Available online at www.sciencedirect.com
SCIENCE DIRECT
ELSEVIER
Journal of Magnetism and Magnetic Materials 272–276 (2004) e647–e648
Journal of magnetism and magnetic materials
www.elsevier.com/locate/jmmm

Magnetic order and moment distribution in doped spin-chain systems

Sebastian Eggert[a,*], Ian Affleck[b]

[a] Institute of Theoretical Physics, Chalmers University of Technology, S-412 96 Göteborg, Sweden
[b] Department of Physics, University of British Columbia, Vancouver, BC, V6T 121 Canada

Abstract

We consider the effect of doping on the magnetic order in quasi one-dimensional (1D) antiferromagnets. First the detailed magnetic response of finite spin-$\frac{1}{2}$ chains in the presence of a staggered field is determined, which by itself shows an interesting crossover as function of length and field strength. We can then understand the ordering by including an effective coupling between the chains, which results in a Néel-ordered phase at low temperatures, but with a broad distribution of magnetic moments that has to be determined self-consistently.

PACS: 75.10.Jm; 75.20.Hr

Keywords: Spin chain; Antiferromagnetic order; Impurity

Doping and impurity effects in low-dimensional antiferromagnets remain of strong interest in the condensed matter physics community, spurred by high-T_c superconductivity and other exotic effects in those systems. Typically, antiferromagnetic three-dimensional Néel order does exist at extremely low temperatures, but is easily destroyed in such systems by a combination of quantum fluctuations, temperature fluctuations, and disorder effects. In this paper, we study how static impurities affect the Néel order in quasi-1D antiferromagnets, which are modelled by spin-$\frac{1}{2}$ chains with a weak coupling $J' \ll J$ to the neighboring chains $\vec{\delta}$ (before doping)

$$H = \sum_{j,\vec{y}} \left(J\vec{S}_{j,\vec{y}} \cdot \vec{S}_{j+1,\vec{y}} + \sum_{\vec{\delta}} J'\vec{S}_{j,\vec{y}} \cdot \vec{S}_{j,\vec{y}+\vec{\delta}} \right).$$

In uncoupled chains, it is known that long-range antiferromagnetic order is destroyed by quantum fluctuations even at $T = 0$, which results in antiferromagnetic correlations that decay with a powerlaw. However, a staggered field B can easily induce alternating order $m_{\text{alt}} = 1/L \sum_j (-1)^j \langle S_j^z \rangle$ throughout the sample since the staggered susceptibility diverges at $T = 0$ [1].

In the case of quasi-1D antiferromagnets the coupling to the neighboring chains plays the role of an effective staggered field from the antiferromagnetic background $B = zJ'm_{\text{alt}}$, which always implies an ordered state at $T = 0$ [1]. Here, z is the number of neighboring chains. Note, that the effective field neglects quantum fluctuations between neighboring chains, but within each chain we are able to determine the alternating moment by a full quantum mechanical solution $m_{\text{alt}}(B)$. We can then study the ordered state by solving the effective field equation self-consistently for a non-zero solution m

$$m = m_{\text{alt}}(zJ'm). \tag{1}$$

For the undoped case it is known that the alternating magnetization is given by a scaling law $m_{\text{alt}}(B) = aB^{1/3}$ up to logarithmic corrections [2], which results in $m = a^{2/3}\sqrt{zJ'}$ [3] in good agreement with experiments [4].

In a doped system the impurities effectively cut the chain at low temperatures [5]. It is therefore necessary to calculate the alternating moment for finite chains and average over the disorder in order to arrive at a

*Corresponding author. Tel.: +46-31-772-3190; fax: +46-31-772-3204.
E-mail address: eggert@fy.chalmers.se (S. Eggert).

0304-8853/$ - see front matter
doi:10.1016/j.jmmm.2003.12.1088

self-consistent distribution of moments m in Eq. (1). Previous results have shown that finite chains have a different staggered susceptibility as a function of T depending if they contain an even or odd number of spins [6], which can be traced to the contribution of the zero-modes in the correlation functions [7]. Moreover, it has been found that the response is lower for finite chains which yields a distinct drop of the Néel temperature with increased doping [6] in agreement with existing experiments [4]. The undoped value of T_N scales roughly with J' [1] up to logarithmic corrections which we have quantitatively determined to give $0.6 \lesssim T_N/zJ' \lesssim 1$ in the range $0.1 > J'/J > 0.00001$.

The alternating moment in a finite field at $T = 0$ in Fig. 1 shows again a distinct difference between even and odd chains and obeys a scaling behavior of the form

$$m_{\mathrm{alt}}(B) = L^{-1/2} f(L^{1/2} B^{1/3}) \tag{2}$$

in agreement with a dimensional scaling analysis. Assuming a sharp distribution of lengths $L \approx 1/p$ Eq. (2) also implies a scaling form for the average alternating moment

$$m = L^{-1/2} g(zJ'L). \tag{3}$$

The low doping limit $\lim_{x\to\infty} f(x) \to ax$ recovers the $B^{1/3}$ scaling behavior with a length-independent solution for $m = a^{2/3}\sqrt{zJ'}$, which we see as a sharp peak in the moment distribution for low doping levels in the inset of Fig. 1. For larger doping p we expect a broader distribution, but the difference between even and odd chains also becomes important. The self-consistent solution to Eq. (1) shows two distinct peaks corresponding to the even and odd chain segments as displayed in the inset of Fig. 1. Interestingly, the peak for the odd chains shifts to higher moments (increased order parameter) as the doping increases, even though the Néel temperature is known to drop. In fact we know from Fig. 1 that $m_{\mathrm{alt}} \propto L^{-1/2}$ diverges for short odd chains. However, in that limit quantum fluctuations between the shorter chains also become more important so it is not clear if this exotic "increased order from disorder" effect is robust or if the order parameter always decreases with increasing doping. Qualitatively, however, the peak will indeed split for larger doping $p \gtrsim zJ'/10$ and the shape of the distributions in the inset is adequate, except for a doping dependent rescaling of m.

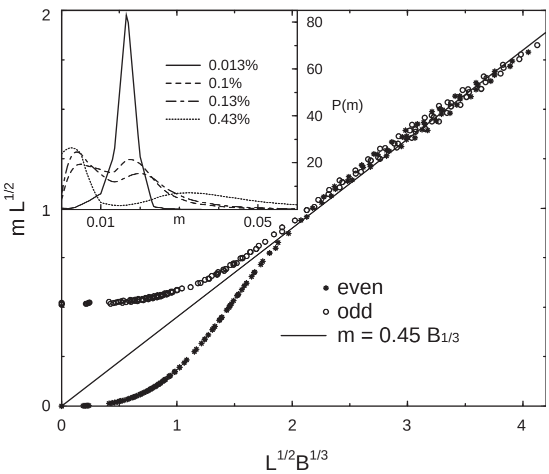

Fig. 1. The alternating magnetization as a function of staggered magnetic field B and length L from numerics for open chains with $L \leqslant 27$ and $B \leqslant 0.5J$. Inset: The corresponding distribution of moments in units of $\hbar g\,\mu_B$ according to Eq. (1) for $J' = 0.0008J$. The non-uniform distribution of m along the chains was taken into account by including the known behavior near the edges [6,8].

In summary, we have studied the doping dependence of the Néel ordered phase at $T = 0$ in quasi-1D antiferromagnets and showed explicitly how the order parameter is modified in the presence of static disorder. The distribution of the magnitude of alternating moments broadens with doping and we find a characteristic double peak structure for $p \gtrsim zJ'/10$.

References

[1] Y. Imry, D. Pincus, D. Scalapino, Phys. Rev. B 12 (1975) 1978.
[2] I. Affleck, M. Oshikawa, Phys. Rev. B 60 (1999) 1038.
[3] I. Affleck, M.P. Gelfand, R.R.P. Singh, J. Phys. A 27 (1994) 7313.
[4] K.M. Kojima, et al., Phys. Rev. Lett. 78 (1997) 1787.
[5] S. Eggert, I. Affleck, Phys. Rev. B 46 (1992) 10866.
[6] S. Eggert, I. Affleck, M.D.P. Horton, Phys. Rev. Lett. 89 (2002) 47202;
S. Eggert, I. Affleck, M.D.P. Horton, Phys. Rev. Lett. 90 (2003) 89702.
[7] A.E. Mattsson, S. Eggert, H. Johannesson, Phys. Rev. B 56 (1997) 15615.
[8] S. Eggert, I. Affleck, Phys. Rev. Lett. 75 (1995) 934.