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SIMULATION OF QUANTUM SPIN-LIQUID PHASES WITH SPECTRAL METHODS

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Abstract

In this work, we combine accurate Chebyshev polynomial expansions [1–3] and thermal pure quantum states (TPQ) [4] 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 [5]. 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.

Introduction

In this work, we use a spectral approach to identify spin-liquid phases. We start by benchmarking the "thermal pure quantum" (TPQ) states method against a novel spectral method that was developed in-house called "Chebyshev polynomial Green function" (CPGF) method. The benchmarking that was carried out so far aims at optimizing numerical efficiency, i.e. computational complexity and energy resolution, which affects the accuracy of these methods. These details crucially affect our ability to effectively simulate quantum spin-liquids (QSLs). The model that was used to verify that QSL phases can be captured by these methods was the Kitaev-Heisenberg model on the honeycomb lattice. This model interpolates between the Heisenberg and Kitaev models, which are both exactly solvable. However, as one moves from one model to the other, there are nontrivial phase transitions. We verified that our methods are perfectly able to capture these transitions, which is a good indication that they could be used to study QSLs. Moreover, we are able to reproduce the behaviour of the specific heat as a function of temperature for the pure Kitaev model, showing a two-peak behaviour.

Main Objectives

1. Identify quantum spin-liquid phases using accurate and efficient spectral methods.
2. Develop software that goes beyond the state-of-the-art calculations for quantum spin models with application to spin-liquids, namely simulating larger systems with controlled convergence properties and statistical error.

Methods

Thermal Pure Quantum States

The idea is to represent an equilibrium state as a pure quantum state. The method is based on an iterative scheme. Given an upper bound on the energy density, u, at each iteration k, a new state $|\psi_{k+1}>$ is computed:

$$|\psi_{k+1}\rangle \equiv \frac{(u-\hat{h})\,|\psi_k\rangle}{||\,(u-\hat{h})\,|\psi_k\rangle\,||}, \tag{1}$$

where $\hat{h}$ is the Hamiltonian divided by the total number of sites. To each iteration, there corresponds a given temperature. Using the states obtained in this way, we can compute quantum averages, such as the energy density, or the spin correlation.

Chebyshev Polynomial Green Function

This method is based on numerically evaluating the resolvent operator $\mathcal{G}(z) = (z-\mathcal{H})^{-1}$, with $z = \varepsilon + i\eta$, where ε is the energy, and the resolution $\eta \gtrsim \delta\varepsilon$, the mean level spacing. We use an expansion in terms of Chebyshev polynomials $T_n(\mathcal{H})$, with coefficients $g_n(\varepsilon,\lambda)$,

$$\mathcal{G}(\varepsilon + i\lambda) = \sum_k \frac{1}{\varepsilon + i\lambda - \varepsilon_k}|k\rangle\langle k| = \sum_{n=0}^{\infty} g_n(\varepsilon,\lambda) T_n(\mathcal{H}). \tag{2}$$

The truncation of the Chebyshev series does not compromise convergence to the target function, i.e. the method is numerically exact. The lattice Green function can be cast as the Chebyshev series

$$\mathcal{G}(z) = \sum_{n=0}^{\infty} g_n(z) T_n(\mathcal{H})\,, \quad \text{with} \quad g_n(z) = \frac{2}{1+\delta_{0,n}} \frac{\left(z - i\sqrt{1-z^2}\right)^n}{i\sqrt{1-z^2}}. \tag{3}$$

Observables may then be written in terms of the Green function and computed using this method. The advantages of this approach include: ability to fix the desired resolution; numerically exact, fast convergence. However, it requires target energy/resolution, unknown a priori. Hence, we use TPQ to estimate the ground state energy and then use that as an input of CPGF in a hybrid approach.

Results

We study the ferromagnetic Kitaev model [6] and the Kitaev-Heisenberg model of Ref.[5], whose results we reproduce (see Fig.1). Both models are considered on the honeycomb lattice.

The Hamiltonian is constituted by Heisenberg and Kitaev terms on each nearest neighbour pair i, j.

$$\mathcal{H}^{(\gamma)}_{Heis\;ij} = J_H \mathbf{S}_i \cdot \mathbf{S}_j \qquad \mathcal{H}^{(\gamma)}_{Kit\;ij} = J_K S_i^{\gamma} S_j^{\gamma}, \tag{4}$$

for $\gamma = x, y, z$, and each of the 3 nearest neighbours on the honeycomb lattice corresponds to one of the directions x, y, z. Here, $J_H = (1-\alpha)$ and $J_K \equiv J = -2\alpha$. In Fig.2, we take $\alpha = 1$.

For the Kitaev model, our two-peak structure of the temperature dependence of the specific heat is consistent with previous studies, namely Refs.[7–9] (see Fig.2).

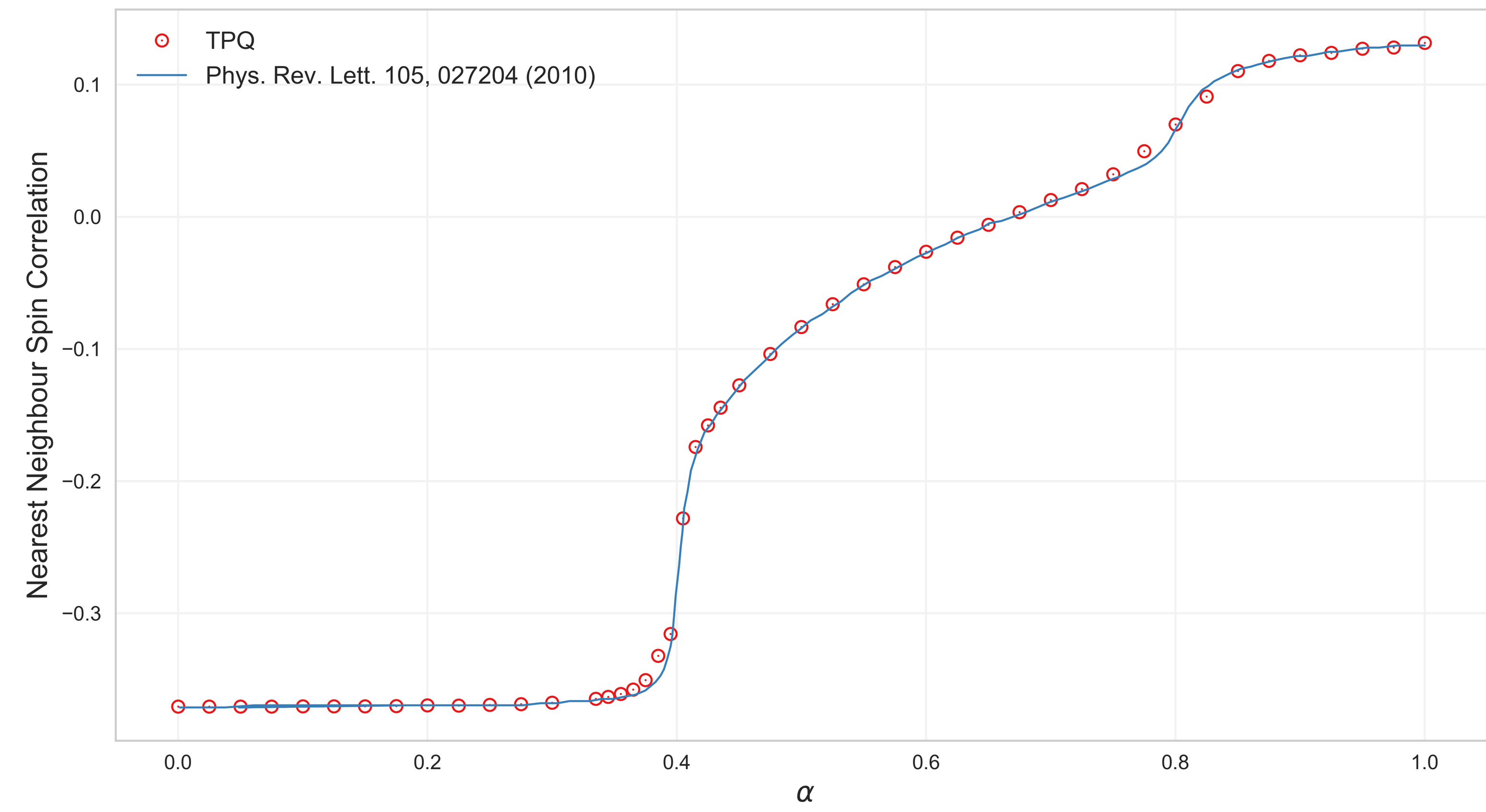

Figure 1: Nearest Neighbour Spin Correlations for the Kitaev-Heisenberg model on the honeycomb lattice, computed using TPQ with 24 spins. The results coincide with those of Ref.[5], showing two phase transitions: from an antiferromagnetic state in the Heisenberg limit to a stripy antiferromagnetic phase at about $\alpha = 0.4$, and from the stripy phase to the spin-liquid phase close to $\alpha = 0.8$.

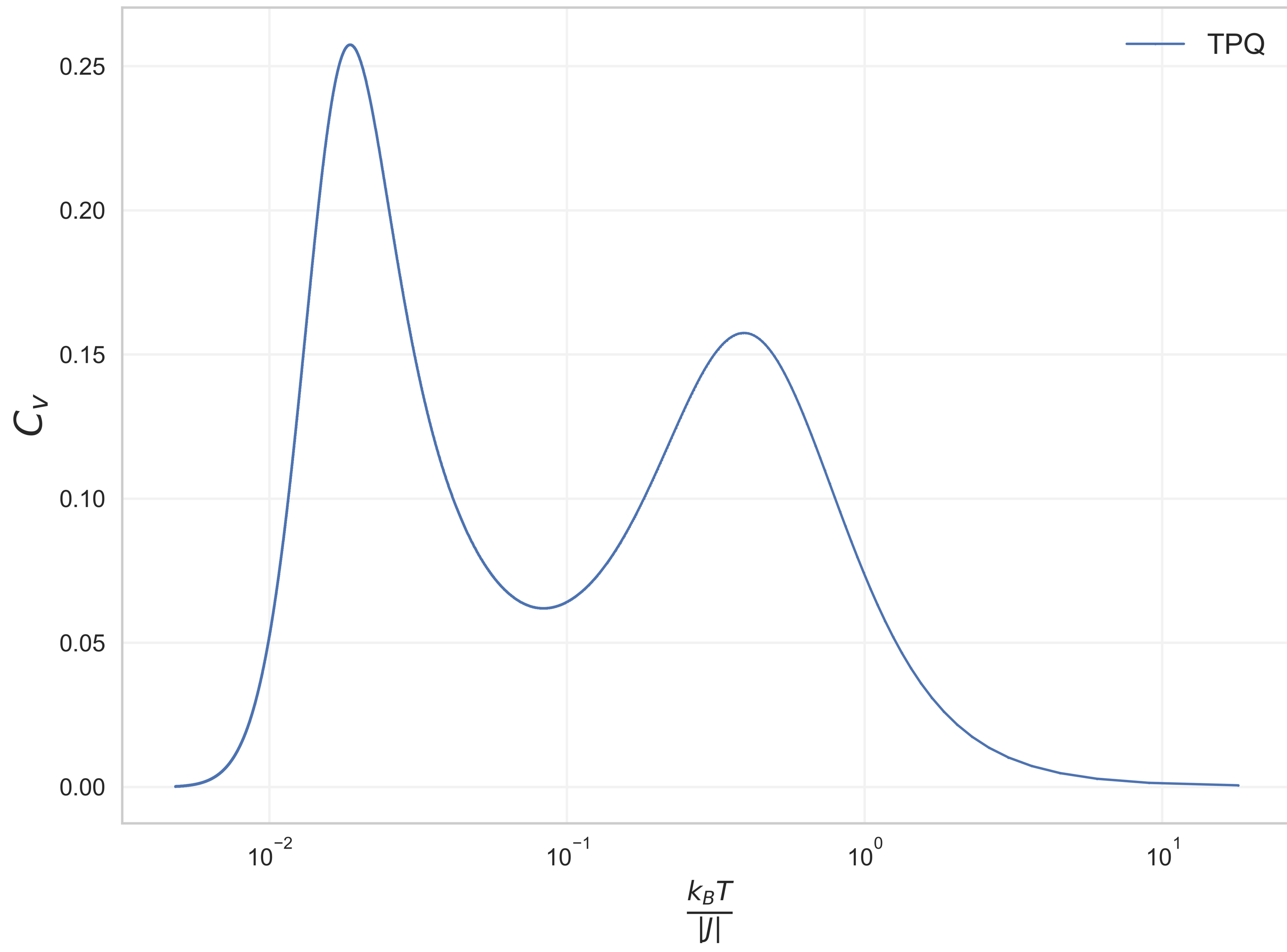

Figure 2: Dependence of the specific heat per site on temperature for the ferromagnetic Kitaev model on the honeycomb lattice, computed using TPQ with 18 spins. It shows the typical two-peak profile that is associated with the spin-liquid phase.

Conclusion

- We have implemented a hybrid TPQ-CPGF method, which is advantageous compared with TPQ.
- CPGF allows direct control of the resolution and temperature.
- The convergence and accuracy of CPGF can be reliably controlled.
- We successfully identified a quantum spin-liquid phase using our approach.

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