NUMERICAL STUDIES OF THE COLLECTIVE EXCITATIONS OF Rb2MnxCr1-xCl4 MIXED CRYSTALS
D. Sieger, W. Ching, D. Huber, R. Geick

To cite this version:
D. Sieger, W. Ching, D. Huber, R. Geick. NUMERICAL STUDIES OF THE COLLECTIVE EXCITATIONS OF Rb2MnxCr1-xCl4 MIXED CRYSTALS. Journal de Physique Colloques, 1988, 49 (C8), pp.C8-1021-C8-1022. <10.1051/jphyscol:19888465>. <jpa-00228666>

HAL Id: jpa-00228666
https://hal.archives-ouvertes.fr/jpa-00228666
Submitted on 1 Jan 1988

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
NUMERICAL STUDIES OF THE COLLECTIVE EXCITATIONS OF Rb$_2$Mn$_{x}$Cr$_{1-x}$Cl$_4$ MIXED CRYSTALS

D. Sieger (1), W. Y. Ching (2), D. L. Huber (3) and R. Geick (4)

(1) Physikalisches Institut Universität Würzburg, D-8700 Würzburg, F.R.G.
(2) Department of Physics, University of Missouri-Kansas City, Kansas City, Missouri 64110, U.S.A.
(3) Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, U.S.A.

Abstract. - The spin dynamics of the random quasi-two-dimensional magnetic system Rb$_2$Mn$_x$Cr$_{1-x}$Cl$_4$ has been studied by a computer simulation employing the equation-of-motion method. The resulting $S(q, \omega)$ data correspond qualitatively to the experimentally observed excitation frequencies of wavelike magnons and cluster modes. The disorder effects can be related shown to the classical equilibrium configuration.

Rb$_2$Mn$_x$Cr$_{1-x}$Cl$_4$ is a random quasi-two-dimensional magnetic system with competing exchange interactions and competing anisotropies leading to disorder and frustration effects. For intermediate concentrations $x \cong 0.5$, Rb$_2$Mn$_x$Cr$_{1-x}$Cl$_4$ shows spin glass behaviour. For concentrations $x > 0.6$, the systems exhibit random antiferromagnetic behaviour, and for $x < 0.4$ random ferromagnetic behaviour. For all these cases, there is no well defined ground state. Of particular interest are the magnetic excitations in this system.

Numerical calculations, using the equation-of-motion method [1] have been performed for $x = 0.70, 0.59, 0.25$. Samples of Rb$_2$Mn$_x$Cr$_{1-x}$Cl$_4$ with these concentrations have previously been investigated by inelastic neutron scattering [2].

For calculating the excitations with the equation-of-motion method we have assumed the Hamiltonian to be of the Heisenberg form.

$$H = -\frac{1}{2} \sum J_{jk} S^j S^k.$$ (1)

Were $J_{jk}$ are the exchange constants with values known from experiments [2] and $S^j$ the spins ($j = 1, \ldots, N$).

The ground state was calculated for a $40 \times 40$ spin array with a statistical distribution of Mn and Cr ions on the lattice sites according to the concentration under consideration. Classical equilibrium spin configurations were obtained [3] by successively rotating the spins into the directions of their local fields until the total energy stabilizes to 1 part in 100 million.

For the calculation of the excitations, we consider the spin operators with the quantisation axes ($z$-axis) in the directions of the equilibrium spin orientations introducing thus a local Cartesian coordinate system for each ion. Then linearized equations of motion for the spin operators are derived by treating deviations of the spin operators from the classical equilibrium orientations as small quantities. Essentially, what is done is to make Holstein-Primakoff expansions in the local coordinate system. By expressing the spin–spin correlation function in the form of a Green’s function, the dynamic structure factor can be calculated on the basis of the microscopic properties of the Hamiltonian of our mixed systems. The operator equations of motion are used to obtain equations of motion for the Green’s functions which are then integrated numerically. The dynamic structure factor can then be expressed as a linear combination of the Fourier transform of the time dependent Green’s functions.

For all three samples ($x = 0.25, 0.59, 0.70$) the experimentally determined excitation spectrum shows spin wave branches which are almost the same as for the pure end members and, in coexistence with them in the same frequency range, dispersionless cluster modes. The reason for this behaviour are disorder-induced frustration effects which can be visualized already from the ground state. Figure 1 shows an example of a calculated ground state ($10 \times 10$ array, ferromagnetic sample, $x = 0.25$). It is evident, there are regions with well defined ferromagnetic order and areas with highly disordered spins (bottom side in Fig. 1).

![Fig. 1. A part (10 x 10 array) of the calculated ground state of Rb$_2$Mn$_{0.25}$Cr$_{0.75}$Cl$_4$ in the $S_x$, $S_y$-plane showing ordered and disordered spin regions. Mn-ions denoted as circles and Cr-ions as crosses.](http://dx.doi.org/10.1051/jphyscol:19888465)
This disordered area which is decoupled from the ordered regions is the source of the dispersionless modes whereas the wave-like magnon is based on the ordered region.

In figure 2 the calculated dynamical structure factor (also for $x = 0.25$ and for several reduced wavevectors $q$) is plotted versus the energy. For each wavevector, we have extracted the peaks and shoulders (see arrows in Fig. 2) as the center frequencies of the various excitations. For comparison, these data are shown as crosses within the experimentally determined dispersion relations (dots).

Within the experimental errors, there is a fairly good agreement of the calculated points with the experimental data. Both theory and experiment give dispersionless modes in coexistence with a ferromagnetic spin wave branch, of nearly the same dispersion as in pure Rb$_2$CrCl$_4$.

For the antiferromagnetic and spin glass samples the correspondence between theory and experiment is similar.

Hence, we may conclude that the experimentally observed excitation spectrum can be calculated numerically from a harmonic model and that both the spin waves and the cluster modes are linear excitations.

Fig. 2: Numerically calculated dynamical structure factor $S(Q, \omega)$ for Rb$_2$Mn$_{0.25}$Cr$_{0.75}$Cl$_4$ at several reduced wavevectors $q$.

Fig. 3: Dispersion relation of Rb$_2$Mn$_{0.25}$Cr$_{0.75}$Cl$_4$ showing experimental points (dots) and calculated points (crosses).

Acknowledgements

Two of us (D. S., R. G.) acknowledge financial support of the German Fed. Minister for Research and Technology under contract number 03-Ge1Wue-6.