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Density matrix renormalization group study of the competition between spin and quadrupolar correlations in the bilinear-biquadratic spin-1 model

Ultracold gases of alkali metal atoms have attracted a lot of attention recently both in experiment and theory. The SU(2) symmetric bilinear-biquadratic (BLBQ) spin-1 Heisenberg Hamiltonian is able to model the behavior of such systems with $F = 1$:

H = $\sum_i [(\vec{S}_i \otimes \vec{S}_{i+1}) \cos\theta + (\vec{S}_i \otimes \vec{S}_{i+1})^2 \sin\theta]$.

In the range $-\pi < \theta \leq \pi$ this model exhibits four quantum phases: the ordered ferromagnetic phase, the symmetry protected topological Haldane phase, the dimer phase, and the critical phase. The properties of the system in the critical phase have not been studied extensively so far. It was clarified, though, that the quadrupolar correlator of the system is larger than the spin correlator, therefore this phase was referred to as ”quadrupolar phase” [1].

We study the competition between spin and quadrupolar correlations in the system comprehensively in *all* phases, both in coordinate and momentum space. The properties of BLBQ spin *rings* (which are translational invariant) are studied. To this end, we use our version of density matrix renormalization group (DMRG) with SU(2) symmetry for periodic boundary conditions (PBC) [2]. Incorporation of SU(2) symmetry allows for formulation of the PBC algorithm in terms of reduced tensors only and reduces memory requirements significantly. It is also particularly useful in the ferromagnetic phase due to ability to capture the entire ground state multiplet in a single DMRG run.

From our numerical results we deduce approximate analytical expressions for the correlators inside and close to the ferromagnetic phase. In particular, we find that the spin correlator $S(r) = 0$ for any $r > 0$ at the phase transition point $\theta = -3\pi/4$ and in the ferromagnetic phase, while the quadrupolar correlator $Q(k)$ diverges at the momentum $k = 0$ in the same area and therefore plays the decisive role there. In fact, our results indicate that the spin correlations dominate only in the area $-\pi/2 < \theta < \pi/4$.

Furthermore, we simulate numerically the power law decay of both correlation functions with distance ($|S(r)| \sim r^{-\alpha}$, $|Q(r)| \sim r^{-\beta}$) in the entire critical phase, which has not been done before. The critical exponents show opposite behavior when increasing θ: α increases monotonously while β decreases. We prove analytically and numerically that $\alpha = 2$ at the first-order transition point $\theta = \pi/2$, and find a discontinuous jump of both correlation functions there.

[1] S. R. Manmana *et al.*, Phys. Rev. B 83, 184433 (2011).
[2] M. V. Rakov, M. Weyrauch, J. Phys. Commun. 1, 015007 (2017).
[3] M. V. Rakov, M. Weyrauch, manuscript in preparation.

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