o.m5.o1 Structural aspects of low-dimensional magnetic and electronic crystals.

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Low-dimensional metals may exhibit a phase transition at T_{CDW} towards a Charge-density wave (CDW) state at low temperatures. The CDW modulation at q,? = 2k,? $_F$ is often incommensurate, because the Fermi wavevector k,? $_F$ is not necessarily related to the lattice periodicities of the average structure. The CDW in the conduction band is coupled to a displacement wave of the atomic positions. Accordingly x-ray scattering and structure analysis can be used to study the CDW state.

Crystals with localized magnetic moments may transform from a paramagnetic state at high temperatures towards a state with ferromagnetic or anti-ferromagnetic order at low temperatures. The magnetic order is not accompanied by a structural distortion. In low-dimensional magnets, several types of states with magnetic order may form. One is the spin-Peierls state, in which structural distortions are responsible for the magnetic order. Furthermore, it has been found that in many of these materials, magnetic order is related to charge-order. Again, the latter is connected with structural distortions. In both instances, x-ray scattering provides information on the nature of the ordered states.

Here, we will give a brief overview of the superspace approach as a tool to study both incommensurate and commensurate superstructures. Several ecamples are presented. For the 1D CDW crystal $NiTa_2Se_7$ it will be shown that the x-ray structure provides essential information on the character of the primary and secondary components of the CDW. The 2D CDW in the phosphate bronzes $(PO_2)_4(WO_3)_{2m}$ will be discussed[1]. The CDW state will be characterized, and the relation between the two phase transitions will be discussed. Finally, the implications will be analysed of the the low-temperature superstructure of the 2D magnet NaV_2O_5 for the understanding of the phase transition and of the properties of the low-temperature phase[2,3]. It will be shown that the superspace approach was essential to solve this simple - fold superstructure.

[1] Lüdecke J. Jobst, A. and van Smaalen S. "The CDW structure of the m = 4 phosphate bronze $(PO_2)_4(WO_3)_{2m}$", Europhys. Lett. (2000) **49**: 357-361.
[2] Van Smaalen, S. "Structural aspects of spin-chain and spin-ladder oxides", Z. Kristallogr. (1999) **214**: 786-802.
[3] van Smaalen S. and Lüdecke J. "The valence states of vanadium in the low-temperature superstructure of NaV_2O_5", Europhys. Lett. (2000) **49**: 250-254.

o.m5.o2 The fiel induced soliton lattice in CuGeO.

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The spin-Peierls materials provide an interesting example of a non-trivial coherent quantum ground state. The magneto-elastic coupling to the 3D lattice allows an S = 1/2 chain to form a non-magnetic ground state of dimerized spin singlets. This is the case in $CuGeO_3$, where below T_{sp} = 14 K the S = 1/2 Cu ions dimerize long the crystallographic c-direction, producing satellite reflections at (1/2,1,1/2)-type reflections. Though most of the predictions for a spin-Peierls material have been verified experimentaly, the exact form of the microscopic model in terms of phonon-interactions and second neighbour and inter-chain magnetic interactions .

This makes it interesting to investigate the high-field phase, for which the predictions depend only on the spin-wave velocity v_s and spin-excitation gap Δ_0, both of which can be determined xperimentally with-out assumptions about the microscopic model. The high-field phase at H_c = 12.5 T is reached when the magnetic field becomes strong enough to break a dimer-bond. The two S = 1/2 spins of a broken dimer will be smeared and repel each other to form an incommensurate soliton lattice.

At HMI, Germany, we have performed neutron scattering studies of the magnetic soliton structure in $CuGeO_3$, using a 14.5 T cryomagnet[1]. The incommensurability is in perfect agreement with the soliton theory. The occurrence of odd and even harmonics enabled us to test the analytic solution for the soliton structure (see below). The amplitudes m_u = 0.097(3) and m_s = 0.019(3) of respectively the uniform and the staggered components agree with theory . The rapid decrease of the soliton width Γ just above Hc is not contained in the theory, but the minimum value Γ = 9.2c is consistent with field theory, and the slow increase at higher fields has been observed in density matrix calculations.

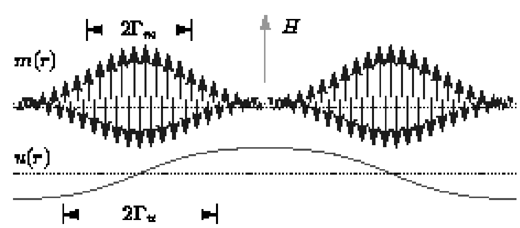

Fig. 1: One period of the soliton structure as etermined by neutron diffraction. The maximum amplitude of the magnetic structure corresponds to 0.1 μ_B.

[1] H. M. Rønnow, M. Enderle, D. F. McMorrow, L.-P. egnault, G. Dhalenne, A. Revcolevschi, A. Hoser, K. Prokes, P. Vorderwisch nd H. Schneider, ``Neutron scattering study of the field-induced soliton lattice in $CuGeO_3$", To appear in Phys. Rev. Lett.