

Spin-Ice State of the Quantum Heisenberg Antiferromagnet on Pyrochlore Lattice



Yuan Huang^{1,2}, Kun Chen^{1,2}, Youjin Deng^{1,2}, Nikolay V. Prokof'ev^{1,3}, and Boris V. Svistunov^{1,3}

¹ University of Massachusetts

² University of Science and Technology of China

³ National Research Center "Kurchatov Institute, Moscow"



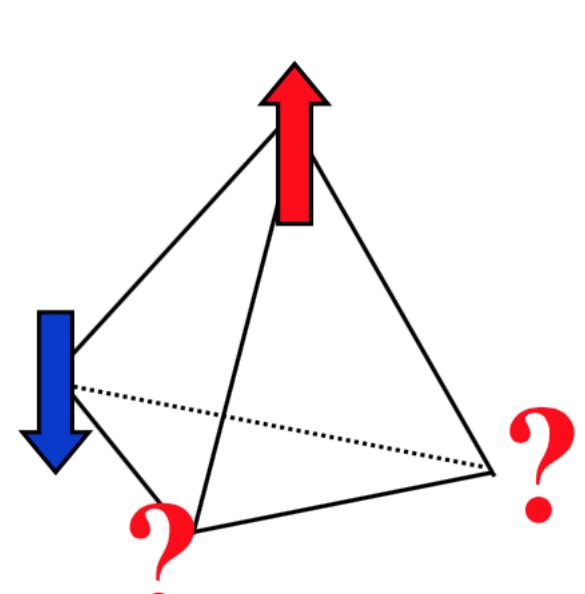
Abstract

We study the low-temperature physics of the spin-1/2 Heisenberg antiferromagnet on a pyrochlore lattice and find a “fingerprint” evidence for the thermal spin-ice state in this frustrated quantum magnet. The identification of the spin-ice state is done through a remarkably accurate microscopic correspondence for static structure factor between the quantum Heisenberg and classical Heisenberg/Ising models, and the characteristic bow-tie pattern with pinch points. The dynamic structure factor is consistent with diffusive spinon dynamics at pinch points.

Frustrated Magnets

Frustration

- (classical) massive degenerate ground state
- strong correlations/fluctuations
- novel phases, including spin liquids
- common in many real materials
- typical example in 3D: pyrochlore lattice

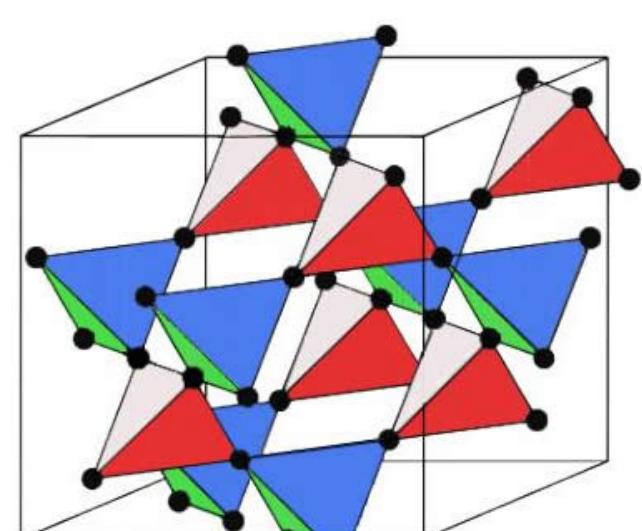


Model

AF quantum Heisenberg model on pyrochlore lattice

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (J > 0)$$

no controlled method to study the low temperature physics so far



Diagrammatic Monte Carlo

Spin Fermionization

$$H = \frac{J}{4} \sum_{\substack{\langle i,j \rangle \\ \alpha\beta\gamma\delta}} (f_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} f_{i\beta}) \cdot (f_{j\gamma}^\dagger \boldsymbol{\sigma}_{\gamma\delta} f_{j\delta}) - \frac{i\pi T}{2} \sum_i (n_i - 1)$$

- complex chemical potential term: exact cancellation of all unphysical contributions in grand-canonical statistics
- interacting flat-band fermionic Hamiltonian

Feynman Diagrams & DiagMC

Full Green's function: expansion of Feynman diagrams in bare Green's function and coupling constant

Dyson equations:

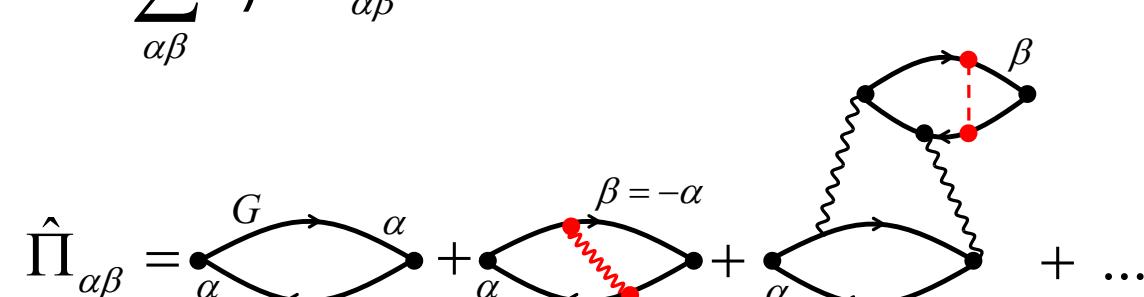
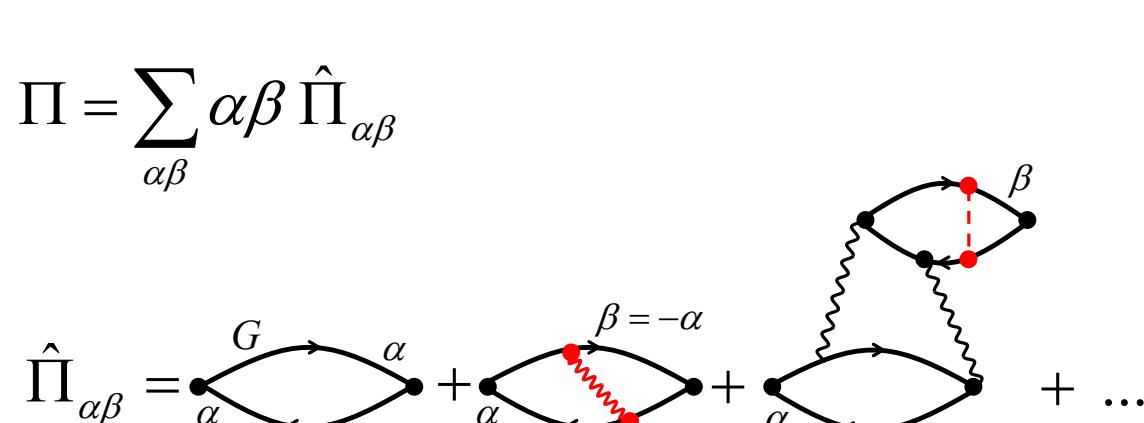
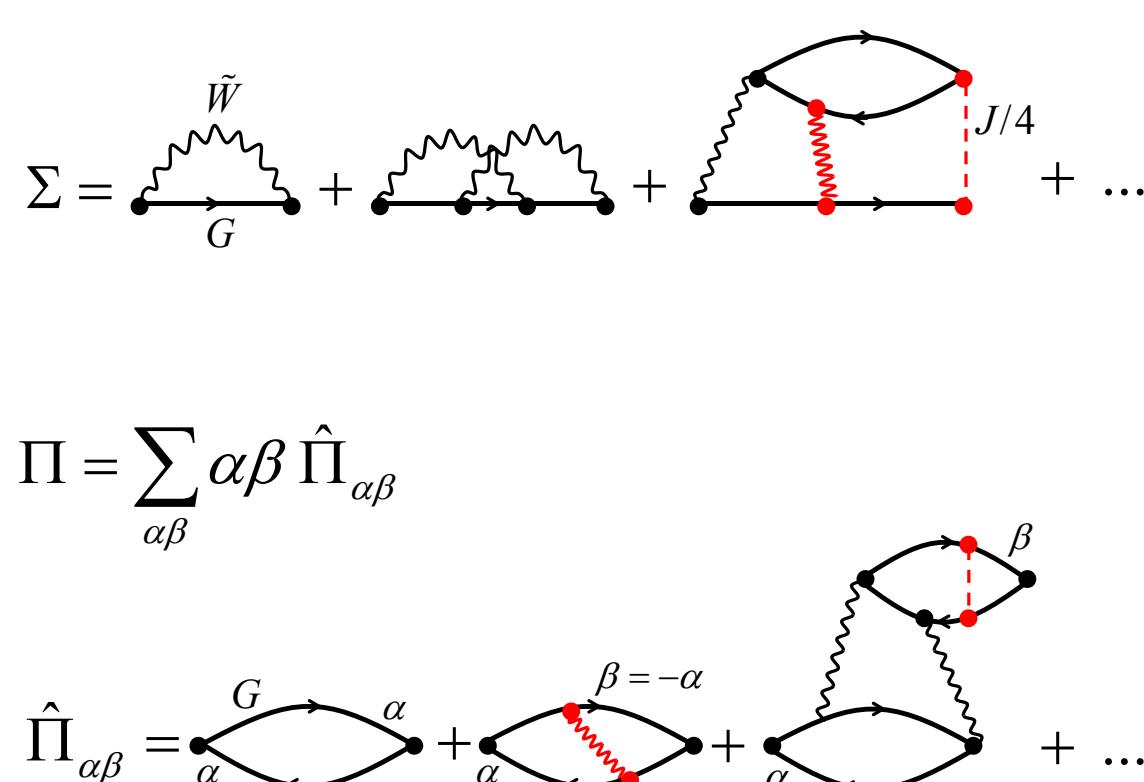
$$G_\alpha = G_\alpha^{(0)} + G_\alpha^{(0)} \Sigma_\alpha G_\alpha$$

$$\hat{U} = \hat{J} - \hat{J} \cdot \hat{\Pi} \cdot \hat{U}$$

Susceptibility:

$$\chi(\mathbf{r}, \tau) = \langle \mathbf{S}(\mathbf{r}_i, 0) \cdot \mathbf{S}(\mathbf{r}_j, \tau) \rangle$$

Dyson-like equation $\hat{\chi} = \hat{\Pi} + \hat{\Pi} \cdot \hat{J} \cdot \hat{\chi}$



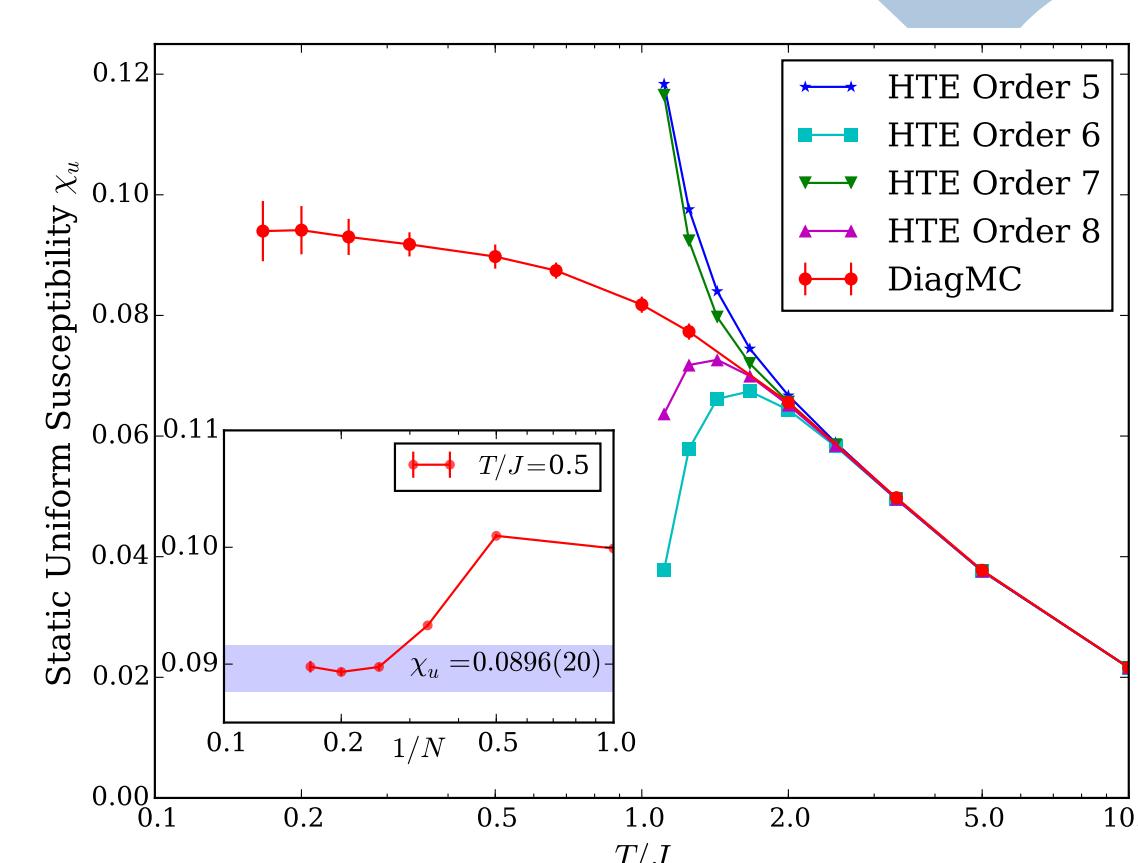
Series Convergence

Uniform susceptibility χ_u

$$\chi_u = \sum_r \int_0^\beta d\tau \chi(\mathbf{r}, \tau)$$

- High temperature expansion diverges at $T < J$
- DiagMC converges down to $T/J \approx 1/6$
⇒ **strongly correlated regime!**
- Convergence after 6th order diagrams
⇒ cancellation of 113824 diagrams

HTE: H. J. Schmidt, A. Lohmann, and J. Richter, P. R. B 84, 104443 (2011).

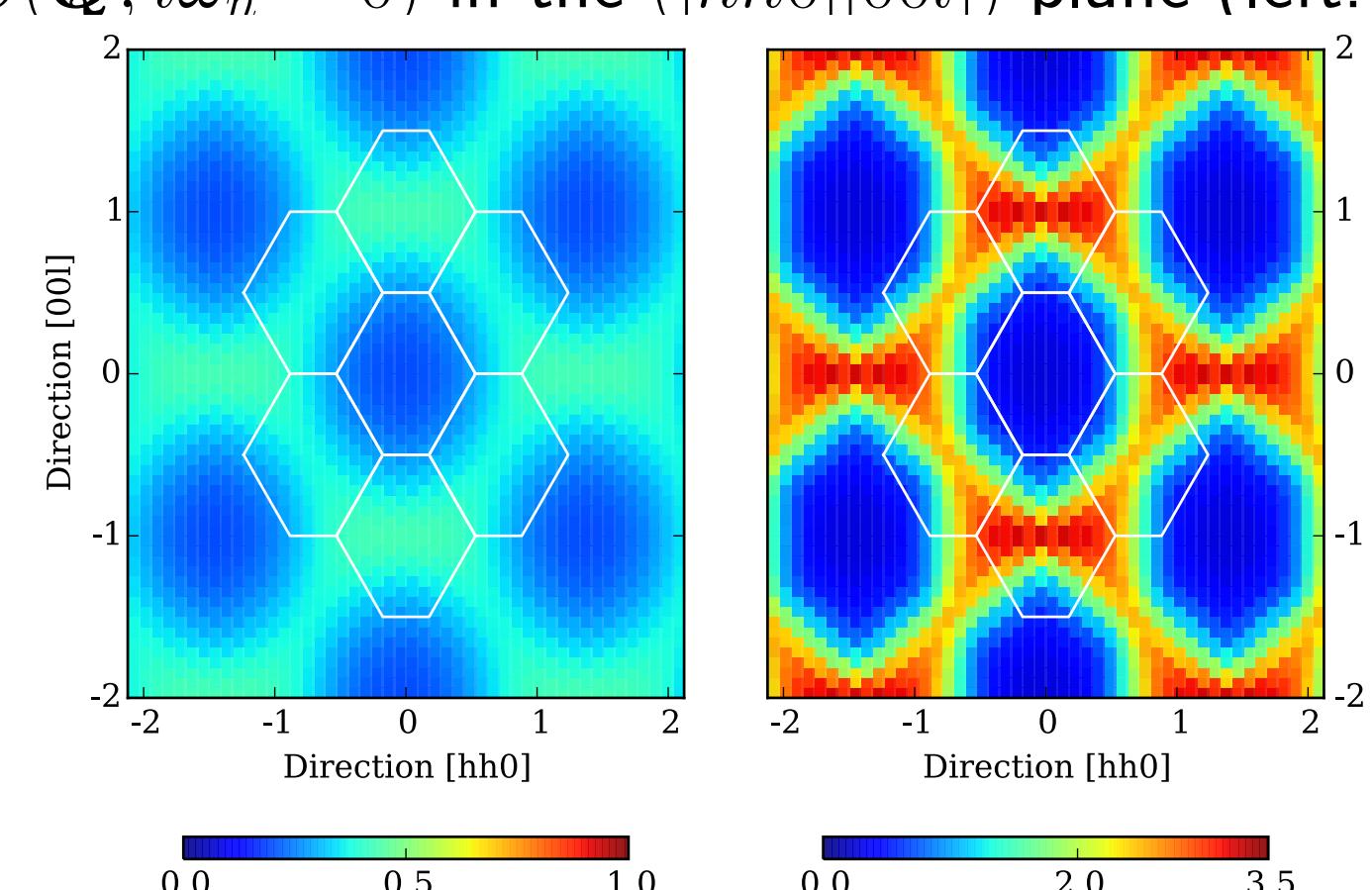


Spin Ice: Static Structure Factor

Structure factor in the momentum–Matsubara-frequency domain

$$S(\mathbf{Q}, i\omega_n) = \frac{1}{V} \sum_{i,j} \int_0^\beta d\tau \chi(\mathbf{r}_i, \mathbf{r}_j; \tau) e^{-i[\mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{r}_i) + \omega_n \tau]}$$

$S(\mathbf{Q}, i\omega_n = 0)$ in the $([hh0][00l])$ plane (left: $T = 2J$; right: $T = J/6$)



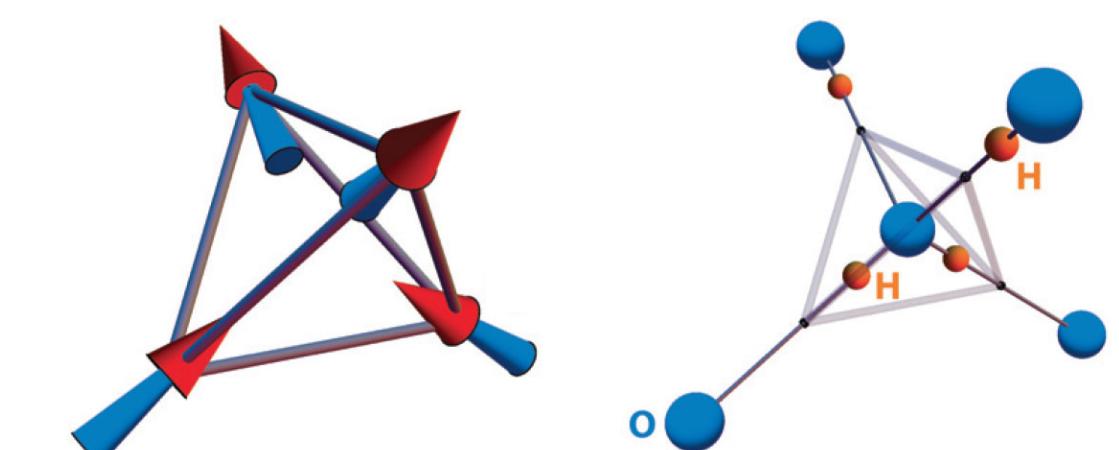
- high-T($2J$): checkerboard pattern
- low-T($J/6$): bow-tie pattern with pinch points

Spin Ice: Static Structure Factor

Pinch points are direct consequences of '2-in/2-out' ice rule.

Around the pinch points, structure factor has pseudo-dipolar singularities:

$$S(\mathbf{Q}_{\text{pinch}} + \mathbf{q}) \propto \frac{q_\perp^2}{q_\parallel^2 + q_\perp^2}$$



Spin Ice: Quantum-to-Classical Correspondence

Static spin-spin correlation function:

$$\chi(\mathbf{r}) \equiv \int_0^\beta d\tau \chi(\mathbf{r}_0, \mathbf{r}_i; \tau)$$

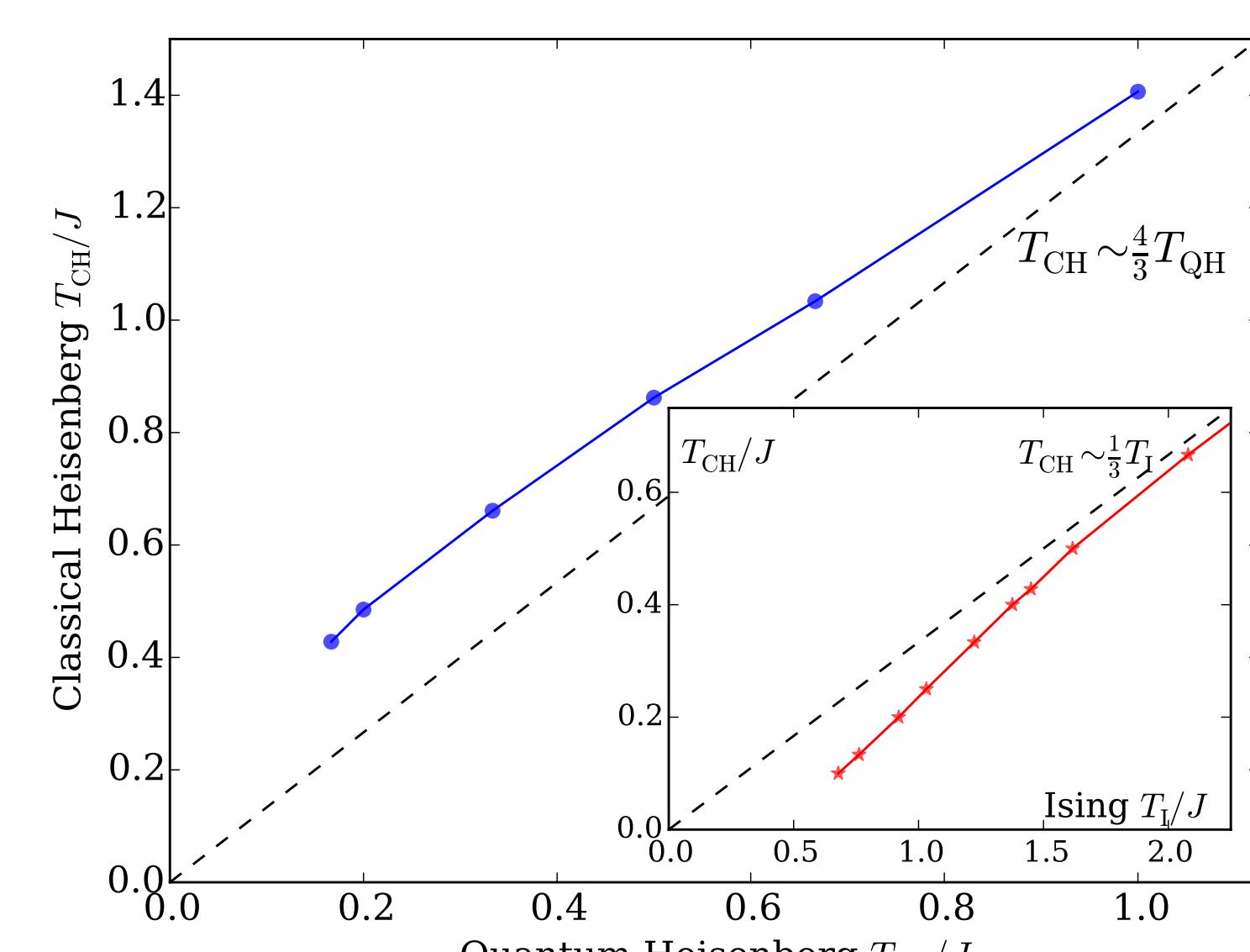
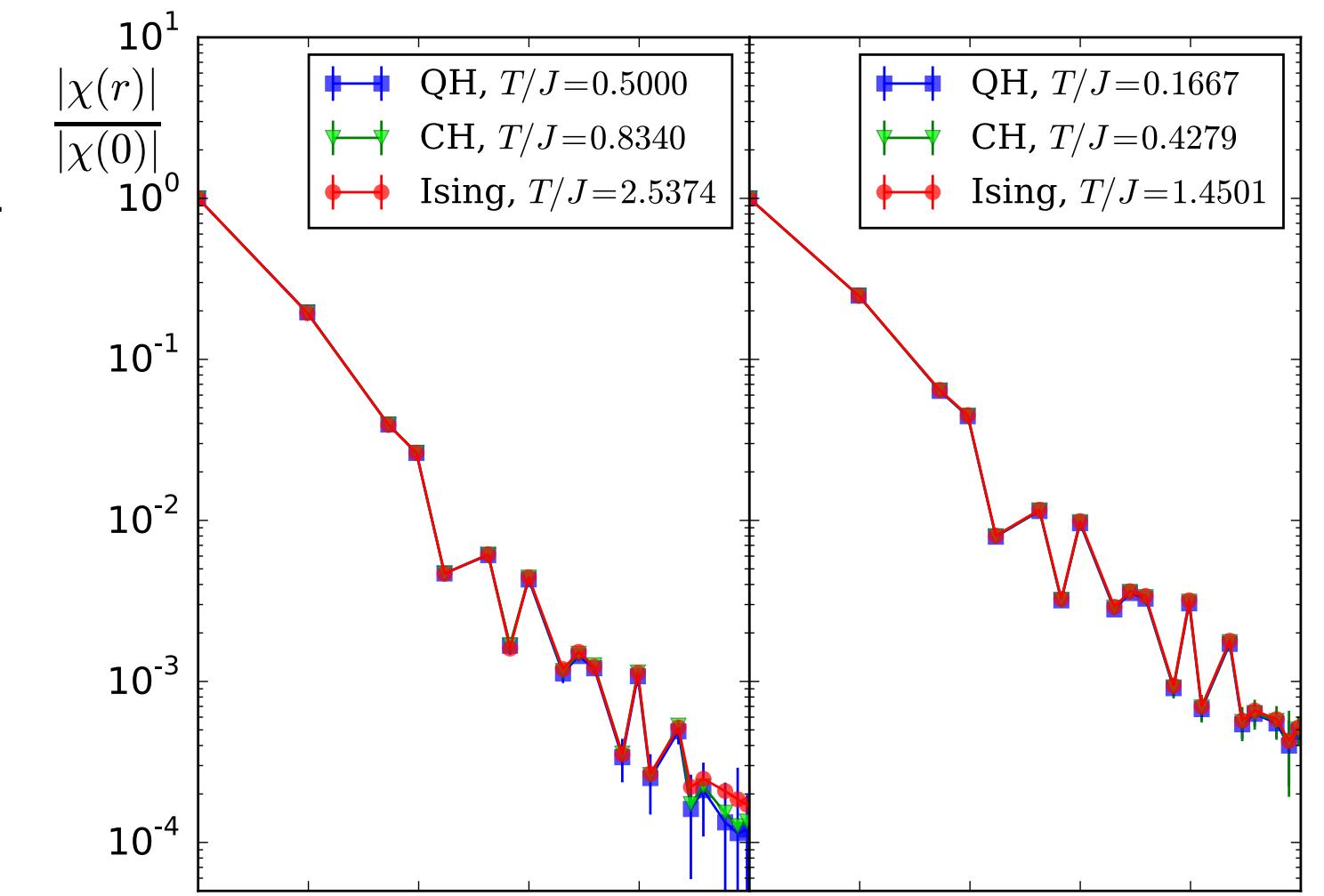
Compare the normalized static correlator $f(\mathbf{r}) = \frac{\chi(\mathbf{r})}{\chi(0)}$ in

- quantum Heisenberg model (QH)
- classical Heisenberg model (CH)
- Ising model

The QCC holds for:

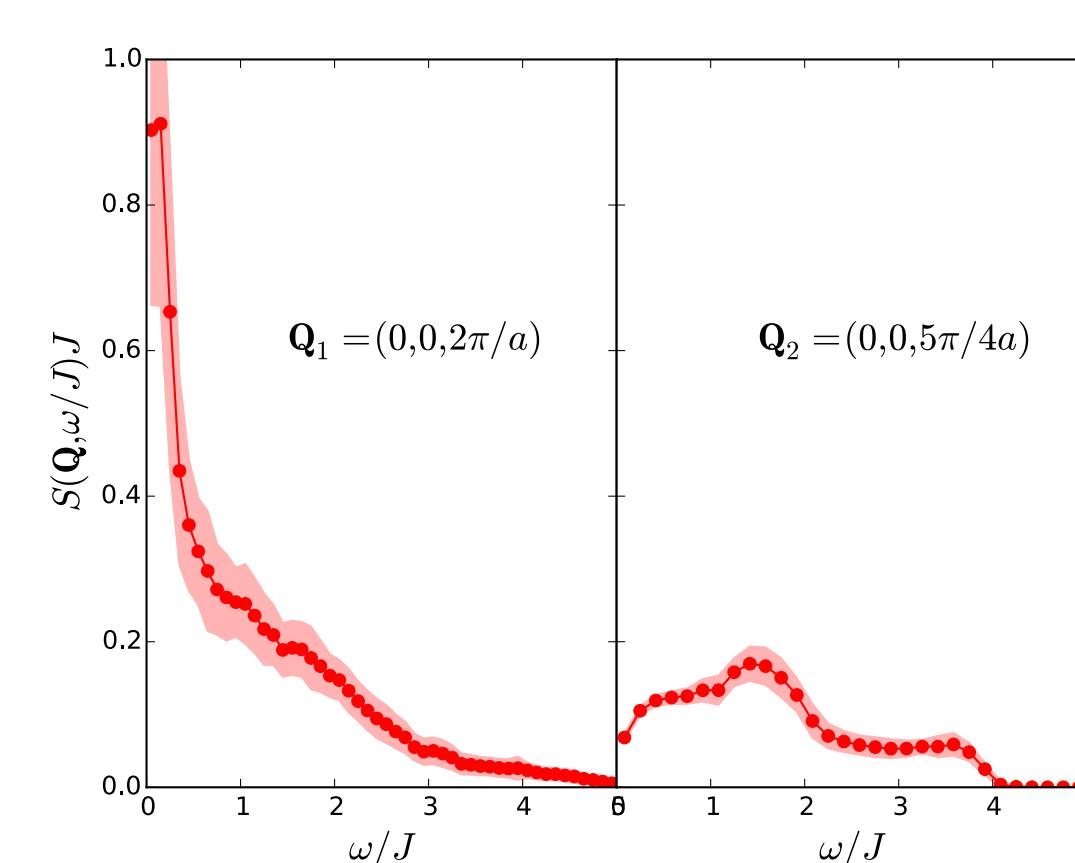
- only static correlations, but not for equal-time correlations
- all distances starting from the nearest-neighbor sites
- not only high-T limit but also intermediate temperature regime (down to $J/6$)

* Similar QCC between quantum and classical Heisenberg model was also found on triangular and square lattice [?]



Spin Ice: Dynamics

Dynamic structure factor $S(\mathbf{Q}, \omega)$



From Matsubara frequency functions to real frequency (numerical analytic continuation):

$$S(\mathbf{Q}, i\omega_n) = \frac{1}{\pi} \int_0^\infty \frac{(1 - e^{-\beta\omega})\omega}{\omega_n^2 + \omega^2} S(\mathbf{Q}, \omega) d\omega$$

- \mathbf{Q}_1 (pinch point): diffusive (Drude-type) spinon peak
- \mathbf{Q}_2 (on the nodal line): spinon contributions get suppressed due to ice rule; a broad continuum originating from local spin fluctuations

References & Acknowledgments

- [1] Y. Huang, K. Chen, Y. Deng, N. V. Prokof'ev, and B. V. Svistunov, Phys. Rev. Lett. **116**, 177203 (2016).
- [2] S. A. Kulagin, N. V. Prokof'ev, O. A. Starykh, B. V. Svistunov, and C. N. Varney, Phys. Rev. Lett. **110**, 070601 (2013); Phys. Rev. B **87**, 024407 (2013).
- [3] N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. B **84**, 073102 (2011).



SIMONS
FOUNDATION



NSFC