

LOW TEMPERATURE PROPERTIES OF THE ANISOTROPIC FERROMAGNET

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A new model of anisotropic Heisenberg ferromagnet is examined by the Green's function method in the low temperature case. Magnetization evaluated up to  $T^4$  shows renormalization of Dyson's coefficients due to the anisotropy. Zero point deviations and energy gap are calculated too.

The anisotropic Heisenberg ferromagnet receives great attention recently, because it is evident now, that even in the systems which could be treated as isotropic, there always remains a certain degree of anisotropy, which has to be taken into account at low temperatures.

We studied the low temperature behaviour of the specific anisotropic model proposed by Belorizky et al.<sup>1,2)</sup>, which describes a system of magnetic ions on the simple cubic lattice with the ground state  $\sqrt{6}$  or  $\sqrt{7}$  doublet. For  $C_{4h}$ ,  $C_{4v}$ ,  $D_4$  or  $D_{4h}$  symmetry of the bond, introducing pseudo spin 1/2, the most general Hamiltonian of the system in the absence of anisotropy field, but in an external magnetic field  $\mathcal{H}$  in z-direction, is given by

$$H = -J \sum_{\vec{n}, \vec{m}} \hat{S}_{\vec{n}}^x \hat{S}_{\vec{m}}^x + J' \sum_{\vec{n}} \sum_r \hat{S}_{\vec{n}}^r \hat{S}_{\vec{n}+\vec{a}_r}^r - g\mu_B \mathcal{H} \sum_{\vec{n}} \hat{S}_{\vec{n}}^z \quad (1)$$

$r = x, y, z.$

$\vec{a}_r$  denotes the lattice vector connecting the given site with its nearest neighbour along r-axis. We considered only the ferromagnetic configuration of the ions<sup>1,2)</sup> which appears for  $J > 0, |J'| < J$ , in the limit  $\frac{J'}{J} = \delta \ll 1$ .

In the case of low temperatures, it is sufficient to

work with the Dyson-Maleev boson representation for spin operators<sup>3,4)</sup> in order to obtain the magnetization up to  $T^4$ . The Hamiltonian expressed in terms of Bose operators was used to obtain the system of the equations for boson Green's functions  $\langle\langle B_{\vec{k}}^+ | B_{\vec{k}}^+ \rangle\rangle$  and  $\langle\langle B_{-\vec{k}}^+ | B_{\vec{k}}^+ \rangle\rangle$ . Higher order GF were decoupled in the linear approximation, for example:

$$\langle\langle B_{\vec{z}}^+ B_{\vec{\beta}} B_{\vec{k}+\vec{z}-\vec{\beta}} | B_{\vec{k}}^+ \rangle\rangle \approx \langle B_{\vec{z}}^+ B_{\vec{z}} \rangle (\delta_{\vec{k},\vec{\beta}} + \delta_{\vec{z},\vec{\beta}}) \langle\langle B_{\vec{k}}^+ | B_{\vec{k}}^+ \rangle\rangle + \langle B_{\vec{\beta}} B_{-\vec{\beta}} \rangle \delta_{\vec{k},-\vec{z}} \langle\langle B_{-\vec{k}}^+ | B_{\vec{k}}^+ \rangle\rangle.$$

In this way, we have obtained a set of self-consistent equations for the energy and the magnetization (calculated up to  $\delta^2$ ):

$$E(\vec{k}) = \sqrt{X_{\vec{k}}^2 - Y_{\vec{k}}^2}; \quad (2)$$

$$\begin{aligned} X_{\vec{k}} &= g\mu_B \mathcal{H} + \frac{J}{2} (\gamma_0 - \gamma_{\vec{k}}) - J'(1 - \alpha_{\vec{k}}) + \\ &+ \frac{J}{2N} \sum_{\vec{q}} \left[ \frac{X_{\vec{q}}}{E(\vec{q})} \coth \frac{E(\vec{q})}{2k_B T} - 1 \right] [M(\vec{k}, \vec{q}) - \delta M'(\vec{k}, \vec{q})] + \\ &+ \frac{J'}{2N} \sum_{\vec{q}} \frac{Y_{\vec{q}}}{E(\vec{q})} \coth \frac{E(\vec{q})}{2k_B T} (W_{\vec{k}} + 2W_{\vec{q}}); \end{aligned} \quad (3)$$

$$\begin{aligned} Y_{\vec{k}} &= J' W_{\vec{k}} - \frac{J}{N} \sum_{\vec{q}} \frac{Y_{\vec{q}}}{E(\vec{q})} \coth \frac{E(\vec{q})}{2k_B T} (\gamma_{\vec{k}+\vec{q}} - \gamma_{\vec{k}-\vec{q}} + \\ &+ 2\delta \cos(k_z - q_z)a - \delta' \alpha_{\vec{k}}); \end{aligned} \quad (4)$$

$$\delta = \frac{\langle S^z \rangle}{S} = 1 - \frac{1}{N} \sum_{\vec{k}} \left[ \frac{X_{\vec{k}}}{E(\vec{k})} \coth \frac{E(\vec{k})}{2k_B T} - 1 \right]; \quad (5)$$

where:

$$\begin{aligned} \gamma_{\vec{k}} &= \sum_{n.n.} e^{i\vec{k}\vec{n}}; \quad \alpha_{\vec{k}} = \cos k_x a + \cos k_y a; \quad W_{\vec{k}} = -\frac{1}{2} (\cos k_x a - \cos k_y a); \\ M(\vec{k}, \vec{q}) &= \gamma_{\vec{k}} + \gamma_{\vec{q}} - \gamma_0 - \gamma_{\vec{k}-\vec{q}}; \quad M'(\vec{k}, \vec{q}) = \alpha_{\vec{k}} + \alpha_{\vec{q}} - 2\cos(k_z - q_z)a - 2. \end{aligned}$$

In the approximation linear in  $\delta$  the relative magnetization  $\hat{b}$  is given by:

$$\begin{aligned} \hat{b} = & 1 - Z_{3/2}(\varepsilon)(1-\delta)S^{3/2} - \frac{3\pi}{2}Z_{5/2}(\varepsilon)(1-\frac{5}{3}\delta)S^{5/2} - \\ & - \frac{33}{16}\pi^2 Z_{7/2}(\varepsilon)(1-\frac{149}{66}\delta)S^{7/2} - \delta[Z_{1/2}(\varepsilon)Z_{5/2}(\varepsilon) + \\ & + Z_{3/2}(\varepsilon)]S^3 + \{-6\pi Z_{3/2}(\varepsilon)Z_{5/2}(\varepsilon) + \delta[\frac{5\pi}{4}Z_{1/2}(\varepsilon)Z_{7/2}(\varepsilon) + \\ & + \frac{143}{8}\pi Z_{3/2}(\varepsilon)Z_{5/2}(\varepsilon)]\}S^4 + O(S^{9/2}); \quad (6) \\ S = & \frac{k_B T}{2\pi J}; \quad \varepsilon = -\frac{g\mu_B \mathcal{H}}{k_B T}; \quad Z_p(\varepsilon) = \sum_{n=1}^{\infty} -\frac{e^{-n\varepsilon}}{n^p}. \end{aligned}$$

It can be seen that each of Dyson's coefficients has been renormalized by the anisotropy and even more important effect of the anisotropy is the appearance of the term proportional to  $T^3$ .

Anisotropic systems have interesting properties at  $T=0$  K. They manifest spin deviations, i.e.  $\hat{b} \neq 1$ , and for this model we have:

$$\Delta \hat{b}(T=0) = \frac{1}{N} \sum_{\vec{k}} \left[ \frac{X_{\vec{k}}}{E(\vec{k})} - 1 \right] = \delta^2 \frac{I_3}{(1 - I_1 + I_2)^2} \quad (7)$$

$$I_1 = \frac{1}{(2\pi)^3} \iiint_{-\pi}^{\pi} d^3v \frac{\cos^2 v_1}{3 - \sum_i \cos v_i}; \quad I_2 = \frac{1}{(2\pi)^3} \iiint_{-\pi}^{\pi} d^3v \frac{\cos v_1 \cos v_2}{3 - \sum_i \cos v_i};$$

$$I_3 = \frac{1}{(2\pi)^3} \iiint_{-\pi}^{\pi} d^3v \left( \frac{\cos v_1 - \cos v_2}{3 - \sum_i \cos v_i} \right)^2;$$

which was evaluated numerically to give  $\Delta \hat{b}(T=0) = 0.06 \delta^2$ .

Another consequence of the anisotropy is energy gap appearing for  $\vec{k} \rightarrow 0$ . In our approximation, we obtained

$$\lim_{k \rightarrow 0} E(\vec{k}) = J \cdot 0,095 \delta^2 \quad (8)$$

It is important to note that the result that the effect of the anisotropy in zero-point deviations and energy gap manifests only in second order in  $\delta$ , agrees with the results obtained by Belorizky et al.<sup>5)</sup> at least qualitatively, while the values of coefficients are different, due to the choice of another boson representation.

Recently, the whole phase diagram of the model was reproduced in the mean field approach<sup>6)</sup>, and it turned out that other region (not ferromagnetic) are very important because the only known material that can be described by this model is antiferromagnetic  $KCoF_3$  with  $T_N=114$  K, so the investigation in this direction is in progress.

#### R e f e r e n c e s

- 1) E.Belorizky, R.Casalengo, P.Fries and J.J.Niez, Jour. de Physique 39 (1978) 1305.
- 2) E.Belorizky, R.Casalengo and P.Fries, phys.stat.sol.(b) 77 (1976) 495.
- 3) F.J.Dyson, Phys.Rev. 102 (1956) 1217, 1230.
- 4) S.V.Maleev, Zh. eksper. teor. Fiz. 33 (1957) 1010.
- 5) E.Belorizky, R.Casalengo and J.J.Niez, Phys. stat.sol. (b) (1980) (to be published).
- 6) E.Belorizky, R.Casalengo, J.Sivardière, J.Magn. & Magn. Mat. 15-18 (1) (1980) 309.