FERROMAGNETIC CRYSTAL WITH A DISLOCATION AT $T \neq 0$

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The effect on magnetization produced by local and quasilocal levels arising as the result of a dislocation is considered. It is shown that at temperatures at which the mean thermal energy is of the order of the energy of these levels, the latter begin to fill up rapidly. This results in a sharp drop of magnetization of the atoms at the dislocation. Since under some assumptions regarding the exchange interaction there will always be virtual levels near the very bottom of the spin-wave band, the spins of the atoms of the dislocation may be strongly deflected. The Holstein-Primakoff formalism is therefore inapplicable and the theory is based on the two-time temperature Green functions. In these functions the effective interaction between the spin waves is taken into account by renormalization of their energy with temperature. It is also taken into account that the number of spin deflections at each site should not exceed the magnitude of the spin itself.

If there are local perturbations in a macroscopic system with a quasicontinuous spectrum of elementary excitations, an unusual reorganization of the energy spectrum of the system takes place. This question was first investigated by I. Lifshitz,[1] who showed that the local perturbation gives rise either to isolated discrete levels split away from the band of the quasicontinuous spectrum, or to a certain redistribution of the levels inside the band, leading to so-called quasilocal states.

The theory of a Heisenberg ferromagnet of simple cubic symmetry having a linear dislocation at zero temperature as a defect was developed in[2,3]. The dislocation was assumed directed along the z axis, and the Hamiltonian of the system could be written in the form

$$H = -J\sum_{\mathbf{j}}\sum_{\boldsymbol{\delta}} \mathbf{S}_{\mathbf{j}}\mathbf{S}_{\mathbf{j}+\boldsymbol{\delta}} - 2(J'-J)\sum_{\mathbf{i}}\sum_{\boldsymbol{\delta}'} \mathbf{S}_{\mathbf{i}}\mathbf{S}_{\mathbf{i}+\boldsymbol{\delta}'} - (J''-J)\sum_{\mathbf{i}}\sum_{\boldsymbol{\delta}''} \mathbf{S}_{\mathbf{i}}\mathbf{S}_{\mathbf{i}+\boldsymbol{\delta}''}, \tag{1}$$

where $\mathbf{i}$ is the dislocation axis, $\boldsymbol{\delta}'$ are the nearest neighbors in the plane z = const, $\boldsymbol{\delta}''$ are the nearest neighbors along the dislocation axis, and $\boldsymbol{\delta} = \boldsymbol{\delta}' + \boldsymbol{\delta}''$.

Because of the dislocation, there appear among the spin-wave excitations of such a crystal localized states (above the band of the quasicontinuous spectrum) and resonance states (within it). All of these states can be classified according to the irreducible representations A_{1g}, B_{1g}, E_u of the group $C_{4v} \times C_i$, which is the symmetry group of a simple cubic crystal with a linear dislocation. They may be denoted as s-, p-, and d-states.

At low temperatures the bottom of the spin-wave band is of physical interest. As was shown in[2], a whole band of virtual levels arises there, the energies of which are given by

$$\frac{E}{2JS} - f_z^2 = \pm \varkappa_0^2 \exp\left\{-\frac{4\pi J}{(J-J'')f_z^2}\right\}, \tag{2}$$

where S is the atomic spin, κ_0 is some constant of the order of the limiting wave vector of longitudinal vibrations (the lattice constant is taken as unity), and f_z is the z component of the wave vector of the spin wave, which plays the role of a parameter. For a fixed f_z, as can be seen from (2), there are in fact two levels, one "local" (minus sign in (2)), and one "quasilocal" (plus sign). Both levels may lie very close to the bottom of the spin-wave band. The quasilocal level is very narrow; its width is

$$\Gamma_s \approx \varkappa_0^2 \exp\left\{-\frac{4\pi J}{(J-J'')f_z^2}\right\} \ll 1,$$

$$\frac{\Gamma_s}{E_s} \approx 4\pi\varkappa_0^2 f_z^{-2} \exp\left\{-\frac{4\pi J}{(J-J'')f_z^2}\right\} \ll 1.$$

The spontaneous magnetic moment in the spin-wave approximation is

$$M = N^3\mu_0 gS - \mu_0 g\sum_{\mathbf{n}} \langle a_{\mathbf{n}}^+ a_{\mathbf{n}}\rangle,$$

where $\langle\ldots\rangle$ signifies the average statistical value over a Gibbs ensemble with the Hamiltonian (1), μ_0 is the Bohr magneton, and g is the Landé factor. We assume that

$$\langle a_{\mathbf{n}}^+ a_{\mathbf{n}}\rangle = \int_{-\infty}^{+\infty} \frac{1}{\exp(E/T)-1}\frac{1}{\pi}\operatorname{Im} G_{\mathbf{nn}}(E-is)\,dE, \quad s = 0^+,$$

$$\sum_{\mathbf{n}} \langle a_{\mathbf{n}}^+ a_{\mathbf{n}}\rangle = \int_{-\infty}^{+\infty} \frac{\nu(E)}{\exp(E/T)-1}\,dE,$$

where

$$\nu(E) = \nu_0(E) + \frac{1}{\pi N^3}\sum_{f_z}\left\{\operatorname{Im}\frac{\Delta_s(f_z,E)}{\Delta_s} + 2\operatorname{Im}\frac{\Delta_p(f_z,E)}{\Delta_p} + \frac{\Delta_d(f_z,E)}{\Delta_d}\right\}$$

(see[3]). Calculating the corresponding integrals, we find an expression for M in the long-wave approximation. The result obtained differs from the Bloch law only in a change of the factor in front of $(T/T_C)^{3/2}$:

$$\frac{M}{N^3\mu_0 g} = S - \left\{1 + \frac{1}{N^2}\left[\frac{1-J''/J}{2(J'/J-1)} - \frac{J'/J-1}{1+0.36(J'/J-1)}\right]\right\}\gamma_0\left(\frac{T}{T_c}\right)^{3/2};$$

γ_0 is the Bloch constant. It is impossible to use this result, however, if there are virtual states in the interval $E \lesssim T$. When $J < J''$ there are no such states, but if $J > J''$, "local" and quasilocal states arise near the lower boundary of the spin-wave band. The latter satisfy the condition $\operatorname{Re}\Delta_S(E_S) = 0$. Expanding Δ_S near the point E_S, we obtain

$$\operatorname{Re}\Delta_s = (E - E_s)\operatorname{Re}\Delta_s'(E_s) + \ldots$$

and consequently the change in the density function is

$$\Delta\nu_s(f_z)=\frac{1}{\pi}\frac{\Gamma_s}{(E-E_s)^2+\Gamma_s^2},\qquad \Gamma_s=-\frac{\operatorname{Im}\Delta_s}{\operatorname{Re}\Delta_s},$$

i.e., those values of E near E_S will make the principal contribution to the integral for M. For them, in view of the smallness of Γ_S, the quantity Δ_S behaves like a δ-function. The contribution of the local vibrations will be still greater, since for them Γ = 0. However, even with such a treatment it is impossible to find the true change of magnetization. The fact is, the virtual levels are very close to the lower boundary of the spin-wave band of the ideal crystal, and as soon as the temperature begins to rise, the spins of the matrix atoms will still be weakly excited, but the spins of the dislocation atoms can be strongly deflected. This result is completely understandable theoretically, since the virtual states that arise near a defect must fill up. In this case the Holstein-Primakoff formalism no longer holds and we must use the method of the temperature Green functions.

The temperature theory uses single-particle Green functions, taking into account the effective interaction of the spin waves by a renormalization of their energy with temperature and that the number of spin deflections at each site should not exceed the magnitude of the spin itself. In our case we introduce into the treatment the two-time advanced Green function

$$\langle\langle S_g^+(t)\,|X_k(t')\rangle\rangle\equiv i\theta(t'-t)\langle[S_g^+(t),X_k(t')]\rangle,$$
$$X_k=(S_k^z)^nS_k^-,\qquad n=0,1,\ldots,2s-1.$$

Setting up the equations of motion and expressing the more complicated Green functions appearing therein in terms of the one written out above, and in the random phase approximation,

$$\langle\langle S_g^+(t)S_p^z(t)\,|X_k(t')\rangle\rangle=\langle S_p^z\rangle\langle\langle S_g^+(t)\,|X_k(t')\rangle\rangle,$$

we obtain

$$EG_{gk}=\delta_{gk}+2J\sum_\delta[\langle S_{g+\delta}^z\rangle G_{gk}-\langle S_g^z\rangle G_{g+\delta,k}]$$
$$-2(J'-J)\sum_{\delta'}\{[\langle S_g^z\rangle G_{g_zk}-\langle S_g^z\rangle G_{gk}]\delta_{g'\delta'}$$
$$+[\langle S_{g_z}^z\rangle G_{g_z+\delta',k}-\langle S_{g_z+\delta}^z\rangle G_{g,k}]\delta_{g'0}\},$$
$$-(J''-J)\{\langle S_g^z\rangle G_{g_z+\delta'',k}-2\langle S_{g_z+\delta''}^z\rangle G_{g,k}+\langle S_{g_z}^z\rangle G_{g_z+\delta'',k}\}\delta_{g'0}.$$

Here

$$G_{g,k}=\langle\langle S_g^+|X_k\rangle\rangle/\langle[S_g^+,X_k]\rangle.$$

As a consequence of the translational symmetry along the z axis we assume that

$$G_{g,k}=G_{g',k'}(f_z)\exp\{if_z(g_z-k_z)\}$$
$$g=(g',g_z),\qquad k=(k',k_z),$$

and we shall seek a solution of the equation obtained in the form of an expansion of $G_{g',k'}$ in terms of the unperturbed functions $G^0_{g',k'}$. The latter satisfy the equation

$$EG^0_{g'k'}=\delta_{g'k'}+4J\sigma(1-\cos f_z)\sum_{\delta'}(G^0_{g',k'}-G^0_{g'+\delta',k'})$$

and have the form

$$G^0_{g'k'}=\frac{1}{N^2}\sum_{\varkappa}\frac{\exp\{i\varkappa(g'-k')\}}{E-E_f},$$

where

$$E_f=4J\sigma(3-\cos f_x-\cos f_y-\cos f_z),$$

$\sigma\equiv\langle S_g^z\rangle_{id}$ is the average value of the spin at any site at the given temperature of an ideal crystal. Thus we find that $G_{g',k'}$ obeys the Dyson equation

$$G_{g'k'}=G^0_{g'k'}+\sum_{pn}G^0_{g'p}V_{pn}G_{nk'}. \tag{3}$$

Here the strictly k-energy part of V depends on the sites through $\langle S_g^z\rangle$ and hence is not localized. In this aspect the problem becomes immense. However, since the virtual levels are near the very bottom of the spin-wave band, we can assume that there is a difference in the temperature dependence of the magnetization of the spins lying at a dislocation and the matrix spins. Then we can neglect the difference in the magnetization of different sites of the matrix and obtain

$$V=\begin{pmatrix}8(J'-J)\sigma+4(J''-J)(1-\cos f_z)\sigma' & -2(J'-J)\sigma' & -2(J'-J)\sigma' & -2(J'-J)\sigma' & -2(J'-J)\sigma'\\ -2(J'-J)\sigma & 2(J'-J)\sigma' & 0 & 0 & 0\\ -2(J'-J)\sigma & 0 & 2(J'-J)\sigma' & 0 & 0\\ -2(J'-J)\sigma & 0 & 0 & 2(J'-J)\sigma' & 0\\ -2(J'-J)\sigma & 0 & 0 & 0 & 2(J'-J)\sigma'\end{pmatrix},$$
$$\sigma'=\langle S_0^z\rangle.$$

The assumption made must be confirmed by the result, i.e., the magnetization of the matrix atoms must differ from σ insignificantly even near a dislocation.

To determine the average values of the spin at a specific site we may use the formula

$$\langle S_n^z\rangle=\frac{(S_n-\Phi_n)(1+\Phi_n)^{2S_n+1}+(1+S_n+\Phi_n)\Phi_n^{2S_n+1}}{(1+\Phi_n)^{2S_n+1}-\Phi_n^{2S_n+1}}, \tag{4}$$

which can be brought in by using the connection between the Green functions and the correlation functions (see, for example,[4])

$$\Phi_n=\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\operatorname{Im}G_{nn}(E'-is)}{\exp(E/T)-1}dE. \tag{5}$$

To find σ′ it is necessary to find the value of Φ_0. It will consist of two parts, one of which takes into account the effect of quasilocal, the other, of local vibrations. For the quasilocal levels

$$\frac{1}{\pi}\operatorname{Im}G_{00}^{ql}=16\varkappa_0^2\left(1-\frac{J''}{J}\right)^{-2}\int f_z^{-4}\exp\left[-\frac{4\pi J}{(J-J'')f_z^2}\right]$$
$$\times\frac{\Gamma_s}{(E-E_s)^2+\Gamma_s^2}df_z$$

and consequently

$$\Phi_0^{ql}=\frac{8\varkappa_0^2}{\pi}\left(1-\frac{J''}{J}\right)^{-2}\int_{-\infty}^{+\infty}dE\left[\exp\left(\frac{E}{T}\right)-1\right]^{-1}\cdot$$
$$\times\int_{-\infty}^{+\infty}f_z^{-4}\exp\left[-\frac{4\pi J}{(J-J'')f_z^2}\right]\frac{\Gamma_s}{(E-E_s)^2+\Gamma_s^2}df_z.$$

Small values of f_z make the principal contribution to the integral; hence the limits of integration may be extended to infinity. By changing the order of integration, i.e., integrating first over E and bearing in mind that the factor $\Gamma_S/[(E-E_S)^2+\Gamma_S^2]$ behaves like $\delta(E-E_S)$, we find

$$\Phi_0^{ql}=\gamma_1\frac{T}{T_c},\qquad \gamma_1=\frac{3}{16\pi^2}\varkappa_0^2\left(1-\frac{J''}{J}\right)^{1/2}\left(\frac{\sigma'}{\sigma}\right)^{5/3},\qquad T_c=2\pi J\sigma.$$

For the local vibration we have

$$\frac{1}{\pi}\operatorname{Im}G_{00}^{l}=\frac{1}{2\pi}\int\operatorname{Im}\left(\frac{1}{E-E_s-is}\right)\frac{1}{\pi}\frac{G^0_{0'0'}}{\Delta_s'(E_s)}df_z.$$

Since the first factor is $\delta(E - E_S)$, we obtain, using (5),

$$\Phi_0 = \gamma_1 T/T_c,$$

i.e., exactly the same expression as in the case of the quasilocal level. Substituting $\Phi_0 = \Phi_0^{ql} + \Phi_0^{l}$ into (4), we find, after iterating,

$$\sigma' \equiv \langle S_0^z \rangle = S - \gamma T / T_c, \quad \gamma = 2\gamma_1|_{\sigma'=\sigma}. \tag{6}$$

As is seen from (6), at low temperatures the magnetization of atoms lying at a dislocation falls proportionately to the first power of T/T_c, i.e., faster than in the Bloch law.

Let us now consider the magnetization at sites nearest the dislocation. According to (4),

$$\langle S_{nd}^z \rangle = S - \Phi_1 \approx \sigma - \Delta\Phi_1$$

where

$$\Delta\Phi_1 = \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{dE}{\exp(E/T)-1} \int_{-\infty}^{+\infty} \operatorname{Im} g_{11}(f_z)\, df_z,$$

$$g_{11} = \frac{JS}{\Delta_s}\left\{\left(\frac{J''}{J}-1\right)\frac{\sigma'}{\sigma}f_z^2 + \left(\frac{J'}{J}-1\right) - \left(\frac{J'}{J}-1\right)\left[1-\frac{1}{8}\left(\frac{J''}{J}-1\right)\frac{\sigma'}{\sigma}f_z^2\right]\eta + \frac{1}{4}\left(\frac{J'}{J}-1\right)\eta^2\right\}(G_{01}^0)^2$$

$$\eta = 2 - \frac{E}{4J\sigma} + \frac{1}{2}f_z^2$$

(see[3]). In our approximation we have Im $g_{11} = 0$ near the lower boundary of an ideal crystal; hence

$$\langle S_{nd}^z \rangle = \sigma,$$

i.e., the magnetization of the sites next to the dislocation coincides with the magnetization of the atoms of the ideal matrix. This justifies the assumption made earlier in determining the strictly energetic part of V.

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[1] I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **17**, 1017, 1076 (1947); **18**, 293 (1948); UMN **7**, 170 (1952); Nuovo Cimento **3**, Suppl. **4**, 716 (1956).

[2] Kh. I. Pushkarov, Vestnik MGU (in press).

[3] Kh. I. Pushkarov, A. M. Savchenko, and V. V. Tarasenko, Zh. Eksp. Teor. Fiz. **54**, 571 (1968) [Sov. Phys.-JETP **27**, 307 (1968)].

[4] A. I. Akhiezer, V. G. Bar'yakhtar, and S. V. Peletminskiĭ, Spinovye volny (Spin Waves), "Nauka", 1967.

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