9.7 cm

THE MARSHALL-PEIERLS SIGN RULE IN FRUSTRATED HEISENBERG CHAINS: THE INFLUENCE OF THE SPIN QUANTUM NUMBER

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We consider the frustrated quantum antiferromagnetic Heisenberg spin chain with spin $s = \frac{1}{2}, 1, \frac{3}{2}$ and 2 with regard to the Marshall-Peierls sign rule (MPSR) . The MPSR determines the **sign** of the Ising basis states building the ground-state wave function and has been proven exactly for bipartite lattices and arbitrary site spins by Lieb and Mattis. As pointed out in several papers the knowledge of the sign is of great importance in different numerical methods as quantum Monte-Carlo, variational wave function calculations and density matrix renormalization group calculations. Using analytic expressions and exact diagonalization data we investigate the breakdown of the MPSR in dependence on frustration. In particular we analyze the breakdown not only in the ground-state ($S = 0$) but also for the lowest eigenstates in higher subspaces of the total spin ($S > 0$). Though there is numerical evidence that in the ground-state for $s = \frac{1}{2}$ the MPSR holds exactly for a small finite frustration we find that for higher spins the influence of frustration on the MPSR is stronger. In particular our calculations suggest that for higher spin $s > 1$ there is no finite frustration where the MPSR is still exactly fulfilled. However, even for large frustration our results show that the weight of the non-Marshall states remains rather small so that the MPSR can be used approximately in the above mentioned numerical technics.

13.4 cm

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