Probing the stability of the spin-liquid phases in the Kitaev-Heisenberg model using iPEPS

Juan Osorio
Institute for Theoretical Physics
ETH Zürich

Philippe Corboz
Institute for Theoretical Physics
University of Amsterdam

Matthias Troyer
Institute for Theoretical Physics
ETH Zürich
Tensor Networks

Entanglement-based approach

M. Hastings, arXiv:0705.2024
F. Brandao, M. Horodecki, arXiv: 1206.2947

Area Law for Entanglement Entropy

$S(A) \sim A$

Matrix Product State (MPS)
Efficient Representation
Tensor Networks

Entanglement-based approach

Hilbert Space

$H \sim V^N$

Exponential growth

low entanglement corner

$S(A) \sim A$

Area law growth for entanglement entropy
iPEPS

- **infinite** Projected Entangled-Pair States
- Define arbitrary structure and size of unit cell.
- Include effect of infinite system via so-called environment tensors.

Typically perform ground state search using imaginary-time evolution.

*Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)*
Contracting the network

Corner Transfer Matrix (CTM)

\[ C(D, \chi) \sim \chi^3 D^4 \]

**PEPS contraction**

Cost \( \sim \) \( \exp(N) \)

**Approximations Required!**

Nishino, Okunishi, JPSJ65 (1996)

Orus, Vidal, PRB 80 (2009)
Proposed by Chaloupka et al. as effective model for (layered) Iridate compounds $A_2IrO_3$ ($A = \text{Li, Na}$).

- Nearest-neighbor (pseudo-)spin interactions composed of isotropic Heisenberg + anisotropic Kitaev terms.

Small system studies show that (zigzag) magnetic order found in Iridate compounds is natural ground state of KH model.

The Hamiltonian

$$H_{i,j}^{(\gamma)} = \cos \varphi \ \vec{S}_i \cdot \vec{S}_j + 2 \sin \varphi \ S_i^{(\gamma)} S_j^{(\gamma)}$$

The general procedure is as follows. Let us represent the site index \( a \) as:

\[
H = -J_x \sum_{x\text{-links}} \sigma^x_j \sigma^x_k - J_y \sum_{y\text{-links}} \sigma^y_j \sigma^y_k - J_z \sum_{z\text{-links}} \sigma^z_j \sigma^z_k
\]

where \( \sigma^x, \sigma^y, \sigma^z \) are Pauli operators and \( J_x, J_y, J_z \) are model parameters.

Gapless (B) phase hosts non-abelian anyonic excitations.

Perfect benchmark.
Isotropic $J_x=J_y=J_z$ point (B-phase).

- Exact energy per site: $-0.3936$.
- iPEPS energy:
  - $D=7$ (AFM): $-0.3933$
  - $D=7$ (FM): $-0.3931$
- Monotonic decrease with $D$.

Spin liquid ground state $\Rightarrow$ Zero magnetization expected.

- iPEPS results:
  - $D=7$ (AFM): $0.01$
  - $D=7$ (FM): $0.02$
- Monotonic decrease with $D$.
- Infinite D extrapolation yields vanishing magnetization.

Results from Baskaran et al. show that only NN correlations of corresponding bond type are non-vanishing, eg.

\[ \gamma(i, j) = x \rightarrow \langle \sigma^x_i \sigma^x_j \rangle = 0.525 \]
\[ \langle \sigma^y_i \sigma^y_j \rangle = 0 \]
\[ \langle \sigma^z_i \sigma^z_j \rangle = 0 \]

Data not shown < 10^{-3}.
Systematic improvement upon increasing bond dimension.

Kitaev's Honeycomb model
Spin-Spin Correlations

Kitaev-Heisenberg model

Previous Results

- Type of transition observed in 4th quadrant differed for small systems vs SP Mean-Field study.
- Survival of QSL phases in TD limit remained under debate.
- Type of phase transitions from AQSL to symmetry broken not certain.

\[ H_{i,j}^{(\gamma)} = \cos \varphi \, \vec{S}_i \cdot \vec{S}_j + 2 \sin \varphi \, S_i^{(\gamma)} S_j^{(\gamma)} \]
Kitaev-Heisenberg model

iPEPS Approach

Energy crossing + OP analysis

• Perform initial runs mapping out phases arising in phase diagram.
• Find representative states deep inside each phase.
• Compare energies + OP of different phases in the vicinity of phase transitions.
• “Hysteretic” behavior will hint towards 1st order type transitions.

Spin Liquid to Stripy Transition

- Weak energy crossing at $\varphi \sim -80^\circ$ (D=6) suggests 1st order phase transition.
- Transition point shifts towards lower $\varphi$ with increasing D.

Kitaev-Heisenberg model
Spin Liquid to Stripy Transition
Energy Crossings

**Kitaev-Heisenberg model**

**Spin Liquid to Stripy Transition**

**Magnetic Order Parameters**


- Discontinuous behavior for Magnetization/Stripy order parameters in GS (red diamonds/cyan circles).
- Green/blue data show OP values for each of the phases.
- Discontinuity expected to remain finite in infinite D limit.
Kitaev-Heisenberg model

Spin Liquid to Stripy Transition

Bond Order Parameter

Dominant NN Correlations

\( \phi \) [deg]

\( \Delta E_{\text{Bond}} \)

\( \langle \sigma \rangle \)

\( \langle \sigma \rangle \)

\( \chi = 51 \)

\( \text{Ground State (D=6 – } \chi = 51) \)

\( \text{Stripy Ordered (D=6 – } \chi = 51) \)

\( \text{Spin Liquid (D=6 – } \chi = 51) \)

\( \text{XX (D=6 – } \chi = 51) \)

\( \text{YY (D=6 – } \chi = 51) \)

\( \text{ZZ (D=6 – } \chi = 51) \)

\( \text{JOL, P. Corboz, M. Troyer, arXiv:1408.4020.} \)
Kitaev-Heisenberg model

FM Spin Liquid to Symmetry-broken

FSL - Ferro

FSL - Stripy

Kitaev-Heisenberg model
AFM Spin liquid to symmetry broken

**ASL - Néel**

**ASL - Zigzag**

Kitaev-Heisenberg model

Summary

| ASL - Néel | 88° | 88° |
| ASL - Zigzag | 92° | 92° |
| FSL - Stripy | -80° | -76° |
| FSL - Ferro | -102° | -108° |
| Ferro - Zigzag | 161° | 162° |
| Stripy - Néel | -33° | -34° |