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QMC simulations of Heisenberg ferromagnet*

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We use the Quantum Monte Carlo Stochastic Series Expansion (SSE) algorithm to investigate the properties of the one-dimensional Heisenberg ferromagnet. We consider the model for two spin values $s = \frac{1}{2}$ and $s = 1$ and study the dependence of the specific heat, magnetisation, magnetic susceptibility and correlation functions on temperature and magnetic field. Obtained results are compared to those derived by analytical methods (Bethe ansatz, Green's function, Random Phase Approximation). In particular, the surprising prediction of a double-peak structure in the specific heat at low temperatures and small magnetic fields can be confirmed.

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1. Introduction

The study of low-dimensional quantum ferromagnets is mainly motivated by progress in the synthesis of new materials which can be described by effective one-dimensional (1D) [1, 2] or two-dimensional (2D) [3, 4, 5, 6] spin $s = \frac{1}{2}$ Heisenberg Hamiltonians. In a recent paper [7] Green's function analytical methods were applied to such systems. It was claimed that, within the employed approximation, the heat-capacity curve for the (isotropic) $s = \frac{1}{2}$ Heisenberg chain shows an unexpected double peak at very low temperatures. Additionally it was shown that the field dependent position of the maxima and the heights of the specific heat and magnetic susceptibility fit to power laws.

The Monte Carlo simulations we carried out confirm these predictions for $s = \frac{1}{2}$. Additionally we have investigated the model for spin $s = 1$. Our simulations show that a similar scaling behaviour can be expected also in that case. The double peak in the specific heat is visible as well. However, the magnetic field range where it appears is shifted in comparison to the $s = \frac{1}{2}$ case.

The outline of the paper is as follows. A brief definition of the model is given in section 2. The section 3 contains an outline of the SSE algorithm, which we employed in the simulations. Example tests of the method's correctness are shown in section 4. The results of the simulations of the $s = \frac{1}{2}$ system are collected in section 5, and the results of the $s = 1$ system in section 6. Finally, section 7 contains our summary.

2. The model

We consider the standard 1D Heisenberg ferromagnet (FHM), which can be described by the following Hamiltonian:

$$H = J \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - h \sum_i \hat{S}_i^z, \tag{2.1}$$

where $\langle ij \rangle$ denotes a pair of spin operators $\hat{\mathbf{S}}_i = \{\hat{S}_i^x, \hat{S}_i^y, \hat{S}_i^z\}$ placed on the nodes of a 1D chain. The coupling constant J is negative, $J < 0$, and the magnetic field h is directed along the z-axis. We assume periodic boundary conditions, i.e., a ring of spins.

3. The algorithm

The numerical simulations were carried out by means of the directed loop algorithm, a particular version of the stochastic series expansion (SSE) [8] method. The detailed description of this algorithm can be found elsewhere (see for example Ref. [9]), but for completeness we briefly present its key points.

The SSE algorithm is based on a power-series expansion of the partition function:

$$Z = \mathrm{Tr}\, e^{-\beta H} = \sum_{\alpha} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle \alpha | H^n | \alpha \rangle . \tag{3.1}$$

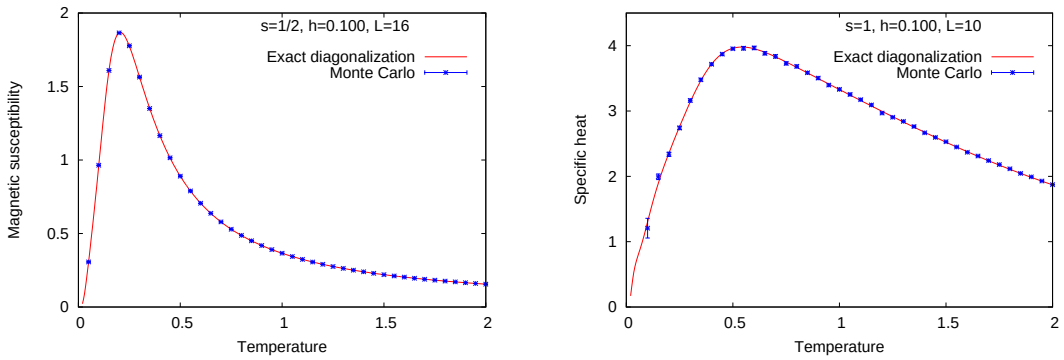

Figure 1: Comparison of Monte Carlo and direct diagonalization results for: magnetic susceptibility of the $s = \frac{1}{2}$, $L = 16$ system in magnetic field $h = 0.1$ (left), and specific heat for $s = 1$, $L = 10$, $h = 0.1$ (right).

It is convenient to use the eigenvectors of the operator $\hat{S}_i^z$ as a base $|\alpha\rangle$, and express the Hamiltonian as a sum of bond operators:

$$H = J \sum_{b=1}^{L} H_b = J \sum_{b=1}^{L} (H_{1,b} + H_{2,b}), \tag{3.2}$$

where L is the number of nodes. Each bond operator is a sum of diagonal part:

$$H_{1,b} = C + \hat{S}_{i(b)}^z \hat{S}_{j(b)}^z - \frac{h}{2J}[\hat{S}_{i(b)}^z + \hat{S}_{j(b)}^z], \tag{3.3}$$

and off-diagonal part:

$$H_{2,b} = \frac{1}{2}[\hat{S}_{i(b)}^+ \hat{S}_{j(b)}^- + \hat{S}_{i(b)}^- \hat{S}_{j(b)}^+], \tag{3.4}$$
$$\hat{S}_i^{\pm} = \hat{S}_i^x \pm \hat{S}_i^y.$$

To ensure that all $H_{1,b}$ matrix elements are positive, the additional C constant has been inserted. Finally the partition function is expressed as

$$Z = \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} \frac{(-J\beta)^n}{n!} \langle \alpha | \prod_{i=1}^{n} H_{a_i,b_i} | \alpha \rangle, \tag{3.5}$$

where

$$S_n = [a_1, b_1], [a_2, b_2], ..., [a_n, b_n] \tag{3.6}$$

denotes the sequence of n diagonal ($a_i = 1$) and off-diagonal ($a_i = 2$) operators living on bonds b_i. After introducing an additional cut-off for the maximal number of operators, $n = n_{\max}$, this expression can be used to simulate the system on a finite $L \times n_{\max}$ lattice.

4. Tests

One of the tests for correctness of our simulation program is the comparison of the Monte Carlo data with results obtained by other methods. For very small systems (up to $L = 16$ spins for $s = 1/2$,

and up to $L = 10$ spins for $s = 1$) we were able to diagonalize the Hamiltonian matrix. This allowed us to calculate all interesting quantities exactly. An example comparison of the Monte Carlo data and the direct diagonalization results is shown in fi gure 1, demonstrating perfect agreement (within the statistical error bars of the Monte Carlo method).

5. Results for spin $s = 1/2$

We compare the results of the Monte Carlo simulations of the spin $s = \frac{1}{2}$ system with the Bethe-ansatz results for the infi nite chain [10]. As an example we show in fi gure 2 the magnetisation and the specifi c heat as a function of temperature, obtained by these two methods. As it can be seen, already for the size $L = 128$, the fi nite-size effects are so small that, in the shown temperature range, the Monte Carlo and Bethe-ansatz results are in perfect agreement. The double maximum in the specifi c-heat curve can be seen for small magnetic fi elds $h < 0.01$, as it was claimed in Ref. [7] using the Green's function approximation.

We checked the dependence of the temperature for which the specifi c heat maximum appears, $T^C_{\max}$, and the maximum height $C_{\max}$ on the magnetic fi eld. If in the range of small fi elds $h < 0.01$, where the double maximum occurs, the left (lower temperature) maximum is taken into account,

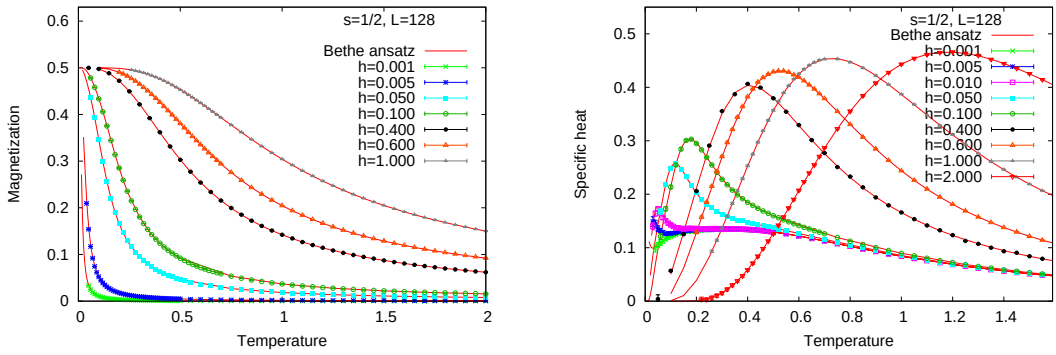

Figure 2: The dependence of the magnetisation (left) and the specific heat (right) on the temperature, for the $s = \frac{1}{2}$ and $L = 128$ system, in various magnetic fields. The Bethe ansatz results are plotted by solid lines.

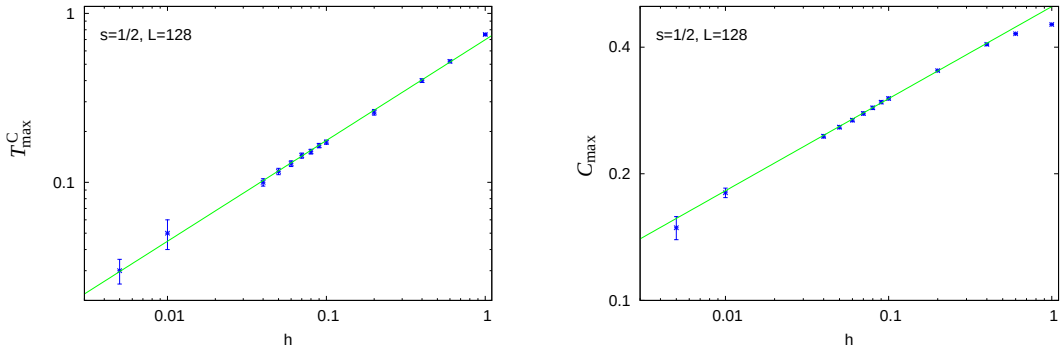

Figure 3: The dependence of the position of the specific-heat maximum (left) and the maximal value (right) on the magnetic field for $s = \frac{1}{2}$, $L = 128$. The fitted power-law ansatz is shown by a dashed line.

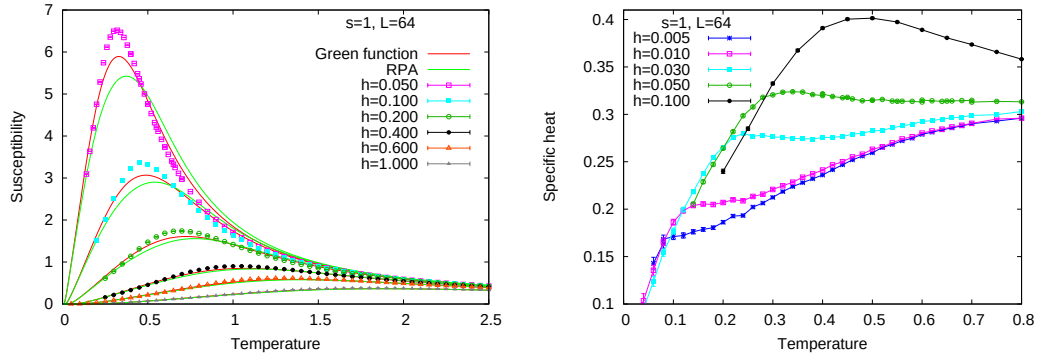

Figure 4: Magnetic susceptibility (left) and specific heat (right) of the $s = 1$, $L = 64$ system as a function of temperature. On the left plot, the analytical results (Green's function, random phase approximation (RPA)) are shown by solid lines.

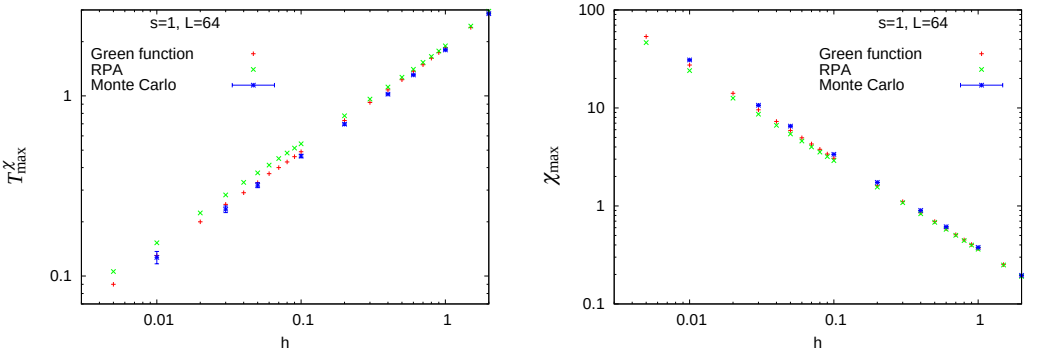

Figure 5: The dependence of the position of the susceptibility maximum (left) and the maximal value (right) on the magnetic field for spin $s = 1$, calculated by three different methods (Green's function, random phase approximation (RPA), and Monte Carlo simulations).

the scaling with fi eld obeys a power-law behaviour as demonstrated in the log-log plots of fi gure 3. By fi tting a power-law ansatz in the range $0 < h < 1.0$, we obtain the following dependence:

$$T^C_{\max} = 0.70(1)h^{0.60(1)}, \qquad C_{\max} = 0.50(1)h^{0.22(1)}. \tag{5.1}$$

This can be compared with results obtained by the Green's function method [7]:

$$T^C_{\max} = 0.596h^{0.542}, \qquad C_{\max} = 0.513h^{0.228}. \tag{5.2}$$

6. Results for spin $s = 1$

We compare the results of the spin $s = 1$ Monte Carlo simulations with the results obtained by Green's function [7] and random phase approximation (RPA) [11] methods. The fi gure 4 shows the dependence of the magnetic susceptibility and specifi c heat on the temperature. In the plot showing the susceptibility, Green's function and RPA results are also depicted. The agreement is quite good; small differences are only visible for small magnetic fi elds.

The double maximum in the specific heat curve is visible, but in contrast to the $s = \frac{1}{2}$ case it does not appear for very small fields. The range where it is visible starts at $h \approx 0.01$ (for spin $s = \frac{1}{2}$ it starts already at $h = 0$).

In the log-log plots of figure 5 the scaling behaviours of the position and height of the magnetic susceptibility maximum as a function of the magnetic field are shown. Again, all three methods show power-law scaling.

7. Summary

The results of our Monte Carlo simulations of the 1D Heisenberg ferromagnet were briefly presented. A comparison with other analytical methods shows good agreement. Therefore the existence of the double peak in the specific-heat curve and the power-law scaling of the positions and heights of the specific heat and magnetic susceptibility maxima have been confirmed.

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References

[1] M. Takahashi, P. Turek, Y. Nakazawa, M. Tamura, K. Nozawa, D. Shiomi, M. Ishikawa, and M. Kinoshita, *Phys. Rev. Lett.* **67** (1991) 746.

[2] C.P. Landee and R.D. Willett, *Phys. Rev. Lett.* **43** (1979) 463.

[3] N. Read and S. Sachdev, *Phys. Rev. Lett.* **75** (1995) 3509.

[4] C. Timm, S.M. Grivin, P. Henelius, and A.W. Sandvik, *Phys. Rev. B* **58** (1998) 1164.

[5] S. Feldkemper, W. Weber, J. Schulenburg, and J. Richter, *Phys. Rev. B* **52** (1995) 313.

[6] H. Manaka, T. Koide, T. Shidara, and I. Yamada, *Phys. Rev. B* **68** (2003) 184412.

[7] I. Junger, D. Ihle, J. Richter, and A. Klümper, *Phys. Rev. B* **70** (2004) 104419.

[8] A.W. Sandvik and J. Kurkijärvi, *Phys. Rev. B* **43** (1991) 5950.

[9] O.F. Syljuasen and A.W. Sandvik, *Phys. Rev. E* **66** (2002) 046701.

[10] A. Klümper, *Eur. Phys. J. B* **5** (1998) 667.

[11] S.V. Tjablikov, in *Methods in the quantum theory of magnetism*, Plenum Press, New York, 1967.