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Objekttyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **62 (1989)**

Heft 6-7

PDF erstellt am: **21.09.2024**

Persistenter Link: https://doi.org/10.5169/seals-116073

Helvetica Physica Acta
Vol. 62 (1989)
0018-0238/89/070735-05$1.50+0.20/0

Critical and paramagnetic spin fluctuations in Heisenberg ferromagnets.

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Abstract

A mode coupling theory which takes full account of the lattice structure and the extended range of the exchange interactions has been used to evaluate the critical and paramagnetic spin correlation functions in several ferromagnetic compounds. The comparison of the theoretical results with the experimental neutron scattering data for EuO, EuS and Pd_2MnSn leads us to conclude that the mode-coupling theory gives an adequate description of the spin dynamics in the disordered phase.

1. Introduction

In recent years a number of papers have reported results of neutron scattering experiments on isotropic ferromagnets in the paramagnetic phase. The high quality of the experimental data offers the possibility to distinguish among the different theoretical predictions and to resolve the distinctive features of each material. A resurgence of theoretical studies on the dynamics of paramagnetic spin fluctuations has been prompted by debate of the features displayed in the new experimental data.

The ferromagnetic materials most frequently used in neutron scattering experiments are the europium compounds EuO and EuS, the Heusler compound Pd_2MnSn and the $3d$ metals Fe and Ni. The europium compounds are good realizations of localized moment ferromagnets [1]; their magnetic lattice structure is fcc and the magnetic interaction is restricted to first and second neighbours. The Heusler compound Pd_2MnSn is an fcc ferromagnet and neutron scattering data on this compound at low temperature appear to be well described by a Heisenberg hamiltonian, but longer range interactions,

up to the eight neighbour, must be considered [2]. Finally Fe is a bcc ferromagnet and the possibility to describe its magnetic properties by an effective Heisenberg hamiltonian is argument of current debate [3].

2. Theory

The static and dynamical properties of the localized moment ferromagnets are usually analyzed in terms of the Heisenberg hamiltonian:

$$H = -\frac{1}{2}\sum_{ij} J_{ij}\vec{s}_i \cdot \vec{s}_j - h\sum_i s_i^z \tag{1}$$

The theoretical task is the evaluation of the normalized Kubo relaxation function:

$$F_q^\alpha(t) = \chi_q^{-1}\int_0^\beta d\lambda(< S_q^\alpha(S_q^\alpha(t+i\lambda))^\dagger >) \tag{2}$$

whose Fourier transform is connected to the frequency and wave vector dependent fluctuation spectrum $S(q,\omega)$ - which is the quantity observed in inelastic magnetic neutron scattering experiments - by the fluctuation-dissipation theorem:

$$S(q,\omega) = \frac{\omega}{1-exp(-\frac{\omega}{k_B T})}\chi_q F_q(\omega) \tag{3}.$$

In eq.(2) $S_q^\alpha(t) = s_q^\alpha(t) - < s_q^\alpha >$, where s_q^α is the Fourier transform of the spin variables, $\beta = \frac{1}{T}$ and χ_q is the isothermal susceptibility.

The time evolution of the relaxation function can be derived from a generalized Langevin equation:

$$\partial_t F(t) = i\omega_q F_q(t) - \int_0^t dt' M_q(t-t')F_q(t') \tag{4}$$

where ω_q is the RPA precession frequency and $M_q(t)$ the memory function.

A satisfactory description of the dynamical behaviour of ferromagnetic systems in the ordered phase has been achieved developing a perturbative approach, but such technique cannot be extended in the critical and paramagnetic regions, because as $T \to T_c$, $\omega_q \to 0$ and we have no more an unperturbed parameter which sets the scale of energy. At the critical point and for long wave length fluctuations the renormalization group technique provides a rigorous prescription of both static and dynamic events. However the results cannot be unambiguously extended to the paramagnetic state and to high wave vectors.

The approximate theories proposed up to now to evaluate the memory function in the paramagnetic phase are a "three pole approximation" and the mode-coupling theory.

The "three-pole approximation" [4] truncates the continued fraction expansion of the Laplace transform of $F_q(t)$ at the third stage, namely:

$$F_q(\omega) = \frac{1}{\pi} \frac{\tau_q \delta_{1q} \delta_{2q}}{\left[\omega \tau_q (\omega^2 - \delta_{1q} - \delta_{2q})\right]^2 + (\omega^2 - \delta_{2q})^2} \tag{5}$$

The parameters δ_{1q} and δ_{2q} are related to the second and fourth frequency moments of $F_q(\omega)$, and therefore can be approximately evaluated from the known exchange interaction constants; τ_q can be expressed by a function of δ_{2q} [5]. The three poles approximation has proved to be very useful to interpret experimental data [5,6,7], expecially when it is used as a fitting function with δ_{1q} and δ_{2q} as free parameters.

The mode-coupling theory [8] gives a more satisfactory approach to the study of spin fluctuations in the paramagnetic phase. It gives the correct dynamical critical behaviour not only for an isotropic Heisenberg ferromagnet, but it also explains the line-shape modifications at very small q, observed in neutron spin-echo experiments, due to the onset of the dipolar interaction [9].

The mode coupling approximation leads to the following nonlinear equation for the spin relaxation function in an isotropic ferromagnet:

$$\partial_t F_q(t) = -2T \sum_k (J_k - J_{q-k})(J_k - J_q)\chi_k \int_0^t dt' F_k(t-t') F_{q-k}(t-t') F_q(t') \tag{6}$$

The use of the mode-coupling theory to interpret neutron scattering data collected out of the critical region, i.e. for high wave-vectors and temperatures, was up to now prevented by the fact that the known solutions of eq. (6) are obtained either analytically, for asymptotically small q [10], or numerically, but only for a simple cubic lattice with magnetic interactions restricted to nearest neighbours [8].

In a recent paper [11] we have described in detail a method to obtain a numerical solution of eq. (6) for the fcc real magnetic lattice of europium compounds, in order to interpret experimental data. Later work extended the calculation to all three cubic lattices and interactions up to ten shells of neighbouring magnetic ions.

3. Results

The comparison of the theoretical line shape derived from mode coupling theory with the experimental data on europium compounds shows a very good agreement

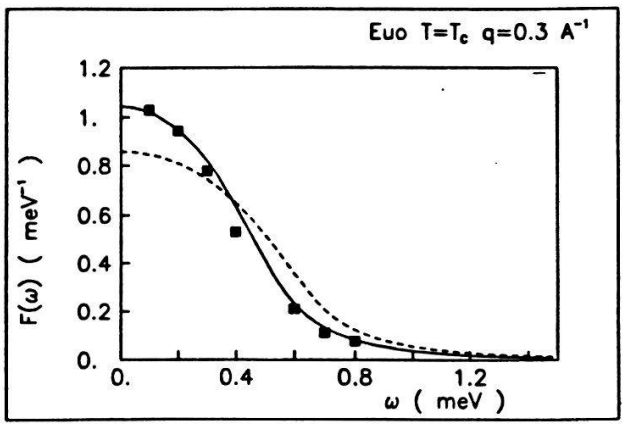

Fig. 1 Experimental data reported in [12] for EuO at its critical temperature and $0.3\ \AA^{-1}$ are compared with results of the mode coupling approximation. The dashed curve is the result for a simple cubic lattice, and it demonstrates the influence of the lattice structure on the dynamic properties even at relatively long wavelengths.

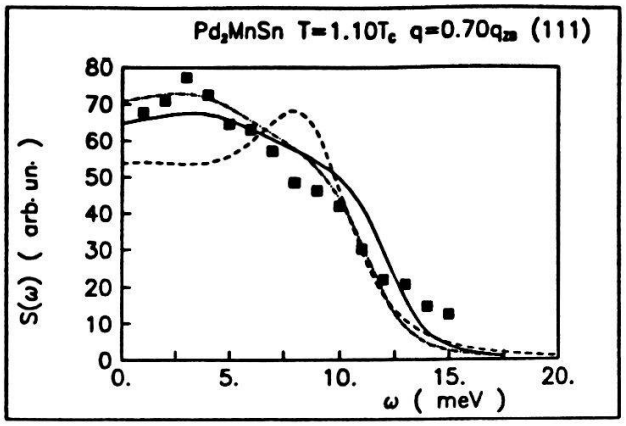

Fig. 2 Experimental data [7] for the Heusler compound Pd_2MnSn at $T = 1.1\ T_c$ and $q = 0.7 q_{ZB}$ in the (111) direction are shown together with results from theoretical calculations. The solid and dash-dot curves are mode coupling calculations with six and eight shells of neighbours, respectively, and the dashed curve is the theoretical three pole approximation. Calculated spectra are convoluted with a resolution function.

throughout the disordered phase [11].

In fig. 1 the theoretical curve for EuO is shown together recent high resolution neutron scattering data by Mezei et al. at $T = T_c$ [12]; the importance of the lattice structure and range of interactions is apparent. Only for very small wave vectors and at the critical temperature, i.e. well within the critical region, is the line shape predicted by the mode coupling theory for an isotropic ferromagnet substantially different from that one observed in spin echo experiments. This puzzle can be solved within the framework of mode coupling theory if the dipolar interaction is taken into account [9]. The most interesting features displayed by the solution obtained for EuS is the change of the line shape at the zone boundary as the direction of the wave vectors is varied.

The numerical solution of eq. (6) for Pd_2MnSn has been obtained using six or all the eight exchange constants obtained in [2] by fitting the spin wave spectra. The comparison with the experimental data for intermediate wave vector is reported in fig. 2, which shows that the mode coupling line shape reproduces the experimental data much better than a theoretical three pole function.

The tolerable agreement obtained for the metallic compound Pd_2MnSn prompted us to solve the mode coupling equation also for an effective Heisenberg hamiltonian proposed in literature to model bcc iron. The calculation has shown that different sets of

exchange parameters, which give comparable macroscopic properties, such as the critical temperature or the spin wave stiffness constant, give spectra which differ significantly both in the energy width and in the shape. The most interesting result has been obtained by using the effective hamiltonian derived in [13] from a theoretical calculation. The calculated spectra are almost entirely confined below $100meV$ and the shape of the spectra do not change appreciably with wave vector in the second half of the range in the (011) and (111) directions; these results are in qualitative agreement with experimental observations [14].

4. Conclusions

Mode coupling theory is useful for describing quantitatively the neutron scattering spectra at intermediate and high wave vectors in the entire paramagnetic region. Also the dynamical behaviour of metallic compounds can be described by Heisenberg hamiltonian if long range interactions are taken into account. New experiments can be devised to test the theoretical predictions and to obtain a better description of the magnetic interactions in the paramagnetic region.

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