Thermodynamics of the frustrated ferromagnetic spin-1/2 Heisenberg chain

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Abstract. We studied the thermodynamics of the one-dimensional $J_1$-$J_2$ spin-1/2 Heisenberg chain for ferromagnetic nearest-neighbor bonds $J_1 < 0$ and frustrating antiferromagnetic next-nearest-neighbor bonds $J_2 > 0$ using full diagonalization of finite rings and a second-order Green-function formalism. Thereby we focus on $J_2 < |J_1|/4$ where the ground state is still ferromagnetic, but the frustration influences the thermodynamic properties. We found that their critical indices are not changed by $J_2$. The analysis of the low-temperature behavior of the susceptibility $\chi$ leads to the conclusion that this behavior changes from $\chi \propto T^{-2}$ at $J_2 < |J_1|/4$ to $\chi \propto T^{-3/2}$ at the quantum-critical point $J_2 = |J_1|/4$. Another effect of the frustration is the appearance of an extra low-$T$ maximum in the specific heat $C_v(T)$ for $J_2 \gtrsim |J_1|/8$, indicating its strong influence on the low-energy spectrum.

Introduction: In low-dimensional frustrated quantum magnets thermal and quantum fluctuations strongly influence the low-temperature physics [1,2]. Special attention has been paid to one-dimensional (1D) $J_1$-$J_2$ quantum Heisenberg magnets, see Ref. [3] and references therein. Recent experimental studies have shown that edge-shared chain cuprates, such as LiVCuO$_4$, Li(Na)Cu$_2$O$_2$, Li$_2$ZrCuO$_4$, and Li$_2$CuO$_2$ [4–13], represent a family of quantum magnets for which the 1D $J_1$-$J_2$ Heisenberg model is a good starting point for a theoretical description. The above listed compounds are quasi-1D frustrated spin-1/2 magnets with a ferromagnetic (FM) nearest-neighbor (NN) in-chain coupling $J_1 < 0$ and an antiferromagnetic (AFM) next-nearest-neighbor (NNN) in-chain coupling $J_2 > 0$.

The model: The Hamiltonian of the 1D $J_1$-$J_2$ Heisenberg ferromagnet is given by

$$H = J_1 \sum_{\langle i,j \rangle} S_i S_j + J_2 \sum_{\langle i,j \rangle} S_i S_j,$$

where the first sum runs over the NN bonds and the second sum over the NNN bonds. Henceforth we set $J_1 = -1$. For the model (1) a quantum critical point at $J_2 = 0.25$ exists where the FM ground state (GS) gives way for a singlet GS with spiral correlations for $J_2 > 0.25$ [14–16]. For most of the edge-shared chain cuprates $J_2$ is large enough to realize such a spiral GS. However, several materials considered as model systems for 1D spin-1/2 ferromagnets, such as TMCuCl$_2$[(CH$_3$)$_4$NCuCl$_3$] [17] and p-NPNN (C$_{13}$H$_{16}$N$_3$O$_4$) [18], might have also a weak frustrating NNN interaction $J_2 < 0.25$. Moreover, recent studies [13] lead to the conclusion that Li$_2$CuO$_2$ is a quasi-1D spin-1/2 system with a dominant FM $J_1$ and weak frustrating AFM

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\( J_2 \approx 0.2|J_1| \). Here we focus on the parameter region \( J_2 \leq 0.25 \), i.e. the GS is ferromagnetic. Only at \( J_2 = 0.25 \) the FM GS multiplet is degenerate with a spiral singlet GS [14–16]. On the other hand, the frustrating \( J_2 \) influences the low-energy excitations, in particular, if \( J_2 \) is close to the quantum critical point. Hence, the frustration may have a strong effect on the low-\( T \) thermodynamics. We mention that previous studies [19, 20] of the thermodynamics of the 1D J1-J2 model did not consider values of \( J_2 \) near the quantum critical point \( J_2 \lesssim 0.25 \).

**Results:** To study the thermodynamic properties we use the full exact diagonalization (ED) of finite rings of up to \( N = 22 \) lattice sites, complemented by data obtained by a spin-rotation-invariant second-order Green-function method (RGM) [21–24]. Note that by contrast to ED the RGM is limited to values \( J_2 \leq 0.2 \) [24] but yields results for \( N \to \infty \), that allows the calculation of the correlation length by the RGM. Here we will present data for the spin-spin correlation functions \( \langle S_0 S_n \rangle \), the uniform static spin susceptibility \( \chi \) and the specific heat \( C_v \). For the discussion of the correlation length of the model (1), see Ref. [24]. For the unfrustrated model we will compare our results with available Bethe-ansatz data [25] and transfer-matrix renormalization group (TMRG) results [19].

The temperature dependence of the spin correlation functions \( \langle S_0 S_n \rangle \) is shown for \( n = 1 \) (NN) and \( n = 10 \) for various \( J_2 \) in Fig. 1. With increasing frustration the correlation functions decrease, where the further-distance correlators decay much stronger than the NN correlator. Near and at the quantum critical point the large-distance correlator \( \langle S_0 S_{10} \rangle \) vanishes already at \( T \gtrsim 0.05 \). Interestingly, for \( J_2 = 0.2, 0.24 \), and 0.25 the correlator \( \langle S_0 S_{10} \rangle \) changes the sign and goes through a minimum. This behavior is not affected by finite-size effects, e.g., the correlators \( \langle S_0 S_8 \rangle \) for \( N = 16, 20 \) and \( \langle S_0 S_6 \rangle \) for \( N = 12, 16, 20 \) also change the sign and go through a minimum for \( J_2 = 0.2, 0.24 \), and 0.25.

Next we discuss the low-temperature properties of the susceptibility \( \chi = \lim_{h \to 0} d\langle S_z \rangle/dh \). Due to the FM GS \( \chi \) diverges at \( T \to 0 \). Using Bethe-ansatz for \( J_2 = 0 \) the critical behavior has been determined as \( \chi \propto T^{-2} \) [25]. Using the RGM, recently it has been confirmed that the critical indices for the susceptibility and the correlation length, \( \gamma = 2 \) and \( \nu = 1 \), respectively, are not changed by frustration for \( J_2 < 0.25 \). However, at the quantum critical point \( J_2 = 0.25 \) a change of the low-temperature physics is expected [1]. To study that question we consider the

![Figure 1](image1.png)

**Figure 1.** Spin correlation function \( \langle S_0 S_1 \rangle \) (NN) and \( \langle S_0 S_{10} \rangle \) calculated by ED for \( N = 20 \) sites.

![Figure 2](image2.png)

**Figure 2.** \( \chi T^2 \) versus \( \sqrt{T} \) calculated by ED for \( N = 22 \) (thick lines – calculated data, thin lines – extrapolation to \( T \to 0 \), see Eq. (2) and text) and RGM (circles) as well as Bethe-ansatz data (squares) for \( J_2 = 0 \) from Ref. [25]. The inset shows the coefficient \( y_0 = \lim_{T \to 0} \chi T^2 \) versus \( J_2 \).
related to the existence of the FM critical point at $T = 0$. It has been derived for $J_2 = 0$ in Ref. [25]. For the frustrated system (1) the coefficients $y_0$, $y_1$, and $y_2$ depend on $J_2$. In Fig. 2 we plot $\chi T^2$ versus $\sqrt{T}$. We find a good agreement of the ED data for $\chi T^2$ with Bethe-ansatz results down to quite low temperature $T$. The RGM results for $\chi T^2$ deviate slightly from the Bethe-ansatz results for finite $T$, but approach the Bethe-ansatz data for $T \to 0$, see also Ref. [22]. The behavior of the leading coefficient $y_0$ and the next-order coefficient $y_1$ can be extracted from the results for $\chi T^2$ by fitting them to Eq. (2). For the RGM we use data points up to a cut-off temperature $T = T_{cut} = 0.005$. To deal with finite-size effects in the ED data at very low $T$, we use the specific heat per site $C_v(T)$, see below, to determine that temperature $T_{ED}$ down to which the first four digits of $C_v(T)$ for $N = 20$ and $N = 22$ coincide. Then we fit the ED data in the interval $T_{ED} \leq T \leq T_{ED} + T_{cut}$ to Eq. (2). Note that $T_{ED}$ becomes smaller for increasing $J_2$, we find e.g., $T_{ED} = 0.22, 0.13, 0.09, 0.04, 0.03, 0.02$ at $J_2 = 0.0, 0.1, 0.15, 0.2, 0.24, 0.25$, respectively. For $J_2 = 0$ we found $y_0 = 1/24$ ($y_0 = 0.0418$) for the RGM (ED), which agrees with the Bethe-ansatz results of Ref. [25]. [Note the different definitions of $\chi$ in our paper and in Ref. [25].] Including frustration $J_2 > 0$ we observe a linear decrease of $y_0$ with $J_2$ down to zero at $J_2 = 0.25$ given by

$$y_0 = (1 - 4J_2)/24,$$

(3)

cf. the inset of Fig. 2. The vanishing of $y_0$ at $J_2 = 0.25$ indicates the change of the low-$T$ behavior of the physical quantities at the quantum critical point [1]. Indeed, a polynomial fit according to $y_1 = a_y + b_y J_2 + c_y J_2^2$ yields the finite value $y_1 \approx 0.05 (0.04)$ for RGM (ED). Hence, our data provide evidence for a change of the low-$T$ behavior of $\chi$ from $\chi \propto T^{-2}$ at $J_2 < 0.25$ to $\chi \propto T^{-3/2}$ at the quantum critical point $J_2 = 0.25$. For a a similar discussion of the correlation length $\xi$, see Ref. [24], where it was found that the low-$T$ behavior of $\xi$ changes from $\xi \propto T^{-1}$ at $J_2 < 0.25$ to $\xi \propto T^{-1/2}$ at $J_2 = 0.25$.

In Fig. 3 we present ED results for the specific heat $C_v$. For $J_2 = 0$ we found a broad maximum at $T \approx 0.332$ and a steep decay to zero starting at about $T = 0.05$ in accord with the TMRG [19]. For $J_2 \geq 0.125$ the specific heat exhibits a minimum located at around $T = 0.2$, and two maxima, namely a high-$T$ maximum at around $T = 0.6$ and an additional low-$T$ maximum at $T < 0.1$. If $J_2$ approaches $J_2 = 0.25$, a further quite sharp peak at very low $T$ appears,
that is, however, strongly size dependent, see Fig. 4. From Fig. 4 it is obvious that the extra low-$T$ finite-size peak behaves monotonously with $N$. Hence, we have performed a finite-size extrapolation to $N \to \infty$ of the height $C\nu$ and the position $T\nu$ of the peak in $C\nu(T)$ using the formula $a(N) = a_{\infty} + a_1/N^2 + a_2/N^4$. The extrapolated values $C\nu_{\infty}$ and $T\nu_{\infty}$ are shown in the insets of Fig. 4. Obviously, $C\nu_{\infty}$ > 0 even near the quantum critical point $J_1 = 0.25$, where $C\nu_{\infty} \approx 0.05$. On the other hand, $T\nu_{\infty}$ decreases with $J_2$ and becomes very small near $J_2 = 0.25$. This behavior suggests that a characteristic steep decay of $C\nu(T)$ down to zero starts at very low $T$ when approaching $J_2 = 0.25$.

**Summary:** We discussed the thermodynamics of frustrated FM spin-1/2 $J_1$-$J_2$ Heisenberg chains and found as prominent features (i) a change of the low-$T$ critical behavior at the quantum critical point $J_2 = |J_1|/4$, (ii) and an additional low-$T$ maximum in the specific heat for $|J_1|/4 > J_2 > |J_1|/8$.

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