Available online at www.sciencedirect.com
ScienceDirect
C. R. Chimie 10 (2007) 79–81
COMPTES RENDUS CHIMIE
http://france.elsevier.com/direct/CRAS2C/

Preliminary communication / Communication

Order-from-disorder in a spin-dimer magnet

Wolfram Brenig

Institute for Theoretical Physics, Technical University of Braunschweig, Braunschweig, Germany

Received 24 May 2006; accepted after revision 28 November 2006
Available online 16 January 2007

Abstract

We study the magnetism of a two-dimensional model of coupled spin dimers in the presence of disorder. Using a quantum Monte-Carlo approach, we evaluate the staggered structure factor as a function of the exchange coupling strength and for various disorder concentrations. We show that substitutional disorder in terms of non-magnetic defects leads to long-range magnetic order at zero temperature. ***To cite this article: W. Brenig, C. R. Chimie 10 (2007).***

Keywords: Spin models; Quantum critical points; Disorder

There is a growing suspicion that thermodynamic properties of many novel materials at finite temperatures may be a consequence of their vicinity to quantum critical points, i.e. changes of the ground-state symmetry as a function of some intrinsic parameter p. Such quantum phase transitions (QPTs) may play a key role in the high-temperature cuprate superconductors, in heavy fermion materials, and in low-dimensional quantum magnets. Regarding the latter, antiferromagnetically (AFM) coupled spin-1/2 dimer magnets are of particular interest. Many molecular magnetic materials can be understood in terms of one-, two- and three-dimensional networks of spin dimers [1]. In dimer magnets, p can be identified with the ratio J/j of the intra-dimer exchange to an effective inter-dimer coupling. For $|p| \gg 1$ and $J > 0$, the ground state can be understood in terms of a product state of weakly interacting spin-singlets which display no magnetic long-range order (MLRO). However, as p is lowered to $|p| \sim 1$ and in spacial dimensions $D \geq 2$, a QPT to MLRO may arise with a commensuration vector $\mathbf{Q}$ depending on the details of the inter-dimer coupling. In this context, the impact of disorder has become a recent topic. Here we focus on the effects of substitutional disorder arising from non-magnetic defects. In molecular dimer magnets, such defects can be introduced in a controlled way, as e.g. in the coupled ladder compound $[Ph(NH_3)](18C_6)[Ni(dmit)_2]_{1-x}[Au(dmit)_2]_x$, where the $[Ni(dmit)_2]^-$ ion leads to spin-1/2, while for Ni → Au spin-0 results [2]. To be specific, we study the 2D version of the so-called Kondo-necklace model of coupled spin-1/2 dimers:

$$H_{SKN} = j \sum_{lm} \mathbf{S}_{Pl} \cdot \mathbf{S}_{Pm} + J \sum_{l} \mathbf{S}_{Pl} \cdot \mathbf{S}_{ll}, \qquad (1)$$

shown in Fig. 1. The clean limit of this model has been discussed in Refs. [3–5].

E-mail address: w.brenig@tu-bs.de

1631-0748/$ - see front matter
doi:10.1016/j.crci.2006.11.008

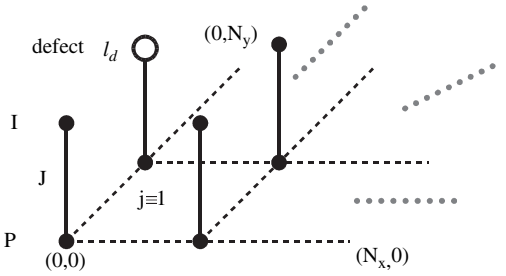

Fig. 1. 2D Kondo-necklace with $2 \times N_x \times N_y$ sites (periodic boundary conditions assumed). Spin-1/2 moments are located on the solid bullets. Solid (dashed) lines refer to inter(intra)-dimer exchange $J(j \equiv 1)$.

The disorder we consider amounts to a random removal of spins from sites l_d of the upper layer 'I' of Fig. 1, thereby introducing *non-magnetic defects* at a concentration c. It has been conjectured that generically such defects in AFM quantum spin systems will enhance local AFM spin correlations and therefore stabilize or trigger MLRO on unfrustrated lattices [6,7]. To test this conjecture in the present case, we have evaluated the AFM order parameter, i.e. the longitudinal staggered structure factor:

$$S_n(\mathbf{Q}) = \left\langle \left(m^z_{n\mathbf{Q}} \right)^2 \right\rangle \tag{2}$$

where $m^z_{n\mathbf{Q}} = \sum_l S^z_{nl} \exp(i\mathbf{Q}\cdot\mathbf{r}_l)/N_n$ is the staggered magnetization, with $\mathbf{Q} = (\pi, \pi, \pi)$. $m^z_{n\mathbf{Q}}$ selects between $n = P, I, A$, for which $\mathbf{r}_l$ runs over the lower (upper) layer for $n = P(I)$ and all sites for $n = A$. The calculation of $S_n(\mathbf{Q})$ proceeds via a quantum Monte-Carlo (QMC) technique, namely the stochastic series expansion (SSE) with loop-updates introduced in Refs. [8,9]. Details will be reported elsewhere.

Fig. 2 summarizes our results. It shows the low-temperature squared staggered moment $M^2_{\mathbf{Q}} = 3S_n(\mathbf{Q})$ vs. J for various defect concentrations and for fixed inter-dimer exchange $j \equiv 1$ at a system size of $N = 2 \times N_x \times N_y = 2 \times 24 \times 24$. Extensive finite-size scaling analysis has been performed at various J and c to ensure that the systematic finite-size corrections to $M^2_{\mathbf{Q}}$ are on the order of, or less than $\sim 10\%$ and have no impact on the results discussed here [10]. Moreover, the inverse temperature $\beta = 1/T$ has been chosen such as to represent the zero-temperature limit. At $c = 0$, $M^2_{\mathbf{Q}}$ is finite below a critical value of $J = J_c$ and drops to approximately zero for $J > J_c$. Extrapolation of $M^2_{\mathbf{Q}}(J < J_c)$ by a power law leads to $J_c \approx 1.41(2)$. We identify J_c with the QPT and expect AFMLRO for $J < J_c$ in the thermodynamic limit at $T = 0$. For $J > J_c$ we find no other transitions, i.e.

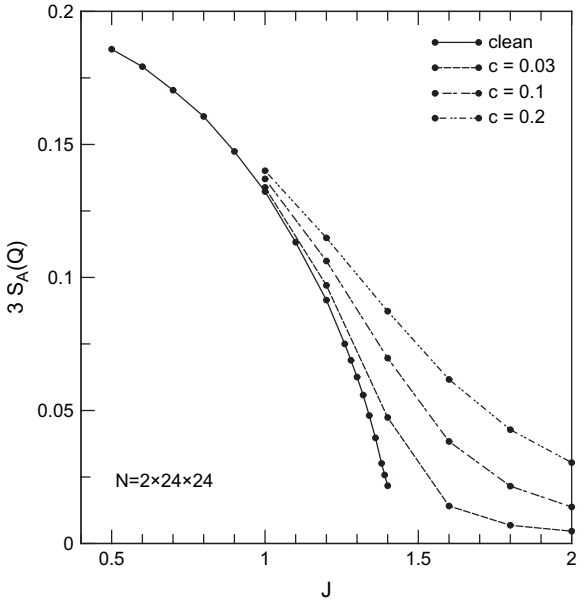

Fig. 2. Staggered structure factor $S_A(\mathbf{Q})$ vs. J close to the QPT for various defect concentrations c. Inverse temperatures $\beta = 1/T$ are $\beta = 100$ at $c = 0$ and $\beta = 1024$ at $c = 0.03$, 0.1, and 0.2. Disorder results include averages over ~ 900 system realizations each. Statistical errors are less than the solid-circle marker size.

the systems connect adiabatically to the limit of $J = \infty$. Therefore, it is in a dimerized state with no MLRO. For a finite defect density, $c > 0$, the situation changes dramatically. For all values of J investigated, we find that the staggered moment, i.e. the order parameter of the AFM state remains finite, also for $J > J_c$. Our results do not rule out a large upward renormalization of the QPT as a function of c, i.e. beyond the range of J considered here. However, it is rather likely that the QPT is suppressed by the disorder and $J_c(c \neq 0) = \infty$ for all c. In any case Fig. 2 demonstrates the main point of this short note, i.e. that non-magnetic disorder can induce MLRO in a state which is non-magnetic otherwise in the clean limit, i.e. we find *order-from-disorder*.

Acknowledgement

Part of this work has been funded by the German Science Foundation, DFG, under Grant Nos. BR 1084/2-2 and BR 1084/4-1.

References

[1] O. Kahn, Molecular Magnetism, Wiley-VCH, 1993.
[2] S. Nishihara, T. Akutagawa, T. Hasegawa, T. Nakamura, Chem. Commun. 5 (2002) 408.

[3] Y. Matsushita, M.P. Gelfand, C. Ishii, J. Phys. Soc. Jpn 66 (1997) 3648.
[4] M. Feldbacher, C. Jurecka, F.F. Assaad, W. Brenig, Phys. Rev. B 66 (2002) 045103.
[5] W. Brenig, preprint cond-mat/0502489.
[6] G.B. Martins, M. Laukamp, J. Riera, E. Dagotto, Phys. Rev. Lett. 78 (1997) 3563.
[7] H.-J. Mikeska, U. Neugebauer, U. Schollwöck, Phys. Rev. B 55 (1997) 2955.
[8] A.W. Sandvik, Phys. Rev. B 59 (1999) R14157.
[9] O.F. Syljuasen, A.W. Sandvik, Phys. Rev. E 66 (2002) 046701.
[10] W. Brenig, Int. J. Mod. Phys. B 20, in press.