A dynamic theory of the nonmagnetic phase of singlet magnets

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A nonlinear microscopic theory of the low-temperature nonmagnetic phase of singlet magnets is constructed, which makes it possible to calculate the spectrum of collective oscillations, the spin correlation functions, the asymptotic behavior of the thermodynamic functions, the magnitude of the critical field and the criterion for ferromagnetism.

1. INTRODUCTION

It is well known that many magnetic compounds consisting of ordered arrays of magnetic ions which interact via an exchange interaction of fixed sign and intensity nevertheless remain nonmagnetic at all temperatures down to $T=0$. The reason that magnetic order is absent in these cases is the existence of a single-ion anisotropy (SIA) which is strong compared to the exchange force.

As was shown in Ref. 1, these structures are spin-ordered despite the absence of magnetic order; furthermore, this ordering has tensor characteristics. For this reason, the properties of such structures differ from those of pure (disordered) paramagnets (PMs); in particular, their properties are found to be close to those of antiferromagnets (AFMs) (specifically, uniaxial AFMs in a field parallel to the anisotropy axis). In order to describe such tensor structures, a generalized Maleev-Dyson transformation was proposed in Ref. 1 and a spin-wave theory was developed; however, in view of its crudeness, this theory can only be regarded as a first step in the investigation of such systems.

The goal of this article is to construct a first-principles microscopic theory of these PMs at low temperatures, which correctly takes into account the quasiparticle interactions. The model we will investigate is a spin structure with isotropic exchange and an "easy plane" (EP) SIA in an external field perpendicular to the EP. This structure is described by the Hamiltonian

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

(The sign of D is chosen so that the ground state of an isolated ion is a singlet). For the case that the ratio $\xi=D/2J_0$ ($J_0=\Sigma_j J_{ij}$) exceeds some critical value ξ_{cr} (in the molecular-field approximation $\xi_{cr}=1$ when $S=1$), this model gives rise to a nonmagnetic quadrupole-ordered (QO) ground state in the region of fields $0<h<h_{c1}$ (see Fig. 2 below).

In this paper we will determine the spin correlation function, the spectrum of collective oscillations, the low-temperature asymptotic behavior of the free energy, the magnetization, the specific heat, the value of the critical field h_{c1} and the criterion for ferromagnetism for this model.

In order to calculate temperature-dependent anharmonic corrections, we use the Born approximation; it is well-known that this level of approximation correctly includes all the qualitative characteristics of the temperature behavior. Calculations at $T=0$, where the system properties are especially quantum-mechanical, must be carried out more carefully; in particular, we must take into account the very large renormalizations of the bare spin-wave values which follow from calculations in the first Born approximation. Toward this end, we set up a formalism involving a nonunitary self-consistent u-v transformation; the self-consistency allows us to obtain an exact integral equation for the functions which generate this transformation. We then set up an iterative scheme to solve this equation.

The calculation is carried out for $S=1$, which is the minimum value of spin for which tensor structures can exist; consequently, the quantum features appear with special clarity for this case.

Note that two different approaches are used in the course of these calculations, both of which are applicable to the description of spin structures with tensor-vector order parameters: a quasiparticle approach based on the generalized Maleev-Dyson transformation,[1] and a diagrammatic technique based on Wick's theorem for Hubbard operators, with a view to comparing these results. (Specifically, in this paper we set up a low-temperature variant of the diagrammatic technique for Hubbard operators which is close to the standard technique used for Bose systems.[2]) Both approaches imply a prior transition to local coordinates, because the simple connection between the Hubbard operators and the Bose systems proposed in Ref. 1, and also Wick's theorem for the Hubbard operators, hold only in these coordinates.

2. HAMILTONIAN

The concept of local coordinates for a system with tensor interactions and the technique for transforming to them are described in detail in Ref. 1. It was shown there that when investigating the nonmagnetic phase of a magnetic insulator described by the Hamiltonian (1), the local coordinates coincide with the original coordinates. Therefore we can use the connection between spin operators and Hubbard operators which obtains in local coordinates, and which for $S=1$ takes the form:

$$S^z=X^{11}-X^{-1-1}, \quad S^+=-(X^{10}+X^{0-1}), \quad S^-=-(S^+)^+,$$

$$O_2^0=(S^z)^2-{}^2/_3, \quad O_2^1=X^{10}-X^{0-1},$$

$$O_2^2=X^{1-1}, \quad O_2^{-m}=(-1)^m(O_2^m)^+, \tag{2}$$

and substitute them into (1), to obtain the required Hamiltonian in local coordinates in terms of Hubbard operators:

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$$\tilde{\mathcal{H}} = y_a \sum_i X_i^{-1-1} X_i^{0-1} + y_b \sum_i X_i^{10} X_i^{01} + \sum_{ij} \{ V_{ij}^{bb} X_i^{10} X_j^{01} + V_{ij}^{aa} X_i^{-1-1} X_j^{0-1} + V_{ij}^{ab} X_i^{10} X_j^{-1-1} + V_{ij}^{ba} X_i^{01} X_j^{0-1} + V_{ij}^{zz} (X_i^{11} - X_i^{-1-1}) (X_j^{11} - X_j^{-1-1}) \},$$

$$V_{ij}^{aa} = V_{ij}^{bb} = V_{ij}^{ab} = V_{ij}^{ba} = 2V_{ij}^{zz} = -J_{ij}, \quad y_{a,b} = D \mp h. \tag{3}$$

3. LOW-TEMPERATURE MODIFICATION OF THE DIAGRAMMATIC TECHNIQUE FOR HUBBARD OPERATORS

A. Rules for the diagram technique

It is well-known that in the presence of tensor interactions, in particular SIA, Wick's theorem for spin operators—which lies at the base of the Vaks-Larkin-Pikin (VLP) technique—does not hold; however, an analogous theorem holds for Hubbard operators under the condition that the Hamiltonian of the system can be written in local coordinates. The diagrammatic technique of Refs. 3,4 is based on this modified Wick's theorem.

In the low-temperature limit, the diagrammatic technique for Hubbard operators can be simplified and is close to the diagrammatic technique for Bose systems.[2] Just as in the low-temperature variant of the technique for spin operators,[5] this simplification is possible because the contribution from diagrams containing disconnected elements in blocks is found to be exponentially small at low temperatures, and we need take into account only diagrams containing Green's function lines which are continuously linked with each other. The difference lies in the fact that these Green's functions are defined by Hubbard operators and not by spin operators. In what follows, the following matrix Green's function will be important:

$$\hat{G}(l, \tau; l', \tau') = \begin{pmatrix} G_{aa} & G_{ab} \\ G_{ba} & G_{bb} \end{pmatrix} \tag{4}$$

with components

$$G_{aa}(l, \tau; l', \tau') = \langle T X_l^{-1-1}(\tau) X_{l'}^{0-1}(\tau') \rangle,$$
$$G_{ab}(l, \tau; l', \tau') = \langle T X_l^{-1-1}(\tau) X_{l'}^{10}(\tau') \rangle,$$
$$G_{ba}(l, \tau; l', \tau') = \langle T X_l^{01}(\tau) X_{l'}^{0-1}(\tau') \rangle,$$
$$G_{bb}(l, \tau; l', \tau') = \langle T X_l^{01}(\tau) X_{l'}^{10}(\tau') \rangle. \tag{5}$$

In zero-order approximation its Fourier transform equals

$$\hat{G}^{(0)}(\mathbf{k}, \omega_n) = \begin{pmatrix} b_a K_{aa}^{(0)} & 0 \\ 0 & b_b K_{bb}^{(0)} \end{pmatrix}, \tag{6}$$

where

$$K_{\mu\mu}^{(0)} = [\beta(y_\mu - i\omega_n)]^{-1} \quad (\beta = 1/k_B T),$$

$$b_a = \langle X^{-1-1} - X^{00} \rangle_0, \quad b_b = \langle X^{00} - X^{11} \rangle_0. \tag{7}$$

There are also different diagrams of vertex-block type which in the present case are determined by pairing of the Hubbard operators.

On the whole, the topology of diagrams and general rules of the diagrammatic technique are found to be close to those for the low-temperature modification of the VLP technique. These rules are as follows:

1. Each diagram is made up of lines corresponding to the Green's function (7) linked continuously with each other and included in a block.

2. A factor b_a or b_b is associated with the block, depending on the subscript of the Green's functions standing at the right end of the link.

3. Within the block all the lines are "thick," i.e., each bare Green's function, as determined by Eqs. (7), is replaced by a spin-wave function. The equations for the Green's function in the spin-wave approximation take the form

$$K_{aa}(\mathbf{k}, \omega_n) = u_\mathbf{k}^2/[\beta(\omega_\mathbf{k}^- + i\omega_n)] + v_\mathbf{k}^2/[\beta(\omega_\mathbf{k}^+ - i\omega_n)],$$
$$K_{bb}(\mathbf{k}, \omega_n) = u_\mathbf{k}^2/[\beta(\omega_\mathbf{k}^+ - i\omega_n)] + v_\mathbf{k}^2/[\beta(\omega_\mathbf{k}^- + i\omega_n)],$$
$$K_{ab}(\mathbf{k}, \omega_n) = K_{ba}(\mathbf{k}, \omega_n) = u_\mathbf{k} v_\mathbf{k} \{1/[\beta(\omega_\mathbf{k}^- + i\omega_n)] + 1/[\beta(\omega_\mathbf{k}^+ - i\omega_n)]\}, \tag{8}$$

where the spin-wave frequencies and functions $u_\mathbf{k}$, $v_\mathbf{k}$ equal

$$\omega_\mathbf{k}^\pm = \varepsilon_\mathbf{k} \pm h = [D(D - 2J_\mathbf{k})]^{1/2} \pm h,$$
$$u_\mathbf{k}^2 = {}^1/_2[(D - J_\mathbf{k})/\varepsilon_\mathbf{k} + 1], \quad v_\mathbf{k}^2 = {}^1/_2[(D - J_\mathbf{k})/\varepsilon_\mathbf{k} - 1]. \tag{9}$$

they are obtained from the relation between the Green's function $\hat{G}(\mathbf{k}, \omega_n)$ and Larkin's diagrams for the irreducible part of $\hat{\Sigma}(\mathbf{k}, \omega_n)$:

$$\hat{G}(\mathbf{k}, \omega_n) = \{\hat{I} - \hat{\Sigma}(\mathbf{k}, \omega_n)\hat{V}(\mathbf{k})\}^{-1}\hat{\Sigma}(\mathbf{k}, \omega_n), \tag{10}$$

The form of the interaction matrix is

$$\hat{V}(\mathbf{k}) = \begin{pmatrix} V^{aa} & V^{ab} \\ V^{ba} & V^{bb} \end{pmatrix}$$

[The potentials V^{aa}, V^{ab}, V^{ba}, V^{bb} are defined by Eq. (3)] and the zero-order approximation for $\hat{\Sigma}(\mathbf{k}, \omega_n)$:

$$\hat{\Sigma}^{(0)}(\mathbf{k}, \omega_n) = \hat{G}^{(0)}(\mathbf{k}, \omega_n).$$

In this case, we introduce through the relations

$$\begin{pmatrix} G_{aa} & G_{ab} \\ G_{ba} & G_{bb} \end{pmatrix} = \begin{pmatrix} K_{aa} & K_{ab} \\ K_{ba} & K_{bb} \end{pmatrix} \begin{pmatrix} b_a & 0 \\ 0 & b_b \end{pmatrix} \tag{11}$$

the Green's function $K_{\mu\nu}$ defined without the factors b_a, b_b which are characteristic of the block as a whole. The Green's function (8) is represented by boldface continuous lines with subscripts μ, ν at their ends ($\mu, \nu = a, b$).

4. Wavy lines with subscripts denote the interactions $V^{\mu\nu}$ ($\mu\nu = a, b$) or V^{zz} as defined by the Hamiltonian (3).

5. The types of vertex blocks are detemined by all possible pairings in the SU(3) algebra. There are three types of vertices: vertices with one entering or leaving line, vertices in which two lines intersect and finally vertices in which three lines intersect. Since the internal vertices, i.e., vertices of the latter two types, are always linked by interaction lines in the low-temperature technique, by indicating the subscripts of the latter we simultaneously and unequivocally indicate the types of operators corresponding to a given internal vertex. The type of operator corresponding to an external vertex is determined by the Green's function subscript.

6. A factor of 2 goes with vertices in which three Green's functions of the same type ($\mu = \nu = \nu'$) converge,

while for all the others this factor is 1.

7. For low T the relations $b_a \approx -1$, $b_b \approx 1$ are approximately valid.

B. Green's function and polarization operator in the Born approximation

Taking into account the quasiparticle interactions leads to a renormalization of the Green's function $\hat{\tilde{K}}(\mathbf{k},\omega_n)$, defined as usual by the Dyson equation

$$\hat{\tilde{K}}=\hat{K}+\hat{K}\hat{\Pi}\hat{\tilde{K}},$$

where $\hat{K}$ is the matrix of the unperturbed spin-wave Green's function (8), and $\hat{\Pi}$ is the matrix polarization operator whose components $\Pi_{\mu\nu}$ are described as usual by graphs which cannot be divided along a single spin-wave line, and which have entering vertices of type μ and exiting vertices of type ν. The solution to the Dyson equation is

$$\hat{\tilde{K}}^{-1}=\hat{K}^{-1}-\hat{\Pi}. \tag{12}$$

The explicit form of the graphs for components of the polarization operator Π_{aa}, Π_{ab} in Born approximation is shown in Fig. 1. To it correspond the analytic expressions

$$\frac{\Pi_{aa}(\mathbf{k})}{\beta}=-\frac{1}{N}\sum_{\mathbf{p}}\{[2(J_{\mathbf{k}}+J_{\mathbf{p}})-(J_0+J_{\mathbf{k}-\mathbf{p}})]n_{\mathbf{p}}$$
$$+(J_{\mathbf{k}}+J_{\mathbf{p}}+J_0)N_{\mathbf{p}}+3J_{\mathbf{p}}\mu_{\mathbf{p}}\},$$
$$\frac{\Pi_{ab}(\mathbf{k})}{\beta}=-\frac{1}{N}\sum_{\mathbf{p}}\{(J_{\mathbf{k}}+J_{\mathbf{p}})N_{\mathbf{p}}+(J_{\mathbf{p}}+2J_{\mathbf{k}})n_{\mathbf{p}}+(2J_{\mathbf{p}}+J_{\mathbf{k}-\mathbf{p}})\mu_{\mathbf{p}}\}. \tag{13}$$

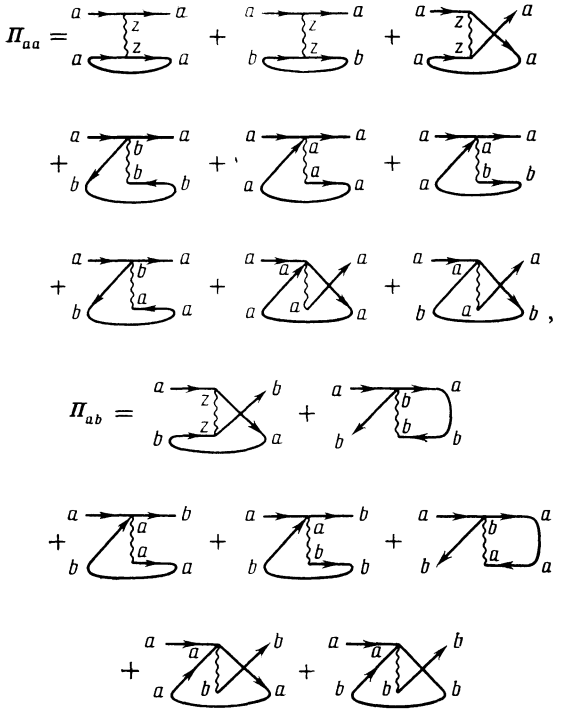

FIG. 1. Graphical representation of components of the polarization operator in Born approximation.

The equations for Π_{bb} and Π_{ba} are easily obtained from the equations for Π_{aa} and Π_{ab} respectively by replacing the subscript a by the subscript b and conversely. The correlation functions entering into (13) are defined by the relations

$$n_{\mathbf{p}}=\lim_{\tau\to 0^-}\sum_{\omega_n}K_{aa}(\mathbf{p},\omega_n)e^{i\omega_n\tau},\qquad N_{\mathbf{p}}=\lim_{\tau\to 0^+}\sum_{\omega_n}K_{bb}(\mathbf{p},\omega_n)e^{i\omega_n\tau},$$
$$\mu_{\mathbf{p}}=\lim_{\tau\to 0^-}\sum_{\omega_n}K_{ab}(\mathbf{p},\omega_n)e^{i\omega_n\tau}=\lim_{\tau\to 0^+}\sum_{\omega_n}K_{ba}(\mathbf{p},\omega_n)e^{i\omega_n\tau} \tag{14}$$

and equal

$$n_{\mathbf{p}}=u_{\mathbf{p}}^2n(\omega_{\mathbf{p}}^-)+v_{\mathbf{p}}^2n(\omega_{\mathbf{p}}^+)+v_{\mathbf{p}}^2,$$
$$N_{\mathbf{p}}=u_{\mathbf{p}}^2n(\omega_{\mathbf{p}}^+)+v_{\mathbf{p}}^2n(\omega_{\mathbf{p}}^-)+v_{\mathbf{p}}^2,$$
$$\mu_{\mathbf{p}}=u_{\mathbf{p}}v_{\mathbf{p}}[1+n(\omega_{\mathbf{p}}^+)+n(\omega_{\mathbf{p}}^-)],\quad n(\omega_{\mathbf{p}}^{\pm})=[\exp(\beta\omega_{\mathbf{p}}^{\pm})-1]^{-1} \tag{15}$$

C. Spectrum of collective excitations, critical field and criterion for ferromagnetism in Born approximation

The spectrum of collective excitations renormalized by the Born approximation is determined by the zeroes of the function $\hat{\tilde{K}}^{-1}$, which is related to the polarization operator by Eq. (12), or in explicit form by the equation

$$\tilde{\omega}_{\mathbf{k}}^{\pm}=\Big\{D(D-2J_{\mathbf{k}})-D\frac{1}{2\beta}(\Pi_{aa}+\Pi_{bb})(\mathbf{k})+J_{\mathbf{k}}\frac{1}{2\beta}(\Pi_{aa}+\Pi_{bb}$$
$$-\Pi_{ab}-\Pi_{ba})(\mathbf{k})\Big\}^{1/2}\pm\Big\{h-\frac{1}{\beta}\frac{1}{2}(\Pi_{aa}-\Pi_{bb})(\mathbf{k})\Big\}. \tag{16}$$

Substituting the values of the components of the polarization operator, we obtain explicit expressions for the two branches of the spectrum in the Born approximation, which we write out in the limit of small quasimomentum:

$$\frac{\tilde{\omega}_{\mathbf{k}}^{\pm}}{D}=\Big\{\bar{H}_{c1}^{\,2}(0)+\delta^{(1)}H_{c1}(T)+\frac{\bar{A}}{\xi}(1-\gamma_{\mathbf{k}})\Big\}^{1/2}$$
$$\pm\{H-\delta^{(2)}H_{c1}(T)\}. \tag{17}$$

The constants entering into (17) equal

$$\bar{H}_{c1}^{\,2}(0)=H_{c1}^{\,2}+\delta(\xi)/\xi,$$
$$H_{c1}^{\,2}=1-\frac{1}{\xi},\qquad \delta(\xi)=\frac{1}{N}\sum_{\mathbf{p}}[(3+2\gamma_{\mathbf{p}})v_{\mathbf{p}}^2+3\gamma_{\mathbf{p}}u_{\mathbf{p}}v_{\mathbf{p}}]; \tag{18}$$

$$\delta^{(1)}H_{c1}(T)=\frac{1}{2\xi}\frac{1}{N}\sum_{\mathbf{p}}\{(3+2\gamma_{\mathbf{p}})(u_{\mathbf{p}}^2+v_{\mathbf{p}}^2)+6\gamma_{\mathbf{p}}u_{\mathbf{p}}v_{\mathbf{p}}\}$$
$$\cdot\{n(\omega_{\mathbf{p}}^+)+n(\omega_{\mathbf{p}}^-)\},$$

$$\delta^{(2)}H_{c1}(T)=\frac{1}{4\xi}\frac{1}{N}\sum_{\mathbf{p}}\{n(\omega_{\mathbf{p}}^{+})-n(\omega_{\mathbf{p}}^{-})\}, \tag{19}$$

$$\bar{A}=1+\delta A(0)+\delta A(T),$$

$$\delta A(0)=-\frac{1}{N}\sum_{\mathbf{p}}\{(3-\gamma_{\mathbf{p}})v_{\mathbf{p}}^{2}+u_{\mathbf{p}}v_{\mathbf{p}}\},$$

$$\delta A(T)=-\frac{1}{N}\sum_{\mathbf{p}}\left\{\frac{1}{2}(3-\gamma_{\mathbf{p}})(u_{\mathbf{p}}^{2}+v_{\mathbf{p}}^{2})+u_{\mathbf{p}}v_{\mathbf{p}}\right\}$$

$$\cdot\{n(\omega_{\mathbf{p}}^{+})+n(\omega_{\mathbf{p}}^{-})\},$$

The remaining symbols are: $\gamma_{\mathbf{k}}=J_{\mathbf{k}}/J_0$, $H+h/D$. The meaning of the notations in Eq. (17) becomes clear if we note that the condition for softening of the frequency $\omega_{\mathbf{k}}^{-}$ for $\mathbf{k}=0$ determines the line of critical fields:

$$\tilde{H}_{c1}(T)=\{\tilde{H}_{c1}^{2}(0)+\delta^{(1)}H_{c1}(T)\}^{1/2}+\delta^{(2)}H_{c1}(T) \tag{20}$$

i.e., a line of second-order orientational phase transitions (OPTs) from the nonmagnetic phase to the angular ferromagnetic ($FM_<$) phase (see Fig. 2).

The numerical value of the correction $\delta(\xi)$ to the bare critical field H_{c1} at $T=0$ depends on a single parameter ξ, which decreases monotonically as ξ grows on the interval (ξ_{cr}, ∞). The bare value ξ_{cr} is $\xi_{cr}^{(0)}=1$. Since $\delta(\infty)=0$, and $\delta(1)$, which we have calculated for a simple cubic (SC) lattice, equals

$$\delta(1)=0.261, \tag{21}$$

we obtain the upper and lower estimates $0\leqslant\delta(\xi)\leqslant 0.261$.

The value (21) allows us to determine more accurately the value of ξ_{cr} itself in Born approximation. In fact, according to (18) and the condition $\tilde{H}_{c1}(0)=0$ for $\xi=\xi_{cr}$, we have

$$\xi_{cr}=1-\delta(\xi_{cr}). \tag{22}$$

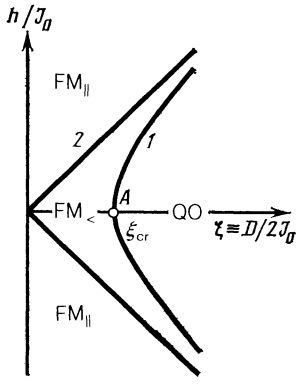

FIG. 2. Phase diagram at $T=0$. 1—second-order OPT line $h=\tilde{h}_{c1}(0)$ between the nonmagnetic QO phase and the $FM_<$ phase, as described by Eq. (18) ($\tilde{h}_{c1}(0)\equiv D\tilde{H}_{c1}(0)$), 2—the second-order OPT line $h=\tilde{h}_{c2}(0)$ between the angular and collinear ($FM_\parallel$) ferromagnetic phases, described by the equation $\tilde{h}_{c2}/J_0=2\xi$, see Ref. 1 ($\tilde{h}_{c2}(0)=h_{c2}(0)$). A is the multicritical point with coordinates $(0, \xi_{cr})$.

Using estimate (21) at $\xi=\xi_{cr}^{(0)}$, we obtain the Born approximation value

$$\xi_{cr}=0.739, \tag{23}$$

a value which differs considerably from the bare ξ_{cr}. We must then ask how accurate this value is; a discussion of this question will be presented in Sec. 4.

Let us note that the value of ξ_{cr} is an important characteristic of the system. First of all, it constitutes a more precise criterion for ferromagnetism, i.e., it is the value of $\xi=D/2J_0$ above which ferromagnetism is absent all the way down to $T=0$ (in the absence of an external field). Secondly, this quantity determines the critical point of the phase diagram (point A of Fig. 2), i.e., the point of nonanalyticity of the spectrum at $k=0$, $T=0$.

In point of fact, it follows from (17) that at the point where $\tilde{H}_{c1}(0)=0$ the dispersion law of the soft mode is linear in k for small k, whereas at the other points on the phase line, say, point 1 where $\tilde{H}_{c1}(0)\neq 0$, it is quadratic in k as $k\to 0$. (The nonanalyticity of the spectrum leads, e.g., to the fact that the values of such quasiparticle characteristics as the sound velocity, scattering amplitude etc. depend at this point on the order in which the limits $k\to 0$, $\Delta\xi=\xi_{cr}-\xi\to 0$ are taken; this question will be discussed in detail in Sec. 4.) What is important for us now is that the different qualitative character of the dispersion law for $H_{c1}-H\ll ak\ll H_{c1}$ and $H_{c1}\ll ak\ll +1$ determines the different character of the thermal corrections to the spectrum and the critical field in the two limiting cases: for $\theta\gg H_{c1}$, where they equal

$$\delta^{(1)}H_{c1}(T)=\theta^{2}\left(\frac{\alpha}{\xi}\right)^{-1/2}\zeta(2)\left(5-\frac{1}{\xi}\right)\Big/4\xi\pi^{2}\quad\left(\theta\equiv\frac{k_{B}T}{D}\right),$$
$$\delta^{(2)}H_{c1}(T)=-H\theta^{2}\left(\frac{\alpha}{\xi}\right)^{-1/2}\zeta(2)/2\xi\pi^{2}, \tag{24}$$
$$\delta A(T)=-\theta^{2}\left(\frac{\alpha}{\xi}\right)^{-1/2}\zeta(2)\left(1-\frac{1}{4\xi}\right)\Big/\pi^{2},$$

and for $H_{c1}-H\ll\theta\ll H_{c1}$, where Eqs. (17) reduce to

$$\tilde{\omega}_{\mathbf{k}}^{\pm}/D=\bar{\Delta}^{\pm}+(\bar{A}/2\xi H_{c1})(1-\gamma_{\mathbf{k}}),$$
$$\bar{\Delta}^{\pm}=H_{c1}\pm H+\delta(\xi)/2\xi H_{c1}+\delta\Delta^{\pm}(T) \tag{25}$$

and $\delta\Delta^{-}(T)$, $\Delta A(T)$ equal

$$\delta\Delta^{-}(T)=(2\xi\theta/\alpha)^{1/2}(H_{c1})^{-1/2}\Gamma(3/2)\zeta(3/2)/4\xi\pi^{2},$$
$$\delta A(T)=-(2\xi\theta/\alpha)^{1/2}(H_{c1})^{1/2}\left(1-\frac{1}{4\xi}\right)\Gamma(3/2)\zeta(3/2)/4\pi^{2} \tag{26}$$

($\zeta(p)$ is the Riemann zeta function, $\alpha=(1-\delta_{\mathbf{k}})/k^{2}$). For all the remaining cases the thermal corrections are exponentially small in T.

It also follows from (24), (26), and (20) that far from the point A the thermal corrections to the critical field are $\sim T^{3/2}$, whereas near this point we have

$$\tilde{H}_{c1}(T)\sim T. \tag{27}$$

D. Born corrections to the free energy and thermodynamic functions

The basic spin wave corrections to the free energy are given by closed-loop graphs, with which is associated the

standard expression for the free energy of noninteracting quasiparticles

$$\beta F^{\text{c-B}} = \sum_{\mathbf{k}\mu} \ln[1 - \exp(-\beta\omega_{\mathbf{k}}^{\mu})].$$

The correction due to interaction in the first Born approximation is determined by the diagrams from Fig. 3. The corresponding analytic expression is conveniently represented using the components of the polarization operator (13):

$$\Delta F_{int} = -\frac{1}{\beta N}\sum_{\mathbf{k}} \{\Pi_{aa}(\mathbf{k})n_{\mathbf{k}} + \Pi_{bb}(\mathbf{k})N_{\mathbf{k}} + [\Pi_{ab}(\mathbf{k}) + \Pi_{ba}(\mathbf{k})]\mu_{\mathbf{k}}\}$$

$$= \Delta F(0) + \Delta F(T). \tag{28}$$

For the temperature-independent corrections we obtain the equation

$$\Delta F(0) = \frac{2}{N^2}\sum_{\mathbf{kp}} \{[3(J_{\mathbf{k}}+J_{\mathbf{p}}) - J_{\mathbf{k}-\mathbf{p}}]v_{\mathbf{k}}^2 v_{\mathbf{p}}^2 + (2J_{\mathbf{p}}+J_{\mathbf{k}-\mathbf{p}})u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{p}}v_{\mathbf{p}} + 2u_{\mathbf{k}}v_{\mathbf{k}}v_{\mathbf{p}}^2(3J_{\mathbf{k}}+J_{\mathbf{p}})\}, \tag{29}$$

and for the temperature-dependent corrections the equation

$$\Delta F(T) = -\frac{1}{\beta N^2}\sum_{\mathbf{kp}} \{\Gamma_0^{\alpha\alpha}(\mathbf{k},\mathbf{p})n(\omega_{\mathbf{k}}^{\alpha})n(\omega_{\mathbf{p}}^{\alpha}) + \Gamma_0^{\beta\beta}(\mathbf{k},\mathbf{p})n(\omega_{\mathbf{k}}^{\beta})n(\omega_{\mathbf{p}}^{\beta}) + \Gamma_0^{\alpha\beta}(\mathbf{k},\mathbf{p})[n(\omega_{\mathbf{k}}^{\alpha})n(\omega_{\mathbf{p}}^{\beta}) + n(\omega_{\mathbf{k}}^{\beta})n(\omega_{\mathbf{p}}^{\alpha})]\}, \tag{30}$$

where

$$-\frac{1}{\beta}\Gamma_0^{\alpha\alpha}(\mathbf{k},\mathbf{p}) = -\frac{1}{\beta}\Gamma_0^{\beta\beta}(\mathbf{k},\mathbf{p}) = [2(J_{\mathbf{k}}+J_{\mathbf{p}}) - (J_0+J_{\mathbf{k}-\mathbf{p}})]$$
$$\cdot(u_{\mathbf{k}}^2u_{\mathbf{p}}^2 + v_{\mathbf{k}}^2v_{\mathbf{p}}^2) + (J_{\mathbf{k}}+J_{\mathbf{p}}+J_0)(v_{\mathbf{k}}^2u_{\mathbf{p}}^2 + u_{\mathbf{k}}^2v_{\mathbf{p}}^2)$$
$$+(3J_{\mathbf{k}}+J_{\mathbf{p}})u_{\mathbf{k}}v_{\mathbf{k}}(u_{\mathbf{p}}^2+v_{\mathbf{p}}^2)$$
$$+(3J_{\mathbf{p}}+J_{\mathbf{k}})u_{\mathbf{p}}v_{\mathbf{p}}(u_{\mathbf{k}}^2+v_{\mathbf{k}}^2) + 2(J_{\mathbf{k}-\mathbf{p}}+J_{\mathbf{k}}+J_{\mathbf{p}})u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{p}}v_{\mathbf{p}}, \tag{31}$$

while the expression for $\Gamma_0^{\alpha,\beta}(\mathbf{k},\mathbf{p})$ differs from (31) by the replacement $u_{\mathbf{p}} \to v_{\mathbf{p}}$, $v_{\mathbf{p}} \to u_{\mathbf{p}}$.

An explicit calculation of the temperature correction $\Delta F(T)$ gives for $H_{c1} \gg \theta$,

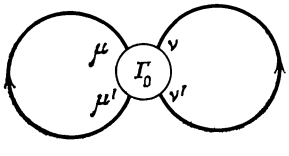

FIG. 3. Graph for the correction to the free energy due to interactions of the collective excitations (Born approximation).

$$\Delta F(T) = J_0\left(\frac{2\xi\theta}{\alpha}\right)^3 H_{c1}\left(\frac{\Gamma(3/2)}{4\pi^2}\right)^2 Z_{\eta_2}^2\left(\frac{H_{c1}-H}{\theta}\right) \cdot\left(Z_p(x) \equiv \sum_{n=1}^{\infty} n^{-p}e^{-nx}\right) \tag{32}$$

while for $H_{c1} \ll \theta$,

$$\Delta F(T) = J_0\theta^4(5-1/\xi)(\alpha/\xi)^{-3}(\zeta(2)/2\pi^2)^2. \tag{33}$$

In the same way, for the anharmonic corrections to the magnetization and spin-induced specific heat—which are related to the free energy by the relations $M_z = \partial F/\partial h$, $C_s = -T\partial^2 F/\partial T^2$—we obtain for $H_{c1} \gg \theta$

$$\delta M_z = -2J_0\theta^2(\alpha/2\xi)^{-3}H_{c1}(\Gamma(3/2)/4\pi^2)^2 Z_{3/2}(x)Z_{1/2}(x), \tag{34}$$
$$\delta C_s = -6J_0\theta^2(\alpha/2\xi)^{-3}H_{c1}(k_B/D)(\Gamma(3/2)/4\pi^2)^2 \cdot\{Z_{\eta_2}^2(x) + 2xZ_{\eta_2}(x)Z_{\eta_2}(x) + {}^1/_3x^2[Z_{1/2}^2(x) + Z_{\eta_2}(x)Z_{-1/2}(x)]\},$$
$$x \equiv (H_{c1}-H)/\theta$$

and for $H_{c1} \ll \theta$

$$\delta M_z = a_1T^2, \quad a_1 = -H\left[\zeta(0) + \frac{\pi}{2}\frac{\theta}{(H_{c1}^2-H^2)^{1/2}}\right]\left(\frac{\alpha}{\xi}\right)^{-3}\frac{1}{2\xi} \cdot\frac{\zeta(2)}{4\pi^4}\left(\frac{k_B}{D}\right)^2\left(5-\frac{1}{\xi}\right), \tag{35}$$
$$\delta C_s = b_1T^3, \quad b_1 = -12J_0\left(\frac{\alpha}{\xi}\right)^{-3}\left(\frac{\zeta(2)}{2\pi^2}\right)^2\left(\frac{k_B}{D}\right)^4\left(5-\frac{1}{\xi}\right)$$

In the limit $H_{c1} - H \ll \theta \ll H_{c1}$, we obtain from (34)

$$\delta M_z = a_2T^{5/2}, \quad a_2 = -\frac{1}{\xi}\frac{H_{c1}}{(H_{c1}-H)^{1/2}}\Gamma(1/2)\zeta(3/2)\left(\frac{\alpha}{2\xi}\right)^{-3} \cdot\left(\frac{\Gamma(3/2)}{4\pi^2}\right)^2\left(\frac{k_B}{D}\right)^{5/2}, \tag{36}$$
$$\delta C_s = b_2T^2, \quad b_2 = -6J_0H_{c1}\left(\frac{\alpha}{2\xi}\right)^{-3}\left(\frac{\Gamma(3/2)\zeta(3/2)}{4\pi^2}\right)^2\left(\frac{k_B}{D}\right)^3.$$

In comparing Eqs. (35), (36) with the results of Ref. 1, we note that the characteristics of the temperature dependence of the Born and spin-wave corrections to the magnetization, susceptibility and specific heat are the same in the limit $H_{c1} \ll \theta$, but for $H_{c1} - H \ll \theta \ll H_{c1}$ they differ qualitatively. It is interesting that in the latter case the Born correction to the specific heat is found to vary as an integer power of T, which allows us to observe its contribution experimentally against the background of the half-integral powers of the spin-wave results.

We note that formally the Born correction $\delta M_z(T)$ goes to infinity at the OPT point $H = H_{c1}$. However, this result must not be understood literally, because in the immediate vicinity of a second-unit OPT point our perturbation-theory calculation becomes inapplicable; it only points up the strengthened role of anharmonicity in the present case.[1)]

As for the actual behavior of the system in the fluctuation region, we can say the following: it is well-known that for arbitrarily small but finite T, in the immediate vicinity of the OPT point the quantum system behaves classically.[7] Correspondingly, in our case within this region we will have scaling behavior characteristic of the three-dimensional classical XY model.

To conclude this section, we note that the quantities $\Gamma_0^{\alpha\alpha}(\mathbf{k},\mathbf{p})$, $\Gamma_0^{\beta\beta}(\mathbf{k},\mathbf{p})$, $\Gamma_0^{\alpha\beta}(\mathbf{k},\mathbf{p})$ entering into (30) have the meaning of forward scattering amplitudes of α- and β-quasiparticles. (Beginning at this point in the article, we will transform the notation $\omega_{\mathbf{k}}^{-}\to\omega_{\mathbf{k}}^{\alpha}$, $\omega_{\mathbf{k}}^{+}\to\omega_{\mathbf{k}}^{\beta}$.) In the long-wavelength limit they equal

$$-\frac{1}{\beta}\Gamma_0^{\mu\nu}(\mathbf{k},\mathbf{p})=\frac{J_0}{2}\frac{5-1/\xi}{(H_{c1}^2+(1-\gamma_{\mathbf{k}})/\xi)^{1/2}(H_{c1}^2+(1-\gamma_{\mathbf{p}})/\xi)^{1/2}}\mp\frac{J_0}{2}\qquad(\mu,\nu=\alpha,\beta)\tag{37}$$

(The upper sign refers to the case $\mu=\nu$, the lower to $\mu\neq\nu$.) We will say more about scattering amplitudes in the following section, where an alternate method will be used in the investigation—the quasiparticle formalism. In this section we will also present an investigation of the ground state which is more accurate than the Born approximation, and compare the results of the two different approaches used.

4. QUASIPARTICLE FORMALISM

As usual, for low T the original spin Hamiltonian can be reduced to an effective Hamiltonian for interacting Bose particles. In order to do this, we must use a transformation from spin to Bose operators, which in the case of systems with tensor interactions is implemented by using the generalized Maleev-Dyson transformation presented in Ref. 1. It consists of a transformation to local coordinates and from them to Hubbard operators, and the introduction of Bose operators into the latter according to the equations

$$\begin{aligned}&X^{10}=b^+(1-a^+a-b^+b),\quad X^{01}=b,\\&X^{-10}=a^+(1-a^+a-b^+b),\quad X^{0-1}=a,\\&X^{1-1}=b^+a,\ X^{-11}=a^+b,\ X^{11}=b^+b,\ X^{-1-1}=a^+a.\end{aligned}\tag{38}$$

Substituting (38) into (3) and passing to momentum space, we obtain

$$\mathcal{H}=\mathcal{H}_2+\mathcal{H}_4+\mathcal{H}_6,\tag{39}$$

$$\mathcal{H}_2=\sum_{\mathbf{k}}\{(D-h-J_{\mathbf{k}})a_{\mathbf{k}}^+a_{\mathbf{k}}+(D+h-J_{\mathbf{k}})b_{\mathbf{k}}^+b_{\mathbf{k}}-J_{\mathbf{k}}(a_{\mathbf{k}}^+b_{-\mathbf{k}}^++b_{-\mathbf{k}}a_{\mathbf{k}})\},\tag{40}$$

$$\begin{aligned}\mathcal{H}_4=\sum_{\mathbf{kpq}\varkappa}\Big\{\Big[&\frac{1}{2}J_{\mathbf{p}-\mathbf{k}}(a_{\mathbf{k}}^+b_{\mathbf{q}}^+a_{\mathbf{p}}b_{\varkappa}+b_{\mathbf{k}}^+a_{\mathbf{q}}^+b_{\mathbf{p}}a_{\varkappa}-b_{\mathbf{k}}^+b_{\mathbf{q}}^+b_{\mathbf{p}}b_{\varkappa}-a_{\mathbf{k}}^+a_{\mathbf{q}}^+a_{\mathbf{p}}a_{\varkappa})\\&+J_{\varkappa}(a_{\mathbf{k}}^+a_{\mathbf{q}}^+a_{\mathbf{p}}a_{\varkappa}+b_{\mathbf{k}}^+b_{\mathbf{q}}^+b_{\mathbf{p}}b_{\varkappa}+a_{\mathbf{k}}^+b_{\mathbf{q}}^+b_{\mathbf{p}}a_{\varkappa}\\&+b_{\mathbf{k}}^+a_{\mathbf{q}}^+a_{\mathbf{p}}b_{\varkappa})\Big]\delta(\mathbf{k}+\mathbf{q}-\mathbf{p}-\varkappa)\\&+J_{\varkappa}(a_{\varkappa}^+b_{\mathbf{k}}^+a_{\mathbf{q}}^+a_{\mathbf{p}}+a_{\varkappa}^+b_{\mathbf{k}}^+b_{\mathbf{q}}^+b_{\mathbf{p}}+b_{\varkappa}^+a_{\mathbf{k}}^+a_{\mathbf{q}}^+a_{\mathbf{p}}\\&+b_{\varkappa}^+a_{\mathbf{k}}^+b_{\mathbf{q}}^+b_{\mathbf{p}})\delta(\mathbf{k}+\mathbf{q}+\varkappa-\mathbf{p})\Big\},\end{aligned}\tag{41}$$

$$\begin{aligned}\mathcal{H}_6=\sum_{\substack{\mathbf{kpqs}\\\mathbf{lm}}}\{&-J_{\mathbf{q}+\mathbf{s}-\mathbf{m}}(b_{\mathbf{k}}^+a_{\mathbf{p}}^+a_{\mathbf{q}}^+a_{\mathbf{s}}^+a_{\mathbf{l}}a_{\mathbf{m}}+b_{\mathbf{k}}^+b_{\mathbf{p}}^+a_{\mathbf{q}}^+b_{\mathbf{s}}^+b_{\mathbf{l}}b_{\mathbf{m}}\\&+b_{\mathbf{k}}^+a_{\mathbf{p}}^+a_{\mathbf{q}}^+b_{\mathbf{s}}^+a_{\mathbf{l}}b_{\mathbf{m}}+b_{\mathbf{k}}^+b_{\mathbf{p}}^+a_{\mathbf{q}}^+a_{\mathbf{s}}^+b_{\mathbf{l}}a_{\mathbf{m}})\delta(\mathbf{q}+\mathbf{s}+\mathbf{k}+\mathbf{p}-\mathbf{m}-\mathbf{l})\}.\end{aligned}\tag{42}$$

A. Ground state

In order to treat the ground state more precisely, it is convenient first of all to carry out the linear u-v transformation ($a_{\mathbf{k}}$, $b_{\mathbf{k}}\to\alpha_{\mathbf{k}}$, $\beta_{\mathbf{k}}$) so as to diagonalize the quadratic part of the Hamiltonian. In this procedure, the transformation coefficients are determined by the condition that the nondiagonal terms reduce to zero in the bare quadratic Hamiltonian $\mathcal{H}_2$. We can proceed more consistently by introducing a self-consistent transformation which takes into account the fact that after reducing the anharmonic terms to normal form there appear corrections to the quadratic part which themselves depend on the u-v transformation functions. By imposing the condition that the full Hamiltonian, not the bare quadratic Hamiltonian, be diagonalized, we obtain integral equations for the u-v transformation functions. Moreover, because the original Hamiltonian contained a finite number of anharmonic terms, we can thus determine these functions exactly.

What complicates things is the fact that the renormalized quadratic Hamiltonian is formally not self-adjoint. In particular, the coefficients of the Hermitian-conjugate terms $\alpha_{\mathbf{k}}\beta_{-\mathbf{k}}$ and $\beta_{-\mathbf{k}}^{+}\alpha_{\mathbf{k}}^{+}$ are found to be different, which prevents us from selecting conditions on the functions $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ which reduce the coefficients of both terms to zero at the same time.

The reason these coefficients are different is that transformations of Maleev-Dyson type from spin to Bose operators are non-Hermitian. It is easy to confirm that in order to exactly diagonalize the quadratic part with a linear u-v transformation it is necessary also to choose non-Hermitian transformations, i.e., to determine the relation between the original operators $a_{\mathbf{k}}$, $b_{\mathbf{k}}$ and the eigenoperators $\alpha_{\mathbf{k}}$, $\beta_{\mathbf{k}}$ for the collective excitations by the equations

$$\begin{aligned}&a_{\mathbf{k}}^+=u_{\mathbf{k}}\alpha_{\mathbf{k}}^++v_{\mathbf{k}}\beta_{\mathbf{k}},\quad a_{\mathbf{k}}=U_{\mathbf{k}}\alpha_{\mathbf{k}}+V_{\mathbf{k}}\beta_{\mathbf{k}}^+,\\&b_{-\mathbf{k}}^+=u_{\mathbf{k}}\beta_{\mathbf{k}}^++v_{\mathbf{k}}\alpha_{\mathbf{k}},\quad b_{-\mathbf{k}}=U_{\mathbf{k}}\beta_{\mathbf{k}}+V_{\mathbf{k}}\alpha_{\mathbf{k}}^+,\end{aligned}\tag{43}$$

without assuming that $u_{\mathbf{k}}=U_{\mathbf{k}}$, $v_{\mathbf{k}}=V_{\mathbf{k}}$. In order to obtain certain general relations, let us perform this transformation, assuming that the original Hamiltonian is of the form

$$\mathcal{H}_2=\sum_{\mathbf{k}}\{(\tilde{A}_{\mathbf{k}}-h)a_{\mathbf{k}}^+a_{\mathbf{k}}+(\tilde{A}_{\mathbf{k}}+h)b_{\mathbf{k}}^+b_{\mathbf{k}}+\tilde{B}_{\mathbf{k}}a_{\mathbf{k}}^+b_{-\mathbf{k}}^++\tilde{C}_{\mathbf{k}}b_{-\mathbf{k}}a_{\mathbf{k}}\}\tag{44}$$

while not yet specifying the form of $\tilde{A}_{\mathbf{k}}$, $\tilde{B}_{\mathbf{k}}$, and $\tilde{C}_{\mathbf{k}}$. After this transformation, we obtain

$$\begin{aligned}\tilde{\mathcal{H}}_2=\sum_{\mathbf{k}}\{&[\tilde{A}_{\mathbf{k}}(u_{\mathbf{k}}U_{\mathbf{k}}+v_{\mathbf{k}}V_{\mathbf{k}})+\tilde{B}_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}+\tilde{C}_{\mathbf{k}}U_{\mathbf{k}}V_{\mathbf{k}}](\alpha_{\mathbf{k}}^+\alpha_{\mathbf{k}}+\beta_{\mathbf{k}}^+\beta_{\mathbf{k}})\\&+h(\beta_{\mathbf{k}}^+\beta_{\mathbf{k}}-\alpha_{\mathbf{k}}^+\alpha_{\mathbf{k}})+(\tilde{A}_{\mathbf{k}}\cdot 2v_{\mathbf{k}}U_{\mathbf{k}}+\tilde{B}_{\mathbf{k}}v_{\mathbf{k}}^2+\tilde{C}_{\mathbf{k}}U_{\mathbf{k}}^2)\alpha_{\mathbf{k}}\beta_{-\mathbf{k}}\\&+(\tilde{A}_{\mathbf{k}}\cdot 2u_{\mathbf{k}}V_{\mathbf{k}}+\tilde{B}_{\mathbf{k}}u_{\mathbf{k}}^2+\tilde{C}_{\mathbf{k}}V_{\mathbf{k}}^2)\beta_{-\mathbf{k}}^+\alpha_{\mathbf{k}}^+\}.\end{aligned}\tag{45}$$

From the condition that the coefficients of the anomalous terms $\alpha_k\beta_{-k}$ and $\beta^{+}_{-k}\alpha^{+}_{k}$ reduce to zero, we obtain the equations

$$2\tilde{A}_k v_k U_k+\tilde{B}_k v_k^2+\tilde{C}_k U_k^2=0, \quad 2\tilde{A}_k u_k V_k+\tilde{B}_k u_k^2+\tilde{C}_k V_k^2=0, \tag{46}$$

and from the commutation relations the identity

$$u_k U_k-v_k V_k=1. \tag{47}$$

Eqs. (46), (47) allow us to determine the explicit relation between the spectrum of collective excitations, as well as the functions u_k, v_k, U_k, V_k, with the coefficients $\tilde{A}_k$, $\tilde{B}_k$, and $\tilde{C}_k$:

$$\tilde{\omega}_k^{\alpha,\beta}=\tilde{\varepsilon}_k\mp h=(\tilde{A}_k^2-\tilde{B}_k\tilde{C}_k)^{1/2}\mp h, \tag{48}$$

$$u_k U_k={}^1/_2(\tilde{A}_k/\tilde{\varepsilon}_k+1),\ u_k v_k=-{}^1/_2\tilde{C}_k/\tilde{\varepsilon}_k,$$
$$v_k V_k={}^1/_2(\tilde{A}_k/\tilde{\varepsilon}_k-1),\ U_k V_k=-{}^1/_2\tilde{B}_k/\tilde{\varepsilon}_k. \tag{49}$$

Let us turn now to the Hamiltonian (39)–(42). The bare quadratic part $\mathscr{H}_2$ has the form (40), where

$$A_k=D-J_k, \quad B_k=C_k=-J_k. \tag{50}$$

The Hamiltonian $\mathscr{H}_4$ has the form (41). Carrying out the transformation (43) on this Hamiltonian, followed by a reduction to normal ordering in the operators α_k, β_k, and isolating the quadratic part and comparing the result with the form (45), we obtain corrections to the coefficients A_k, B_k, and C_k:

$$A_k^{(4)}=\frac{1}{N}\sum_p\{u_p v_p(J_k+3J_p)+v_p V_p[3(J_k+J_p)-J_{k-p}]\}, \tag{51}$$

$$B_k^{(4)}=\frac{1}{N}\sum_p\{2v_p V_p(3J_k+2J_p)+U_p V_p(2J_p+J_{k-p})\},$$
$$C_k^{(4)}=\frac{1}{N}\sum_p\{u_p v_p(2J_k+J_{k-p})\}.$$

Proceeding in the same way with the Hamiltonian $\mathscr{H}_6$, we obtain

$$A_k^{(6)}=-\frac{1}{N^2}\sum_{pq}\{u_p v_p v_q V_q[3(J_k+3J_p)+3J_q+5J_{k+q+p}]\},$$

$$B_k^{(6)}=-\frac{1}{N^2}\sum_{pq}\{v_p V_p v_q V_q[3(3J_k+J_p)+3J_q+5J_{k+q+p}] \tag{52}$$
$$+2U_p V_p u_q v_q(J_p+3J_{k+q+p})\},$$

$$C_k^{(6)}=-\frac{1}{N^2}\sum_{pq}\{u_p v_p u_q v_q(J_k+3J_{k+q+p})\}.$$

The total values of the coefficients in the quadratic Hamiltonian equal

$$\tilde{A}_k=A_k+A_k^{(4)}+A_k^{(6)}, \quad \tilde{B}_k=B_k+B_k^{(4)}+B_k^{(6)},$$
$$\tilde{C}_k=C_k+C_k^{(4)}+C_k^{(6)}. \tag{53}$$

Thus, the renormalized excitation spectrum for $T=0$ is determined by Eq. (48) after substituting in (53). If in the course of these transformations we extract terms which do not depend on the operators α_k, β_k, we obtain an expression for the ground-state energy:

$$E_0=\Delta E_0^{(2)}+\Delta E_0^{(4)}+\Delta E_0^{(6)}, \tag{54}$$

$$\Delta E_0^{(2)}=\frac{1}{N}\sum_k\{2(D-J_k)v_k V_k-2J_k u_k v_k\},$$

$$\Delta E_0^{(4)}=\frac{2}{N^2}\sum_{kp}\{J_{k-p}(U_k V_k u_p v_p-v_k V_k v_p V_p)+2J_p(3v_k V_k v_p V_p$$
$$+U_k V_k u_p v_p+3v_k V_k u_p v_p+u_k v_k v_p V_p)\},$$

$$\Delta E_0^{(6)}=-\frac{3}{N^2}\sum_{kpq}\{(5J_{q-k-p}+9J_k+6J_p)u_k v_k v_p V_p v_q V_q$$
$$+(J_k+3J_{k+p+q})U_k V_k u_q v_q u_p v_p\}.$$

The functions u_k, v_k, U_k, V_k also determine corrections to the correlation functions for the spin and quadrupole operators at $T=0$. They can be obtained by using the connection between the spin and quadrupole operators and the operators a_k, b_k, after passing in accordance with (43) to the operators α_k, β_k and extracting the temperature-independent part. For example, the quantity $\Delta Q=Q-Q_0^{(0)}$ (where $Q_0=\langle 3(S^z)^2-2\rangle$ is the quadrupole order parameter[1]) characterizes the deviation of the ground state from a state with full quadrupole order $\langle S^\alpha\rangle=0$, $Q_0=-2$ due to the presence of zero-point energy of the oscillations; we obtain for this quantity

$$\frac{\Delta Q_0}{2}=\frac{1}{N}\sum_p 3v_p V_p. \tag{55}$$

It follows from (49) that the functions u_k, v_k, U_k, V_k themselves are determined by a system of three integral equations:

$$v_k V_k={}^1/_2(\tilde{A}_k/\tilde{\varepsilon}_k-1),\ u_k v_k=-\tilde{C}_k/2\tilde{\varepsilon}_k,\ U_k V_k=-\tilde{B}_k/2\tilde{\varepsilon}_k, \tag{56}$$

since all the parameters entering into the right side of (56) can be uniquely expressed in terms of the three independent combinations standing on the left side.

In view of the complicated form of the integral equations, it is expedient to solve them via an iterative method. The zero-order approximation obtained by using the unperturbed values A_k, B_k, and C_k from (50) yields functions which coincide with those given by (9). Using them, we can find more precise values in first approximation to the coefficients $\tilde{A}_k$, $\tilde{B}_k$, and $\tilde{C}_k$; these functions in turn determine the spectrum in first approximation via (48), and also by substituting into the right side of (56) the transformation functions (43) in second approximation. The iterative process is repeated until the desired accuracy is attained.

It is obvious that the computed results will depend on the parameter ξ. The maximum value of the anharmonic correction is attained for minimum ξ, i.e., for $\xi=\xi_{cr}$ (see Fig. 2). Mathematically this follows from the equations we have obtained; physically it corresponds to the increasingly important role of anharmonicity as we approach the multicritical point A. So as to estimate the upper bound of the corrections, let us carry out an explicit calculation for $\xi=\xi_{cr}$ (for a SC lattice), thereby obtaining a self-consistent value for ξ_{cr} itself.

Carrying out this calculation, we verify that the iteration process attains an adequate degree of convergence after only three steps. The result:

$$u_k v_k = 0{,}288\gamma_k \Big/ \frac{\varepsilon_k}{D}, \quad U_k V_k = (0.279\gamma_k - 0.039) \Big/ \frac{\varepsilon_k}{D},$$
$$2v_k V_k = (1{,}127 - 0.602\gamma_k) \Big/ \frac{\varepsilon_k}{D}, \tag{57}$$
$$\frac{\varepsilon_k}{D} = 1{,}11(1-\gamma_k)^{1/2}[1+0{,}03(1-\gamma_k)]^{1/2}$$

can be considered exact to three decimal places and used for further calculations based on the equations obtained in this paper, e.g., for numerical estimates of the ground-state energy, correlation functions etc.

In particular, we obtain the following criterion for ferromagnetism, along with an upper limit on the deviation of the ground state from the state of full quadrupole order

$$\xi_{cr} = 0.762, \quad (\Delta Q_0/2)^{max} \equiv \Delta Q_0(\xi_{cr})/2 = 0{,}055. \tag{58}$$

In conclusion, we note that if we use the zeroth-order approximation (9) in Eqs. (48)–(54) for the u-v transformation functions and then limit ourselves only to terms derived from $\mathscr{H}_4$ in these equations, we obtain exactly the results of the previous section for the $T = 0$ spectrum and the correction $\Delta F(0)$ to the free energy.

B. Thermal corrections and scattering amplitudes

Besides the terms quadratic in α_k, β_k investigated earlier, the Hamiltonian contains fourth- and sixth-order terms which describe quasiparticle scattering processes, e.g., $\tilde{\mathscr{H}}_4$ has the form

$$\tilde{\mathscr{H}}_4 = -\frac{1}{\beta}\sum_{kqpx}\{\Gamma_0^{\alpha\alpha}(x,k;p,q)\alpha_q^+\alpha_p^+\alpha_k\alpha_x + \Gamma_0^{\beta\beta}(x,k;p,q)\beta_q^+\beta_p^+\beta_k\beta_x + \Gamma_0^{\alpha\beta}(x,k;p,q)\alpha_q^+\beta_p^+\alpha_k\beta_x\} + \mathscr{H}_4', \tag{59}$$

where $\mathscr{H}_4'$ contains terms which do not preserve the number of quasiparticles. Without writing out the full expressions for the scattering amplitudes at arbitrary angles $\Gamma_0^{\alpha\alpha}(x,k;p,q)$, $\Gamma_0^{\beta\beta}((x,k;p,q)$, $\Gamma_0^{\alpha\beta}(x,k;p,q)$, we note that in the limit $x = p$, $k = q$, and also when using the zero-order approximation for the functions u_k, v_k, U_k, V_k, these functions lead to the Born-approximation forward-scattering amplitude (31):

$$\Gamma_0^{\mu\nu}(p,k;p,k) = \Gamma_0^{\mu\nu}(k,p) \quad (\mu,\nu = \alpha,\beta). \tag{60}$$

Correspondingly, by investigating fourth-order scattering processes in Born approximation we obtain thermal corrections to the spectrum, critical field, free energy, etc., which precisely coincide with the results obtained using the diagram technique. Taking into account 4-particle processes to higher order leads only to changes in the numerical coefficients in Eqs. (24)–(27), (32)–(36) without changing the character of the temperature dependence (except for the immediate vicinity of the OPT point $H = H_{c1}$). Taking into account 6-particle scattering processes leads to thermal corrections which are higher order in T.

Let us dwell on the behavior of the scattering amplitude in some detail. We remark that, as follows from (37), $\Gamma_0^{\mu\nu}(\mathbf{p},\mathbf{k};\mathbf{p},\mathbf{k}) \propto 1/kp$ at the point A (where $H_{c1} = 0$) and $\Gamma_0^{\mu\nu}(\mathbf{0},\mathbf{0};\mathbf{0},\mathbf{0}) =$ constant at all the remaining points on the line $H = H_{c1}$ (see Fig. 2). On the other hand, in the easy-plane phase (the $FM_<$ phase in the designation of Fig. 2, where the continuous symmetry of the Hamiltonian (1) relative to rotation around the z-axis is spontaneously broken), according to Adler's principle[8] the scattering amplitude with the involvement of Goldstone quasiparticles with frequency ω_k in the long-wavelength limit must have the form

$$\Gamma(\mathbf{p},\mathbf{k};\mathbf{p},\mathbf{k}) = (\alpha\omega_k^2\omega_p^2 + \beta k^2 p^2)/\omega_k\omega_p. \tag{61}$$

Let us discuss how the above-mentioned behavior of the scattering amplitude at the boundary of the $FM_<$ phase agrees with this requirement. We note first of all that if for the $FM_<$ phase the Goldstone quasiparticles have the dispersion law $\omega_k = ck$, then at its boundary $H = H_{c1}$ the velocity of sound reduces to zero and $\omega_k = \mathscr{D}k^2$ for small k. This follows from Eq. (58) of Ref. 1 for the $FM_<$ phase, and agrees with the behavior of the frequency of low-lying modes when we approach from the QO phase side [see Eq. (17)] and is typical behavior for a second-order OPT. Correspondingly, from (61) we obtain the requirement $\Gamma(\mathbf{0},\mathbf{0};\mathbf{0},\mathbf{0})$ = constant, which is also satisfied by the amplitudes we have found.

The exception is at the multicritical point A, for which the behavior is characteristically unique. On the one hand, it follows from (17) and the condition $\tilde{H}_{c1}(0) = 0$ that at this point the velocity of sound remains constant[2)] ($\omega_k^{\pm} = ck$), so that we must have $\Gamma_0^{\mu\nu}(\mathbf{0},\mathbf{0};\mathbf{0},\mathbf{0}) = 0$ at the point $h = 0$, $\xi = \xi_{cr} - 0$. On the other hand, this is a point of nonanalyticity in the spectrum at $k = 0$, so that the result at zero quasimomentum, generally speaking, will depend on the path of approach to this point. Direct calculations for the $FM_<$ phase carried out using the same diagram technique and to the same order of approximation as in Sec. 3 for the QO phase (the corresponding computations will be presented in a separate paper), show that on the line $h = 0$ the scattering amplitude for Goldstone quasiparticles has the form (61) [and consequently $\Gamma(\mathbf{0},\mathbf{0};\mathbf{0},\mathbf{0}) = 0$] for any $\xi \in (0,\xi_{cr})$; however, as we approach the point A this form is valid over and ever-decreasing interval of values of quasimomentum, namely those for which $\omega_k, \omega_p \ll \Delta\xi \equiv \xi_{cr} - \xi$. At the point $h = 0$, $\xi = \xi_{cr}$ itself, Eq. (61) can retain its validity only for $k = p = 0$. However, this depends on the order in which the limits are taken. If the limit is taken for finite values of $\Delta\xi$, i.e., if we first set $k = p = 0$, and then $\Delta\xi = 0$, then the Adler principle is fulfilled and $\Gamma(\mathbf{0},\mathbf{0};\mathbf{0},\mathbf{0}) = 0$. When the limits are taken in the opposite order we obtain a different answer, in which the form is $\Gamma(\mathbf{p},\mathbf{k};\mathbf{p},\mathbf{k}) \sim 1/kp$, which coincides exactly with the result (37) for the scattering amplitude of the QO phase if we set $\xi = \xi_{cr}$ in it. Hence, for this value of ξ we simultaneously satisfy both the conditions for joining the results of the QO phase with the results for the $FM_<$ phase and the Adler principle for the $FM_<$ phase.

It should be noted that when we calculate the velocities of sound of both modes in the spectrum of the QO phase, i.e., $c = \lim \partial\omega_k^{\pm}/\partial k$, we find an analogous dependence of the result on the order of taking the limits $k \to 0$,

$\Delta\xi = \xi - \xi_{cr} \to 0$. Actually, it follows from (17) that $c \sim k/(H_{c1}^2 + \alpha k^2)^{1/2}$, and consequently c equals zero or a constant depending on the order in which we let $k \to 0$, $\Delta\xi \to 0$ (because $H_{c1}^2 \to 0$ as $\Delta\xi \to 0$).

In conclusion we point out that the theory we have constructed applies equally to the cases of bulk FM or AFM. In both cases, for $H < H_{c1}$ a single-sublattice tensor phase results. The difference in spin structures appears only for $H > H_{c1}$, where ordering arises in the XY plane: ferromagnetic for $J_0 > 0$ and antiferromagnetic for $J_0 < 0$.

We also emphasize that, as we have verified , the use of the two independent methods we developed for investigating spin systems with tensor-vector order parameters—the low-temperature variant of the diagram technique for Hubbard operators and the formalism based on the generalized Maleev-Dyson transformation—lead to identical results when used in first-order approximations.

[1)]We note that similar unphysical results are also obtained for other spin systems when the Born approximation is used in the immediate vicinity of a second-order OPT point or of a point of phase instability [see, e.g., the result for low-temperature magnetization near a field-driven instability of the APT phase—Eqs. (34)–(37) of Ref. 6].

[2)]The same thing follows from Eq. (57) of Ref. 1 for the $FM_<$ phase.

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