

# Simulation of Quantum Spin-Liquid Phases with Spectral Methods

Francisco Monteiro de Oliveira Brito

Aires Ferreira

Department of Physics, University of York, York YO10 5DD, United Kingdom

fmob500@york.ac.uk

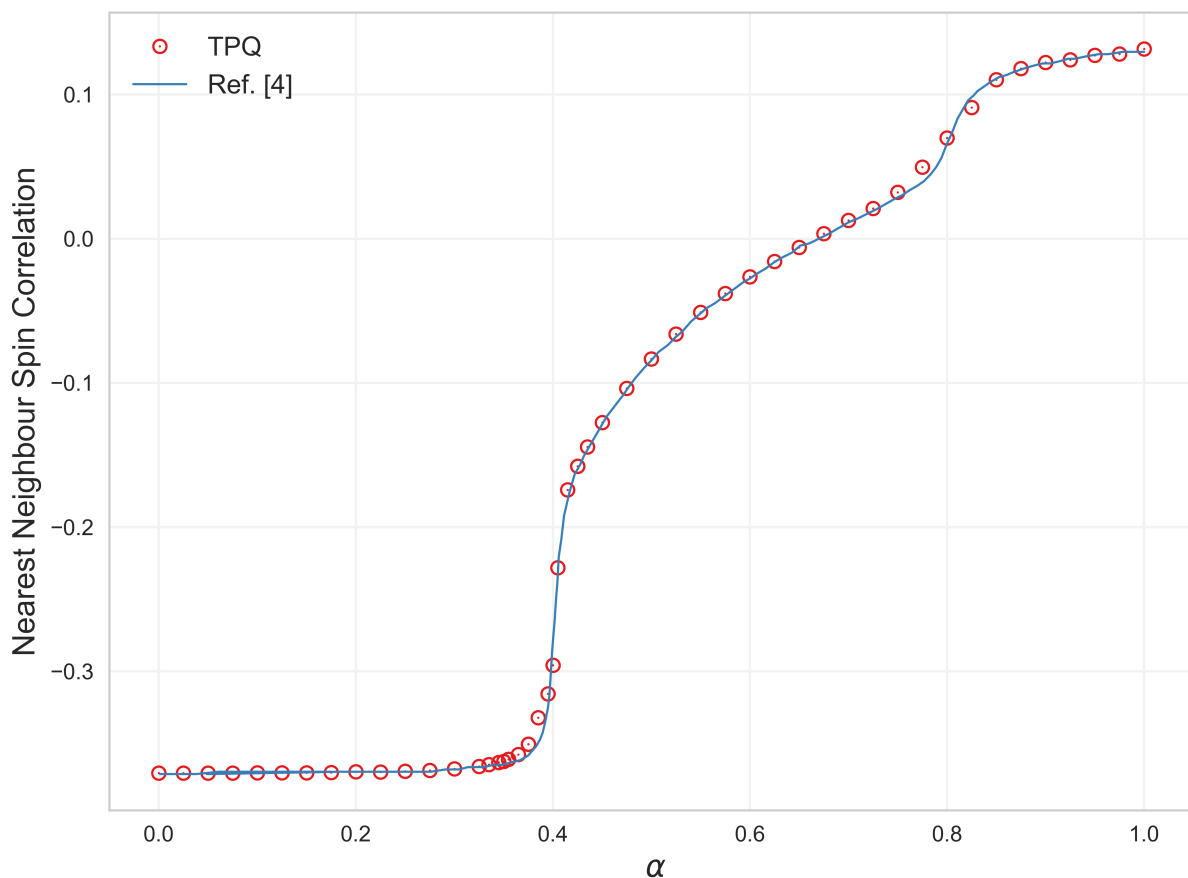
## Abstract

In this work, we combine accurate Chebyshev polynomial expansions [1, 2] and thermal pure quantum states (TPQ) [3] to simulate quantum spin models with highly entangled ground states. We use this hybrid framework to map out in a numerically exact fashion the phase diagram of the Kitaev-Heisenberg model on the honeycomb lattice [4]; see Figure 1. Energy, magnetization and spin correlations are calculated with spectral accuracy in large systems with up to 24 spins. Our method can be easily extended to realistic spin models accommodating impurities, defects and external perturbations. Our results suggest that the hybrid spectral-TPQ approach can provide advantages over pure TPQ and other state-of-the-art methods in probing complex spin systems.

## REFERENCES

1. A. Ferreira, ER. Mucciolo, Phys. Rev. Lett. 115, 106601 (2015), A. Braun, P. Schmitteckert, Phys. Rev. B 90, 165112 (2014)
2. S. M. João et al., Royal Society Open Science, 7, 2 (2020)
3. S. Sugiura and A. Shimizu, Phys. Rev. Lett. 108, 240401 (2012)
4. J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev. Lett. 105, 027204 (2010)

## FIGURES



**Figure 1:** Spin-spin correlations for nearest neighbours for the Kitaev-Heisenberg model on a honeycomb lattice with 24 sites. Here,  $\alpha$  is a parameter that interpolates between the Heisenberg and Kitaev models. For  $\alpha = 0$ , we have the Heisenberg model and for  $\alpha = 1$ , we have the Kitaev model, which is exactly solvable.