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# MARSHALL–PEIERLS SIGN RULE IN FRUSTRATED HEISENBERG CHAINS

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We consider the frustrated antiferromagnetic $s = 1$ Heisenberg quantum spin chain with regard to the Marshall–Peierls sign rule. Using exact diagonalization data we investigate the breakdown of the Marshall–Peierls sign rule in dependence on frustration and compare our findings with data for $s = 1/2$. We calculate a critical value of frustration $J_2^{\mathrm{crit}}$, where the Marshall–Peierls sign rule is violated. The extrapolation of this value to the infinite chain limit holds $J_2^{\mathrm{crit}} \approx 0.016$, lower than in the case of $s = 1/2$ ($J_2^{\mathrm{crit}} \approx 0.027$). This points to a stronger influence of frustration in the case of $s = 1$. Nevertheless, the calculation of the weight of the Ising-states violating the Marshall–Peierls sign rule shows that the latter holds approximately even for a quite large frustration and may be used for numerical techniques.

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## 1. Introduction

The Marshall–Peierls sign rule (MPSR) determines the sign of the Ising-basis-states building the ground-state wave function of a Heisenberg Hamiltonian [1] and has been proven exactly for bipartite lattices and arbitrary site spins by Lieb, Schultz and Mattis [2]. As pointed out in several papers the knowledge of the sign is of great importance in different numerical methods, e.g. for the construction of variational wave functions [3], in quantum Monte-Carlo methods (which suffer from the sign problem in frustrated systems [4]) and also in the density matrix renormalization group method, where the application of the MPSR has the substantially improved method in a frustrated spin system [5].

The MPSR has been analyzed so far for systems with $s = 1/2$. The authors of Ref. [6] studied the frustrated chain and found for the ground state a critical value for the breakdown of the MPSR for the infinite chain limit using exact diagonalization data. For the $J_1 - J_2$ model on the square lattice the violation of the MPSR was considered as an indication for the breakdown of long range order [7, 8]. In the recent paper [9] we extended these investigations to higher subspaces of $S^z$. For linear chains we have shown that for the lowest eigenstates in every subspace $S^z$ there is a finite region of frustration where the MPSR holds.

In this paper we want to analyze the frustrated spin chain with $s = 1$. This spin system has attracted a lot of attention, because of the well-known Haldane conjecture [10]. The unfrustrated $s = 1$ spin chain shows a spin gap and exponential decaying correlations whereas the $s = 1/2$ spin chain has no gap and a power-law correlation decay. Since both systems are qualitatively different one might expect also a different influence of frustration on the MPSR.

## 2. The model and the Marshall–Peierls sign rule

In the following we study the MPSR for the frustrated antiferromagnetic $s = 1$ Heisenberg quantum spin chain

$$\widehat{H} = J_1 \sum_{\langle \mathrm{nn} \rangle} s_i s_j + J_2 \sum_{\langle \mathrm{nnn} \rangle} s_i s_j \,, \tag{1}$$

where $\langle \mathrm{nn} \rangle$ and $\langle \mathrm{nnn} \rangle$ denote nearest-neighbor and next-nearest-neighbor bonds on the linear chain. We set $J_1 = 1$ for the rest of the paper. For this model the MPSR can be exactly proved only for $J_2 \leq 0$.

The Marshall–Peierls sign rule can be described as follows: In the unfrustrated limit of $J_2 = 0$, the lowest eigenstate of the Hamiltonian (1) in each subspace of fixed eigenvalue $M$ of the spin operator $S^z_{\mathrm{total}}$ reads

$$\Psi_M = \sum_m c_m^{(M)} |m\rangle, \qquad c_m^{(M)} > 0. \tag{2}$$

Here the Ising-states $|m\rangle$ are defined by

$$|m\rangle \equiv (-1)^{S_A - M_A} |m_1\rangle \otimes |m_2\rangle \otimes \cdots \otimes |m_N\rangle, \tag{3}$$

where $|m_i\rangle$, $i = 1, \cdots, N$, are the eigenstates of the site spin operator $S^z_i$ $(-s_i \leq m_i \leq s_i)$, $S_A = \sum_{i \in A} s_i$, $M_{A(B)} = \sum_{i \in A(B)} m_i$, $M = M_A + M_B$. The lattice consists of twoequivalent sublattices $A$ and $B$. $s_i \equiv s$, $i = 1, \cdots, N$, are the site spins. The summations in Eq. (2) are restricted by the condition $\sum_{i=1}^N m_i = M$. The wave function (2) is not only an eigenstate of the unfrustrated Hamiltonian $(J_2 = 0)$ and $S^z_{\mathrm{total}}$ but also of the square of the total spin $S^2_{\mathrm{total}}$ with quantum number $S = |M|$. Because $c_m^{(M)} > 0$ is valid for each $m$ from the basis set (3) it is impossible to build up other orthonormal states without using negative amplitudes $c_m^{(M)}$. Hence the ground-state wave function $\Psi_M$ is nondegenerated. As it comes out, the MPSR is still fulfilled not only for the ground state but also for every lowest eigenstate in the subspace $M$ in the unfrustrated case. We emphasize that for $J_2 > 0$ no proof for the above statements can be given and that a frustrating $J_2 > 0$ can destroy the MPSR.

## 3. Results

We have calculated the ground state of the model (1) for $N = 8, \ldots, 14$ varying the frustration parameter $J_2$ by exact diagonalization. While analyzing the ground-state wave function according to the MPSR we found for every system a critical value of frustration $J_2^{\mathrm{crit}}$, where the MPSR starts to be violated. We apply the scaling law proposed by Zeng and Parkinson [6] and extrapolate our data as a function of $1/N^2$. We found a value for the infinite chain limit:

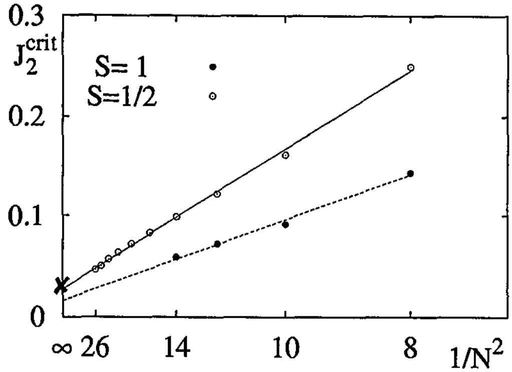


Fig. 1. The critical value of frustration $J_2^{\rm crit}$, where the MPSR starts to be violated as a function of the system size $N$. The cross denotes the value of Zeng and Parkinson [6].

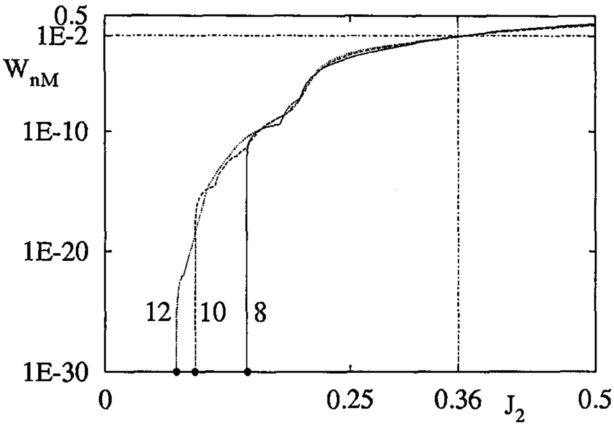


Fig. 2. The weight of non-Marshall-states of the ground-state wave function $W_{nM}$ as a function of frustration $J_2$ for systems with $N = 8, 10, 12$.

$J_2^{\rm crit}(\infty) = 0.016 \pm 0.003$. In Fig. 1 we compare these data with the values for the $s = 1/2$ systems ($N = 8, \ldots, 26$), where the extrapolation yields $J_2^{\rm crit}(\infty) = 0.027 \pm 0.003$. It is also interesting to note that this value is slightly lower than the value of 0.032 found by Zeng and Parkinson [6] using data for $N = 8, \ldots, 20$ only.

We argue that in the case of $s = 1$ the chain is more sensitive to frustration and therefore the MPSR is violated for smaller values of $J_2$. Nevertheless, in numerical methods the MPSR can be used at least approximately for much larger values of frustration. This can be justified by the examination the ground-state wave function according to the Ising-basis-states which violates the MPSR. We call these states non-Marshall-states and denote their weight by $W_{nM}$. In Fig. 2 we show $W_{nM}$ as a function of frustration $J_2$.

As can be seen in Fig. 2, the weight of the non-Marshall-states remains smaller than 1% (1E-2) until $J_2 \approx 0.36$. This result seems to be more or less size independent because all three lines for the systems with $N = 8, 10$, and 12 cross at this point. The points at the bottom line denote the first violation of the MPSR in a given system and coincide with the points given in Fig. 1. The examination of $W_{nM}$ indicates that for a quite large frustration the predominant part of the ground-state wave function fulfills the MPSR. Therefore, the MPSR can be used in numerical methods even if it does not hold strictly.

## 4. Conclusions

We have shown that in the frustrated antiferromagnetic $s = 1$ Heisenberg quantum spin chain the Marshall–Peierls sign rule is violated by frustration. By extrapolation to the infinite chain limit we found a critical value of frustration $J_2^{\mathrm{crit}} \approx 0.016 \pm 0.003$ below which the MPSR still holds exactly. By calculating the weight of the Ising-basis-states of the ground-state wave function which do not fulfill the MPSR we conclude that the MPSR can be used in numerical methods at least approximately until a large frustration of $J_2 \approx 0.36$.

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