k}}}^{\mu})^2 - (u_{\mathbf{k}}^{\mu})^2 \ (\Delta (u_{\mathbf{k}}^{\mu})^2 = \Delta (v_{\mathbf{k}}^{\mu})^2),$$

and  $\tilde{\tilde{u}}_{\mathbf{k}}^{\mu}$  and  $\tilde{\tilde{v}}_{\mathbf{k}}^{\mu}$  are defined by the expressions in Eq. (28) if we substitute  $A_{k}^{\mu}$  and  $B_{k}^{\mu}$  from Eq. (42). The expressions for the corrections in Eq. (60) consist of terms of two types. Those of the first type,  $\Delta \varphi^{\mu}$  and  $\Delta r^{\mu}(T)$  are related to the renormalization of the functions of the u-v transformation, and of the frequencies at T = 0, i.e., they are related to the difference between the effective quasiparticles and those which are unrenormalized and governed by the quadratic Hamiltonian [see Eqs. (12)–(14)]. Together with the term  $\varphi^{\mu} + r^{\mu}(T)$ , which occurs in Eq. (58), they describe the contribution governed by noninteracting quasiparticles which are not unrenormalized but effective. The term of the second type,  $P^{\mu}$ (T), is associated with the dynamic interaction of these quasiparticles. The expressions in Eq. (60) are obtained bearing in mind that the diagonal components of the renormalized Green function are given by Eqs. (23) and (27) subject to the substitutions  $u^{\mu} \rightarrow \tilde{\tilde{u}}^{\mu}, v^{\mu} \rightarrow \tilde{\tilde{v}}^{\mu}$ , and  $\varepsilon^{\mu} \rightarrow \tilde{\tilde{\varepsilon}}^{\mu3}$ , using also the expansion in terms of  $\Delta \varepsilon^{\mu}_{\mathbf{k}}$  under the sign of the sum over  $\omega_n$ , the identity

$$\sum_{\mathbf{e}_{n}} 1/[\beta^{2}(\varepsilon_{k}-i\omega_{n})]^{2}=n(\varepsilon_{k})[1+n(\varepsilon_{k})],$$

and the representation

$$\Delta \varepsilon_{\mathbf{k}^{\mu}}(T) = -\frac{1}{\beta N} \sum_{\mathbf{p}, \mathbf{v}} \{ \Gamma^{\mu\mu}(\mathbf{kp}, \mathbf{pk}) n(\varepsilon_{\mathbf{p}}^{\mu}) + \Gamma^{\mu\nu}(\mathbf{kp}, \mathbf{pk}) n(\varepsilon_{\mathbf{p}}^{\nu}) \}$$

for the temperature Born correction to the frequency.

Explicit calculations give the following expressions for  $P^{\alpha}(T)$ :

$$P^{o}(T) = \theta^{a} \xi f_{i}(\xi) [2\xi(1+\xi)]^{-5} \rho^{-4} \Gamma(3) \Gamma(4) \zeta(2) \zeta(4) / (4\pi^{2})^{2},$$

$$\theta \ll \xi, \, \theta \ll 1 - \xi; \tag{61}$$

$$P^{a}(T) = \theta^{4} \zeta(\frac{3}{2}) \zeta(\frac{5}{2}) (3\pi/2) (4\pi)^{-4}, \quad \xi \ll \theta.$$

The explicit expressions for  $\Delta r^{\mu}(T)$  will not be given: they have the same structure as Eq. (59) with the multipliers  $\Delta c$ ,  $\Delta d$ , and  $\Delta e$  which are numerically small compared with c, d, and e.

The expressions obtained for  $\langle X^{\mu\mu} \rangle$  allow us, firstly, to find the renormalized phase boundary  $\xi_{cr}(T)$  at low temperatures *T*, governed by the condition  $\eta = 1$ , i.e., by the condition  $\xi_{cr} = b_b(\xi_{cr})$ . If we calculate  $b_b$  $= 1 - 2\langle X^{11} \rangle - \langle X^{-1-1} \rangle$  for the unrenormalized value  $\xi_{cr}^{(0)} = 1$ , we obtain the same result as in Ref. 11, where use is made of the condition of softening of the renormalized spectrum of a quadrupole-ordered phase. Secondly, we can readily obtain now the explicit expressions for the magnetization and quadrupole averages employing the expressions in Eq. (10), and the definitions

$$\sigma = \langle X^{ii} - X^{-i-i} \rangle, \quad \lambda = 3 \langle X^{ii} + X^{-i-i} \rangle - 2$$

and the definition of  $\eta$  given by Eq. (5). Outside the direct vicinity of the phase transition point, they are of the form

$$M_{x} = (1 - \xi^{2})^{\frac{1}{2}} \{ 1 - [2\tilde{\varphi}^{b} + \tilde{\varphi}^{a} + \tilde{r}^{a}(T) + P^{a}(T)] \},$$

$$Q_{0} = -(1 + 3\xi)/2 + 3\{ (1 + \xi) [\tilde{\varphi}^{a} + \tilde{r}^{a}(T) + P^{a}(T)] + 2\xi \tilde{\varphi}^{b} \}/2,$$

$$Q_{2} = (1 - \xi)/2 + (\xi - 3) [\tilde{\varphi}^{a} + \tilde{r}^{a}(T) + P^{a}(T)]/2 + \xi \tilde{\varphi}^{b},$$

$$\tilde{\varphi}^{\mu} = \varphi^{\mu} + \Delta \varphi^{\mu}, \ \tilde{r}^{a}(T) = r^{a}(T) + \Delta r^{a}(T),$$
(62)

where the first terms correspond to the self-consistent field approximation at low temperatures T, and the other terms are low-temperature corrections associated with the existence of collective excitations and with their interactions. If  $\xi = 0$ , when  $r^a(T)$  and  $P^a(T)$  are given by Eqs. (59) and (61) in the limiting case of  $\xi \ll \theta$ , whereas  $\Delta r^{\mu}(T)$ ,  $\varphi^{\mu}$  vanish, we obtain the familiar result for an isotropic ferromagnet.

Near a phase transition we cannot use perturbation theory (in particular, the Born approximation) to describe the behavior of thermodynamic functions. Some general conclusions can nevertheless be drawn from an analysis of the behavior of the system in the Gaussian approximation. We note first of all that if the Hamiltonian contains two types of external fields, which are the magnetic  $H^{\alpha}S^{\alpha}$  and quadrupole (single-ion anisotropy) fields  $D^{\pm m}(O_2^m \pm O_2^{-m})$ , the reaction of the investigated system to external perturbations is governed by the isothermal static susceptibility tensor of the  $8 \times 8$  type, which includes the components of the magnetic susceptibility tensor

$$\chi^{\alpha\beta}_{\rm mag} = -\partial^2 F / \partial H^{\alpha} \partial H^{\beta},$$

the components of the quadrupole susceptiblity tensor

$$\chi_{\rm qp}^{mn} = -\partial^2 F / \partial D^m \partial D^n,$$

and the mixed susceptibilities

$$\chi^{\alpha n} = -\partial^2 F / \partial H^{\alpha} \partial D^n.$$

In studies of phase transitions on the basis of the single-ion anisotropy constant  $D \equiv -D^0$  the greatest interest lies in the quadrupole susceptibility  $\chi_{qp}^{00} = -\partial^2 F / \partial D^2$ . It follows from the above definition that the role of this quantity at a phase transition induced by variation of the anisotropy *D* is similar to the role of the specific heat  $C = -T\partial^2 F / \partial T^2$ when a phase transition is induced by variation of temperature. At T = 0 in the Gaussian approximation the quantity  $Q_0 = \langle 3O^0 \rangle$  is given by

$$Q_{0} = -(1+3\xi)/2 + (3/2N) \sum_{\mathbf{p}} \{(1+\xi) (v_{\mathbf{p}}^{a})^{2} + 2\xi (v_{\mathbf{p}}^{b})^{2}\}.$$
(63)

Obviously, the critical behavior of the susceptibility  $\chi^{00}_{qp} = -3\partial Q_0/\partial D$  is governed by the mode  $\varepsilon^b_k$  and not by a Goldstone mode, because

$$\partial (v_{\mathbf{k}}^{a})^{2}/\partial D \sim 1/(1-\gamma_{\mathbf{k}})^{\frac{1}{2}}, \ \partial (v_{\mathbf{k}}^{b})^{2}/\partial D \sim 1/(1-\gamma_{\mathbf{k}}+\Delta\xi)^{\frac{1}{2}}.$$
 (64)

It follows from Eqs. (63) and (64) that in the Gaussian approximation we obtain

$$\chi_{\rm qp}^{00} \sim (\Delta \xi)^{(d-3)/2}, \Delta \xi = \Delta \xi_{\rm cr} - \xi.$$

The behavior described above is of completely different nature from quantum critical behavior (at T = 0) of systems with a two-component order parameter experiencing an orientational phase transition as a result of variation of the field, characterized by  $d_{cr} = 2$  (Ref. 21); it is not a feature of a phase transition induced by variation of the anisotropy constant, but it does characterize a phase transition at T = 0occurring at a multicritical point, representing in particular a consequence of the existence of a critical mode with a linear

dispersion law at the orientational phase transition point. All this applies not only to a single multicritical point Acorresponding to S = 1, but also to all the 2S - 1 multicritical points which exist in this system for arbitrary S and are also characterized by a linear dispersion law of the critical mode<sup>12</sup> (we recall that at an ordinary orientational phase transition of the second order a soft mode obeys a dispersion law  $\varepsilon_{\rm k} \propto k^2$ ). It should be pointed out that for the same reason we can expect specific critical behavior of the system on approach to multicritical points also along other directions, for example, when  $H^{x}$  is varied. This problem and on the whole the behavior of all the components of the isothermal static susceptibility tensor will be discussed elsewhere.<sup>4)</sup> In the case of the critical behavior at  $T \neq 0$ , we find that at all very low but finite values of T there is a small but finite region near the phase transition where the critical behavior obeys the classical scaling laws and outside it we observe the quantum critical behavior described above.

#### CONCLUSIONS

In summarizing the results we must stress that the behavior of the investigated system taken as a whole is governed by two factors. The first is the symmetry which determines the properties common to all the easy-plane systems: a phase with a spontaneously broken symmetry exhibits a Goldstone mode with  $\varepsilon_k \propto k$ , there are definite dependences of the scattering amplitudes of these modes on the quasimomenta, etc. The second factor is associated with the following: the single-ion anisotropy acts as an external quadrupole field and it not only sets the symmetry but also introduces a new qualitative feature associated with broadening of the basis of the operators representing the state of the system, which increases from the three-dimensional basis of the SU(2) algebra to the eight-dimensional basis of the SU(3)algebra, giving rise to specific features of the behavior exhibited only by a system of this kind. For example, the spectrum of collective excitations of a conventional easy-plane ferromagnet consists of three branches (two degenerate branches of transverse oscillations and one branch of longitudinal oscillations), whereas in the case under consideration there are eight branches: six pairwise-degenerate branches of transverse oscillations with frequencies  $\varepsilon_{\mathbf{k}}^{\alpha}$ ,  $\varepsilon_{\mathbf{k}}^{\gamma}$ ,  $\varepsilon_{\mathbf{k}}^{b}$  and two branches of longitudinal oscillations corresponding to  $\tilde{S}_{\mathbf{k}}^{z}$ and  $\widetilde{O}_{\mathbf{k}}^{0}$  (longitudinal oscillations are ignored because they are unimportant at low values of T). The role of the optical modes  $\varepsilon_{\mathbf{k}}^{b}$  and  $\varepsilon_{\mathbf{k}}^{\gamma}$  is very important and, in particular, it is shown that they and not the Goldstone mode  $\varepsilon_{\mathbf{k}}^{\alpha}$  determine the critical behavior of the system.

The interaction of collective excitations is also a characteristic: it changes with  $\xi = D/2J_0$ , and, for example, in the case of long-wavelength Goldstone quasiparticles it varies from attraction at low values of  $\xi$  to repulsion at high  $\xi$ . A change in  $\xi$  alters also the signs and nature of the temperature corrections to the velocity of sound of a Goldstone mode, the anharmonic temperature corrections to the free energy, the magnetization, and other properties. (Transformation of these and other properties due to variation of  $\xi$ reflects the transformation of the structure of the spin order from "pure" ferromagnetic for  $\xi = 0$  to "pure" quadrupole for  $\xi = \xi_{cr}$ .) Finally, it should be pointed out that the critical behavior of the system is special at a phase transition to a quadrupole-ordered phase near a multicritical point. All these special features of the behavior of the investigated system are discussed at the ends of Secs. 2–6.

In describing the various properties we limited ourselves to the Born approximation, which is known to predict correctly all the qualitative effects at low temperatures T(with the exception of the scaling range). As far as the numerical coefficients are concerned, the Born approximation allows for terms up to  $\sim 1/r_0^6$  inclusive (in the case of thermodynamic functions), which is satisfactory in the case of long-range interactions of the RKKY type known to act in systems with a strong single-ion anisotropy (for example, rare-earth magnetic materials).

We shall now make some comments of methodological nature.

1. As pointed out already, the earlier applications of the diagram technique to the Hubbard operators have failed to yield, in an anharmonic theory, the results satisfying the Goldstone theorem and the Adler principle. On the other hand, our attempt to use the same technique<sup>8</sup> yielded directly results correct in respect of the symmetry. Our results indicate that this is not due to some defect of the Hubbard diagram technique, but is a consequence of lack of allowance for transitions between excited states and lack of allowance for the corresponding Green functions, which is a general feature in the development of low-temperature theories. (In the technique described in Ref. 8 all the Green functions are included automatically.) We can allow for these transitions by employing the low-temperature modification of the diagram technique for the Hubbard operators, involving "dressing" of the Green functions  $K_{\mu\nu}$  defined without the factors  $b_{y}$ , because otherwise the relevant Green functions are rejected automatically. The fundamental importance of inclusion of all the Green functions even at low temperatures is demonstrated above by presenting the results in terms of the formalism of the Hubbard diagram technique.

2. The results of the present study demonstrate that the Hubbard diagram technique and the technique of Ref. 8 are equally suitable in the case of low and high values of  $\xi$ , and in particular they reproduce the familiar results when  $\xi \ll 1$  and  $\xi = 0$ . We shall stress this in connection with a review of these methods in Ref. 23, where it is suggested that they are valid when the nonlocal interaction is weak compared with the one-particle interaction, i.e., at high values of  $\xi$ . This is not true because the zeroth-order Hamiltonian is not of the one-particle type, but includes not only external fields but also the molecular field. In particular, if D = 0, it is identical with the zeroth-order Hamiltonian utilized in the Vaks-Larkin–Pikin technique, which is known to describe well an isotropic ferromagnet.

In discussing the Maleev–Dyson, Holstein–Primakoff, or Goldhirsch<sup>24</sup> transformations, we can hardly assume that their use is more natural even when  $\xi \ll 1$ , because then they yield an imaginary unrenormalized spectrum (see the Introduction). The alternative to the diagram technique is the quasiparticle method which can be applied to systems with the single-ion anisotropy and nonlocal tensor interactions and represents a special transformation to the Bose operators of Ref. 6, defined in terms of the SU(n) algebra (n = 2S + 1).

It should be stressed also that all these transformations

to the Bose operators, like the diagram techniques applied to the spin and Hubbard operators, are based on the self-consistent field method as the zeroth approximation; this is clear from the definition  $S^{z} = S - a^{+}a$  of the Maleev–Dyson or Holstein–Primakoff transformation, which implies  $\langle S^z \rangle_0 = S$ , and similar definitions in the case of diagonal operators employed in the case of the transformation proposed in Ref. 6. Moreover, at low temperatures T these diagram techniques degenerate to the corresponding diagram techniques for interacting Bose particles, which are equivalent in the case of the Vaks-Larkin-Pikin technique to quasiparticles introduced by the Maleev-Dyson transformation (see Ref. 16), whereas in the case of the Hubbard diagram technique they are equivalent to quasiparticles introduced by the transformation of Ref. 6 (see Ref. 11). Therefore, the selection of one of the two approaches-diagram techniques for the spin and Hubbard operators or quasiparticle methods-is dictated at low temperatures T simply by convenience. It is important to select them satisfactorily for the task in hand, and in particular, in the presence of the easy-ion anisotropy and nonlocal tensor interactions, we should use the Hubbard diagram technique (or the technique of Ref. 8) and the transformation to the Bose operators defined in the SU(2S + 1) algebra.

systems of this kind, which are characterized by  $d_{\rm cr} = 3$  and have been studied by, for example, numerical experiments in the one-dimensional case<sup>22</sup> or have been deduced from phenomenological considerations.<sup>5</sup>

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<sup>&</sup>lt;sup>1)</sup>Special approaches have also been developed <sup>3,4</sup> beginning from the welldefined unrenormalized quasiparticles, but all of them are limited to the case when  $D/J_0 \ll 1$ .

<sup>&</sup>lt;sup>2)</sup>The condition  $\theta \ge 1 - \xi$  or the more general condition  $\theta \ge \tilde{\xi}_{cr}(0) - \xi$ , where  $\tilde{\xi}_{cr}(0)$  is the renormalized value of the critical anisotropy at T = 0, applies at temperatures outside the range of existence of the easyplane phase, because when H = 0 a multicritical point  $\xi = \tilde{\xi}_{cr}(0)$  corresponds to  $T_c(\xi) = 0$ .

<sup>&</sup>lt;sup>3)</sup>This conclusion is rigorous in the case of the  $\tilde{K}_{bb}$  Green function, but it is only approximately valid in the case of  $\tilde{K}_{aa}$ . The structure of this function differs from the structure of the unrenormalized Green function  $K_{aa}$ , because inclusion of  $\hat{\Pi}$  in the equality  $\hat{K}^{-1} = \hat{K}^{-1} - \hat{\Pi}$  has the effect that the  $4 \times 4 \hat{K}^{(ac)}$  block no longer contains zeros, in contrast to the unrenormalized Green function [see the expressions in Eq. (26)]. This has the effect that the renormalized Green function  $\tilde{K}_{aa}$  contains not only terms  $\sim 1/[\beta(\varepsilon_k^a \pm i\omega_n))$ , but also terms  $\sim 1/\beta(\varepsilon_k^i \pm i\omega_n)$ . However, their contribution is exponentially small when  $\theta \not\in 1$ .

<sup>&</sup>lt;sup>4)</sup>This behavior is in agreement with the current ideas on a phase transition induced by variation of the single-ion anisotropy when H = 0 in