Numerical interchain mean-field theory: application to the specific heat of $MnNi(NO_2)_4(en)_2$ (en = ethylenediamine)

GEORG-AUGUST-UNIVERSITÄT GÖTTINGEN [1]

Andreas Honecker[1], Wolfram Brenig[2], Stefan Süllow[3], Matthias Bleckmann[3], Ralf Feyerherm[4]

[1]Institut für Theoretische Physik, Georg-August-Universität Göttingen

[2]Institut für Theoretische Physik, TU Braunschweig

[3]Institut für Physik der Kondensierten Materie, TU Braunschweig

[4]Helmholtz-Zentrum Berlin für Materialien und Energie

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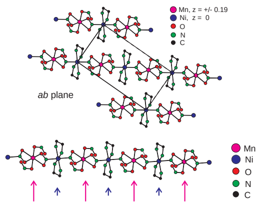
$MnNi(NO_2)_4(en)_2$ (en = ethylenediamine): a ferromagnetic chain compound with alternating spins [1]

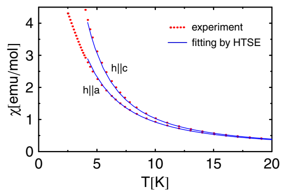
Crystal structure



☞ Alternating spins $S = 5/2$ (Mn), $s = 1$ (Ni)

☞ Ferromagnetic chains, antiferromagnetic coupling

Magnetic susceptibility



Fit by high-temperature series expansion (HTSE)

$\Rightarrow$ $J = 2.8$K, $D = 0.36$K, $J_\perp = 0.072$K [2]

Hamiltonian

$$H_{\text{chain}} = H_{1D} - h\,N\,M$$

with

$$H_{1D} = -J \sum_{x=1}^{N/2} \left(\vec{S}_x \cdot \vec{s}_x + \vec{s}_x \cdot \vec{S}_{x+1} \right) - D \sum_{x=1}^{N/2} (S_x^z)^2$$

and

$$N\,M = \sum_{x=1}^{N/2} (S_x^z + s_x^z)$$

- #spins: N
- average g-factors [1], $J = 2.8$K [2]

$\Rightarrow$ $H = 0.8\text{T} \mathrel{\hat{=}} 0.4\,J$, $H = 1.6\text{T} \mathrel{\hat{=}} 0.8\,J$

Methods

- **exact (full) diagonalization (ED)** for $N \le 10$
- **Quantum Monte Carlo (QMC)**: ALPS 1.3 directed loop application [3] in stochastic series expansion framework [4]

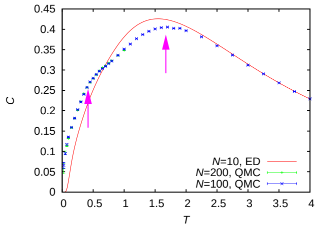
http://alps.comp-phys.org/

ALPS Applications and Libraries for Physics Simulations

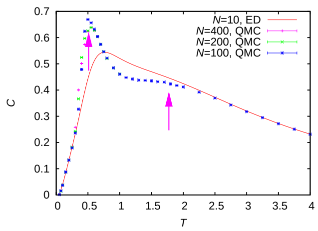
Specific heat per spin: single-chain results

$J_\perp = 0$, normalization: $J = 1$

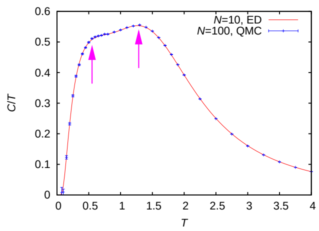
$h = 0$, $D = 0$



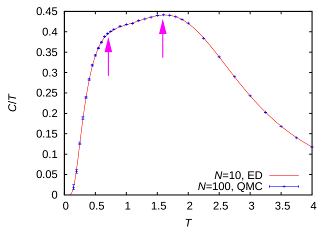
$h = 0$, $D = 0.36/2.8$



$h = 0.4$, $D = 0.36/2.8$



$h = 0.8$, $D = 0.36/2.8$



$\Rightarrow$ $N = 100$ **QMC needed at** $h = 0$ **(sufficient for** $T \gtrsim 0.6\,J$**)**

$\Rightarrow$ $N = 10$ **ED sufficient for** $h = 0.4$ **and** 0.8

Double-peak structure can be traced from $h = 0$, $D = 0$ **to** h, D **finite**

Interchain mean-field theory

Mean-field Hamiltonian (compare also [5]):

$$H^{\text{MF}} = H_{1D} - \underbrace{(h \mp J_\perp \langle M \rangle)}_{= h_{\text{eff.}}} N\,M$$

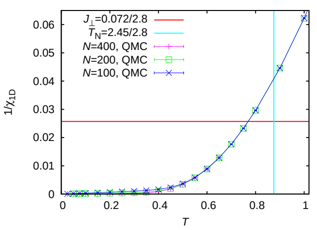
Self-consistency condition:

$$\langle M \rangle = \frac{\text{Tr}\left(M\,\mathrm{e}^{-H^{\text{MF}}/T} \right)}{\text{Tr}\left(\mathrm{e}^{-H^{\text{MF}}/T} \right)}$$

$\Rightarrow$ **magnetic susceptibility** [2, 6, 7]

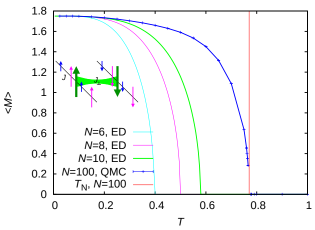
$$\chi_{\text{MF}} = \frac{\mathrm{d}}{\mathrm{d}h} \langle M \rangle = \frac{\chi_{1D}}{1 \pm J_\perp \chi_{1D}} \qquad (\star)$$

Single chain: susceptibility^{-1} at $h = 0$



$J = 1$, $J_\perp = 0$

Self-consistent magnetization at $h = 0$



$J = 1$, $J_\perp = 0.072/2.8$

☞ pole in $(\star)$

$\Rightarrow$ condition for Néel temperature:

$$\frac{1}{\chi_{1D}(T_N)} = J_\perp$$

☞ $N = 100$ QMC at $h = 0$

$\Rightarrow$ $T_N = 0.77\,J \mathrel{\hat{=}} 2.16$K

✔ compare experimental value: $T_N = 2.45$K [1]

✔ insensitive to value of $J_\perp$

☞ finite-size effects at $h = 0$:

$\Rightarrow$ accurate treatment of chains important

Magnetic specific heat: comparison of interchain mean-field results with experiment

Approximations

- without interchain coupling: $J_\perp = 0$
- **interchain mean-field theory**:

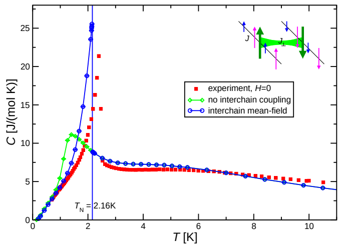
$$C_{\text{MF}} = \frac{1}{N}\frac{\mathrm{d}U}{\mathrm{d}T} = -\frac{\beta^2}{N}\frac{\mathrm{d}}{\mathrm{d}\beta}\left(\langle H^{\text{MF}} \rangle - N \frac{J_\perp}{2} \langle M \rangle^2 \right)$$

$$= \frac{\beta^2}{N}\left(\left\langle \left(H^{\text{MF}} \right)^2 \right\rangle - \left\langle H^{\text{MF}} \right\rangle^2 \right) \pm \beta^3 J_\perp \frac{\mathrm{d}\langle M \rangle}{\mathrm{d}\beta} \left(\langle H^{\text{MF}} M \rangle - \langle H^{\text{MF}} \rangle \langle M \rangle \right)$$

with

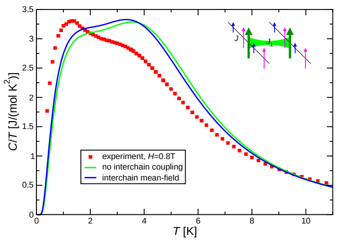
- $\displaystyle \frac{\mathrm{d}\langle M \rangle}{\mathrm{d}\beta} = -\frac{\langle H^{\text{MF}} M \rangle - \langle H^{\text{MF}} \rangle \langle M \rangle}{1 \pm J_\perp \chi_{1D}}$
- $\langle \cdot \rangle$ single-chain expectation values at self-consistently determined magnetization $\langle M \rangle$
- $\beta = 1/T$

$H = 0$, $h = 0$



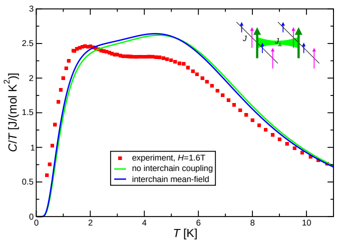
based on $N = 100$ QMC

$H = 0.8\text{T} \| c$, $h = 0.4\,J$



based on $N = 10$ ED

$H = 1.6\text{T} \| c$, $h = 0.8\,J$



based on $N = 10$ ED

Good agreement without adjustable parameters

References

[1] R. Feyerherm, C. Mathonière, O. Kahn, J. Phys.: Condens. Matter **13** (2001) 2639

[2] N. Fukushima, A. Honecker, S. Wessel, W. Brenig, Phys. Rev. B **69** (2004) 174430

[3] F. Alet, S. Wessel, M. Troyer, Phys. Rev. E **71** (2005) 036706

[4] O.F. Syljuåsen, A.W. Sandvik, Phys. Rev. E **66** (2002) 046701

[5] S. Lee, R.K. Kaul, L. Balents, Nature Physics **6**, (2010) 702

[6] H.J. Schulz, Phys. Rev. Lett. **77** (1996) 2790

[7] S. Todo, A. Shibasaki, Phys. Rev. B **78** (2008) 224411

Acknowledgments

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SFB 602 einzelnes Atom kondensierte Materie mikroskopisch makroskopisch 1nm 1 μm

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