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A CONTRIBUTION TO THE THEORY OF A FERROMAGNETIC CRYSTAL WITH TWO SPINS PER SITE *

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The problem of the magnetization and magnetic excitations spectrum of a ferromagnetic crystal has been examined for the case where the total spin moment at each site is due to the combination of two interacting electron spins.

On the basis of a simple model it is shown that, even where the interaction within a site is comparatively weak, of intersite order, the Curie point is close to the maximum level for a hard spin coupling at the site. Besides the usual, "acoustic" branches of magnetic excitations we have also found the high-energy excitations which are connected with transitions between triplet and singlet states at the site, which cannot be derived by examining strongly coupled spins.

The problem of spin interaction within a single site is solved precisely and the self-consistent field approximation is used to take account of site interaction in computing the magnetization, and that of Bogolyubov and Tyablikov in the examination of the magnetic excitation spectrum.

1. The most closely studied model of ferromagnetism is that of Heisenberg (e.g. see [1]), in which it is assumed that exchange-interacting spins are situated at lattice sites. No account is usually taken [2-5] of the fact that the spin of a site with $s > 1/2$ is the resultant of the spins of several electrons of an atom, and the total atomic spin may generally not be preserved on interaction.

It is of definite interest to see what influence the internal spin structure of an atom with $s > 1/2$ has on the magnetic excitation spectrum of a crystal. This problem has been investigated by the approximate second quantization method by Kondorskiy and Pakhomov in [6, 7], and also Izyumov in [8]. The case of several spins per site, where the subsite interaction is much greater than the intersite, has been examined by Izyumov and Yakovlev in [9], using the method of two-time Green's temperature functions. The conditions under which the Heisenberg model may be applied for the case of several magnetic electrons at an atom has been investigated in detail by Irkhin in [10].

In the present work we shall examine the model of a ferromagnetic crystal in each site of which the total spin momentum is the resultant of two interacting electron spins. In section 3 we investigate the temperature dependence of the magnetization of the system in the self-consistent field approximation. In section 4 we shall discuss the exactly solvable problem of two spins in an external field. The results of this examination are used in section 5 to study the magnetic excitation spectrum of the system by means of two-time Green's temperature functions.

2. Let us start from the model Hamiltonian [11]

* *Fiz. metal. metalloved.*, 31, No. 1, 5-12, 1971.

$$\begin{aligned} \mathbf{H} = & -\mu H \sum_{f\alpha} S_{f\alpha}^z - \frac{1}{2} \sum_{f \neq g} \sum_{\alpha, \beta} J(f\alpha; g\beta) (\lambda S_{f\alpha}^+ S_{g\beta}^- + S_{f\alpha}^z S_{g\beta}^z) - \\ & - \frac{1}{2} \sum_{f, \alpha \neq \beta} J(f\alpha; f\beta) (\lambda S_{f\alpha}^+ S_{f\beta}^- + S_{f\alpha}^z S_{f\beta}^z). \end{aligned} \quad (2.1)$$

Here s is the site index ($f = 1 \dots N$); α is the spin number at the site ($\alpha = 1, 2$); $S_{f\alpha}$ is the spin operator $s = \frac{1}{2}$; $J(f\alpha; g\beta)$ is the exchange integral. The case of $\lambda = 1$ corresponds to the isotropic model and that of $\lambda = 0$ to a model of the Ising type. In this work we shall not be concerned with the possibility of antiferromagnetic spin ordering in the lattice and shall therefore assume that the exchange integrals:

$$\begin{aligned} J(f\alpha; f\beta) &= I_1, \quad \alpha \neq \beta; \\ J(f\alpha; g\beta) &\approx J(f; g), \quad f \neq g \end{aligned}$$

are non-negative.

3. Let us use the self-consistent field method for a qualitative examination of the magnetization of the system. In the second term of the (2.1) Hamiltonian, which describes interaction between spins from different sites, let us isolate the quadratic term in the spin deviations from the mean (we shall study the case of $\lambda = 1$ in detail and derive the result for $\lambda = 0$)

$$\begin{aligned} \mathbf{H} = & 2I_2 \sigma^2 N - (2I_2 \sigma + \mu H) \sum_{f\alpha} S_{f\alpha}^z - \frac{1}{2} I_1 \sum_{f, \alpha \neq \beta} S_{f\alpha} S_{f\beta} - \frac{1}{2} \sum_{f \neq g} \sum_{\alpha, \beta} I \times \\ & \times (f\alpha; g\beta) (S_{f\alpha} - \sigma_\alpha) (S_{g\beta} - \sigma_\beta), \end{aligned} \quad (3.1)$$

where $I_2 = \sum_f J(f, g)$ and $\langle S_{f\alpha} \rangle = \sigma_\alpha$, $\sigma_1 = \sigma_2 = \sigma$.

For intersite interaction the problem can be solved in the self-consistent field approximation. As we know [12], the zero approximation of this method is here derived by neglecting the last term in (3.1). In no approximation can interaction between spins within a single site be reduced to the self-consistent field. We shall take accurate account of this interaction. As a result, we get a Hamiltonian of the form

$$\mathbf{H} = \sum_f \mathbf{H}_f,$$

where

$$\mathbf{H}_f = 2I_2 \sigma^2 + (2I_2 \sigma + \mu H) (S_{f1}^z + S_{f2}^z) - I_1 S_{f1} S_{f2}.$$

In this approximation the free energy breaks down into the sum of free energies in a single site

$$F_f = -T \ln Z_f,$$

and the statistical sum Z_f

$$Z_f = \text{Sp} e^{-\beta \mathbf{H}_f} = e^{-2I_2 \sigma^2 \beta} \left\{ e^{(2I_2 \sigma + \mu H) \beta / 4} + e^{\beta I_1 / 4} + e^{-(2I_2 \sigma + \mu H) \beta / 4} + e^{-\beta I_1 / 4} \right\} =$$

$$.1) \quad = e^{-2I_2\sigma^2\beta} e^{\beta I_1\sigma} \{2 \operatorname{ch} y + 1 + e^{-\beta I_1}\}, \quad (3.2)$$

where $\beta = 1/T$; $y = \beta (2I_2\sigma + \mu H)$

Taking account of (3.2), we get

$$\beta F_f = \frac{(y - \beta\mu H)^2}{2I_2\beta} - \beta I_1/4 - \ln\{2 \operatorname{ch} y + 1 + e^{-\beta I_1}\}. \quad (3.3)$$

The mean spin σ is found from the condition of minimum free energy $\partial F_f/\partial\sigma = 0$ and is

$$\sigma = \frac{y - \beta\mu H}{\beta I_2} = \frac{2 \operatorname{sh} y}{2 \operatorname{ch} y + 1 + e^{-\beta I_1}}. \quad (3.4)$$

When the interaction within a site is much greater than the intersite interaction $I_1 \rightarrow \infty$, the equation for the mean spin becomes

$$\sigma = \frac{2 \operatorname{sh} y}{2 \operatorname{ch} y + 1},$$

which is a particular case of the Brillouin function at $s = 1$. In such a system, at $H = 0$ there will be a phase transition for $T_c = 2/3 I_2$, which means that for infinitely large subsite spin interaction we shall get the well known results of the molecular field method for a ferromagnetic crystal with $s = 1$.

In the general case ($H = 0$) the equation for T_c has the form

$$3 + e^{-\beta_c I_1} = 2I_2\beta_c, \quad (3.5)$$

(3.1) where $\beta_c = 1/T_c$. Let us introduce new variables $x = 2I_2\beta_c$ and $\alpha = \frac{1}{2} I_1/I_2$. Then we can rewrite equation (3.5) as

$$3 + e^{-\alpha x} = x. \quad (3.6)$$

After solving (3.6) graphically, it is easy to see that the Curie temperature rises to $T_c = 2/3 I_2$ when the interaction in a site increases (I_2 is fixed). By analogy, it is easy to find the behaviour of the magnetization in a model of the Ising type (in (2.1) $\lambda = 1$). Once again, we find that at fixed intersite interaction ($I_2 = \text{const}$) the Curie temperature rises with I_1 , as far as $T_c = I_2$. The results of the graphical solution of (3.6) for $\lambda = 1$, and the analogous equation for $\lambda = 0$, are given in Fig. 1.

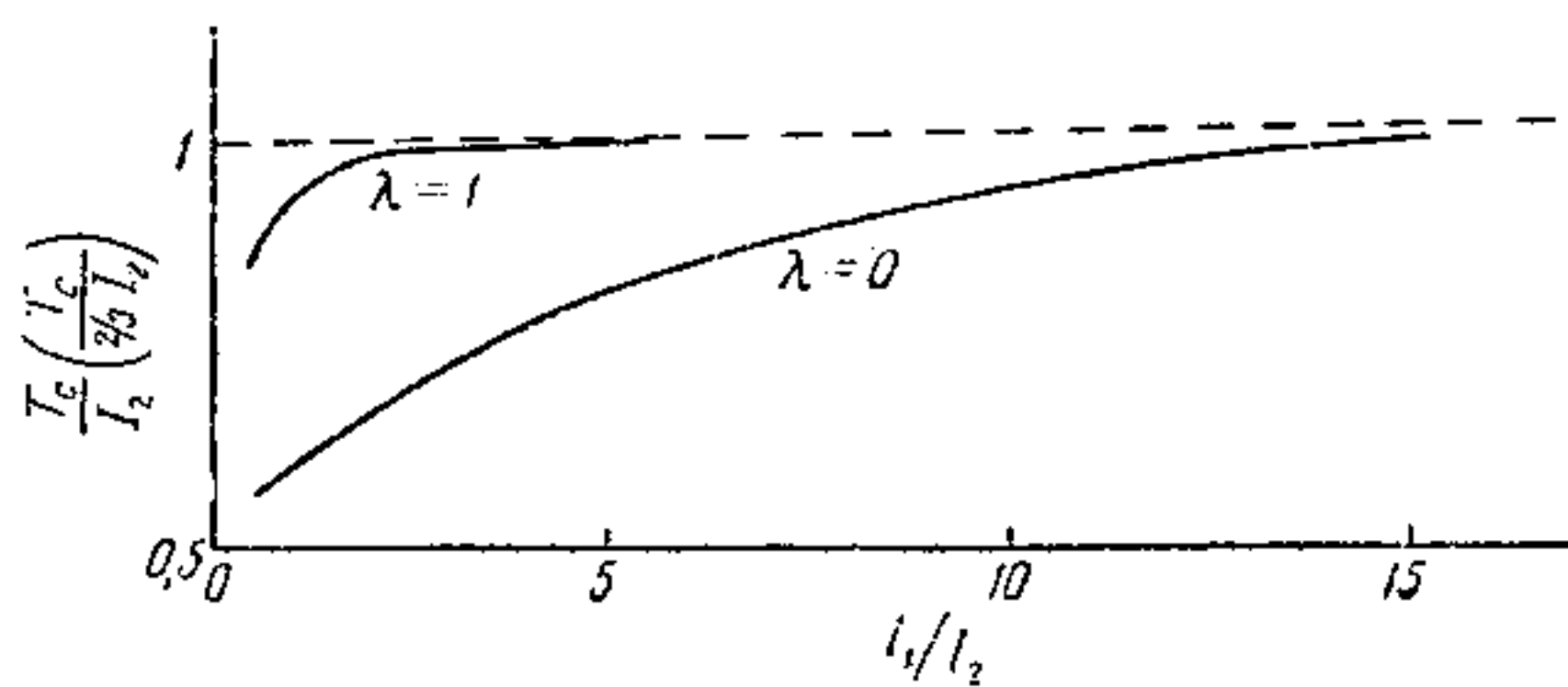


FIG. 1. Critical temperature as a function of the exchange integral relation.

Thus we see that spin motion within a single site has a fairly small influence on the temperature behaviour of the magnetization.

4. We shall use the method of two-time Green's temperature functions [1, 13] to examine the magnetic excitation spectrum of the system.

First let us consider the case of a system in which there is no exchange interaction between the sites. Then the problem is reduced to the exactly solvable problem of two spins interacting in an external field

$$H = -\mu H (S_1^z + S_2^z) - I_1 (S_1 S_2). \quad (4.1)$$

Obviously, the energy spectrum of the system (4.1) can readily be derived by direct solution of the Schrödinger equation. However, for subsequent analysis of the spin excitation spectrum of the system (2.1) we have to find the excitation of system (4.1) by the Green's function method. For such a simple Hamiltonian as (4.1) the system of equations for the Green's functions obviously reduces to two equations and can be solved exactly. We find that the Green's function $\langle\langle S_1^+(t) | S_1^-(0) \rangle\rangle$ has poles μH , and $\mu H - I_1$, the Green's function $\langle\langle S_1^-(t) | S_1^+(0) \rangle\rangle$ has poles $\mu H + I_1$ and $-\mu H + I_1$. Their interpretation is depicted in Fig. 2. The horizontal lines depict the energy levels of the system. The values of the total spin S_t and its projection are given on the left; the intrinsic energy values on the right. The left-hand group of transitions in Fig. 2 corresponds to the poles of Green's function $\langle\langle S_1^+ | S_1^- \rangle\rangle$, the right-hand to the poles of $\langle\langle S_1^- | S_1^+ \rangle\rangle$. We shall not refer to other Green's functions because $\langle\langle S_1^i | S_2^k \rangle\rangle = 0$; $\langle\langle S_1^i | S_1^k \rangle\rangle = \langle\langle S_2^i | S_2^k \rangle\rangle$, where $i, k = \pm, z$, and the rest of them are easily expressed in terms of $\langle\langle S_1^i | S_1^k \rangle\rangle$.

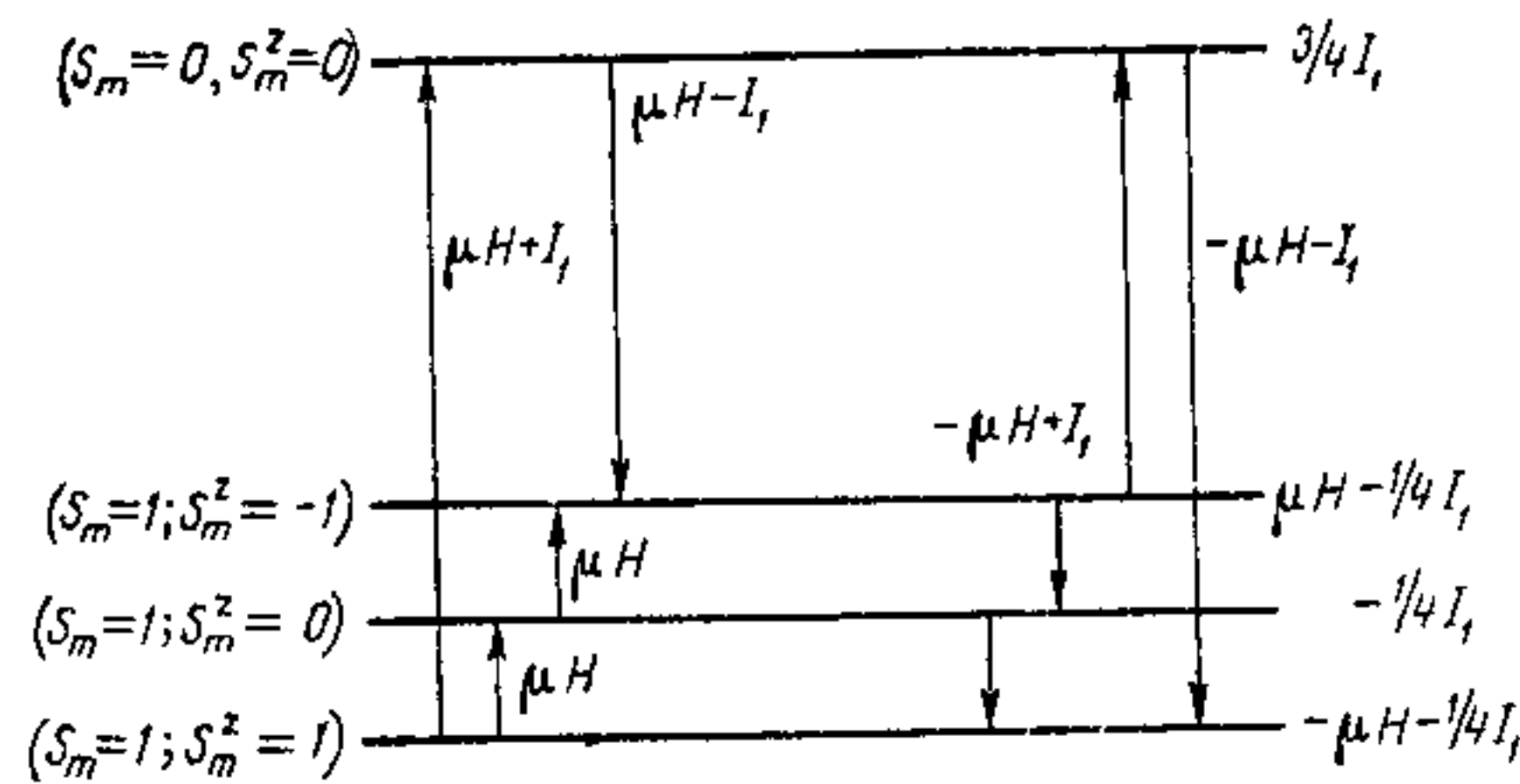


FIG. 2. Spectrum of the magnetic excitations of a two-spin system.

The Green's functions $\langle\langle S_1^+ | S_1^- \rangle\rangle$ and $\langle\langle S_1^- | S_1^+ \rangle\rangle$ describe all the possible transitions in the system involving a change of ± 1 in the total spin projection onto the quantization axis, which is depicted in Fig. 2. Green's function $\langle\langle S_1^z | S_1^z \rangle\rangle$ will, of course, describe transitions in the system without a change in the total spin projection. The spins are parallel to the field ($S_1 = 1, S_1^z = 1$) in the ground state. The poles of Green's function $\langle\langle S_1^+ | S_1^- \rangle\rangle$ which are equal to μH and $\mu H + I_1$, correspond to allowed transitions from ground to excited state, so the corresponding residues are also non-zero at zero temperature. Pole $\mu H - I_1$, which corresponds to transition from the excited state to a lower energy level, has a residue which disappears at zero temperature. This behaviour is because the residues are proportional to the occupation of the initial state. The residues of Green's function poles $\langle\langle S_1^- | S_1^+ \rangle\rangle$ behave in the same way.

5. Now let us determine the magnetic excitation spectrum of the total system (2.1). We shall consider the case of $\lambda = 1$ in detail, and simply give the results for $\lambda = 0$.

We shall examine the following Green's functions:

$$\begin{aligned} \langle\langle S_{m\lambda}^+(t) | S_{n\mu}^-(0) \rangle\rangle &= \theta(t) \langle [S_{m\lambda}^+(t), S_{n\mu}^-(0)] \rangle; \\ \langle\langle S_{m\lambda}^-(t) | S_{n\mu}^+(0) \rangle\rangle &= \theta(t) \langle [S_{m\lambda}^-(t), S_{n\mu}^+(0)] \rangle, \end{aligned} \quad (5.1)$$

where $S_{m\lambda}^\pm(t)$ is the Heisenberg representation of the operator of the transverse components of spin with the total Hamiltonian (2.1) for $\lambda = 1$. Green's function (5.1) describes the dynamic behaviour of the system when the z projection of total spin is altered by unity, the Green's functions poles (5.1) defining the magnetic excitation spectrum of the system.

Now let us define the Green's functions. Using the equation of motion for operator $S_{m\lambda}^+$, for Green's function $\langle\langle S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle$ we shall get the equation

$$\begin{aligned} i \frac{d}{dt} \langle\langle S_{m\lambda}^+(t) | S_{n\mu}^-(0) \rangle\rangle &= i \delta(t) \delta_{mn} \delta_{\lambda\mu} \langle 2S_{m\lambda}^z \rangle + \mu H \langle\langle S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle + \\ &+ \sum_{f \neq m, \alpha} J(f\alpha; m\lambda) \langle\langle S_{f\alpha}^z S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle + \sum_{\alpha \neq \lambda} J(m\alpha; m\lambda) \langle\langle S_{m\alpha}^z S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle - \\ &- \sum_{f \neq m, \alpha} J(f\alpha; m\lambda) \langle\langle S_{m\lambda}^z S_{f\alpha}^+ | S_{n\mu}^- \rangle\rangle - \sum_{\alpha \neq \lambda} J(m\alpha; m\lambda) \langle\langle S_{m\lambda}^z S_{m\alpha}^+ | S_{n\mu}^- \rangle\rangle. \end{aligned} \quad (5.2)$$

Here and below, terms with $f \neq m$ and the term with $f = m$ will be written separately. This is quite natural because the problem is solved exactly for a single site, but approximately for site interaction. In equation (5.2) let us express part of the second Green's functions (for which $f \neq m$) in terms of the first:

$$\begin{aligned} \langle\langle S_{f\alpha}^z S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle &\approx \langle S_{f\alpha}^z \rangle \langle\langle S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle, \quad f \neq m; \\ \langle\langle S_{m\lambda}^z S_{f\alpha}^+ | S_{n\mu}^- \rangle\rangle &\approx \langle S_{m\lambda}^z \rangle \langle\langle S_{f\alpha}^+ | S_{n\mu}^- \rangle\rangle, \quad f \neq m. \end{aligned}$$

Tyablikov is the originator of this uncoupling [1]. We note that, because of translational invariance, the values $\langle S_{f\alpha}^z \rangle$ do not depend on the site index,

$$\langle S_{f_1}^z \rangle = \langle S_{f_2}^z \rangle = \sigma.$$

Since we wish to solve the problem of intrasite interaction exactly, we must examine the equations for the second Green's functions. As we can see from (5.2), we only need to examine equations of motion for Green's functions of the form:

$$\langle\langle S_{m\alpha}^z S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle,$$

in which, besides this, always $\alpha \neq \lambda$. The corresponding equation of motion has the form

$$\begin{aligned} i \frac{d}{dt} \langle\langle S_{m\alpha}^z S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle &= i \delta(t) \langle [S_{m\alpha}^z S_{m\lambda}^+, S_{n\mu}^-] \rangle + \mu H \langle\langle S_{m\alpha}^z S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle - \\ &- \frac{1}{2} \sum_{p \neq m, \gamma} J(p\gamma; m\alpha) \langle\langle S_{m\alpha}^+ S_{p\gamma}^- S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle - \frac{1}{2} \sum_{\alpha \neq \gamma} J(m\gamma; m\alpha) \langle\langle S_{m\alpha}^+ \times \end{aligned}$$

$$\begin{aligned}
& \times S_{m\gamma}^- S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle + \frac{1}{2} \sum_{p=m, \gamma} J(p\gamma; m\alpha) \ll S_{m\alpha}^- S_{p\gamma}^+ S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle + \\
& + \frac{1}{2} \sum_{\alpha \neq \gamma} J(m\gamma; m\alpha) \ll S_{m\alpha}^- S_{m\gamma}^+ S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle + \sum_{p=m, \gamma} J(p\gamma; m\lambda) \ll S_{m\alpha}^z S_{p\gamma}^z \times \\
& \times S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle + \sum_{\gamma \neq \lambda} J(m\gamma; m\lambda) \ll S_{m\alpha}^z S_{m\gamma}^z S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle - \sum_{p=m, \gamma} J(p\gamma; m\lambda) \times \\
& \ll S_{m\alpha}^z S_{m\lambda}^z S_{p\gamma}^+ |S_{n\mu}^- \rangle \rangle - \sum_{\gamma \neq \lambda} J(m\gamma; m\lambda) \ll S_{m\alpha}^z S_{m\lambda}^z S_{m\gamma}^+ |S_{n\mu}^- \rangle \rangle. \tag{5.4}
\end{aligned}$$

Let us examine each of the Green's functions entering this equation in detail:

$$\begin{aligned}
1) & \ll S_{m\alpha}^+ S_{p\gamma}^- S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle \approx 0 \text{ here } p \neq m); \\
2) & \ll S_{m\alpha}^+ S_{m\gamma}^- S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle = \frac{1}{2} \ll S_{m\alpha}^+ |S_{n\mu}^- \rangle \rangle - \ll S_{m\alpha}^+ S_{m\lambda}^z |S_{n\mu}^- \rangle \rangle,
\end{aligned}$$

since it follows from $\gamma \neq \alpha$ and $\alpha \neq \lambda$ that $\gamma = \lambda$ because α, γ and λ assume the values 1 and 2:

$$\begin{aligned}
3) & \ll S_{m\alpha}^- S_{p\gamma}^+ S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle \approx \langle S_{m\alpha}^- S_{m\lambda}^+ \rangle \ll S_{p\gamma}^+ |S_{n\mu}^- \rangle \rangle \text{ where } m \neq p; \\
4) & \ll S_{m\alpha}^- S_{m\gamma}^+ S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle = 0 \text{ (here } \gamma \neq \alpha \text{ и } \alpha \neq \lambda, \text{ hence } \gamma = \lambda); \\
5) & \ll S_{m\alpha}^z S_{p\gamma}^z S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle \approx \langle S_{p\gamma}^z \rangle \ll S_{m\alpha}^z S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle \text{ where } m \neq p; \\
6) & \ll S_{m\alpha}^z S_{m\gamma}^z S_{m\lambda}^+ |S_{n\mu}^- \rangle \rangle = \frac{1}{4} \ll S_{m\alpha}^+ |S_{n\mu}^- \rangle \rangle \text{ (here } \gamma \neq \lambda
\end{aligned} \tag{5.5}$$

and $\alpha \neq \lambda$, therefore $\alpha = \gamma$);

$$7) \ll S_{m\alpha}^z S_{m\lambda}^z S_{p\gamma}^+ |S_{n\mu}^- \rangle \rangle \approx \langle S_{m\alpha}^z S_{m\lambda}^z \rangle \ll S_{p\gamma}^+ |S_{n\mu}^- \rangle \rangle \text{ where } p \neq m;$$

$$8) \ll S_{m\alpha}^z S_{m\lambda}^z S_{m\gamma}^+ |S_{n\mu}^- \rangle \rangle = \frac{1}{2} \ll S_{m\lambda}^z S_{m\alpha}^+ |S_{n\mu}^- \rangle \rangle \text{ (here also } \gamma \neq \lambda$$

and $\alpha \neq \lambda$, hence $\gamma = \alpha$).

Relations 2, 4, 6 and 8 in (5.5) are exact. Such relations are used in the exact solution of the problem of two interacting spins in an external field in section 4. Relation (5) in (5.5) is the approximation of Tyablikov, as in (5.3). Of course, relation 1 is satisfied very well at low temperatures. Determinations 3 and 7 are analogous to those suggested by Callen in [5], with the difference that correlators of spin operators in different sites will be treated as small. Incidentally, under our assumptions the result given below is not altered if, instead of uncouplings 3 and 7, the corresponding Green's functions are simply set equal to zero.

If (5.3) is put into (5.2) and (5.5) the chain of equations for the Green's functions is closed. Going over to Fourier representation we shall see that the Fourier transform of function $\ll S_{m\lambda}^+(t) |S_{n\mu}^-(0) \rangle \rangle$ is:

$$G_{1,1}(\mathbf{k}, \omega) = \frac{i}{2\pi} \frac{\sigma}{\omega - \mu H - (I_2 - I_2(\mathbf{k})) 2\sigma} + \frac{i}{2\pi} \frac{1}{2} \times$$

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$$\begin{aligned} & \times \frac{\sigma - \langle 2S_{m1}^z S_{m2}^z \rangle - \langle S_{m1}^- S_{m2}^+ \rangle}{\omega - \mu H - I_2 2\sigma + I_1} + \frac{i}{2\pi} \frac{1}{2} \times \\ & \times \frac{\sigma + \langle 2S_{m1}^z S_{m2}^z \rangle + \langle S_{m1}^- S_{m2}^+ \rangle}{\omega - \mu H - I_2 2\sigma - I_1}, \end{aligned} \quad (5.6)$$

where $I_2(k) = \sum_{f,m} I(f, m) e^{ik(m-f)}$.

(5.4) Let us analyze the expression we have obtained. The Green's function poles of (5.6) describe the spin excitation spectrum of the system. They have the following form:

$$\omega = \mu H + [I_2 - I_2(k)] 2\sigma; \quad (5.7)$$

$$\omega = \mu H + I_2 2\sigma + I_1; \quad (5.8)$$

$$\omega = \mu H + I_2 2\sigma - I_1. \quad (5.9)$$

If we use the well known relations of [1]:

$$\begin{aligned} \langle\langle A | B \rangle\rangle_E^{(\omega)} &= \frac{i}{2\pi} \int_{-\infty}^{\infty} (e^{\omega/\theta} - \eta) I_{AB}(\omega) \frac{d\omega}{E - \omega - i\epsilon}; \\ \langle\langle B | A \rangle\rangle_{-E}^{(\omega)} &= \frac{i}{2\pi} \int_{-\infty}^{\infty} (e^{\omega/\theta} - \eta) I_{AB}(\omega) \frac{d\omega}{-E - \omega + i\epsilon}, \end{aligned}$$

(5.5)

it is easy to verify that the Green's function $\langle\langle S_{m\lambda}^- | S_{n\mu}^+ \rangle\rangle$ has poles equal to those of (5.7)-(5.9) with the opposite sign. The (5.7) poles represent the energy spectrum of normal spin waves (the gap of which vanishes at $H = 0$) in a ferromagnetic system with a spin of $s = 1$ at each site. The (5.7) spectrum is due to site interaction, which broadens the intersite transition $\omega = \mu H$ (see section 4) into a band.

Excitations (5.8) and (5.9) are analogous to the optical branches in lattice dynamics and are due to transition between triplet and singlet states of the site. In our approximation these excitations do not depend on k and are of a purely local nature. In the case in question site interaction is reduced to the supplementary molecular field $I_2 2\sigma$. It is interesting to note that the quasi-optical excitations in [7] are of an analogous nature if the intersite exchange integrals do not depend on the numbers of the electron state at the site.

For a model of the Ising type (in (2.1) $\lambda = 0$) the spectrum of magnetic excitation has the form:

$$\omega = \mu H + 2I_2\sigma + I_1/2,$$

$$\omega = \mu H + 2I_2\sigma - I_1/2.$$

Such poles have the Green's function $\langle\langle S_{m\lambda}^+ | S_{n\mu}^- \rangle\rangle$. The poles of the conjugated Green's function are equal to these poles with the opposite sign.

We would like to express our gratitude to D. N. Zubarev for his interest in the work and discussion thereof, to Yu. A. Izyumov, N. M. Plakide and B. V. Vasil'yev for interesting discussion; to Ye. N. Yakov for valuable criticism; and also to Doctor E. Praveczi, Doctor V. Tsic and Doctor G. Convent for their interest and useful discussion of the work.

APPENDIX

Using the standard method of [1] it is not hard to derive an equation for the correlation of transverse spin components in a single site

$$\langle S_{m2}^- S_{m1}^+ \rangle = \frac{1}{2} \frac{1}{N} \sum_k \frac{2\sigma}{\exp[\beta(\mu H + 2\sigma(I_2 - I_2(k))) - 1]} - \frac{1}{2} \left(\frac{\sigma - \langle 2S_{m1}^z S_{m2}^z \rangle - \langle S_{m1}^- S_{m2}^+ \rangle}{\exp[\beta(\mu H + I_2 2\sigma - I_1)] - 1} - \frac{\sigma + \langle 2S_{m1}^z S_{m2}^z \rangle + \langle S_{m1}^- S_{m2}^+ \rangle}{\exp[\beta(\mu H + 2I_2\sigma + I_1)] - 1} \right).$$

By analogy, from (5), (6) we get an equation for the relative magnetization

$$1 + 2\sigma = \frac{1}{N} \sum_k \frac{2\sigma}{\exp[\beta(\mu H + 2\sigma(I_2 - I_2(k))) - 1]} - \frac{\sigma - \langle 2S_{m1}^z S_{m2}^z \rangle - \langle S_{m1}^- S_{m2}^+ \rangle}{\exp[\beta(\mu H + I_2 2\sigma - I_1)] - 1} + \frac{\sigma + \langle 2S_{m1}^z S_{m2}^z \rangle + \langle S_{m1}^- S_{m2}^+ \rangle}{\exp[\beta(\mu H + 2I_2\sigma + I_1)] - 1}.$$

To investigate the temperature dependence of the magnetization we need to calculate the correlation functions $\langle S_{m1}^z S_{m2}^z \rangle$ and $\langle S_{m1}^- S_{m2}^+ \rangle$, which go into it. It is, however, no trivial problem to calculate the correlation functions of spin operators (particularly longitudinal) both within a site and between sites (e.g. see [14-16]), for which reason we have not done it here.

REFERENCES

1. S. V. Tyablikov, *Metody kvantovoy teorii magnetizma (Quantum method of magnetism theory)* Moscow, Izd. Nauke (1965).
2. R. A. Tahir-Kheli and D. ter Haar, *Phys. Rev.*, 127, 88 (1962).
3. S. V. Tyablikov, *Fiz. metal. metalloved.*, 16, 321 (1963).
4. E. Praveczi, *Phys. Letters*, 6, 147 (1963).
5. H. B. Callen, *Phys. Rev.*, 130, 890 (1963).
6. Ye. I. Kondorskiy and A. S. Pakhomov, *Dokl. Akad. Nauk. SSSR*, 93, 431 (1953).
7. Ye. I. Kondorskiy and A. S. Pakhomov, *Zh. eksp. teor. fiz.*, 32, 323 (1957).
8. Yu. A. Izyumov, *Zh. eksp. teor. fiz.*, 32, 1058 (1957).
9. Yu. A. Izyumov and Ye. N. Yakovlev, *Fiz. metal. metalloved.*, 9, 667 (1960).
10. Yu. P. Irkhin, *Zh. eksp. teor. fiz.*, 50, 379 (1966).
11. Yu. A. Izyumov, *Fiz. metal. metalloved.*, 8, 3 (1959).
12. V. G. Vaks, A. I. Larkin and S. A. Pikin, *Zh. eksp. teor. fiz.*, 51, 361 (1966).
13. D. N. Zubarev, *UFN*, 71, 71 (1960).
14. R. A. Tahir-Kheli and H. B. Callen, *Phys. Rev.*, 135, A679 (1964).
15. S. H. Liu, *Phys. Rev.*, 139, A1522 (1965).
16. R. A. Tahir-Kheli, *Phys. Rev.* 159, 439 (1967).

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К ТЕОРИИ ФЕРРОМАГНИТНОГО КРИСТАЛЛА С ДВУМЯ СПИНАМИ В УЗЛЕ

Л. А. Максимов и А. Л. Куземский

Рассматривалась задача о намагниченности и спектре магнитных возбуждений ферромагнитного кристалла в случае, когда суммарный спиновый момент в каждом узле образуется в результате сложения двух взаимодействующих электронных спинов.

На основе простой модели показано, что даже при относительно слабом, порядка междоузельного, взаимодействии внутри узла температура Кюри близка к предельной температуре Кюри при жесткой связи спинов в узле. Помимо обычной, «акустической» ветви магнитных возбуждений, найдены высокоэнергетические возбуждения системы, связанные с переходами между триплетным и синглетным состояниями в узле, что невозможно получить при рассмотрении сильно связанных спинов.

Задача о взаимодействии спинов внутри одного узла решается точно, а междоузельное взаимодействие учитывается в приближении самосогласованного поля при вычислении намагниченности и в приближении Боголюбова—Тябликова при исследовании спектра магнитных возбуждений.