Real-space spectral simulation of quantum spin models: Application to the Kitaev-Heisenberg model

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Abstract

The proliferation of quantum fluctuations and long-range entanglement presents an outstanding challenge for the numerical simulation of interacting spin systems with exotic ground states. In this talk, I will present a Chebyshev iterative method [1] that gives access to the thermodynamic properties and critical behavior of frustrated quantum spin models with good accuracy. The computational complexity scales linearly with the Hilbert space dimension and the number of Chebyshev iterations used to approximate the eigenstates. I will show results obtained with this approach for the spin correlations of the Kitaev-Heisenberg model, a paradigmatic model of honeycomb iridates that exhibits a rich phase diagram including a quantum spin liquid phase. The results are benchmarked against exact diagonalization and a popular iterative method based on thermal pure quantum (TPQ) states. All methods accurately predict transitions between paramagnetic, stripy antiferromagnetic and spin-liquid phases for honeycomb layers with antiferromagnetic Heisenberg interactions. Our findings suggest that a hybrid Chebyshev-TPQ approach could open the door to previously unattainable studies of quantum spin models in two dimensions, namely a-RuCl3 in proximity to graphene [2]. This system is promising for quantum computing since it may support bond-directional Kitaev spin interactions.

References

1. Aires Ferreira and Eduardo R. Mucciolo, Phys. Rev. Lett. , 115 (2015) 106601.
2. Sananda Biswas, Ying Li, Stephen M. Winter, Johannes Knolle, and Roser Valentí, Phys. Rev. Lett. 123 (2019), 237201.

Figures

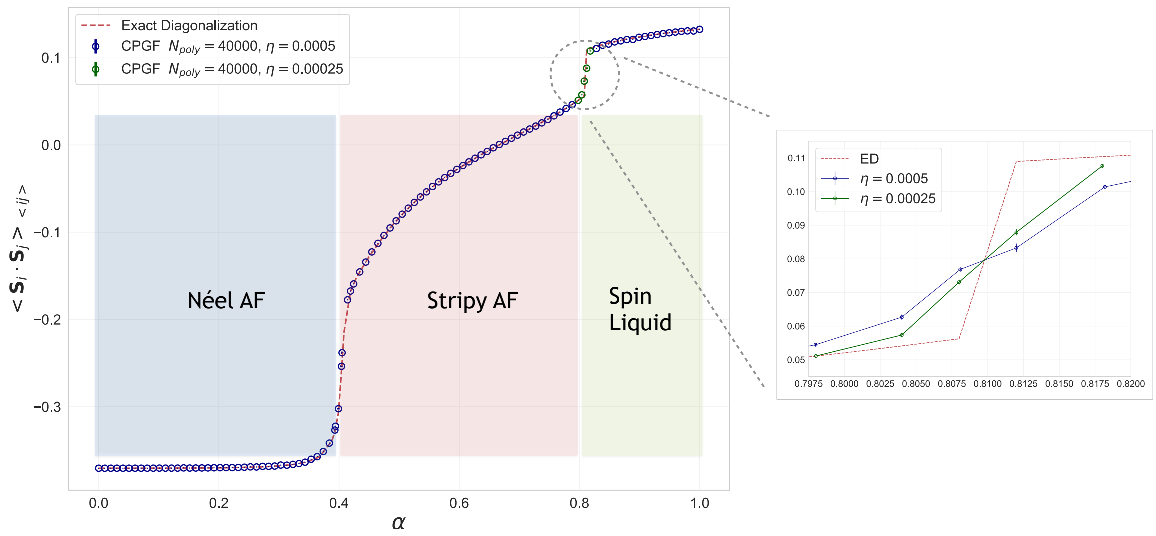

Figure 1: Nearest neighbor spin correlation for the ground state of a 24-site Kitaev-Heisenberg model on the honeycomb lattice with periodic boundary conditions, displaying two phase transitions.