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Quantum Phase Transitions in Frustrated Ferro- and Ferrimagnets

running title: Frustrated Ferrimagnets

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ABSTRACT

We discuss the ground state of the one-dimensional frustrated quantum Heisenberg ferrimagnet. In the limit of weak frustration the ground state has macroscopic total spin and exhibits magnetic long-range order. In the opposite limit of strong frustration the ground state is a singlet ($S = 0$). We find indications that this transition to a singlet state is of first order. We compare the ferrimagnet with the corresponding ferromagnet.

key words: Spin chains, Spin frustration, Quantum phase transitions

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The investigation of ground state (GS) quantum order-disorder transitions in magnetic systems has acctracted much attention. One canonical example is the spin half $J_1 - J_2$ Heisenberg antiferromagnet on the square lattice, where such a transition is driven by the interplay of frustration and quantum fluctuations. Though there are about 100 papers dealing with this two-dimensional frustrated antiferromagnet (see e.g. [1,2]) a quantitative description is still missing. One reason is the failure of the most efficient quantum Monte-Carlo and density matrix renormalistaion group (DMRG) techniques. In order to exploit at least one of these powerful techniques for the discussion of quantum order-disorder transitions one should look for one-dimensional (1d) frustrated quantum spin systems. However, the 1d quantum Heisenberg antiferromagnets do not show magnetic Néel long-range order (LRO). More appropriate are 1d ferro- and ferrimagnets, which exhibit collinear magnetic LRO in the GS if frustration is absent. The existence of LRO in the ferromagnet is trivial because the fully polarized state is an eigenstate of the Hamiltonian. More interesting is the discussion of LRO for the ferrimagnet where the GS wave function is generally not known. This problem has been studied recently (see e.g. [3,4]).

In this paper we study the influence of a frustrating second neighbour bond J_2 on the magnetic ordering of the 1d ferrimagnet and discuss for comparison some known results [5] for the corresponding frustrated 1d ferromagnet. The Hamiltonian of the frustrated 1d ferrimagnet reads

$$H = J_1 \sum_n \mathbf{S}_{1,n}\mathbf{S}_{2,n} + J_2 \sum_n \left(\mathbf{S}_{1,n}\mathbf{S}_{1,n+1} + \mathbf{S}_{2,n}\mathbf{S}_{2,n+1}\right), \qquad (1)$$

where the index n numbers N unitary cells each containing one spin of 'length' S_1 and one of 'length' S_2. In what follows we set $J_1 \equiv 1$ and consider the extreme quantum case $S_1 = 1$ $S_2 = 1/2$. The influence of weak frustration $J_2 \lessapprox 0.23$ on the collinear ferrimagnetic ordering has been discussed by the authors recently [6]. We mention that the corresponding frustrated ferromagnet is obtained by putting $S_1 = S_2 = 1/2$ and $J_1 = -1$. As stated above the GS of model (1) for weak frustration $J_2/J_1 \to 0$ shows ferrimagnetic LRO. On the other hand in the limit $J_2/J_1 \to \infty$ the model represents a system of two decoupled chains (Bethe and Haldane chain) and consequently there is no LRO in this limit. Therefore it is evident that there is an order-disorder transition in the model (1) driven by J_2. A similar situation we have in the corresponding 1d $J_1 - J_2$ ferromagnet [5].

We start with the discussion of the classical version of model (1), i.e. $\mathbf{S}_{1,n}$ and $\mathbf{S}_{2,n}$ are classical vectors of lengths '1' and '1/2'. Then the collinear ferrimagnetic state is stable until a critical $J_{2,c}^{cl} = 1/5$. For $J_2 > J_{2,c}^{cl}$ we have a spiral phase with a pitch angle θ, where cos $\theta = 1/(5J_2)$. Obviously, the collinear – spiral transition is of second order. For $J_2 \to \infty$ we have $\theta = \pi/2$ and the system is composed of two decoupled classical antiferromagnetic chains.

For the quantum model we present exact digonalisation (ED) results for a chain of $N = 8$ unit cells with periodic boundary conditions and DMRG results for $N = 20$ cells with open boundary conditions. To discuss the transition from the collinear ferrimagnetic state to the spiral state we compare the pitch angle θ of the classical and the quantum model. This angle θ is explicitly known as a function of J_2 in the classical case. To calculate the corresponding 'quantum angle' we express the pitch angle by short-range spin correlations [7] and define $K_{cl} = \frac{1}{2}\mathbf{S}_{2,n}\mathbf{S}_{2,n+1}/\mathbf{S}_{1,n}\mathbf{S}_{2,n} = -2\cos\theta + 1/\cos\theta$. The quantum analogue is defined by $K_{qu} = \frac{1}{2}\langle\mathbf{S}_{2,n}\mathbf{S}_{2,n+1}\rangle/\langle\mathbf{S}_{1,n}\mathbf{S}_{2,n}\rangle$. Both quantities are presented in Fig.1. Obviously instead of the continuous classical transition we have in the quantum case a discontinous transition at a critical value $J_{2,c}^{qu}$ larger then the corresponding classical value $J_{2,c}^{cl} = 1/5$. This jump in K_{qu} corresponds to the transition from the GS with macroscopic total spin $S = N/2$ to a singlet GS $S = 0$. We find $J_{2,c}^{qu} = 0.231$ for $N = 20$ and $J_{2,c}^{qu} = 0.229$ for $N = 8$. There are additional steps in K_{qu} for $N = 8$ but not for $N = 20$ indicating strong finite size effects in the region $0.4 \lessapprox J_2 \lessapprox 1.0$.

To illustrate the spiral nature of the correlations in the quantum model we have presented the spin-spin correlations $\langle\vec{S}_{1,n}\vec{S}_{1,n+i}\rangle$ along the spin-one subchain (Fig.2). Clearly we see spiral-like correlations for $J_2 = 0.25$ and $J_2 = 0.5$ with periodicities of about 4 and 3, respectively. For $J_2 = 1.0$ we have antiferromagnetic staggerd correlations at least for short distances indicating a crossover to the regime of weakly coupled subchains (Haldane and Bethe).

Let us summarize our results: (i) The classical 1d ferrimagnet shows a second order transition from a collinear ferrimagnetic state to a noncollinaer spiral state. For the quantum 1d ferrimagnet we find indications for a first order transition from a collinear ferrimagntic state to a noncollinaer spiral-like state. Having in mind the lack of LRO in 1d quantum antiferromagnets we expect that this state is not long-range ordered. This is supported by the fast decay of correlations seen in Fig.2.

The scenario of a first order transition corresponds to the frustrated ferromagnet [5]. (ii) It is known [1,2] that quantum fluctuations favour collinear spin correlations. In accordance with this general observation we find that the collinear quantum ferrimagnetic state is stable beyond the classical transition point, i.e. $J_{2,c}^{qu} > J_{2,c}^{cl}$ for the ferrimagnet. However, this fact is in difference to the reults for the frustrated ferromagnet, where we have $J_{2,c}^{qu} = J_{2,c}^{cl} = 1/4$. For the ferromagnet the coincidence of the classical and the quantum critical value is due to the missing of quantum reduction of the magnetization in the fully polarized ferromagnetic state.

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Figure captions:

Fig.1:

The quantities K_{cl} and K_{qu} for the frustrated ferrimagnet (1) as a function of J_2.

Fig.2:

Spin-spin correlations $\langle\vec{S}_{1,n}\vec{S}_{1,n+i}\rangle$ along the spin-one subchain for various J_2.

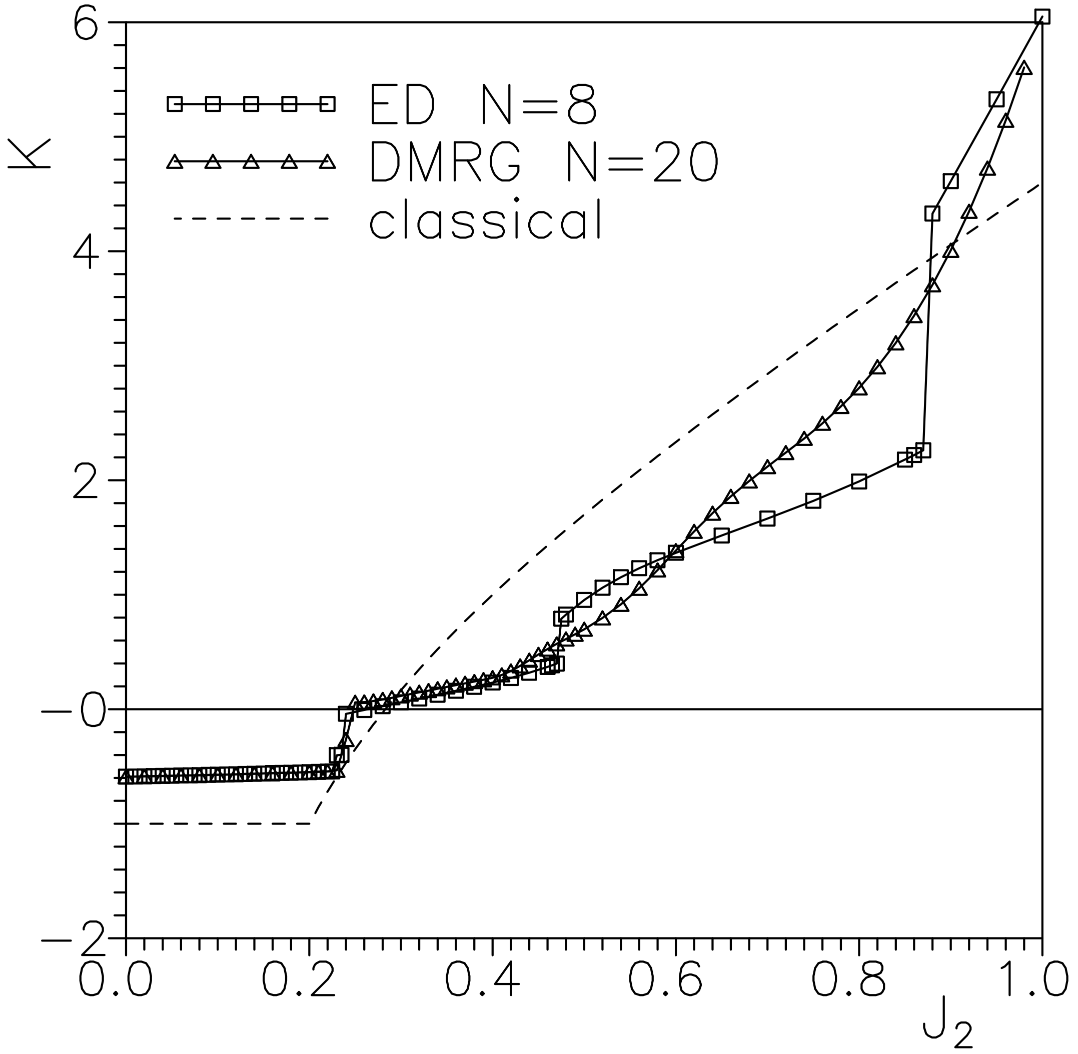
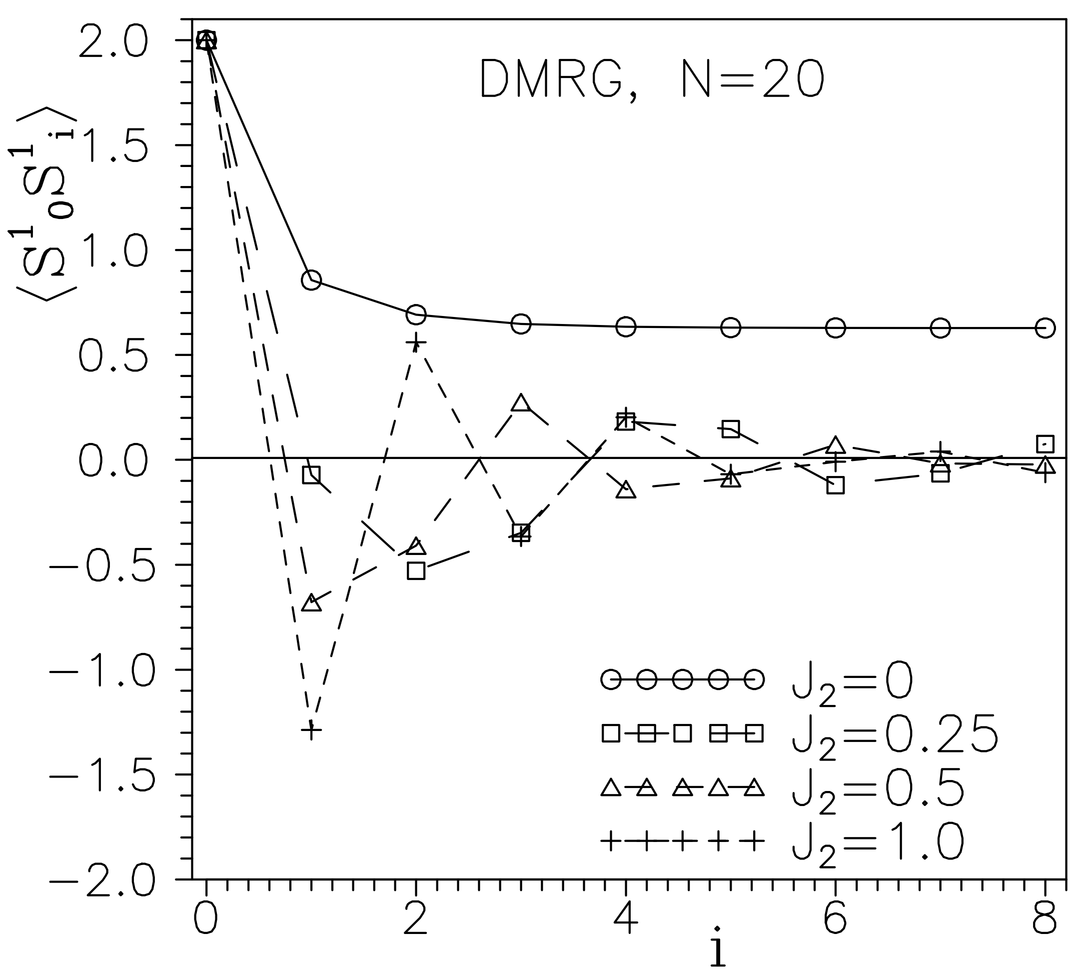


Fig.1



DMRG, N=20
$\langle S^1_0 S^1_i \rangle$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
2
4
6
8
i
$J_2=0$
$J_2=0.25$
$J_2=0.5$
$J_2=1.0$

Fig.2