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CORRELATION THEORY OF ANTIFERROMAGNET Cr_2O_3 FOR $T > T_N$

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A correlation theory is applied to two-sublattice antiferromagnet Cr_2O_3, for $T > T_N$. This theory includes pair correlation effects in a self-consistent calculation of both static and dynamic properties. The two kinds of approximations are assumed: the two-pole approximation for the relaxation function of the random force and the mode-mode decoupling procedure for the static and dynamic higher-order quantities. The formulae for the static susceptibility, line-shape function and magnetic cross-section of the inelastic neutron scattering are given for the case of a non-Bravais two-sublattice antiferromagnet.

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1. Introduction

A correlation theory was introduced by Lindgård and applied to a number of magnets: EuO, EuS [1–3] and Gd [4]. The procedure was based upon the exact Mori formalism [5]. In particular, the theory was applied to a non-Bravais, two-sublattice ferromagnet Gd. In the present work we apply this approach to a non-Bravais, two-sublattice antiferromagnet Cr_2O_3. In the general case the frequency spectrum does not consist of δ-functions because one must include pair correlation effects in a self-consistent calculation of both static and dynamic properties. These effects are taken into account by the above mentioned correlation theory. The basic approximation involved is the use of mode–mode coupling [6] of the self-consistently calculated damped and renormalized spin excitation modes. Cr_2O_3 is non-Bravais crystal, therefore the problem of calculating the static and dynamic properties is more complicated than in the case of the ideal systems such as the Heisenberg ferromagnets EuO and EuS. Finally, we obtain simple formulae for the dynamic relaxation function and for the cross-section of magnetically scattered neutrons. These functions were also calculated in the random phase approximation (RPA) which is a useful zero-order approximation for the correlation theory.

2. The Hamiltonian of the system

For the two sublattices we define inter and intra-sublattice Fourier transformed interactions $J(q)$ and $J'(q)$, respectively, $J(q) = J^*(q)$ but $J'(q)$ may be different from $J'^*(q) = J'(-q)$ [7]. It is further convenient to introduce the so-called uniform and staggered Fourier transformed variables U_q and V_q as

$$U_q^\alpha = \frac{1}{\sqrt{2}}\left[S_A^\alpha(q) + \eta_q^* S_B^\alpha(q)\right], \quad V_q^\alpha = \frac{1}{\sqrt{2}}\left[S_A^\alpha(q) - \eta_q^* S_B^\alpha(q)\right], \tag{1}$$

where $\eta_q = J'(q)/\left|J'(q)\right|$.

In terms of these we can write the Fourier transformed Hamiltonian as

$$H_0 = -\sum_q J^+(q) U_q U_{-q} - \sum_q J^-(q) V_q V_{-q}. \tag{2}$$

where $J^\pm(q) = J(q) \pm \left|J'(q)\right|$ and each subsystem can be discussed separately.

3. The total susceptibility

In the correlation theory we then obtain the susceptibility

$$\chi_u^z(q) = (U_q^z U_{-q}^z) = \frac{1}{R_q^+ - 2J^+(q)}, \tag{3}$$

$$\chi_v^z(q) = (V_q^z V_{-q}^z) = \frac{1}{R_q^- - 2J^-(q)}. \tag{4}$$

The parameters $R_q^\pm$ are expressed by the correlation functions $\langle U_q^z U_{-q}^z\rangle$ and $\langle V_q^z V_{-q}^z\rangle$ which are calculated in the two-pole approximation. The physical meaning of $R_q^\pm$ is that of an inverse susceptibility for a small cluster. This may be q-dependent. In RPA the small cluster is just the single ion. For $T > T_{\mathrm{N}}$, $R_q^+ = R_q^- = A(T)$ is obtained from the sum rule neglecting dynamical corrections, which corresponds to the spherical model.

4. Dynamical properties

In order to obtain the line shape with a finite line width we must solve an exact Mori equation [5] for the frequency dependence of the Laplace-transformed dynamical relaxation function. Then we can obtain the expression for the dynamic relaxation function (line shape) in the two-pole approximation

$$F(q,\omega) = \frac{1}{\pi}\frac{2\beta_q a_q^2}{(\omega^2 - a_q^2)^2 + 4\beta_q^2\omega^2}, \quad a_q^2 = \alpha_q^2 + \beta_q^2 \tag{5}$$

and the static correlation function

$$\langle U_q^z U_{-q}^z\rangle = \chi_u^z(q)\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{2\beta_q a_q^2 \omega \,\mathrm{d}\omega}{\left[(\omega^2 - a_q^2)^2 + 4\beta_q^2\omega^2\right]\left[1 - \exp(-\beta\omega)\right]}. \tag{6}$$

The $\langle V_q^z V_{-q}^z\rangle$ is obtained from Eq. (6) where now $\chi_u^z(q)$ is inserted instead of $\chi_v^z(q)$. We have two parameters: β_q (the damping parameter) and a_q which depend on the wave vector q and temperature. These parameters are determined using equations which are considered in the correlation theory within the two-pole approximation. (All the equations of this theory are given for example in Ref. [8].) The magnetic cross-section for $T > T_N$ is in the form [9]:

$$\left(\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E}\right)^{\mathrm{para}}_{\mathrm{Cr_2O_3}} = \frac{2}{\hbar}\left(\frac{g_N e^2}{m_e c^2}\right)^2 \left[\frac{1}{2}gf(\kappa)\right]^2 \frac{k'}{k_0}\frac{\hbar\omega}{1-\exp(-\hbar\omega\beta)}$$

$$\times\frac{N_0}{g^2\mu_B{}^2}\left\{\chi^z_u(q)+\chi^z_\nu(q)+\frac{1}{2}(\eta_{\tilde{\kappa}}+\eta_{-\tilde{\kappa}})[\chi^z_u(q)-\chi^z_\nu(q)]\right\}$$

$$\times\frac{1}{\pi}\frac{2\beta_q a_q^2}{(\omega^2-a_q^2)^2+4\beta_q^2\omega^2}, \tag{7}$$

where $\boldsymbol{\kappa} = \boldsymbol{k}_0 - \boldsymbol{k}'$ is the change of the neutron wave vector from $\boldsymbol{k}_0$ (incident beam) to $\boldsymbol{k}'$ (scattered beam) and $\tilde{\kappa} = \boldsymbol{\kappa}/|\boldsymbol{\kappa}|$ is the unit vector in the direction $\boldsymbol{\kappa}$. From the above formula we see that in this case we must consider a single line-shape function with the parameters β_q and a_q which corresponds to uniform mode (or the staggered mode) and the total susceptibility consisting of the susceptibility connected with the uniform and staggered ones.

5. Discussion

The magnetic cross-section of inelastic neutron scattering is expressed as a product of the total susceptibility $\chi(q)$ and only one line-shape function $F(q,\omega)$. It has a simple form from the experimental point of view. Looking at formula Eq. (7) we see that the total susceptibility is expressed through the uniform and staggered susceptibility. In the paper [10] the anomaly of the magnetic susceptibility of Cr_2O_3 was investigated using different approximations. The growth of $\chi(q=0)$ above T_N up to about 340 K cannot be explained by the correlation theory within the two-pole approximation, similarly as in the case of RPA and Oguchi methods. Calculated values of $\chi(q=0)$ in the case of the present correlation theory are about two percent higher than in the case of RPA method.

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