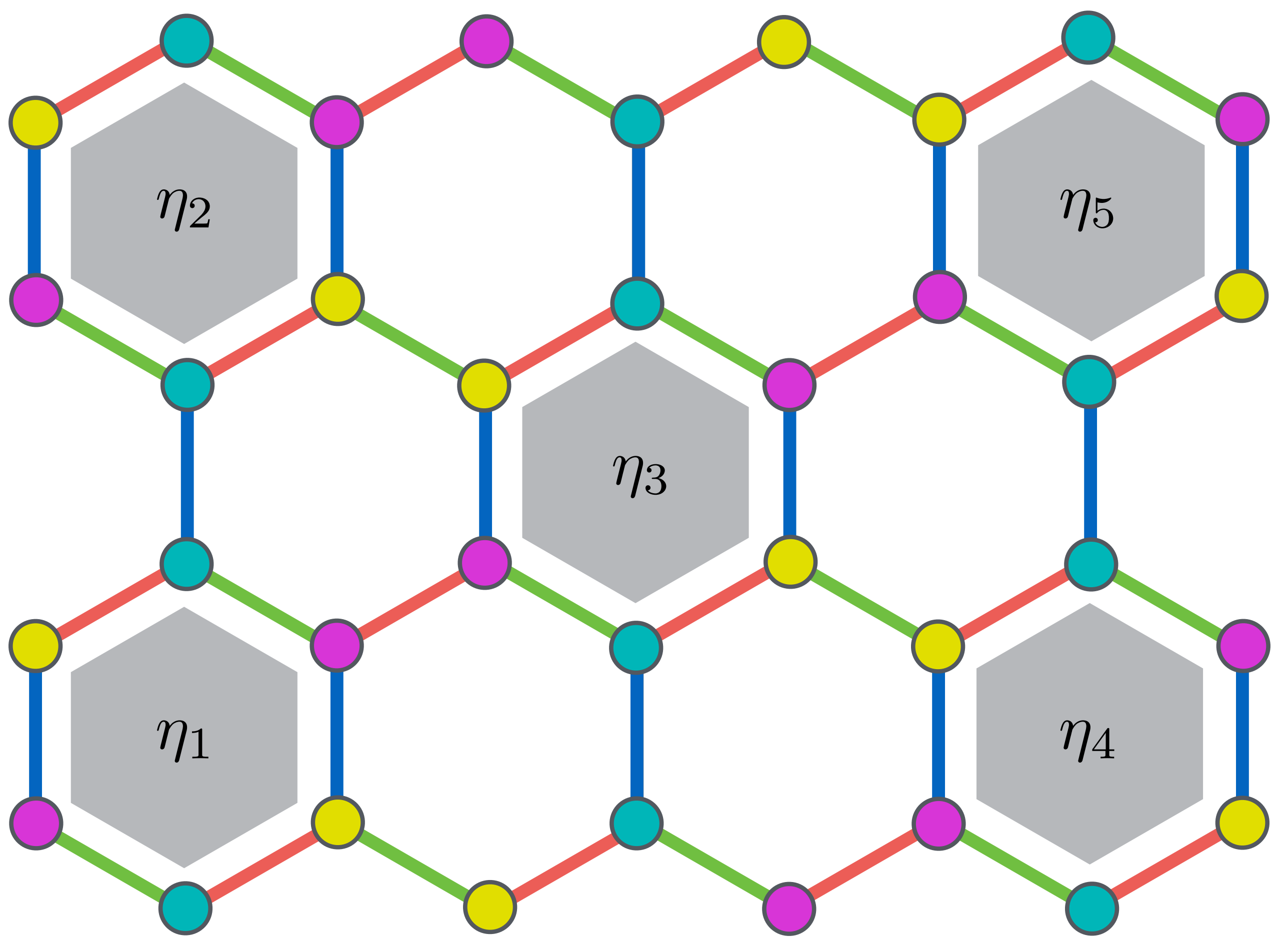
Spin Dynamics and Plaquette Ordering in the Honeycomb Gamma Model



Phys. Rev. Lett. **122**, 257204 (2019)

Gia-Wei Chern

University of Virginia

IBSPCS-KIAS International Workshop - Frustrated Magnetism

Daejeon, Korea, October 18, 2019

Acknowledgment

- Preetha Saha (UVA)
- Depei Zhang (UVA)
- Zhijie Fan (UVA)
- Jing Luo (UVA)
- Seunghun Lee (UVA)
- Kipton Barros (LANL)
- C. D. Batista (UTK/ORNL)
- Zhengtao Wang (UTK)
- Hidemaro Suwa (Tokyo)

- DOE and the Center for Computational Material Spectroscopy and Design at Brookhaven National Lab

Outline

- Numerical methods for dynamical properties of magnetic systems

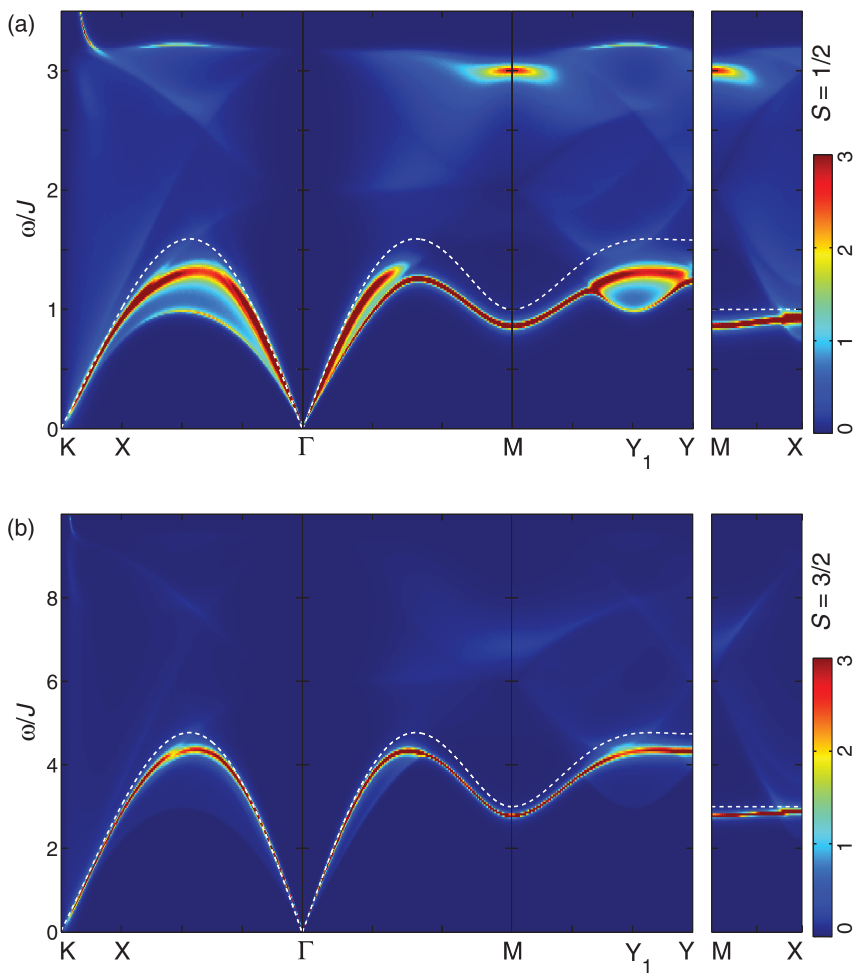
- Plaquette ordering in the honeycomb Gamma model

  1. Thermal order by disorder in frustrated magnets

  2. Hidden plaquette order in the Gamma model

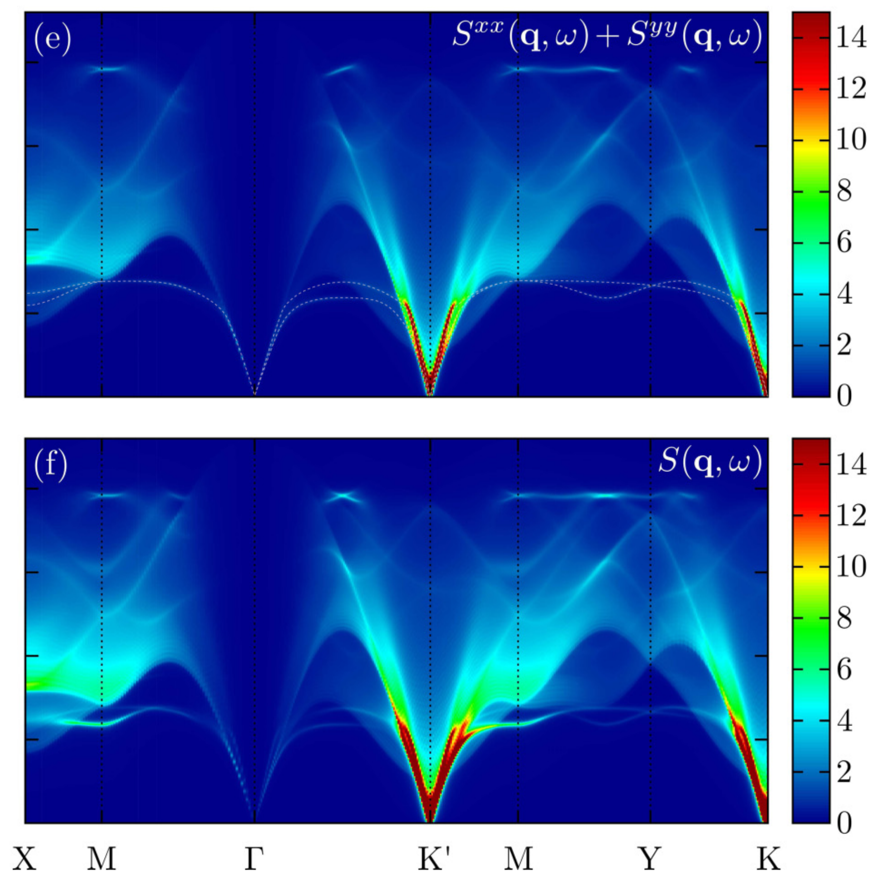
Dynamical Structure Factor

- Holstein-Primarkoff 1/S expansion



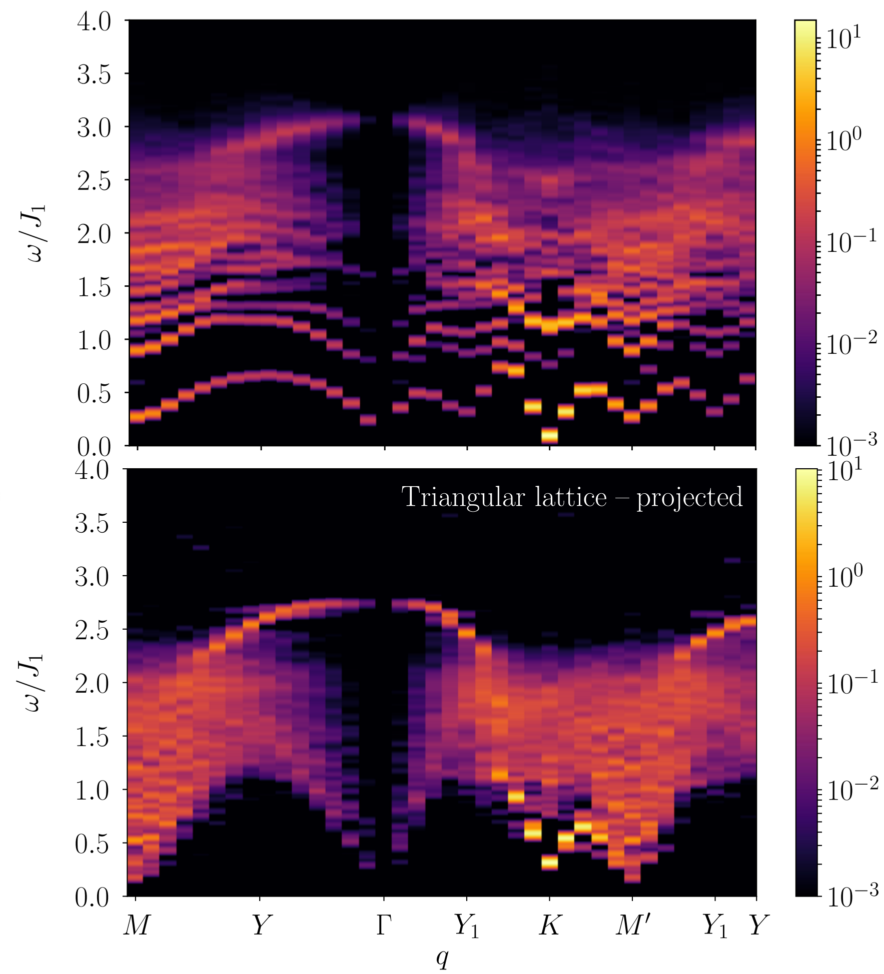
Mourigal, Fuhrman, Chernyshev, Zhitomirsky, PRB **88**, 094407 (2013)

- Schwinger boson



Ghioldi *et al.* PRB **98**, 184403 (2018)

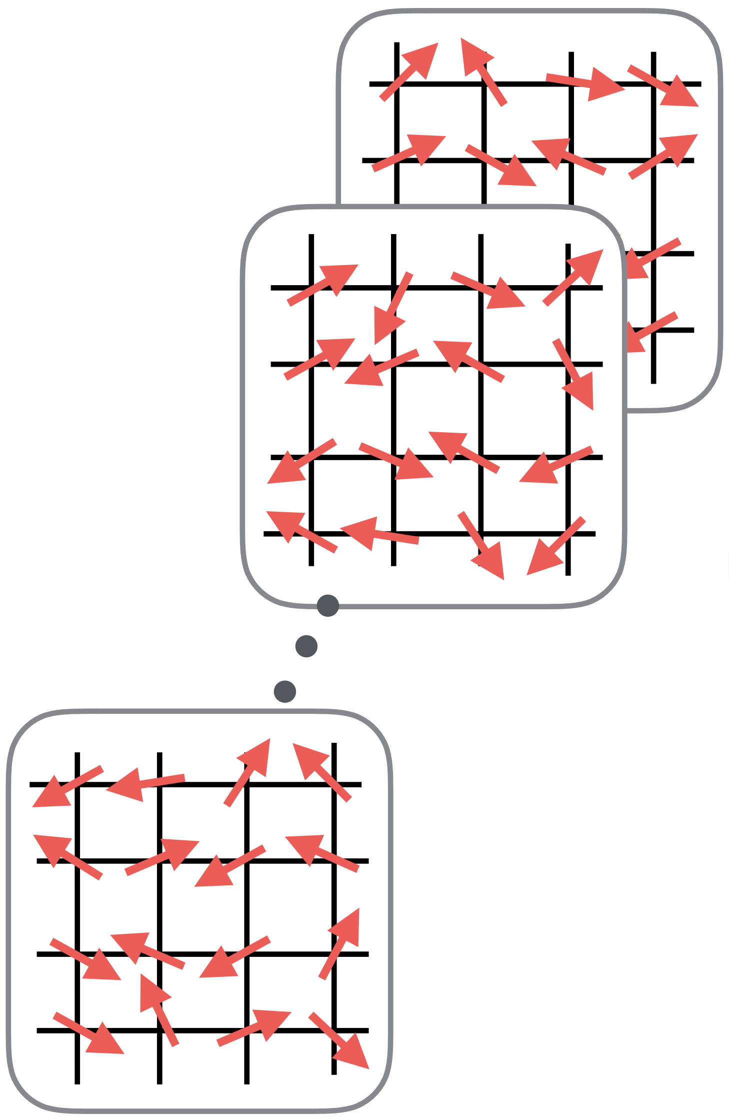
- Variational Monte Carlo



Ferrari and Beca, PRX **9**, 031026 (2019)

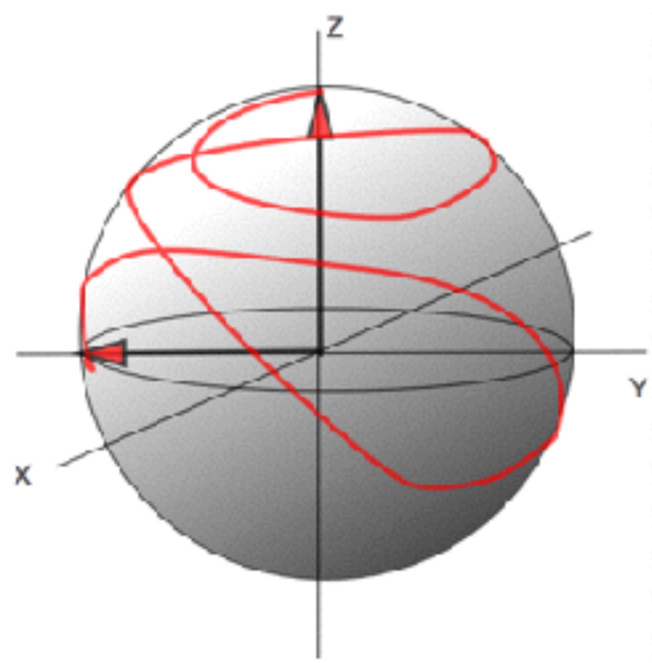
Classical Spin Liquid / Spin Glass?

- Monte Carlo simulations

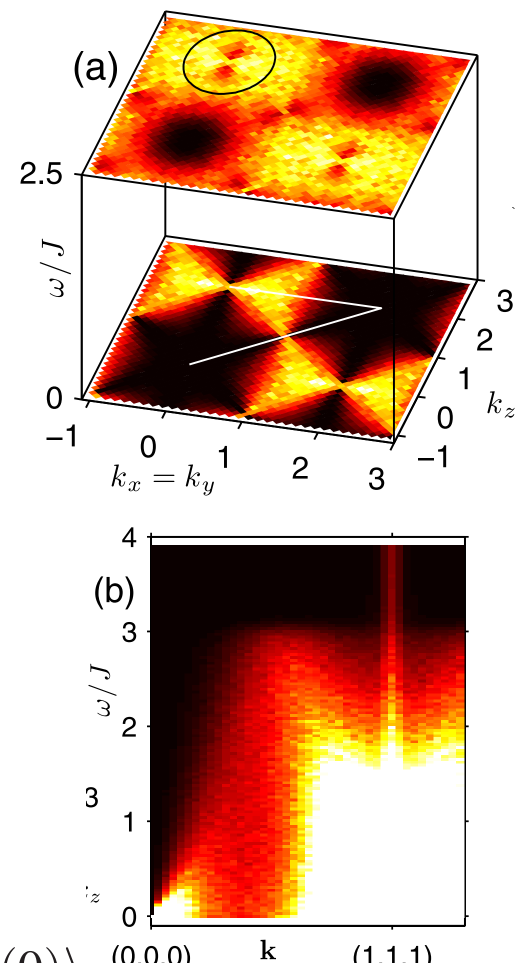


- Landau-Lifshitz equation:

$$\frac{d\mathbf{S}_i}{dt} = -J\mathbf{S}_i \times \sum_j \mathbf{S}_j,$$



- Space-time Fourier transform



$$C^{\gamma\gamma}(\mathbf{r}, t) = \langle S^{\gamma}_{\mathbf{r}}(t) S^{\gamma}_{\mathbf{0}}(0)\rangle$$

$$S^{\gamma\gamma}(\boldsymbol{k}, \omega) = \frac{1}{2\pi}\sum_{\mathbf{r}} \int_{-\infty}^{\infty} e^{i(\omega t - \mathbf{k}\cdot\mathbf{r})} C^{\gamma\gamma}(\mathbf{r}, t)\, dt,$$

VOLUME 60, NUMBER 26 PHYSICAL REVIEW LETTERS 27 JUNE 1988

Anomalous Spin Diffusion in Classical Heisenberg Magnets

Gerhard Müller
Department of Physics, The University of Rhode Island, Kingston, Rhode Island 02881
(Received 4 April 1988)

PRL **101,** 117207 (2008) PHYSICAL REVIEW LETTERS week ending 12 SEPTEMBER 2008

Propagation and Ghosts in the Classical Kagome Antiferromagnet

J. Robert,[1] B. Canals,[2] V. Simonet,[2] and R. Ballou[2]

PRL **102,** 237206 (2009) PHYSICAL REVIEW LETTERS week ending 12 JUNE 2009

Spin Dynamics in Pyrochlore Heisenberg Antiferromagnets

P. H. Conlon[*] and J. T. Chalker

PHYSICAL REVIEW B **96**, 134408 (2017)

Comprehensive study of the dynamics of a classical Kitaev spin liquid

A. M. Samarakoon,[1,2,*] A. Banerjee,[3] S.-S. Zhang,[4] Y. Kamiya,[5] S. E. Nagler,[3,6] D. A. Tennant,[7] S.-H. Lee,[2] and C. D. Batista[1,3,4]

PHYSICAL REVIEW LETTERS **122,** 167203 (2019)

Dynamical Structure Factor of the Three-Dimensional Quantum Spin Liquid Candidate $NaCaNi_2F_7$

Shu Zhang,[1,2] Hitesh J. Changlani,[3,4,1,2] Kemp W. Plumb,[5] Oleg Tchernyshyov,[1,2] and Roderich Moessner[6]

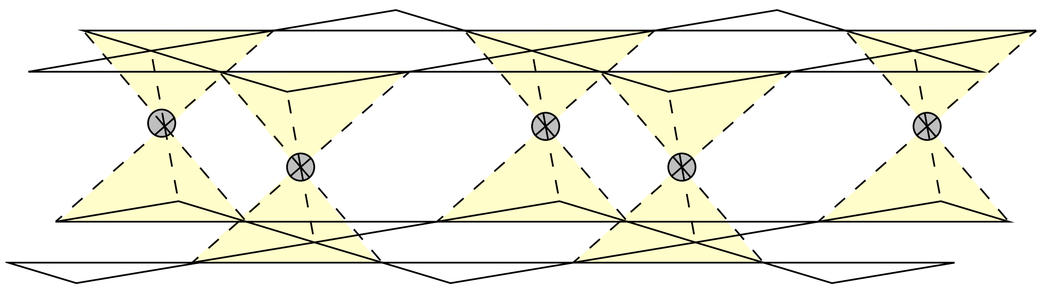
Spin dynamics of the antiferromagnetic Heisenberg model on a kagome bilayer

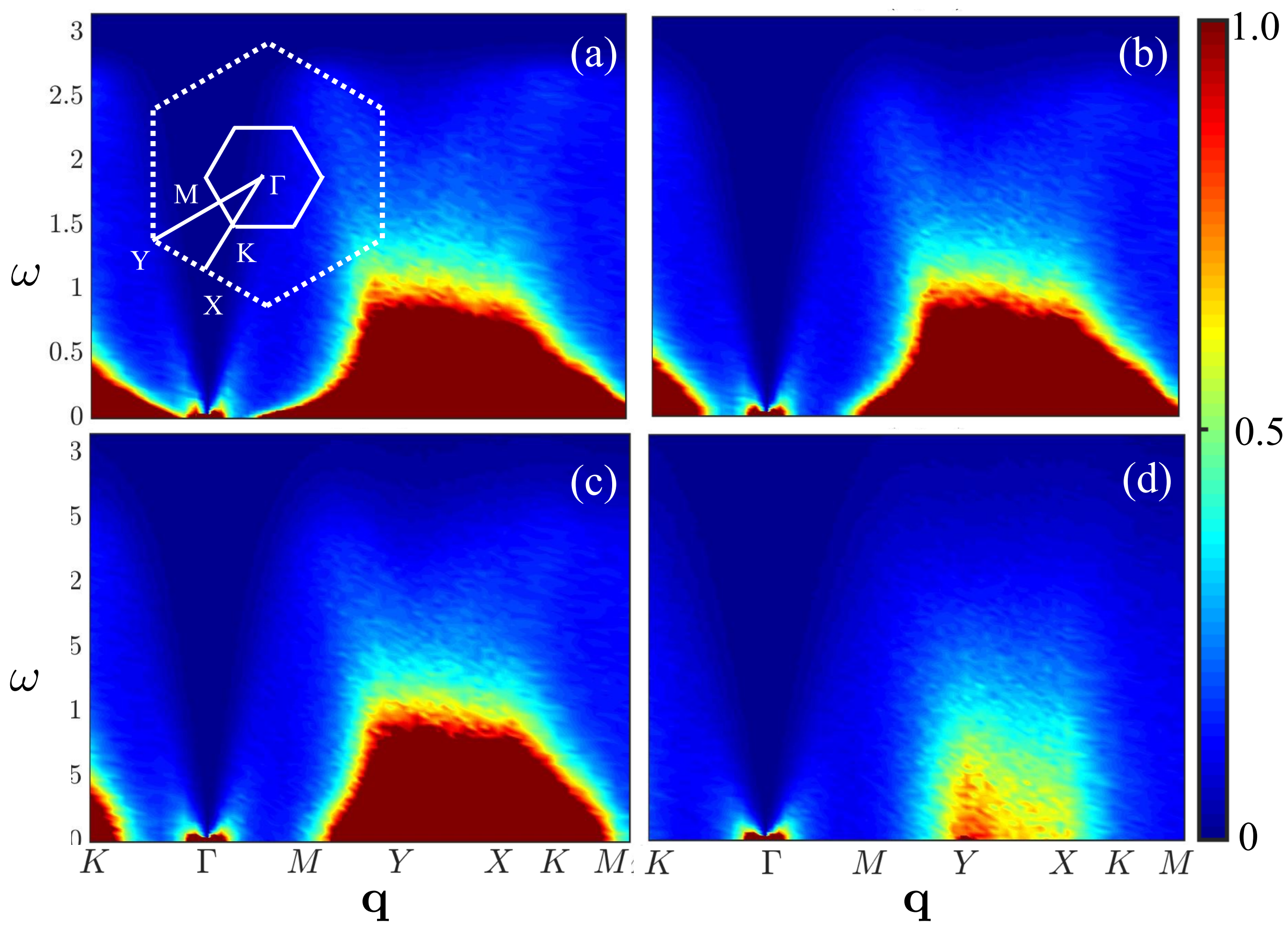
Preetha Saha,[1] Depei Zhang,[1] Seung-Hun Lee,[1] and Gia-Wei Chern[1]

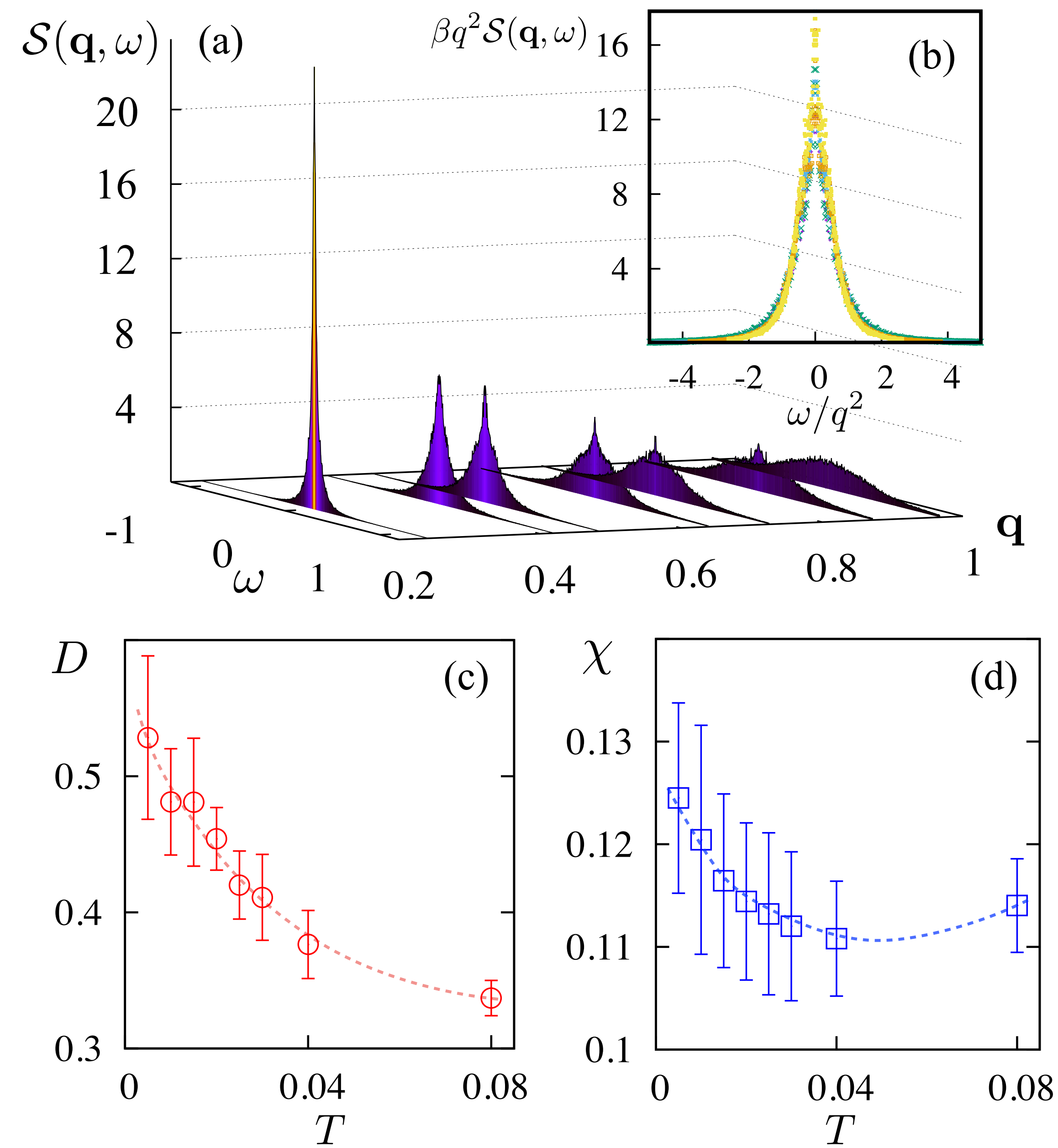
[1] *Department of Physics, University of Virginia, Charlottesville, VA 22904, USA*

(Dated: April 12, 2019)

arXiv:1904.05863v1







nature COMMUNICATIONS

ARTICLE

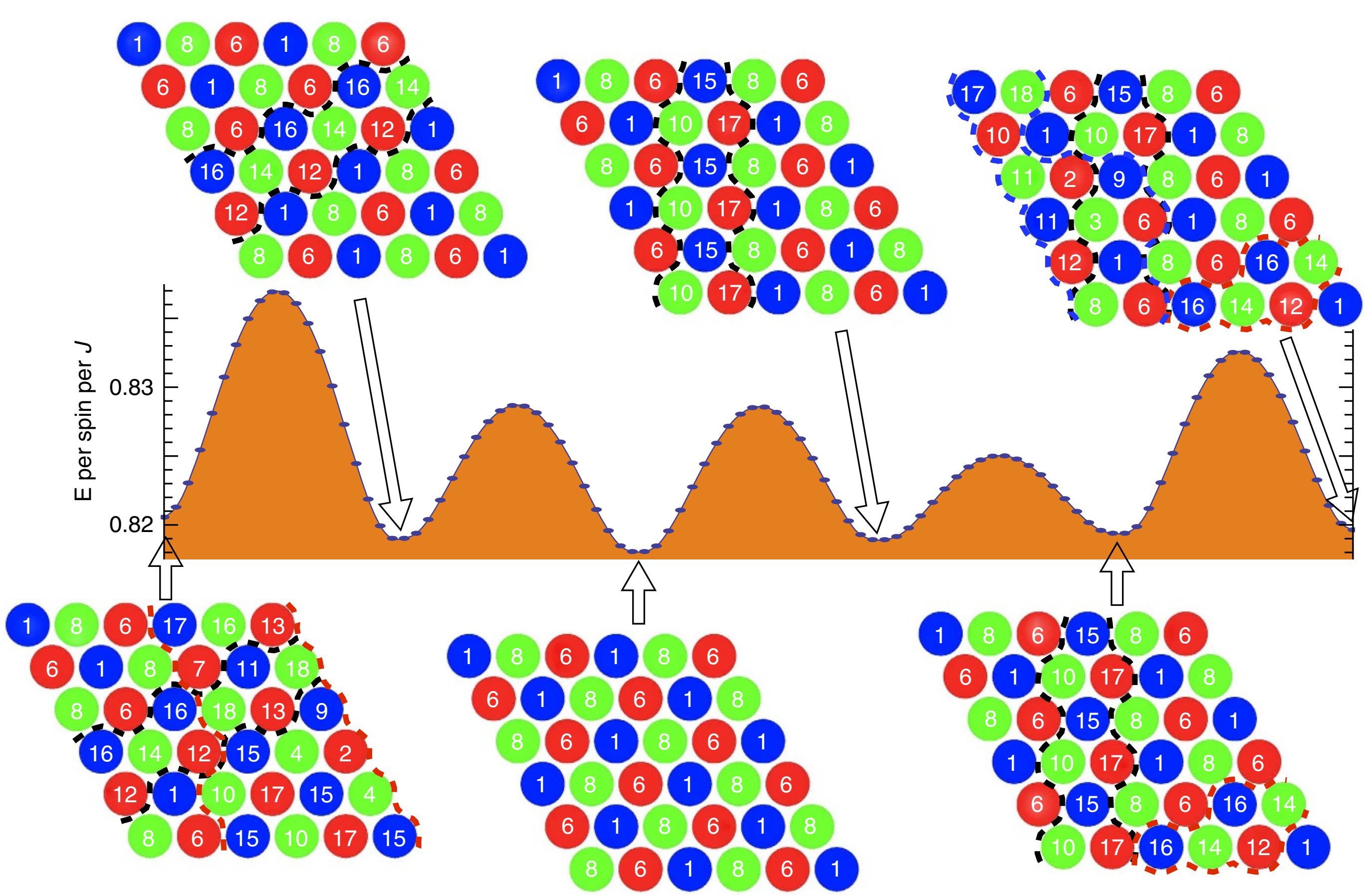
Received 16 Oct 2013 | Accepted 21 Feb 2014 | Published 1 Apr 2014

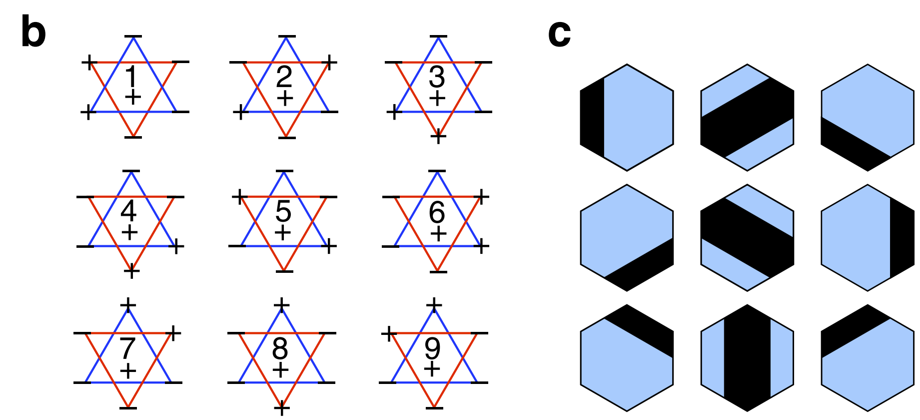
DOI: 10.1038/ncomms4497

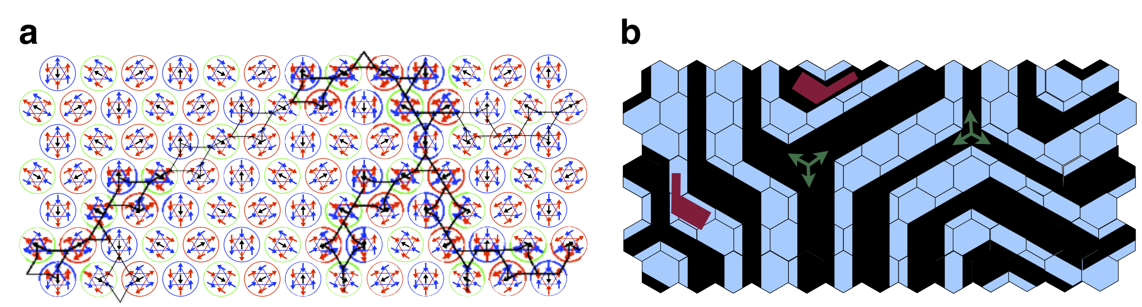
OPEN

Glassiness and exotic entropy scaling induced by quantum fluctuations in a disorder-free frustrated magnet

I. Klich[1,*], S-H Lee[1,*] & K. Iida[1]







Dynamics of Phase Separated States in the Double Exchange Model

Jing Luo[1] and Gia-Wei Chern[1]

[1] *Department of Physics, University of Virginia, Charlottesville, VA 22904, USA*

(Dated: April 11, 2019)

arXiv:1904.05252v1

- Double exchange model on square-lattice close to half-filling:

$$\mathcal{H} = -t \sum_{\langle ij \rangle} \left(c^{\dagger}_{i\alpha} c_{j\alpha} + \text{h.c.} \right) - J \sum_{i} \mathbf{S}_i \cdot c^{\dagger}_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta},$$

- GPU-enabled Langevin dynamics for preparing initial phase separated states

- Landau-Lifshitz + von Neumann dynamics simulations:

$$\frac{d\mathbf{S}_i}{dt} = -\mathbf{S}_i \times \frac{\partial \langle \mathcal{H} \rangle}{\partial \mathbf{S}_i} = J \mathbf{S}_i \times \boldsymbol{\sigma}_{\alpha\beta}\, \rho_{i\beta, i\alpha},$$

$$\begin{aligned} \frac{d\rho_{i\alpha,j\beta}}{dt} &= i(t_{ik}\, \rho_{k\alpha,j\beta} - \rho_{i\alpha,k\beta}\, t_{kj}) \\ &+ iJ(\mathbf{S}_i \cdot \boldsymbol{\sigma}_{\alpha\gamma}\, \rho_{i\gamma,j\beta} - \rho_{i\alpha,j\gamma}\, \boldsymbol{\sigma}_{\gamma\beta} \cdot \mathbf{S}_j). \end{aligned}$$

Dynamics of Phase Separated States in the Double Exchange Model

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[1] *Department of Physics, University of Virginia, Charlottesville, VA 22904, USA*
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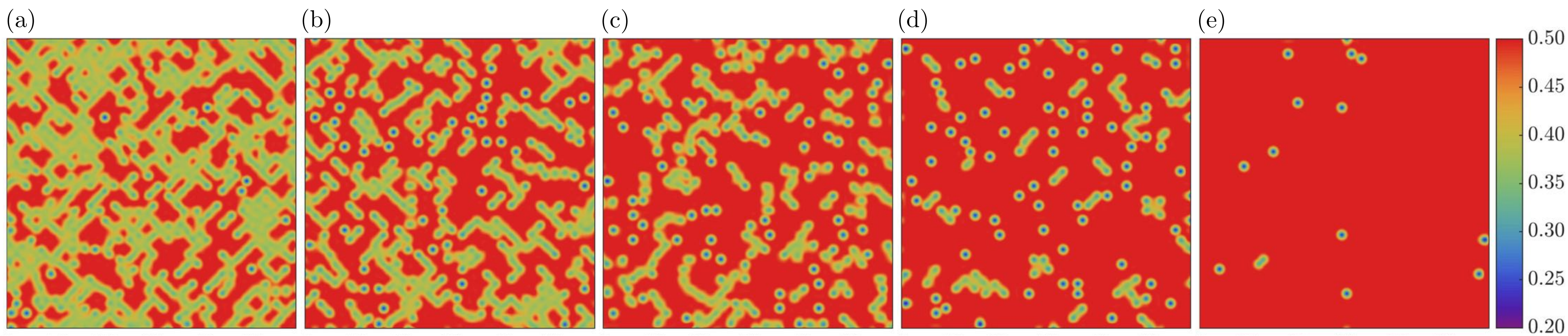


PHYSICAL REVIEW B **97**, 035120 (2018)

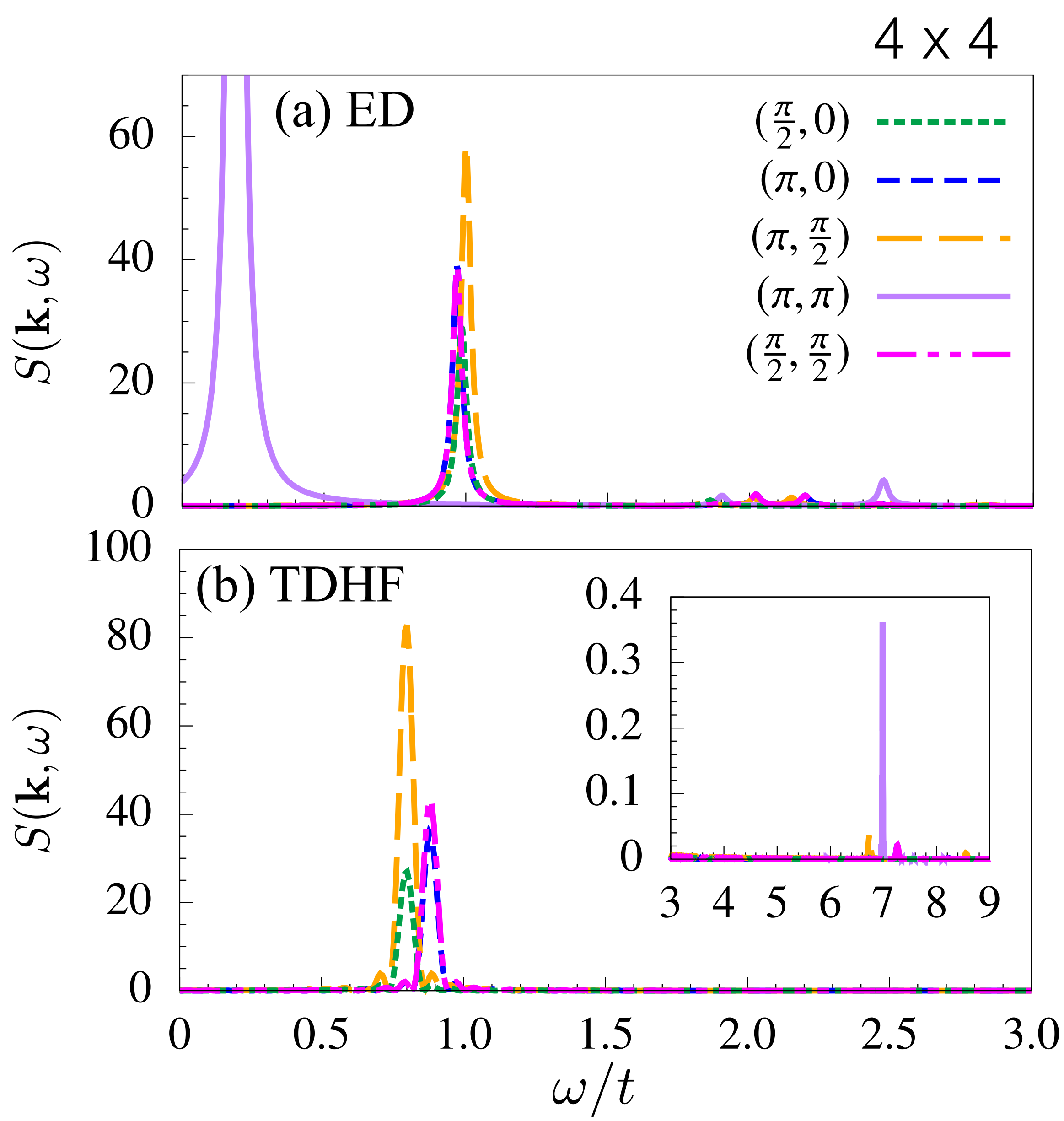
Editors' Suggestion

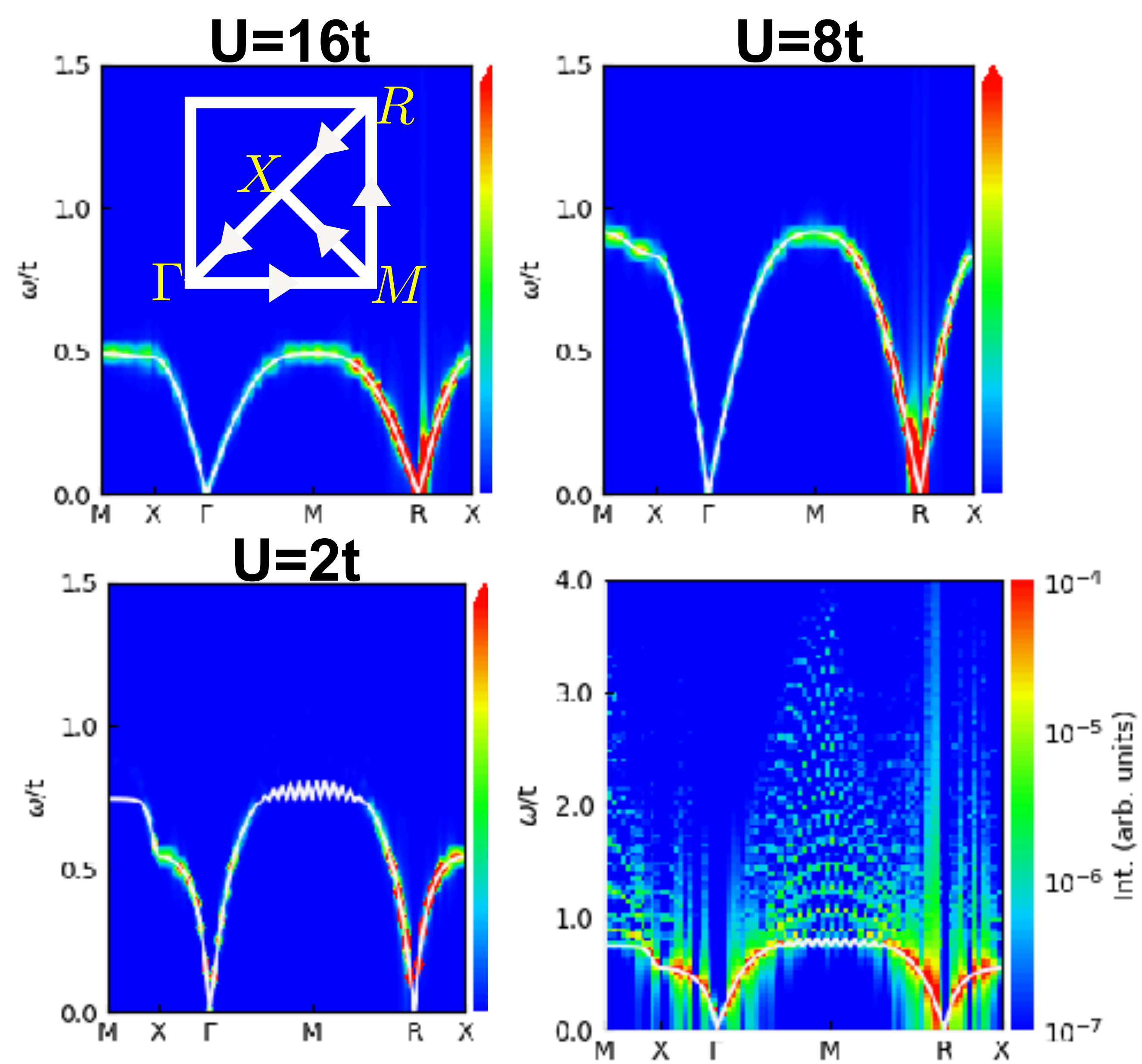
Semiclassical dynamics of spin density waves

Gia-Wei Chern,[1,*] Kipton Barros,[2] Zhentao Wang,[3] Hidemaro Suwa,[3] and Cristian D. Batista[3,4,†]

- Beyond Mott insulators: 2D Hubbard model

48x48





PRL **119,** 157203 (2017) PHYSICAL REVIEW LETTERS week ending 13 OCTOBER 2017

Dynamics of the Kitaev-Heisenberg Model

Matthias Gohlke,[1] Ruben Verresen,[1,2] Roderich Moessner,[1] and Frank Pollmann[1,2]

$$H = \sum_{\langle i,j\rangle_\gamma} K_\gamma S_i^\gamma S_j^\gamma + J \sum_{\langle i,j\rangle} S_i \cdot S_j.$$

- iDMRG to prepare the ground state $|\Phi_0\rangle$
- Initial state: $|\Psi(0)\rangle = S^+_{\mathbf{r}=0}|\Phi_0\rangle$
- Time-dependent DMRG (TEBD, TDVP, etc)

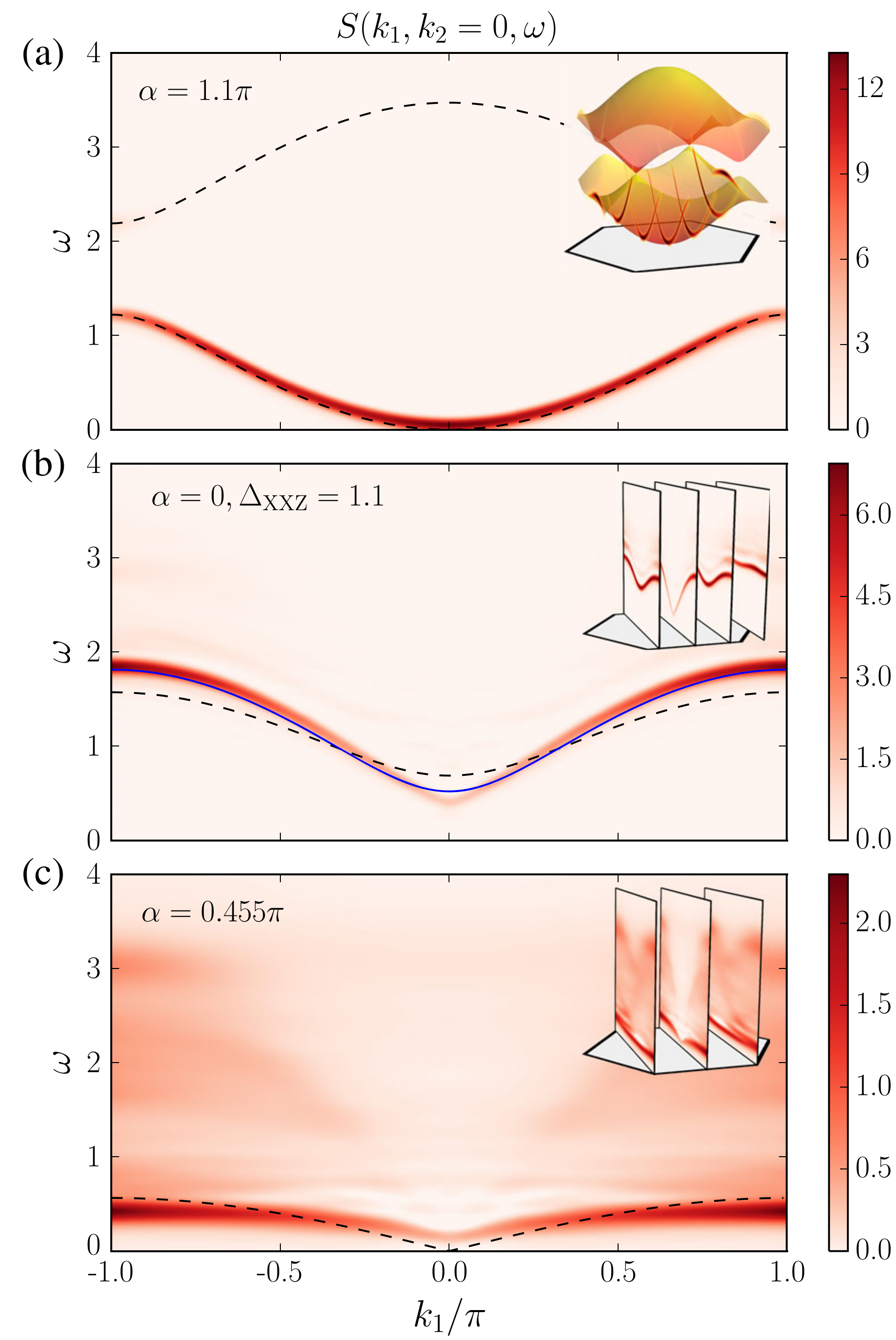
$$|\Psi(t)\rangle = e^{-i\mathcal{H}t/\hbar}|\Psi(0)\rangle$$

- Space-time Fourier Transform:

$$C^{\gamma\gamma}(\mathbf{r},t) = \langle S^\gamma_{\mathbf{r}}(t) S^\gamma_{\mathbf{0}}(0)\rangle$$

$$\mathcal{S}^{\gamma\gamma}(\boldsymbol{k},\omega) = \frac{1}{2\pi}\sum_{\mathbf{r}}\int_{-\infty}^{\infty} e^{i(\omega t - \mathbf{k}\cdot\mathbf{r})} C^{\gamma\gamma}(\mathbf{r},t)\,dt,$$

$J = \cos\alpha$ and $K_\gamma = K = 2\sin\alpha$



$J = -0.95$
$K = -0.62$

$J = 1$
$K = 0$

$J = 0.14$
$K = 1.98$

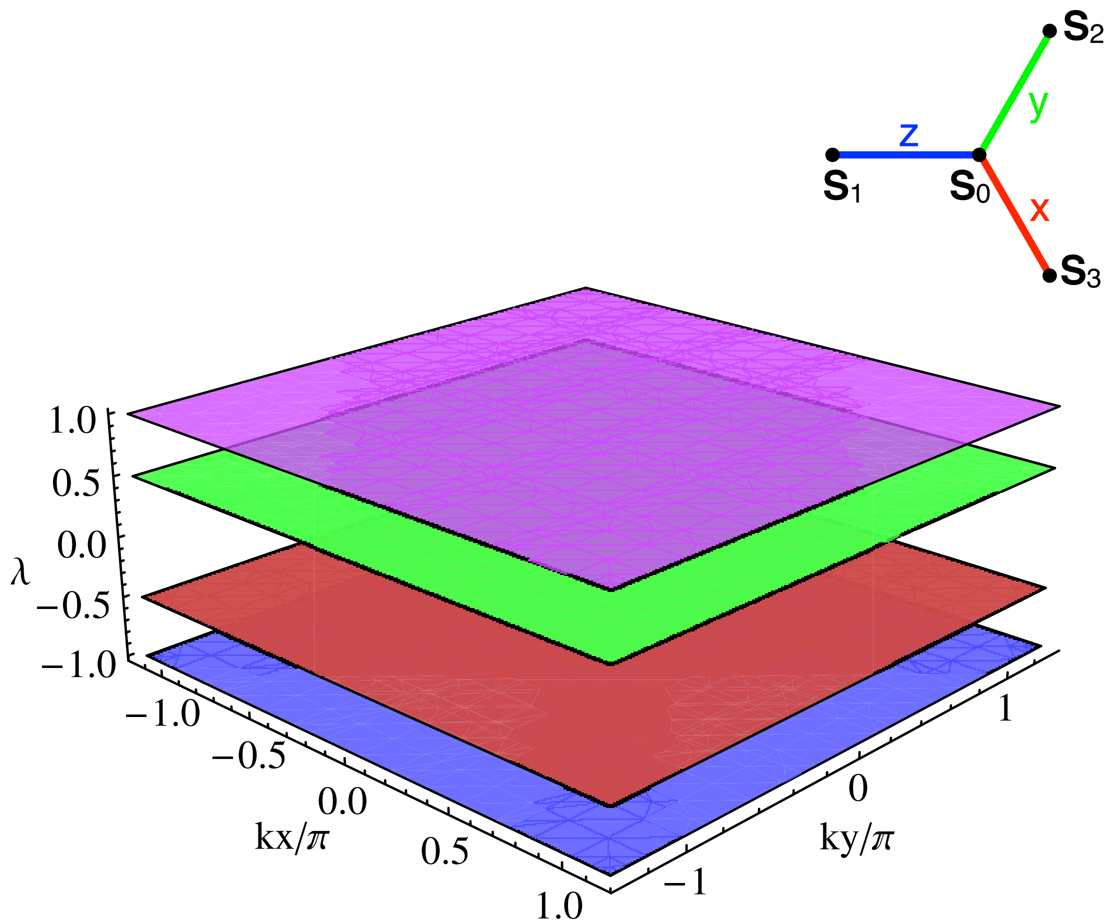
PRL **118,** 147204 (2017) PHYSICAL REVIEW LETTERS week ending 7 APRIL 2017

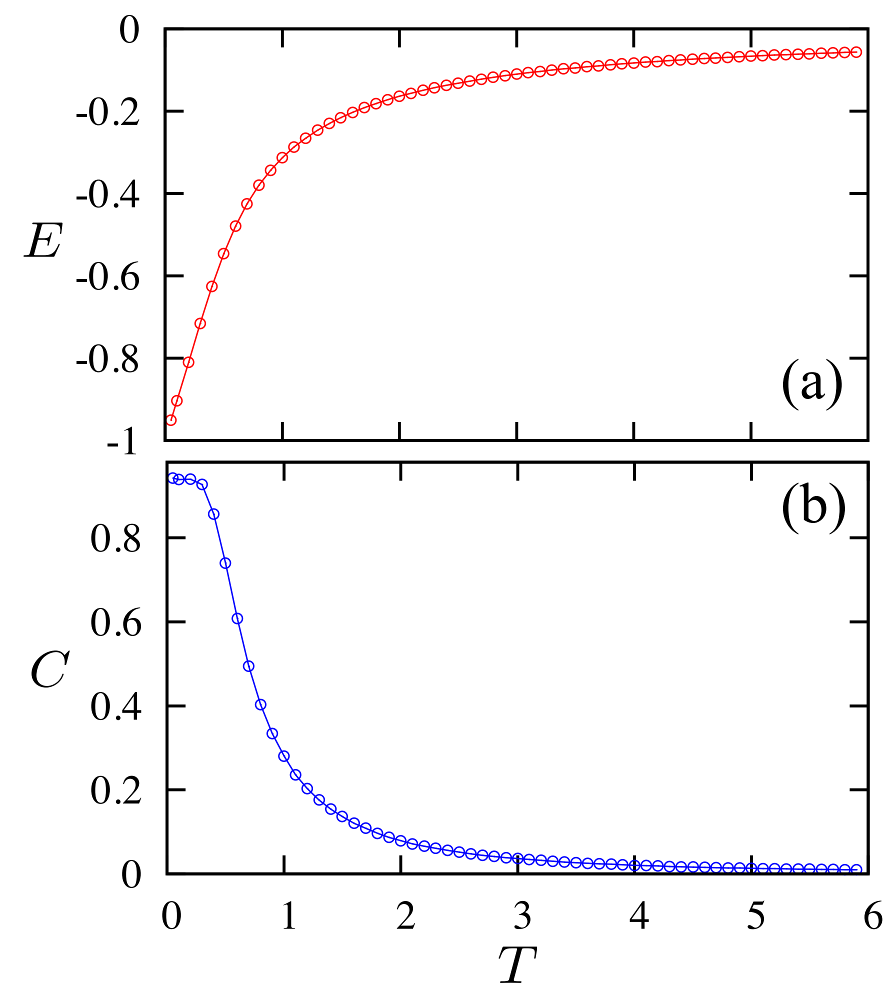
Classical Spin Liquid Instability Driven By Off-Diagonal Exchange in Strong Spin-Orbit Magnets

Ioannis Rousochatzakis and Natalia B. Perkins
School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA

(Received 25 October 2016; published 5 April 2017)

$$\mathcal{H} = \Gamma \sum_{\langle ij\rangle \| x} (S_i^y S_j^z + S_i^z S_j^y) + \Gamma \sum_{\langle ij\rangle \| y} (S_i^z S_j^x + S_i^x S_j^z) + \Gamma \sum_{\langle ij\rangle \| z} (S_i^x S_j^y + S_i^y S_j^x).$$





PRL **118,** 147204 (2017) PHYSICAL REVIEW LETTERS week ending 7 APRIL 2017

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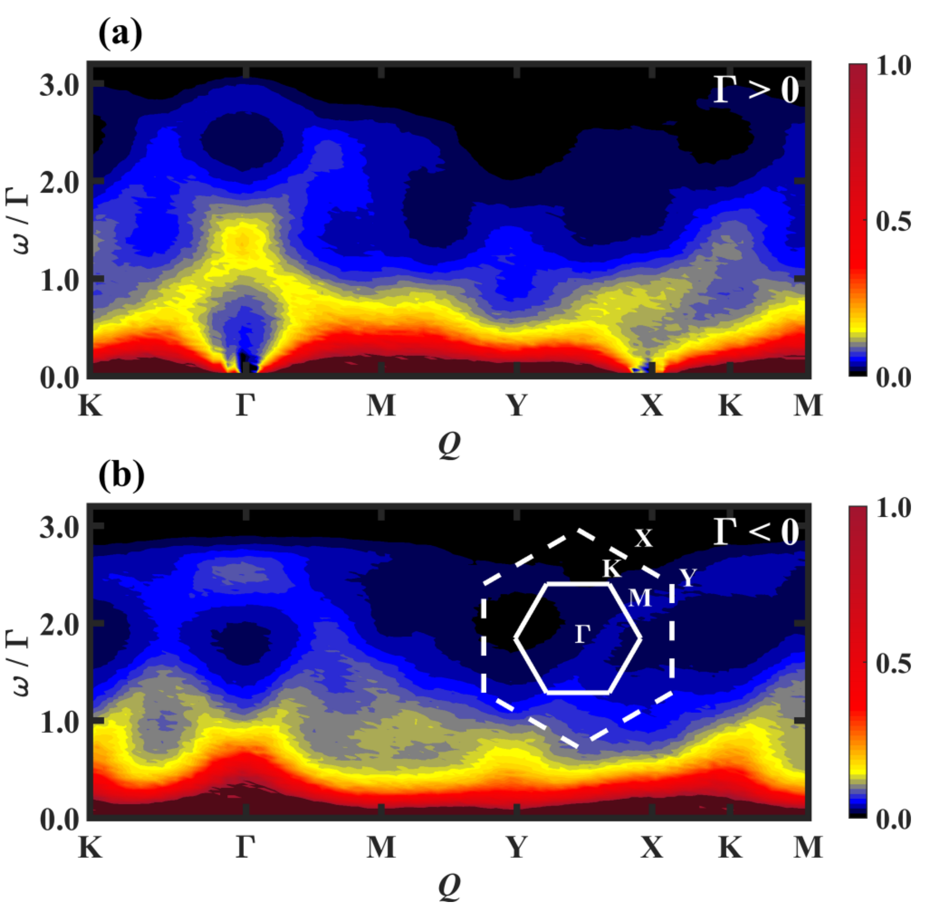
Spin dynamics & dynamical structure factor of this new classical spin liquid?

PHYSICAL REVIEW B **98**, 045121 (2018)

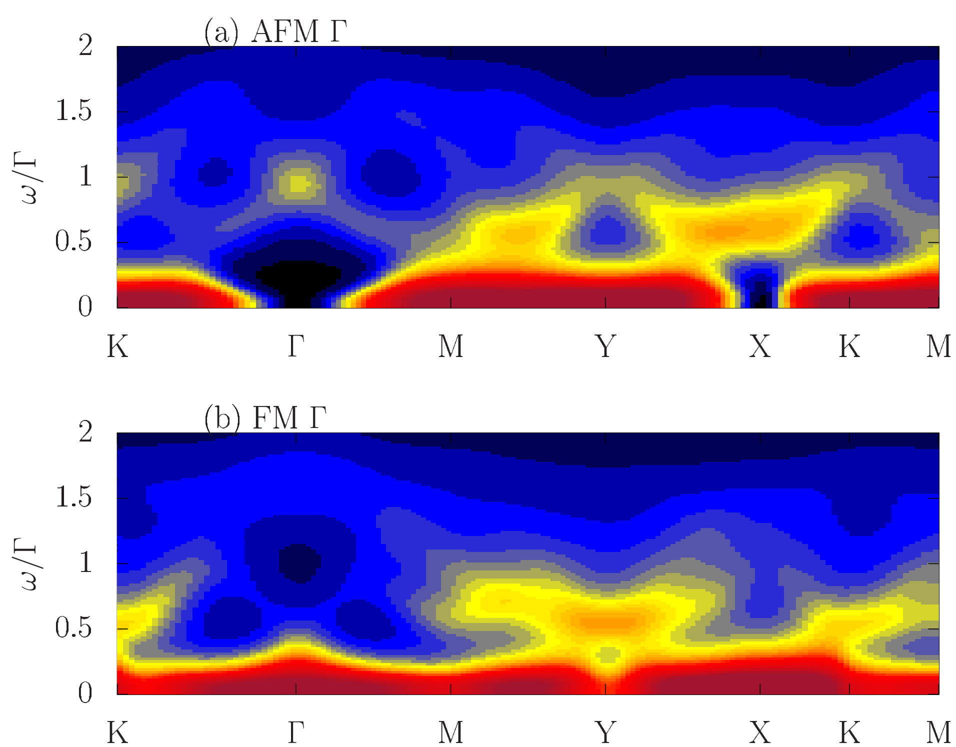
Editors' Suggestion

Classical and quantum spin dynamics of the honeycomb Γ model

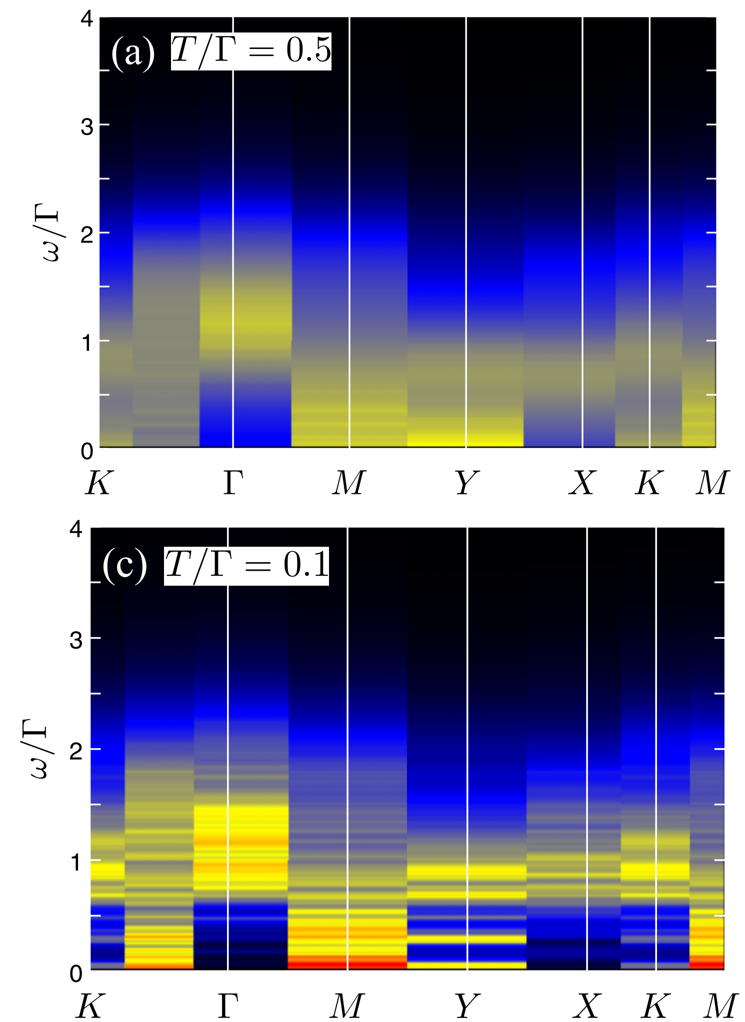
Anjana M. Samarakoon,[1,2] Gideon Wachtel,[3,4] Youhei Yamaji,[5,6] D. A. Tennant,[7,2]
Cristian D. Batista,[1,2,8] and Yong Baek Kim[3,9,10]



Landau-Lifshitz dynamics



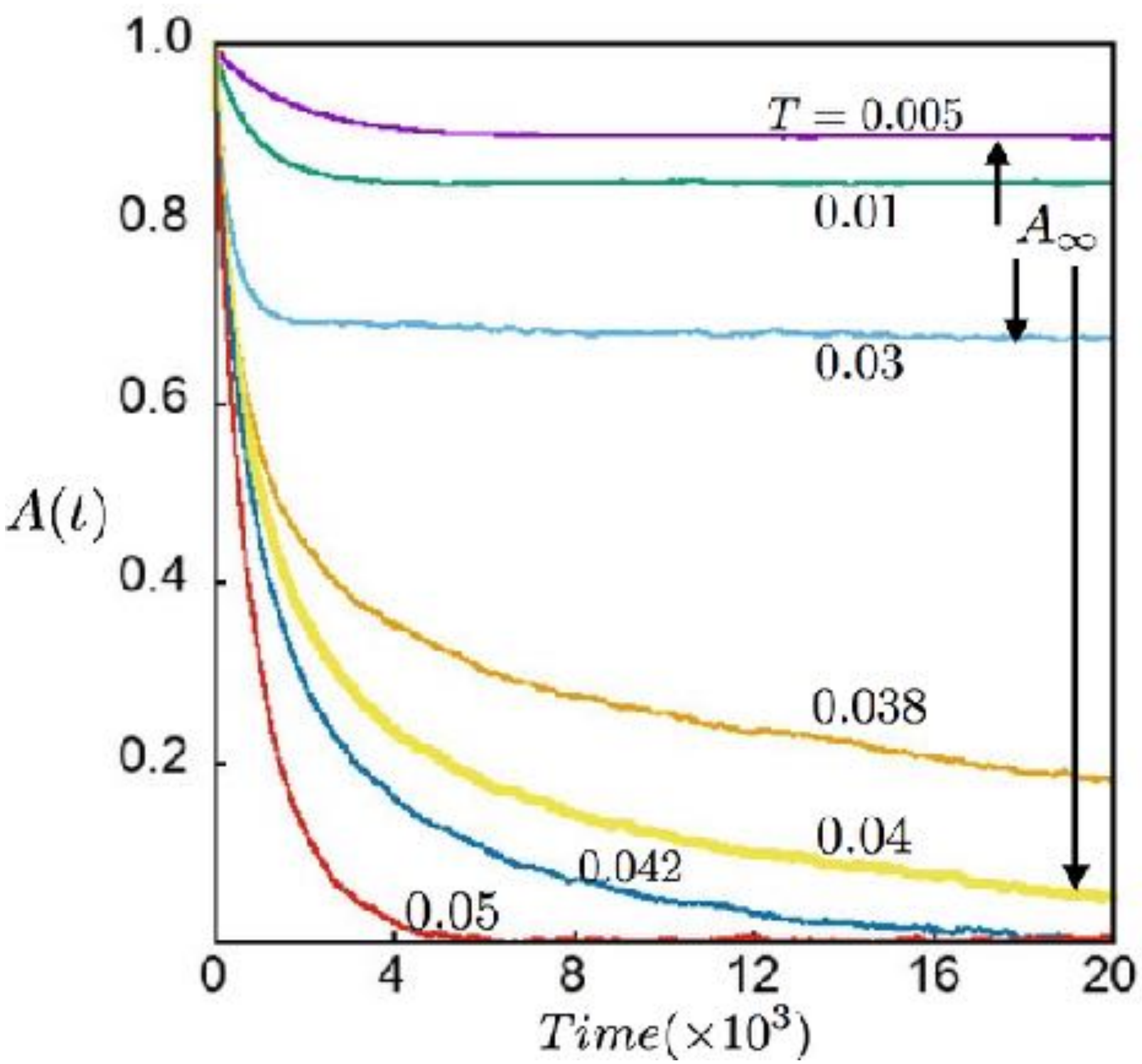
Langevin dynamics with soft spins



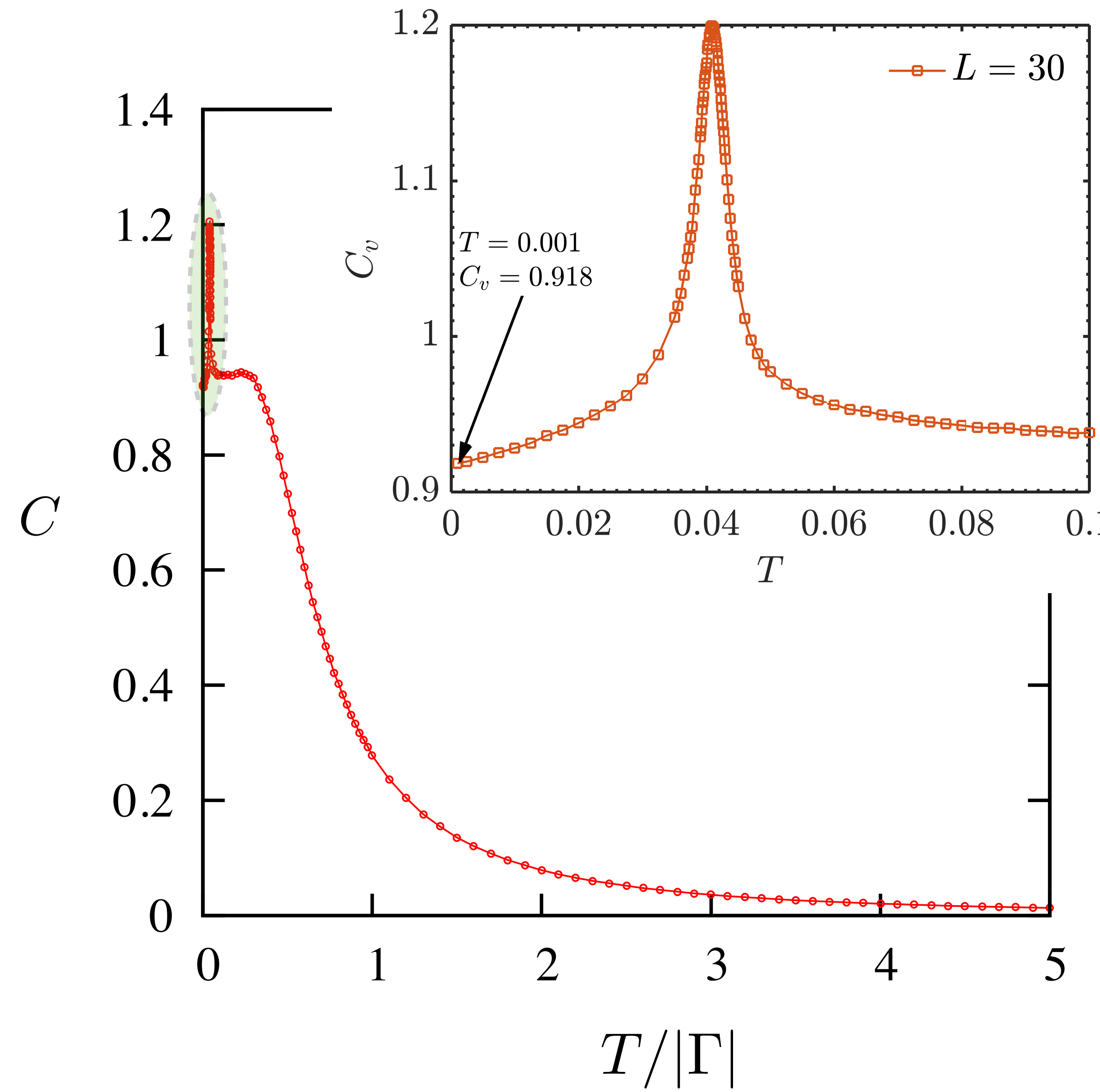
Exact diagonalizaton spin-1/2

Unexpected phase transition

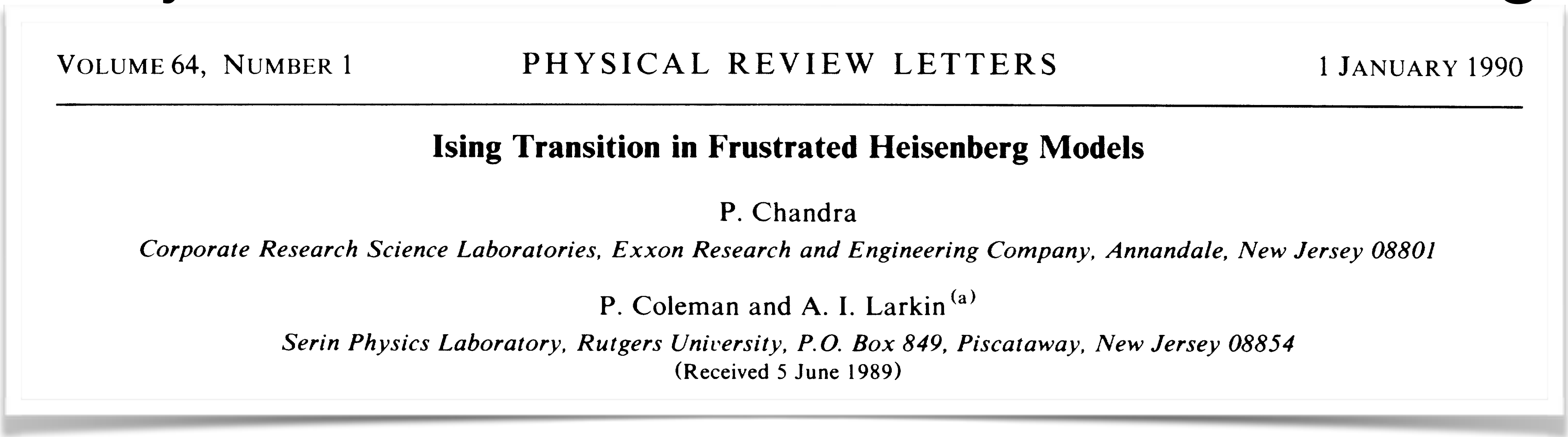
- Autocorrelation function:



- Heat capacity vs T:



Order-by-disorder transition in frustrated magnets

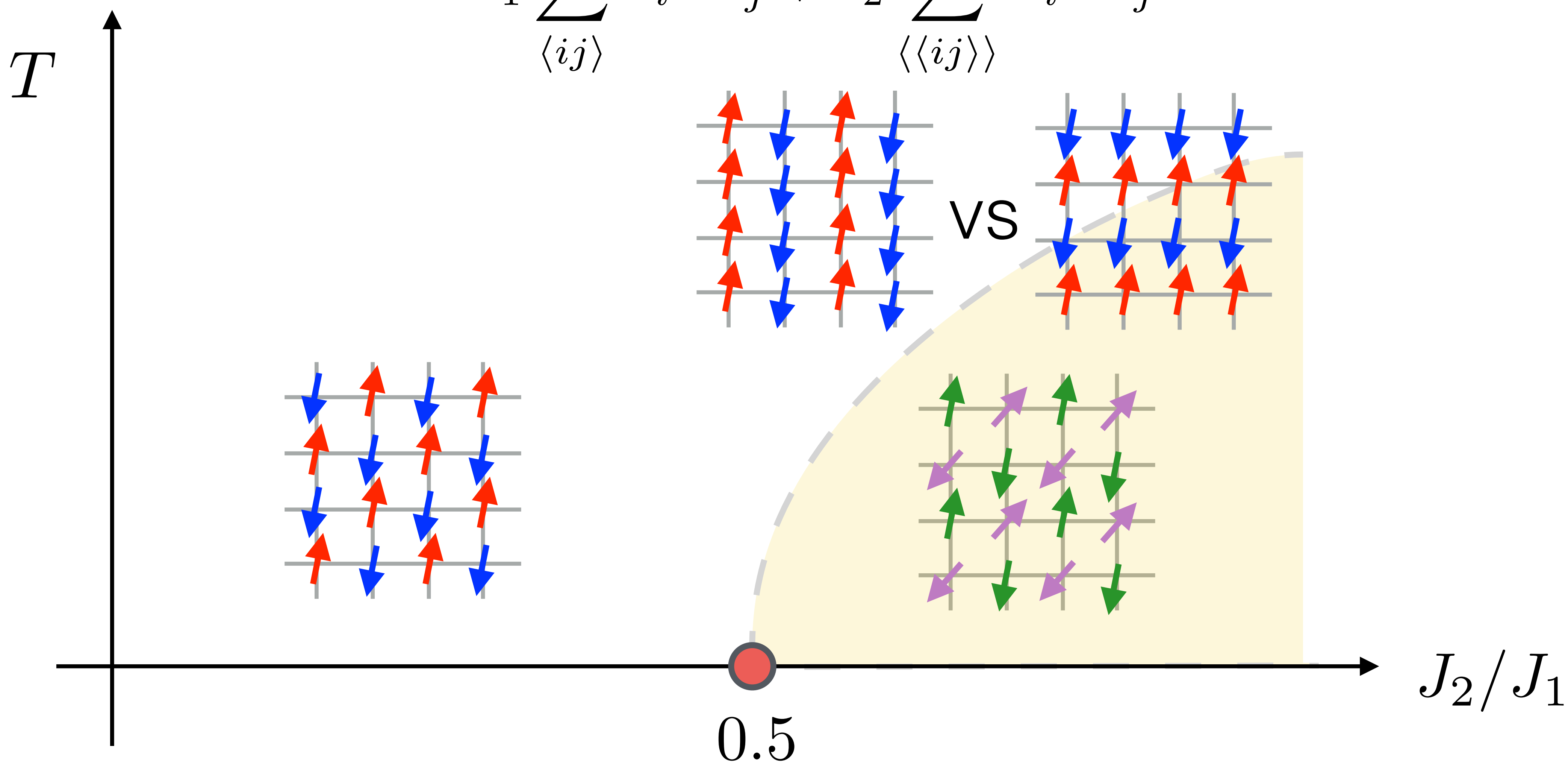

VOLUME 64, NUMBER 1 PHYSICAL REVIEW LETTERS 1 JANUARY 1990

Ising Transition in Frustrated Heisenberg Models

P. Chandra
Corporate Research Science Laboratories, Exxon Research and Engineering Company, Annandale, New Jersey 08801

P. Coleman and A. I. Larkin[a]
Serin Physics Laboratory, Rutgers University, P.O. Box 849, Piscataway, New Jersey 08854
(Received 5 June 1989)

$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

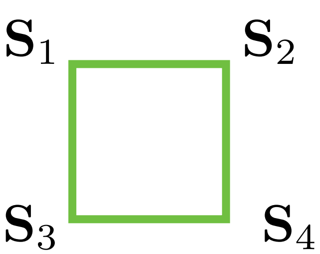


Order-by-disorder transition in frustrated magnets

VOLUME 91, NUMBER 17 PHYSICAL REVIEW LETTERS week ending 24 OCTOBER 2003

Ising Transition Driven by Frustration in a 2D Classical Model with Continuous Symmetry

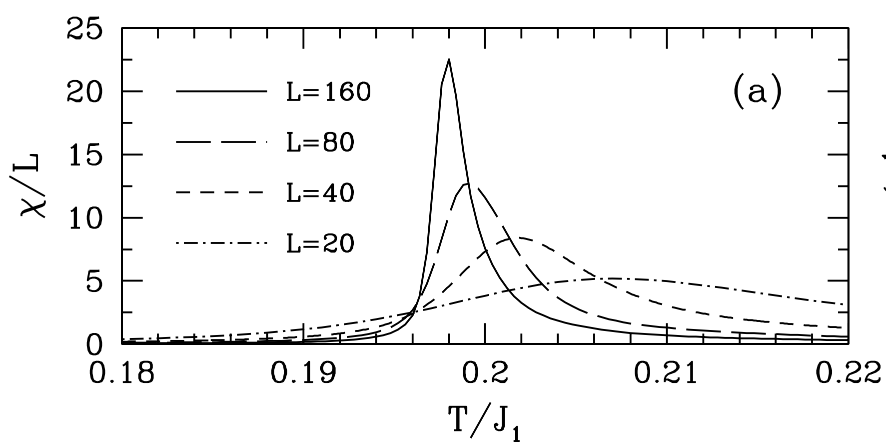
Cédric Weber,[1,2] Luca Capriotti,[3] Grégoire Misguich,[4] Federico Becca,[5] Maged Elhajal,[1] and Frédéric Mila[1]

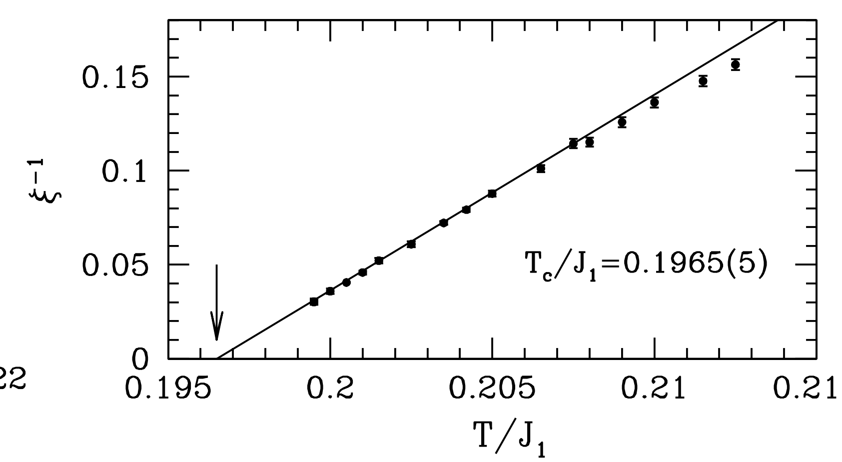


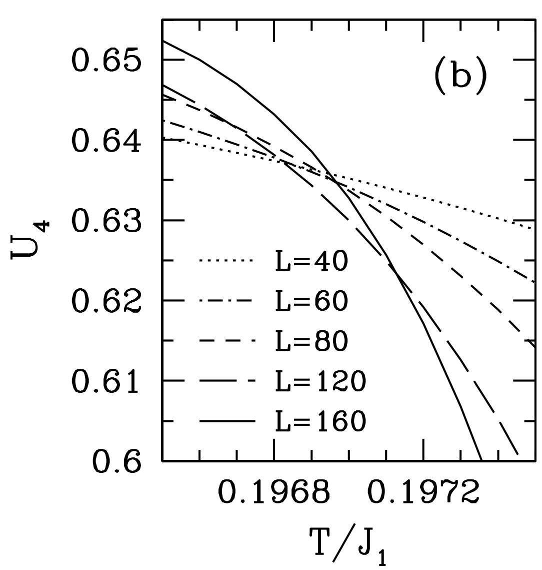
$$\sigma = \frac{\mathbf{S}_1\cdot\mathbf{S}_2 + \mathbf{S}_3\cdot\mathbf{S}_4 - \mathbf{S}_1\cdot\mathbf{S}_4 - \mathbf{S}_2\cdot\mathbf{S}_3}{|\mathbf{S}_1\cdot\mathbf{S}_2 + \mathbf{S}_3\cdot\mathbf{S}_4 - \mathbf{S}_1\cdot\mathbf{S}_4 - \mathbf{S}_2\cdot\mathbf{S}_3|}$$

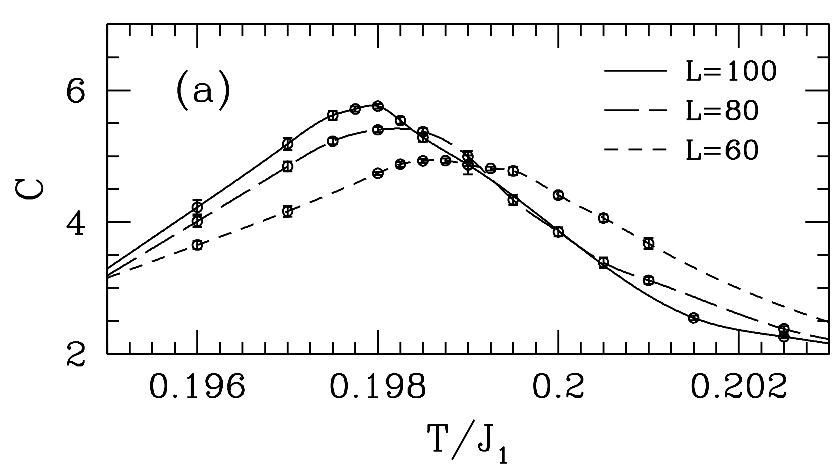
$$M = \frac{1}{N}\sum_{\Box}\sigma_{\Box}$$

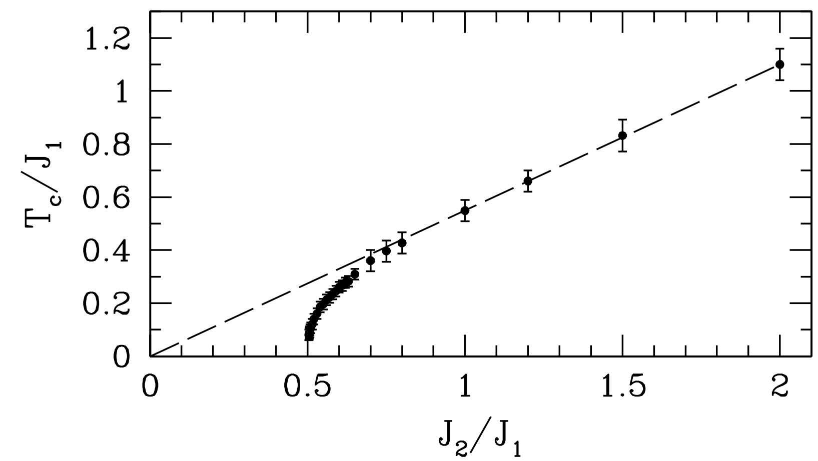
$$\chi = \frac{N}{T}\left(\langle M^2\rangle - \langle|M|\rangle^2\right)$$











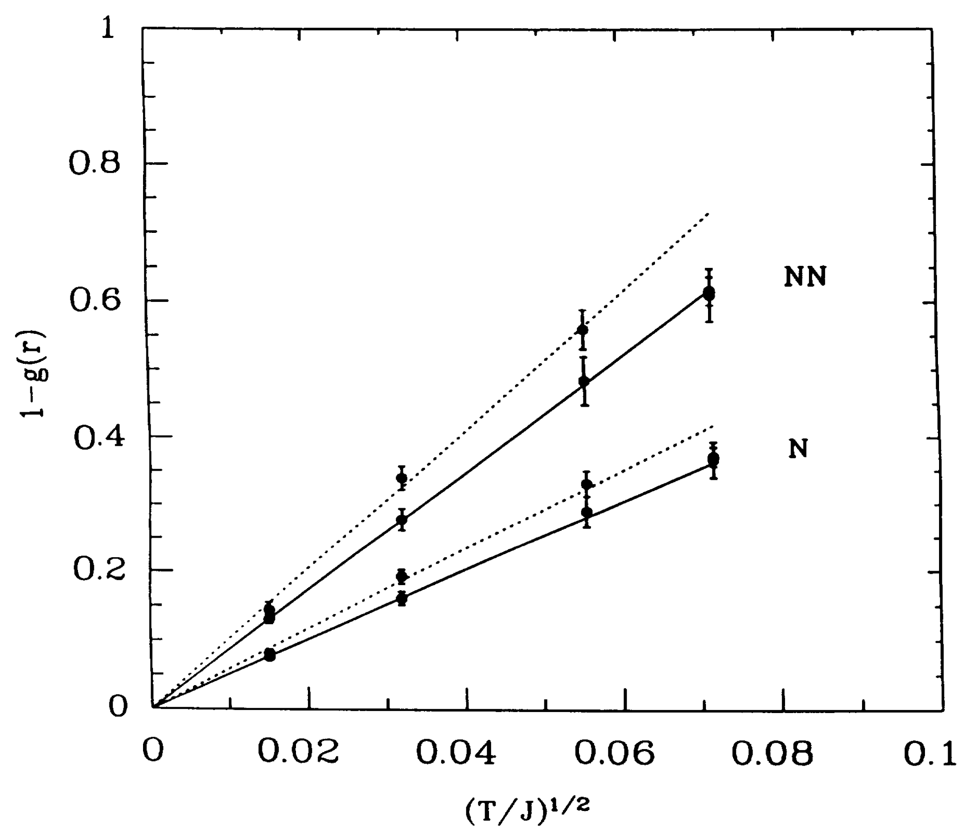
VOLUME 68, NUMBER 6 PHYSICAL REVIEW LETTERS 10 FEBRUARY 1992

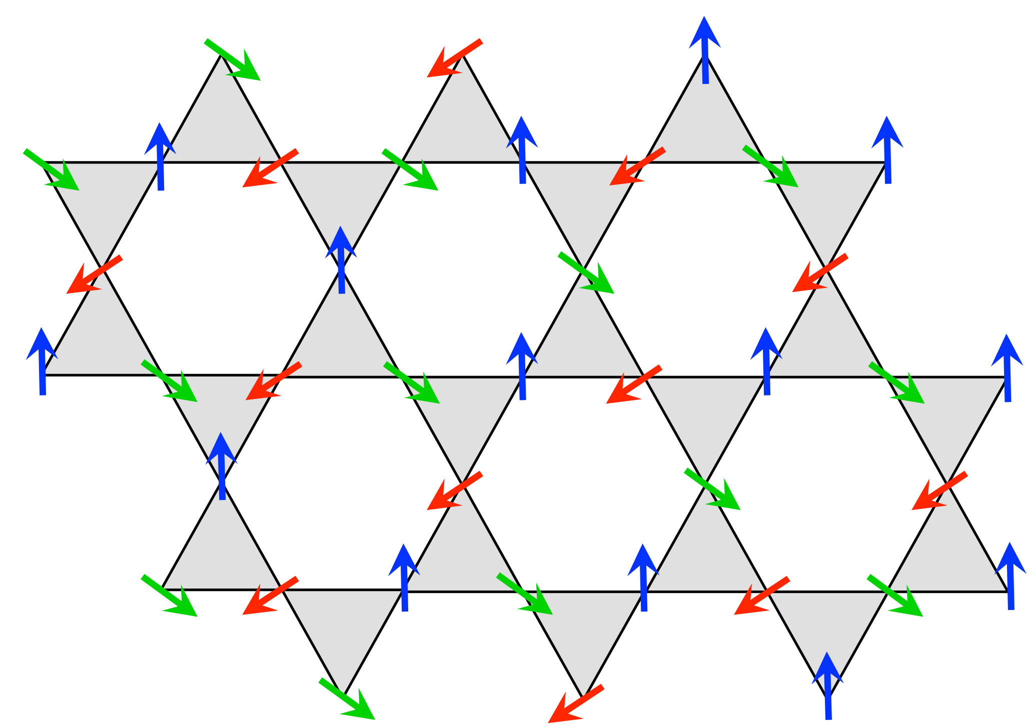
Hidden Order in a Frustrated System: Properties of the Heisenberg Kagomé Antiferromagnet

J. T. Chalker,[(1),(a)] P. C. W. Holdsworth,[(1),(2)] and E. F. Shender[(1),(3),(b)]

- Coplanar vector: $\mathbf{n}_\Delta = \mathbf{S}_1 \times \mathbf{S}_2 + \mathbf{S}_2 \times \mathbf{S}_3 + \mathbf{S}_3 \times \mathbf{S}_1$
- nematic correlations: $g_{ab} = \frac{3}{2}\langle(\mathbf{n}_a \cdot \mathbf{n}_b)^2\rangle - \frac{1}{2}$

$$1 - g_{ab} \sim \sqrt{T}$$





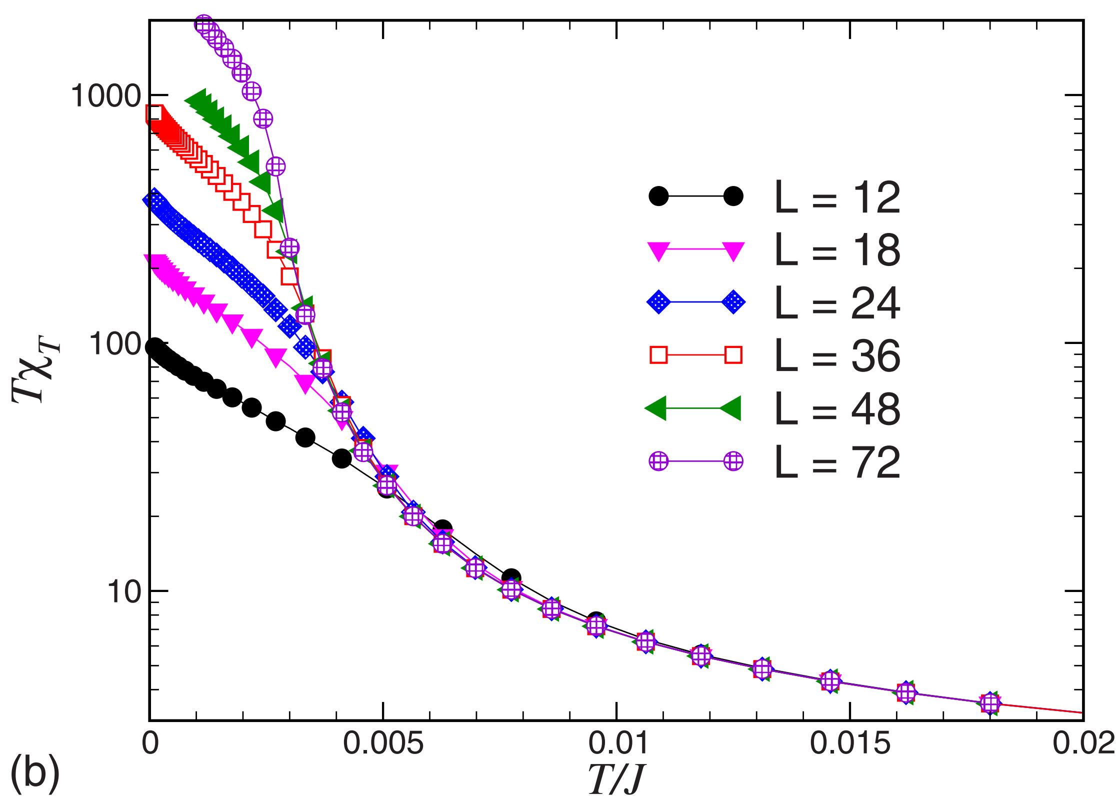
PHYSICAL REVIEW B **78**, 094423 (2008)

Octupolar ordering of classical kagome antiferromagnets in two and three dimensions

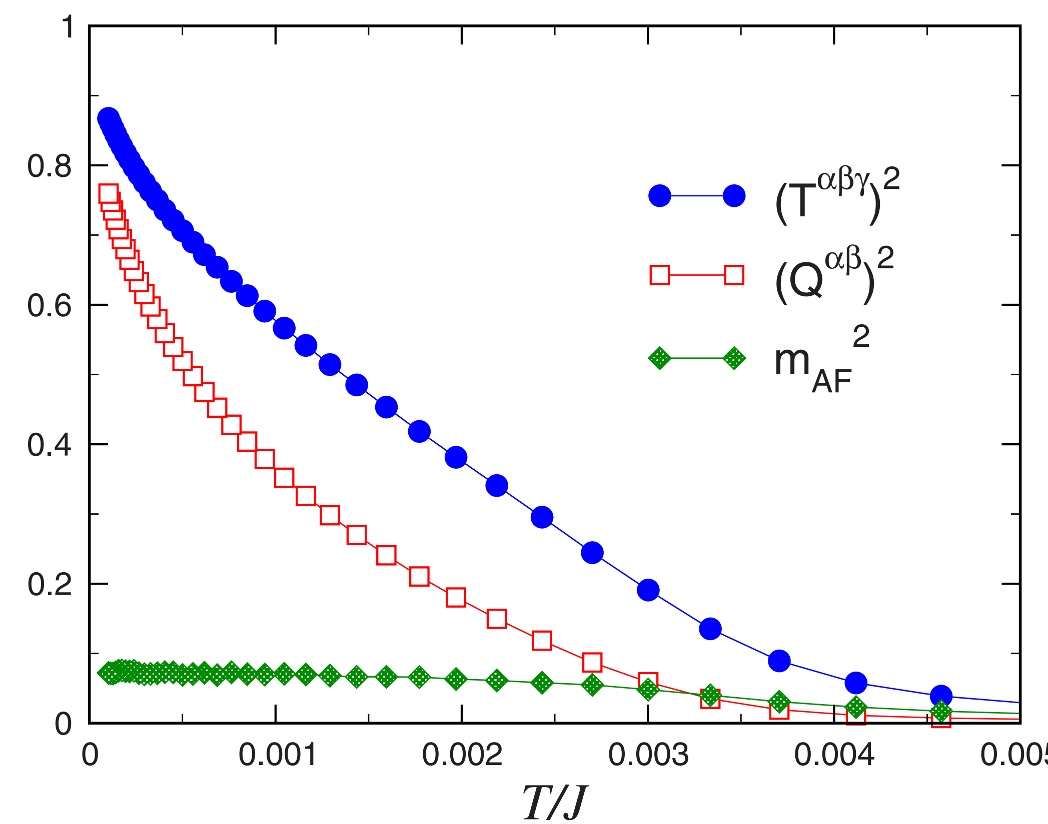
M. E. Zhitomirsky

- coplanar/nematic order = quadrupole order $$Q^{\alpha\beta} = \frac{1}{N}\sum_i \left(S_i^\alpha S_i^\beta - \frac{1}{3}\delta_{\alpha\beta} \right)$$
- Octupolar order: $$T_i^{\alpha\beta\gamma} = S_i^\alpha S_i^\beta S_i^\gamma - \frac{1}{5}S_i^\alpha \delta_{\beta\gamma} - \frac{1}{5}S_i^\beta \delta_{\alpha\gamma} - \frac{1}{5}S_i^\gamma \delta_{\alpha\beta}$$

$$\chi_T = \frac{1}{TN}\sum_{i,j} \langle T_i^{\alpha\beta\gamma} T_j^{\alpha\beta\gamma} \rangle$$



(b)



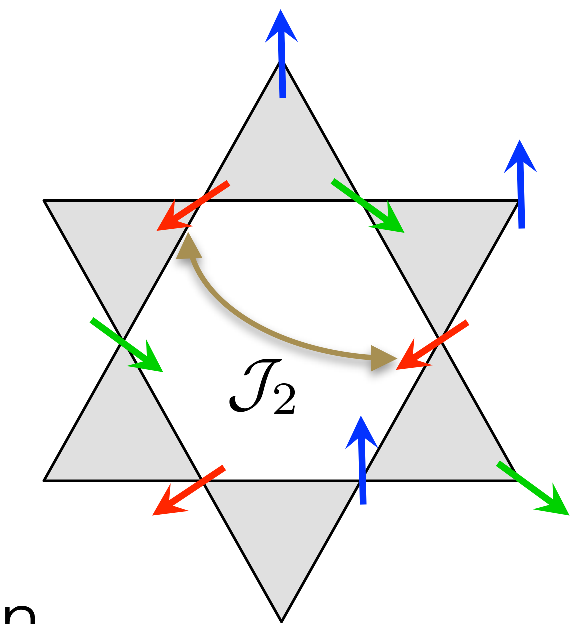
PRL 110, 077201 (2013) PHYSICAL REVIEW LETTERS week ending 15 FEBRUARY 2013

Dipolar Order by Disorder in the Classical Heisenberg Antiferromagnet on the Kagome Lattice

Gia-Wei Chern[1,2,3] and R. Moessner[1]

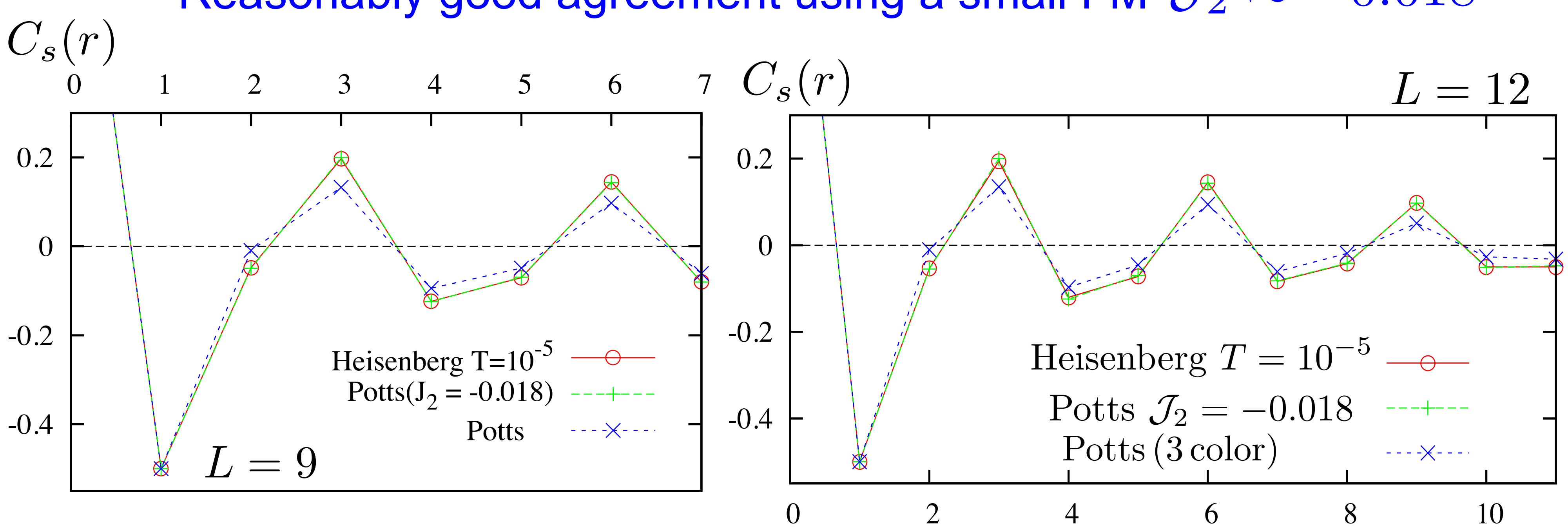
- Effective 3-color (Potts) model with ferromagnetic effective J2 interaction:

$$\mathcal{S}_{\text{eff}} = \mathcal{J}_2 \sum_{\langle\langle ij\rangle\rangle} \delta_{\sigma_i,\,\sigma_j}$$



- Try to fit entropic weight with NNN interaction

Reasonably good agreement using a small FM $\mathcal{J}_2 \approx -0.018$



KT transition

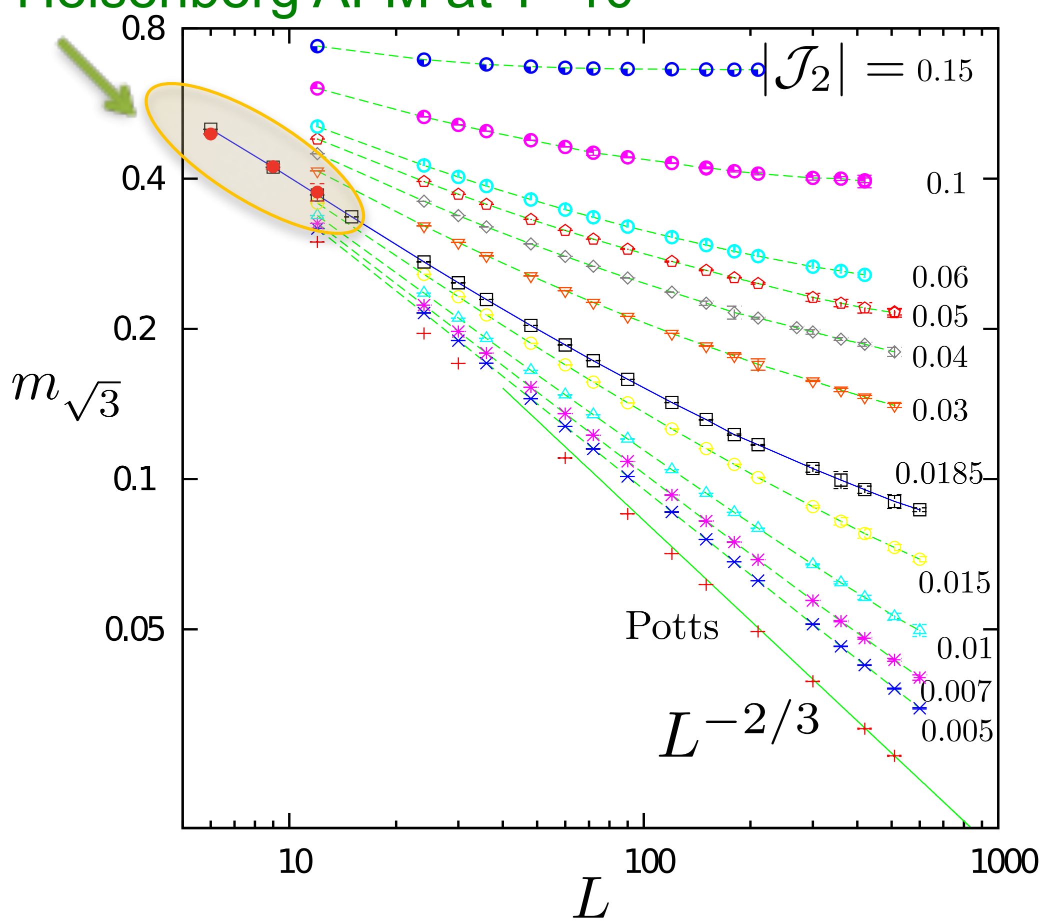
- critical $\mathcal{J}_2^c = 0$: a small negative $\mathcal{J}_2$ increases the stiffness and drive the system into the flat phase

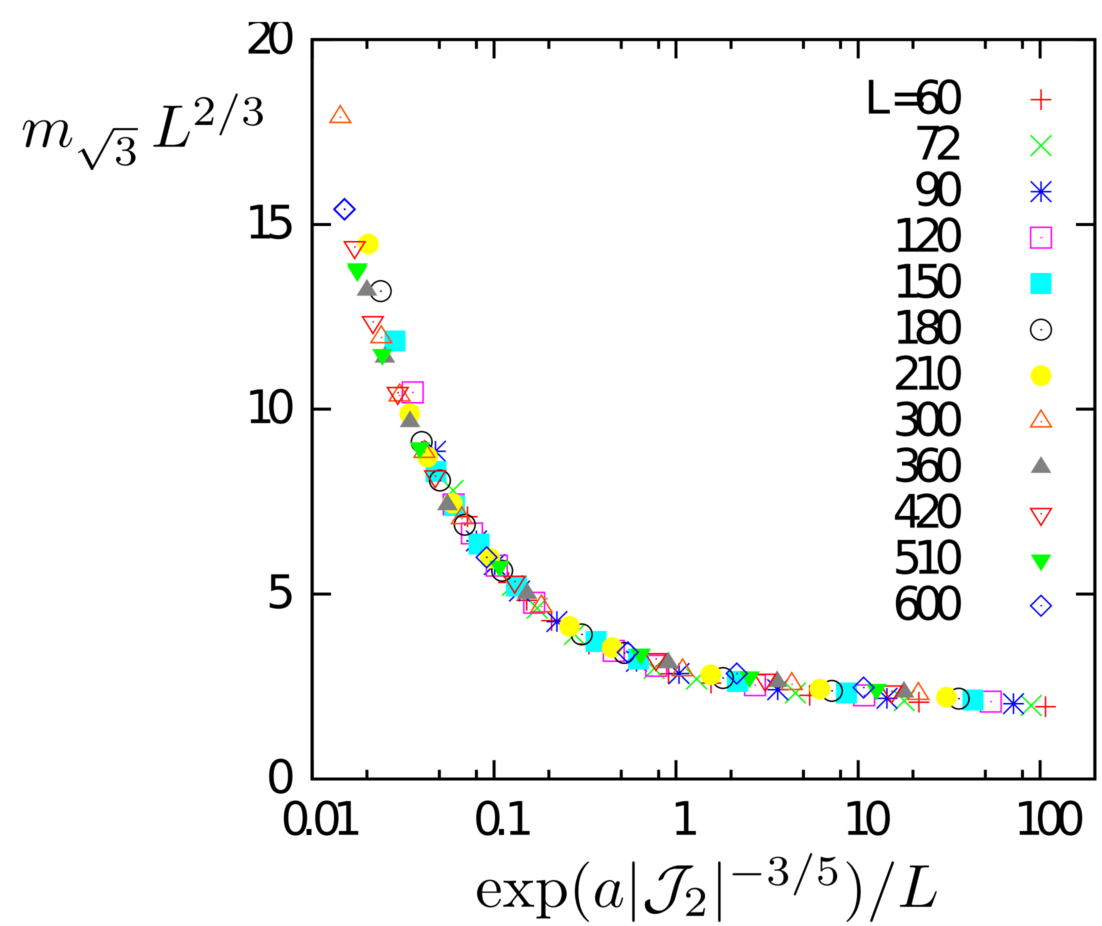
- KT transition: divergence of correlation length $\xi \sim \exp\left(\frac{\text{const}}{|\mathcal{J}_2|^{3/5}}\right)$

(S. Korshunov, '02)

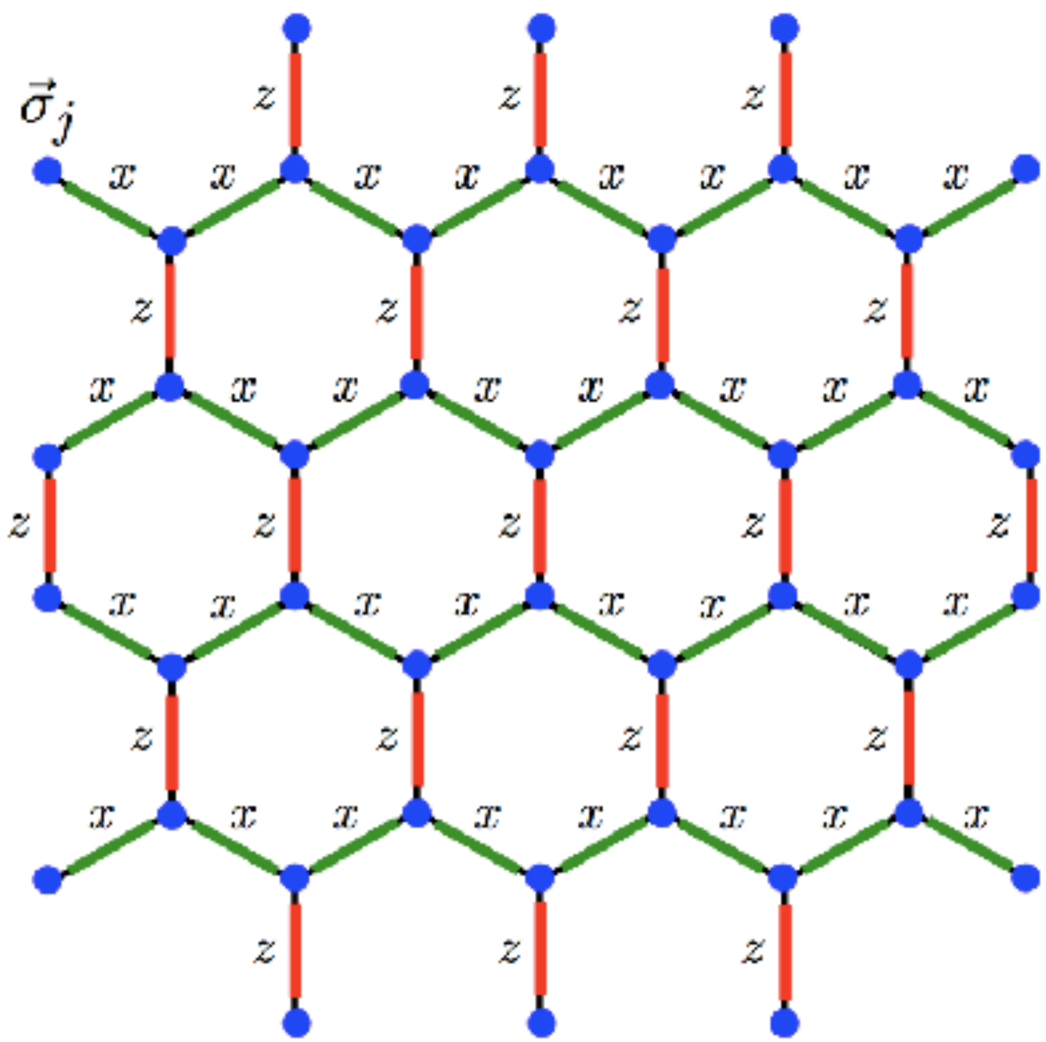
- Finite-size scaling: $m_{\sqrt{3}} L^{2/3} = \mathcal{F}\left(\frac{\xi(\mathcal{J}_2)}{L}\right)$

Heisenberg AFM at T=10^{-5}





Gamma model on honeycomb lattice



- Important interaction in addition to Kitaev and Heisenberg terms in real materials: A_2IrO_3, $RuCl_3$

- A new type of highly frustrated magnets

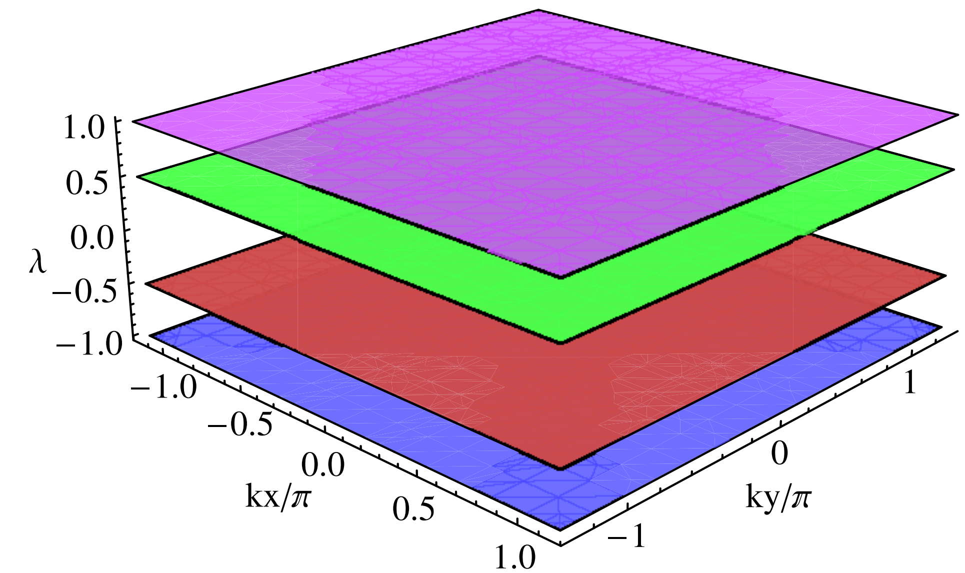
$$\mathcal{H} = \Gamma \sum_{\langle ij \rangle \| x} (S_i^y S_j^z + S_i^z S_j^y) + \Gamma \sum_{\langle ij \rangle \| y} (S_i^z S_j^x + S_i^x S_j^z) + \Gamma \sum_{\langle ij \rangle \| z} (S_i^x S_j^y + S_i^y S_j^x).$$

Macroscopically degenerate ground states

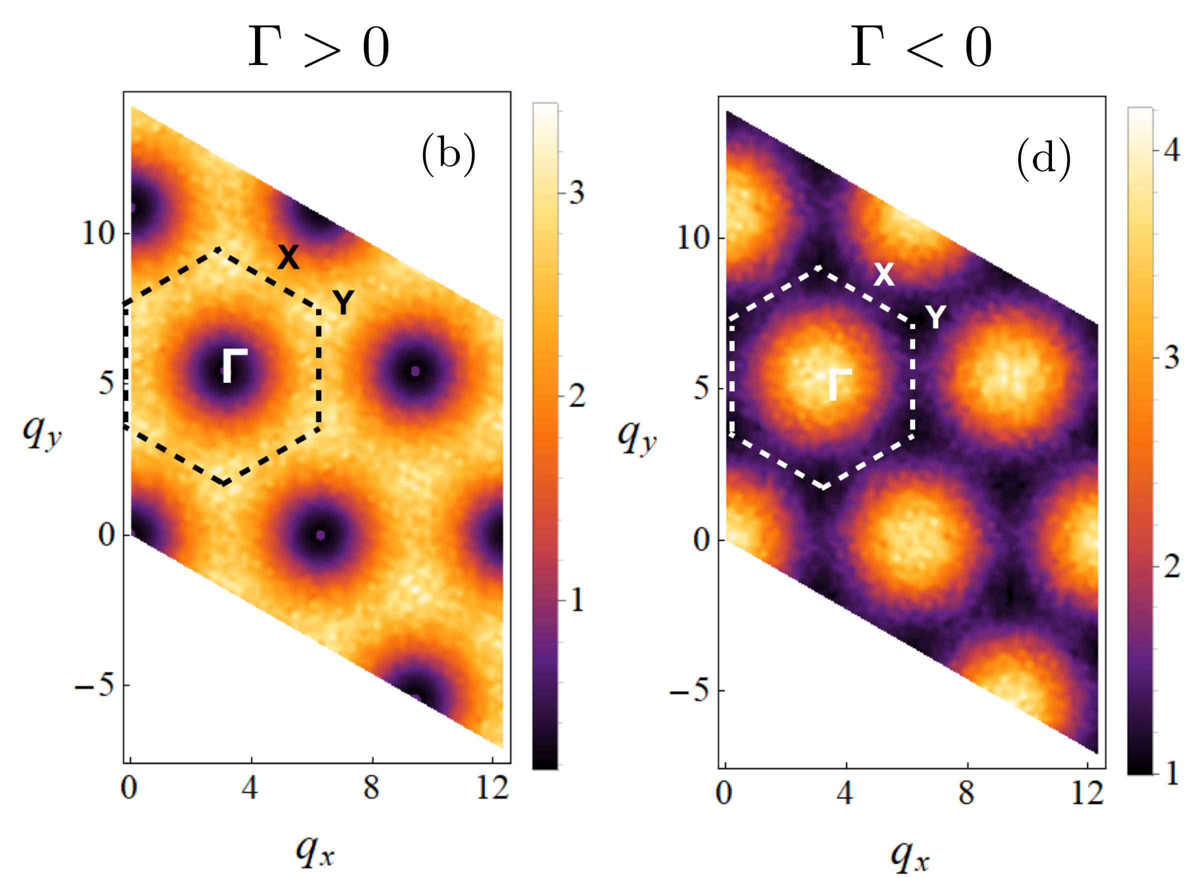
(Rousochatzakis & Perkins, PRL 2017)

- Spectrum under spherical approximation:

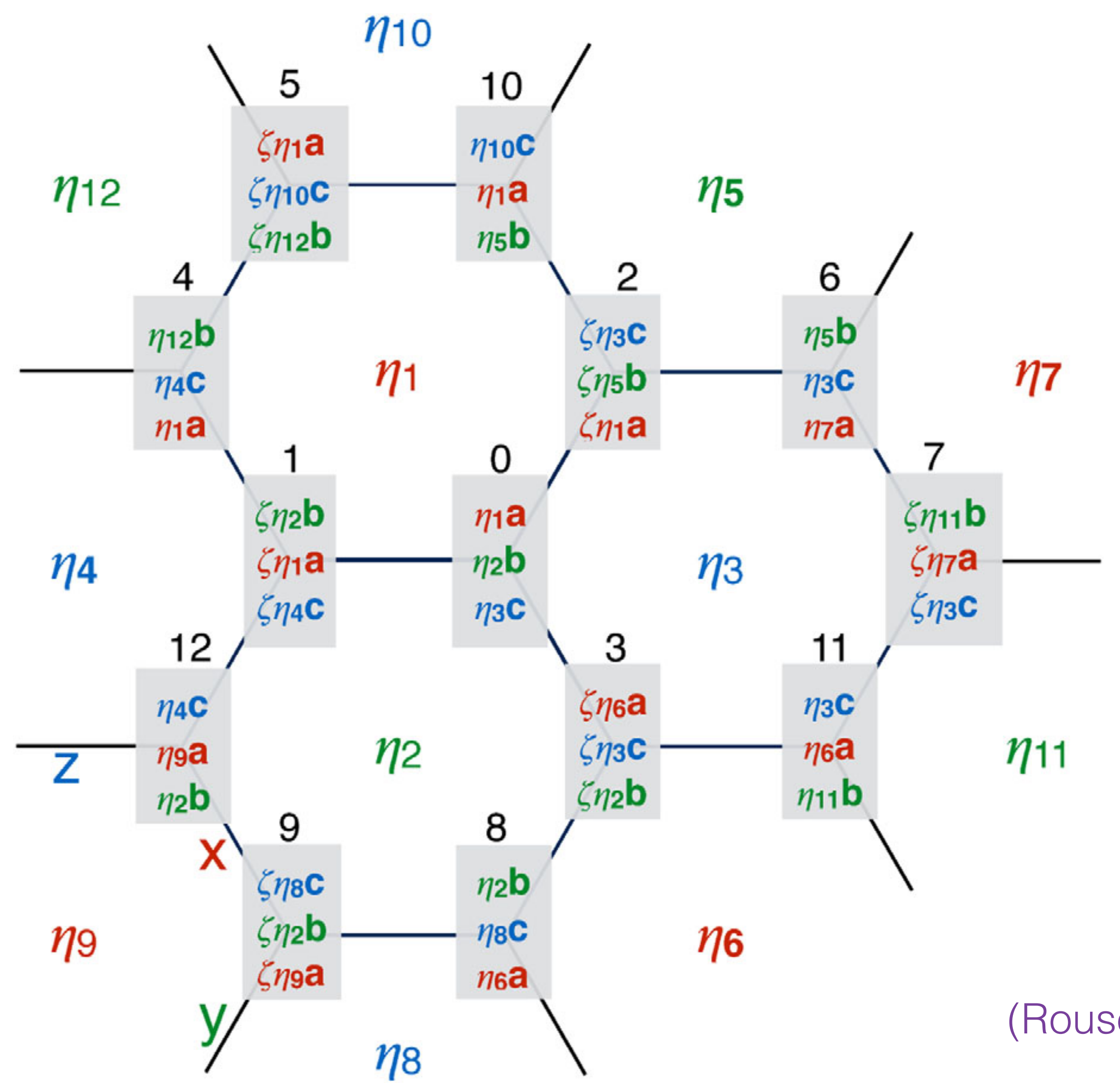
$$\mathcal{H} = \Gamma \sum_{\mathbf{k}} \sum_{ab=1,2} \sum_{\alpha\beta=x,y,z} \mathbb{H}^{ab}_{\alpha\beta}(\mathbf{k}) S^a_\alpha(\mathbf{k}) S^b_\beta(-\mathbf{k})$$



- Static Structure factor S(**q**):



Macroscopically degenerate ground states



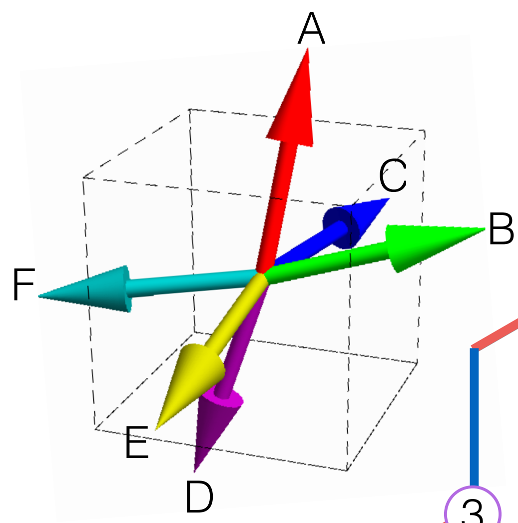
(Rousochatzakis & Perkins, PRL 2017)

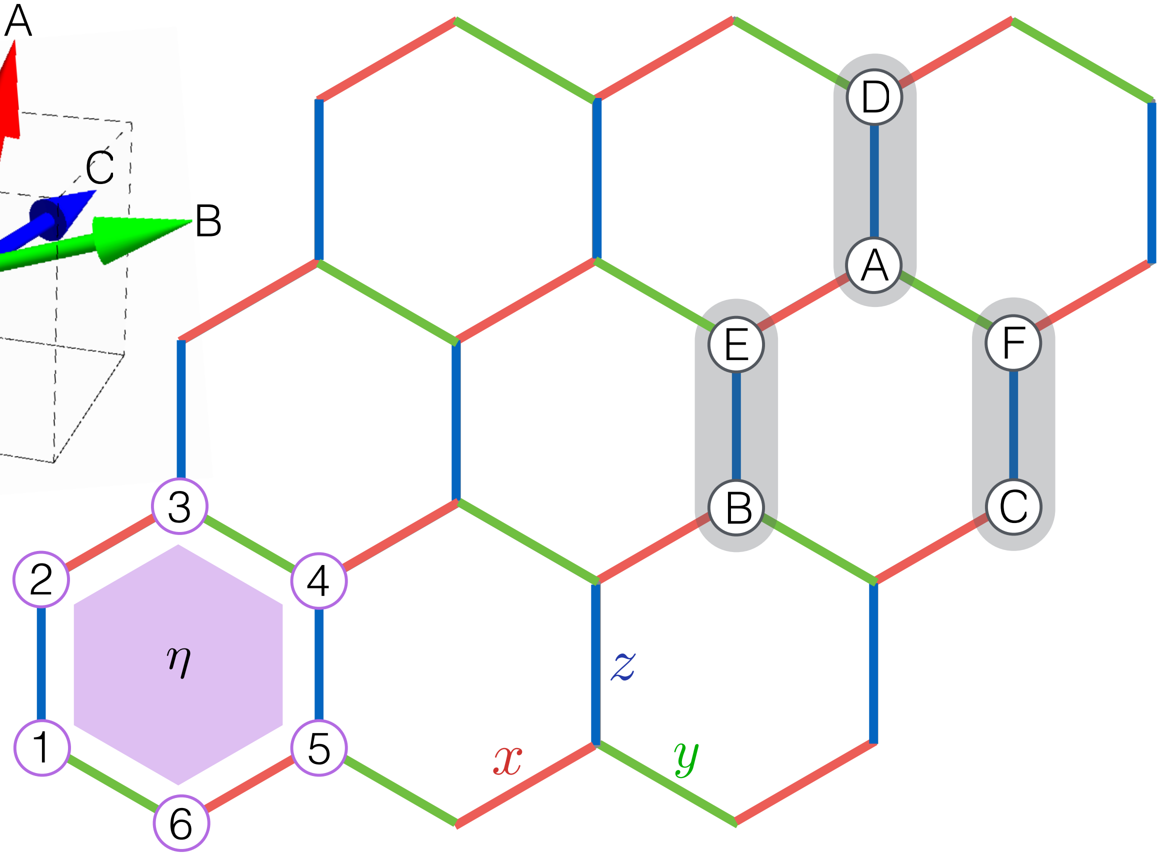
- The degenerate ground states are characterized by continuous variables $\hat{\mathbf{n}} = (a, b, c)$ and a set of discrete Ising variables $\{\eta_i\}$

Macroscopically degenerate classical ground states

$\sqrt{3} \times \sqrt{3}$ order

$$\mathbf{S}_{\mathrm{A}} = (a, b, c)$$
$$\mathbf{S}_{\mathrm{B}} = (c, a, b)$$
$$\mathbf{S}_{\mathrm{C}} = (b, c, a)$$
$$\mathbf{S}_{\mathrm{D}} = \pm(b, a, c)$$
$$\mathbf{S}_{\mathrm{E}} = \pm(a, c, b)$$
$$\mathbf{S}_{\mathrm{F}} = \pm(c, b, a)$$





$$S_1^x \to \eta S_1^x, \quad S_2^y \to \eta S_2^y, \quad S_3^z \to \eta S_3^z,$$

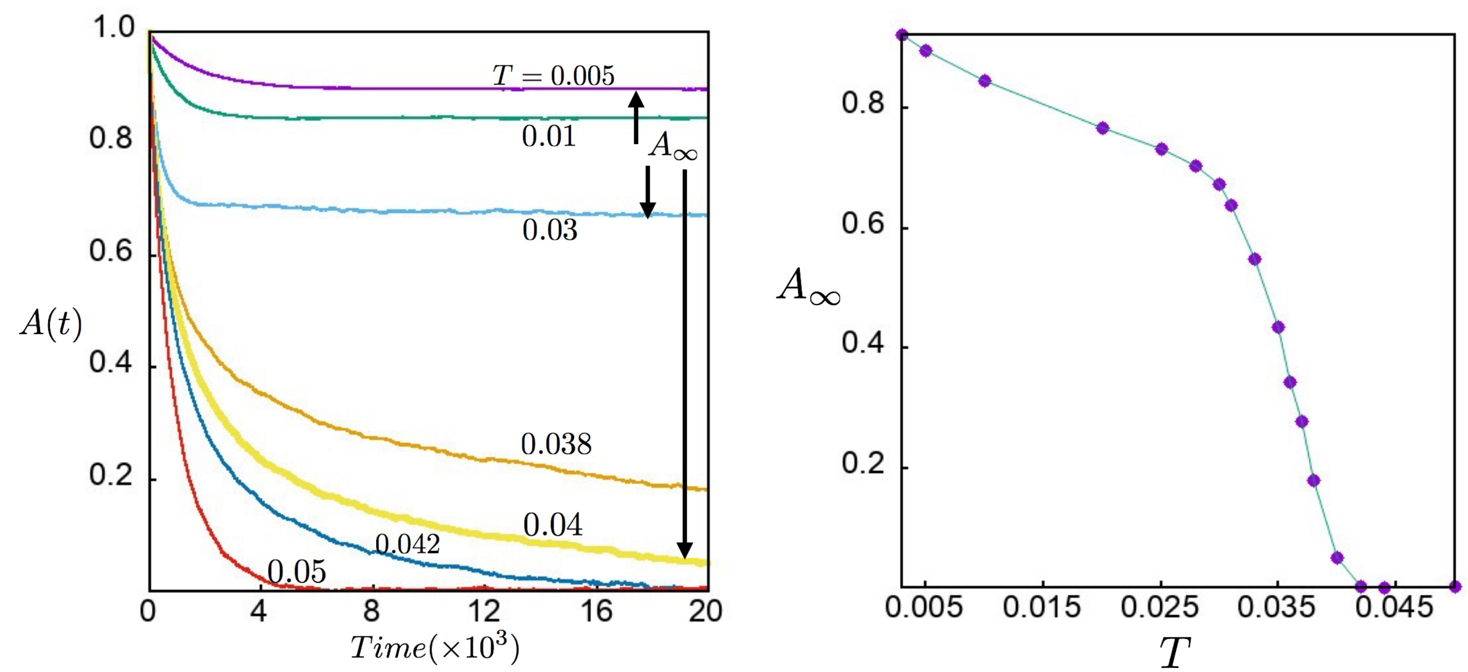
$$S_4^x \to \eta S_4^x, \quad S_5^y \to \eta S_5^y, \quad S_6^z \to \eta S_6^z$$

Thermal order by disorder ?

- Auto-correlation function:

$$A(t) = \frac{1}{N}\sum_i \langle \mathbf{S}_i(t)\cdot\mathbf{S}_i(0)\rangle$$

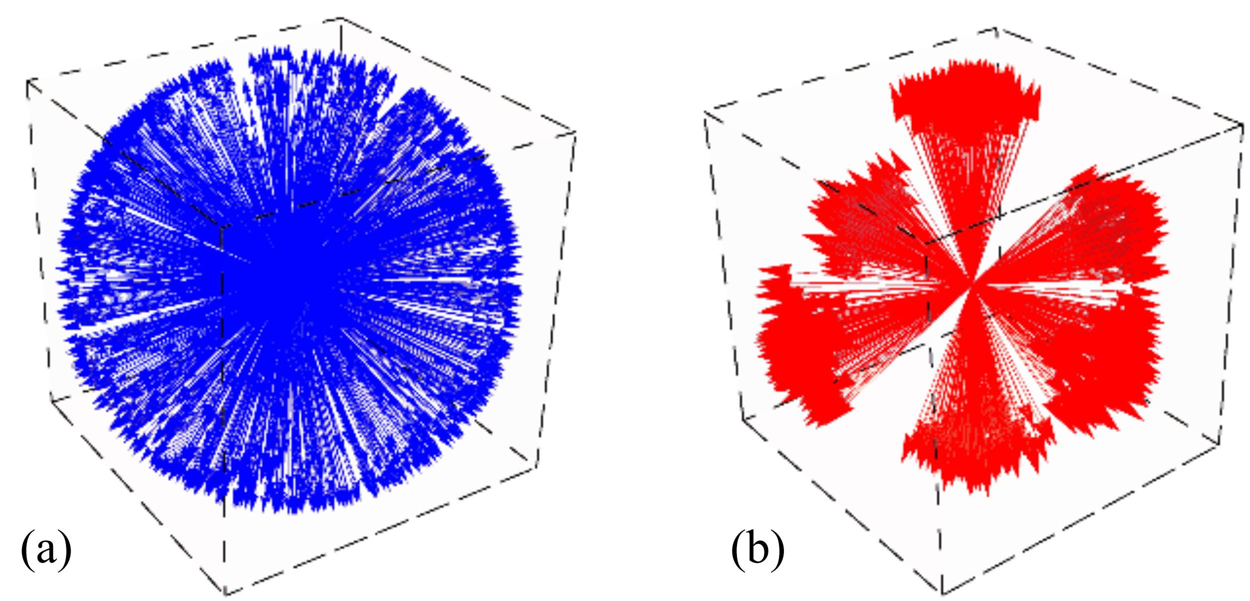
$$\sim A_\infty + (1 - A_\infty)\, e^{-t/\tau}$$



- Snapshots of spins form Monte Carlo simulations

Spins favor cubic directions !

Phase transition ?
Order parameter ?



$T > 0.04|\Gamma|$ $T < 0.04|\Gamma|$

Flux variable

- flux variable on hexagonal plaquettes:

$$W_\alpha = S_1^x\, S_2^y\, S_3^z\, S_4^x\, S_5^y\, S_6^z,$$

- Integrals of motion in the quantum Kitaev model

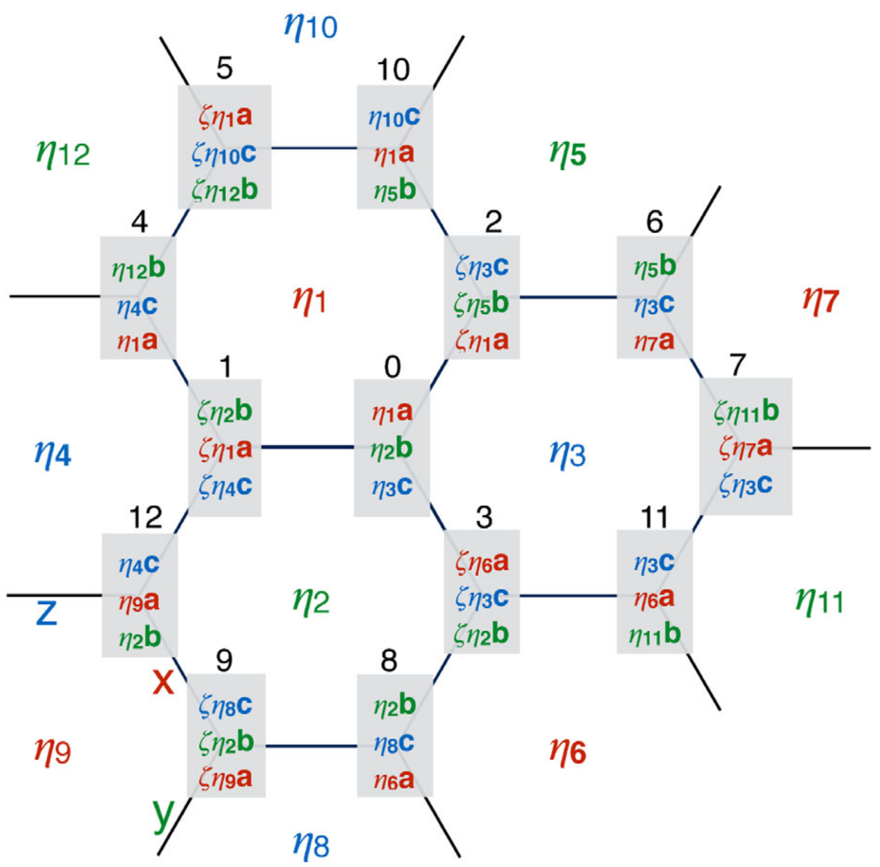
$$[W_\alpha, W_\beta] = 0 \qquad [W_\alpha, \mathcal{H}_{\text{Kitaev}}] = 0$$

- In the classical ground states of the Gamma model:

$$W_{h\in A} = W_{\eta_1} = S_0^x S_1^y S_4^z S_5^x S_{10}^y S_2^z / S^6 = \zeta \tilde{a}^6,$$

$$W_{h\in B} = W_{\eta_2} = S_8^x S_9^y S_{12}^z S_1^x S_0^y S_3^z / S^6 = \zeta \tilde{b}^6,$$

$$W_{h\in C} = W_{\eta_3} = S_{11}^x S_3^y S_0^z S_2^x S_6^y S_7^z / S^6 = \zeta \tilde{c}^6,$$



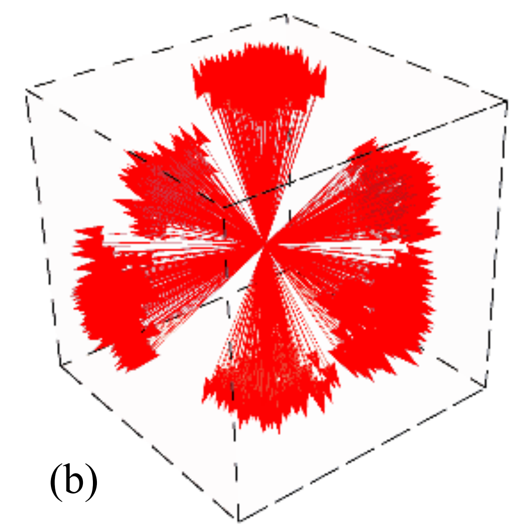
Phase transition: Plaquette ordering

- Flux variables in the "cubic" phase (a, b, c) ~ (1, 0, 0):

$$W_A = a^6 \sim 1$$

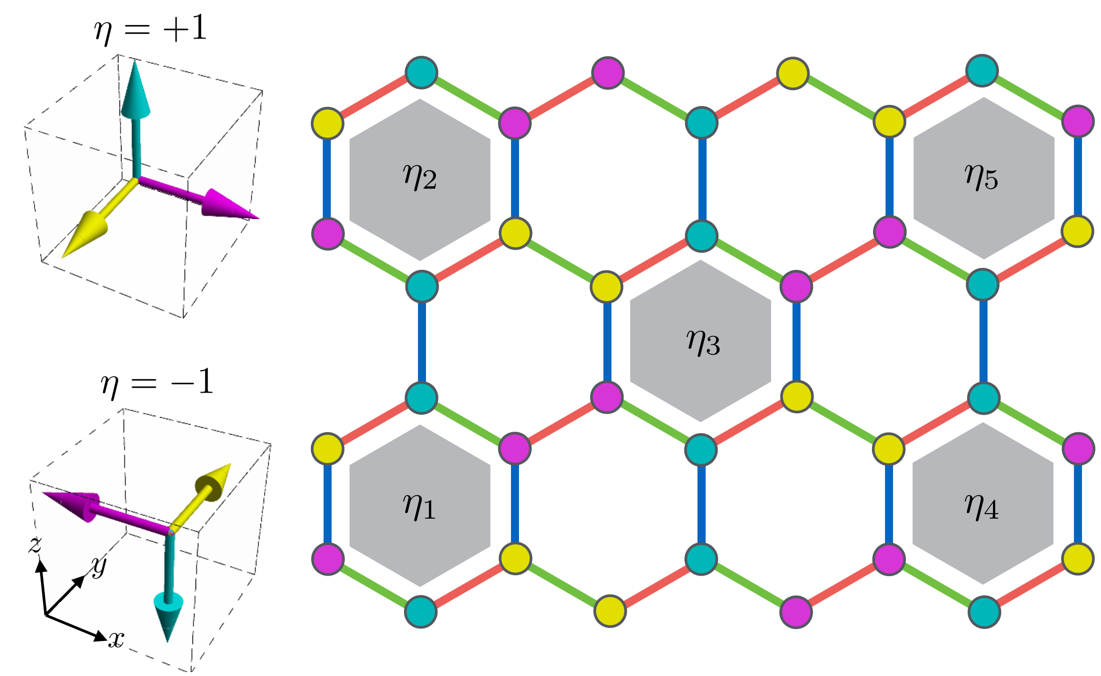
$$W_B = b^6 \sim 0$$

$$W_C = c^6 \sim 0$$



- the flux variables break translation symmetry:

$\sqrt{3} \times \sqrt{3}$ arrangement of the nonzero fluxes

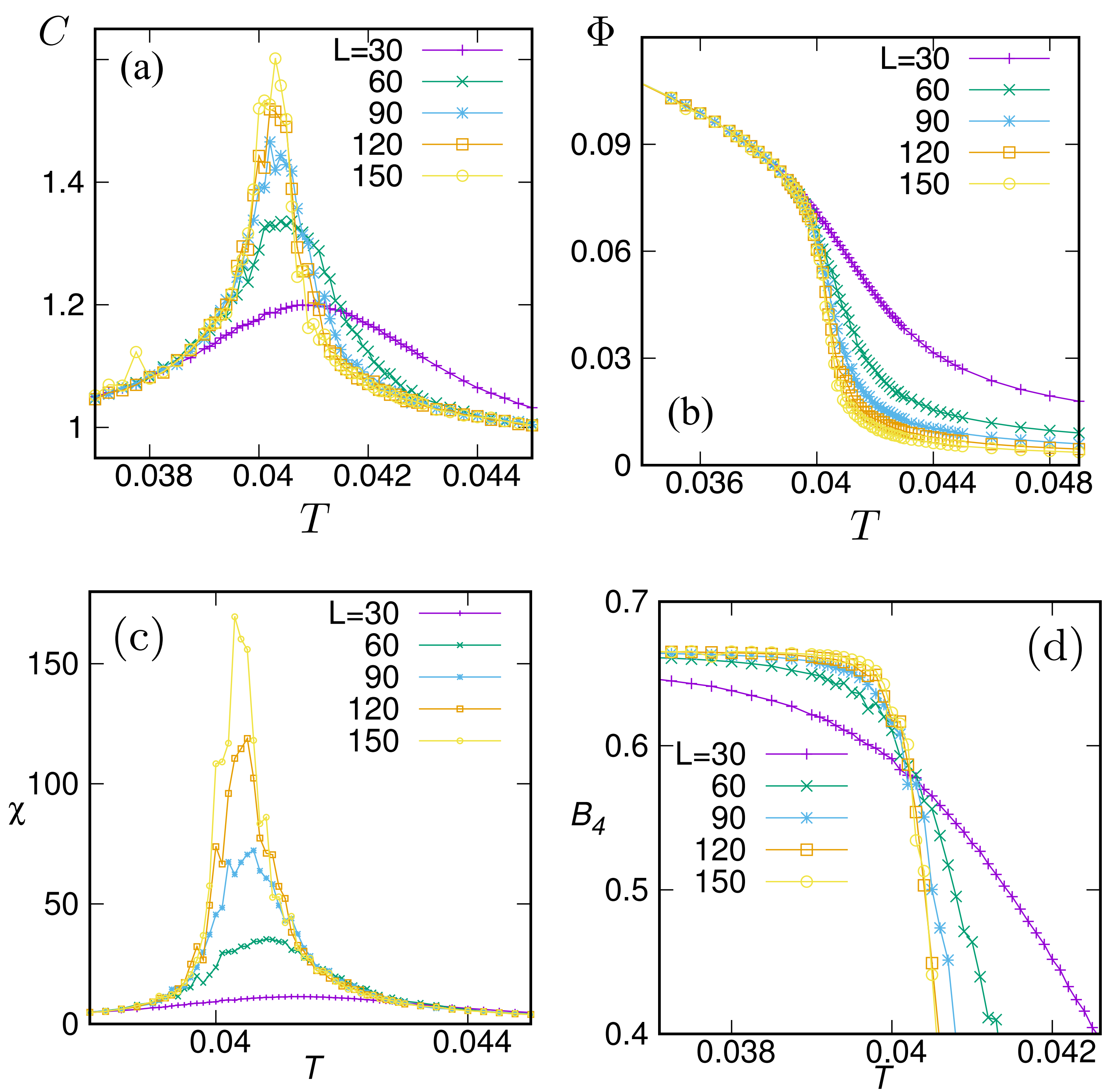


- Order-parameter:

$$\tilde{W}(\mathbf{Q}) = \frac{1}{N}\sum_{\alpha} W_{\alpha}\, e^{i\mathbf{Q}\cdot\mathbf{r}_{\alpha}},$$

ordering wave vector: $\mathbf{Q} = \left(\frac{4\pi}{3}, 0\right).$

Monte Carlo simulations of plaquette ordering



- specific heat

$$C = \frac{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2}{NT^2}$$

- Order-parameter

$$\Phi = \langle |\tilde{W}(\mathbf{Q})| \rangle,$$

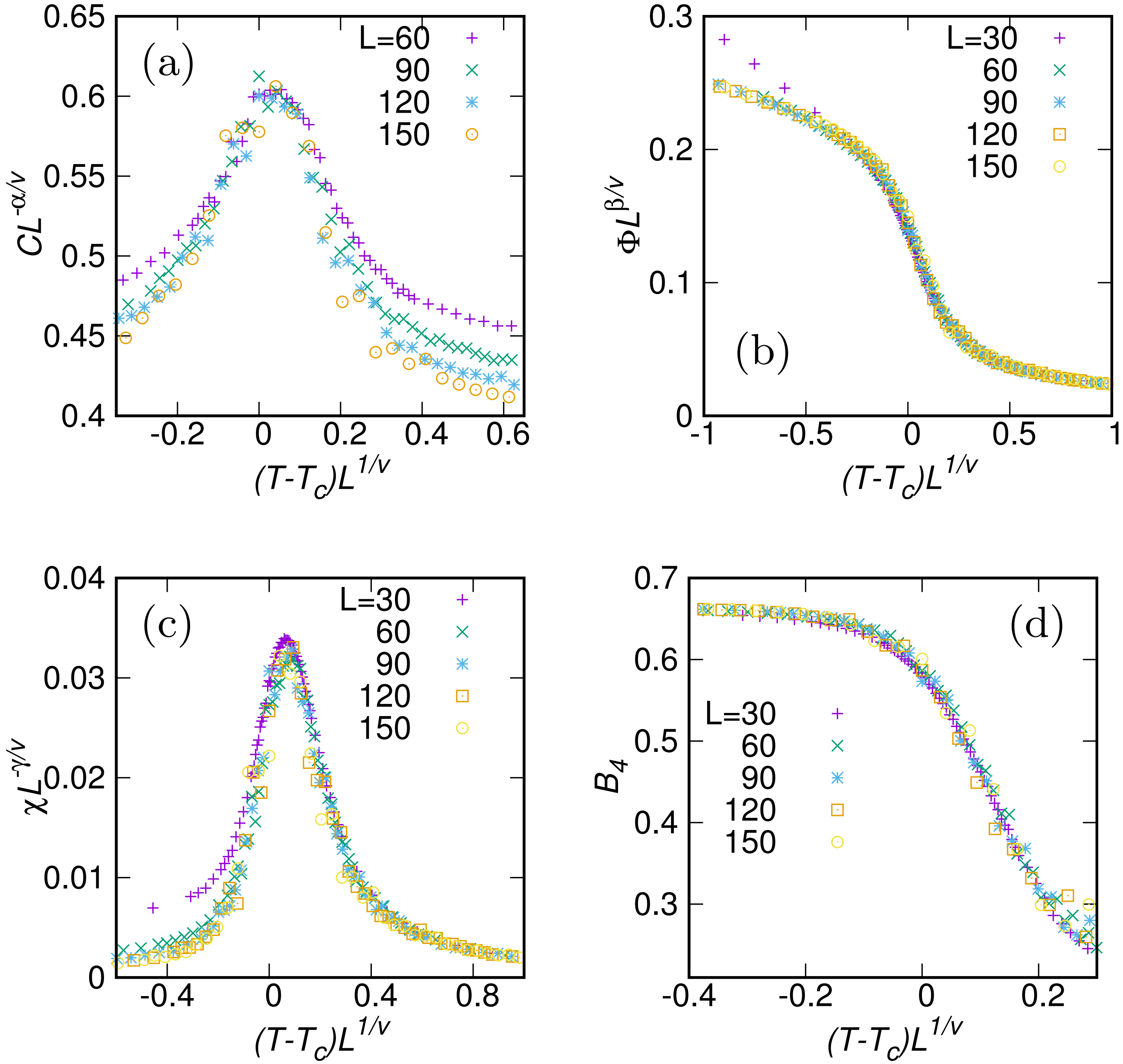
- Susceptibility

$$\chi = N \frac{\langle |\tilde{W}(\mathbf{Q})|^2 \rangle - \langle |\tilde{W}(\mathbf{Q})| \rangle^2}{T}$$

- Binder's cumulant

$$B_4 = 1 - \frac{\langle |\tilde{W}(\mathbf{Q})|^4 \rangle}{3 \langle |\tilde{W}(\mathbf{Q})|^2 \rangle^2}$$

Finite size scaling analysis



- critical exponents

$$\alpha = 0.167$$
$$\beta = 0.177$$
$$\gamma = 1.47$$
$$\nu = 0.863$$

- 2D 3-state Potts universality class:

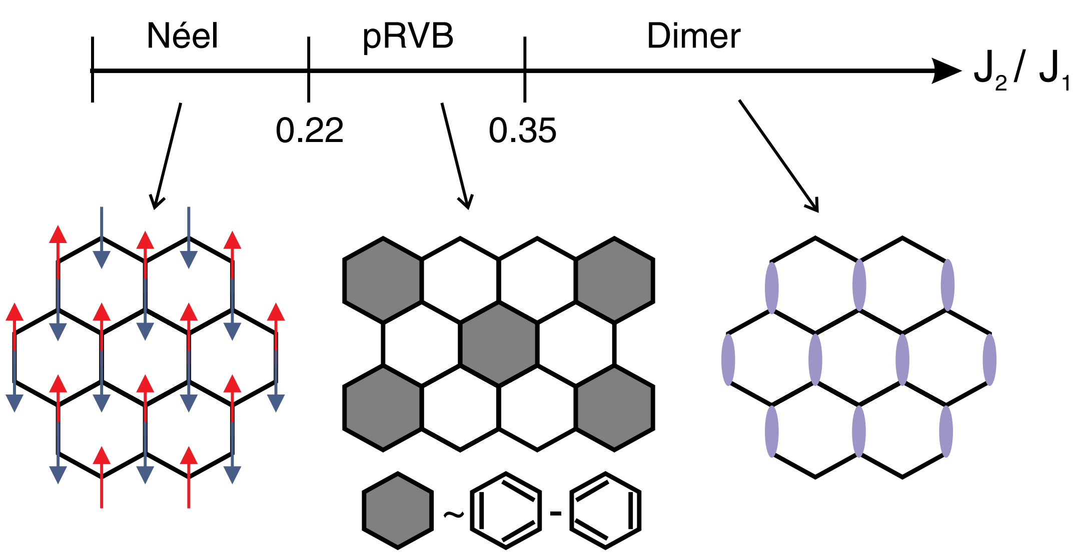
$$\alpha = 1/3 = 0.333$$
$$\beta = 1/9 = 0.111$$
$$\gamma = 13/9 = 1.444$$
$$\nu = 5/6 = 0.833$$

Plaquette ordering in quantum models

- J1-J2 antiferromagnetic Heisenberg model on honeycomb lattice:

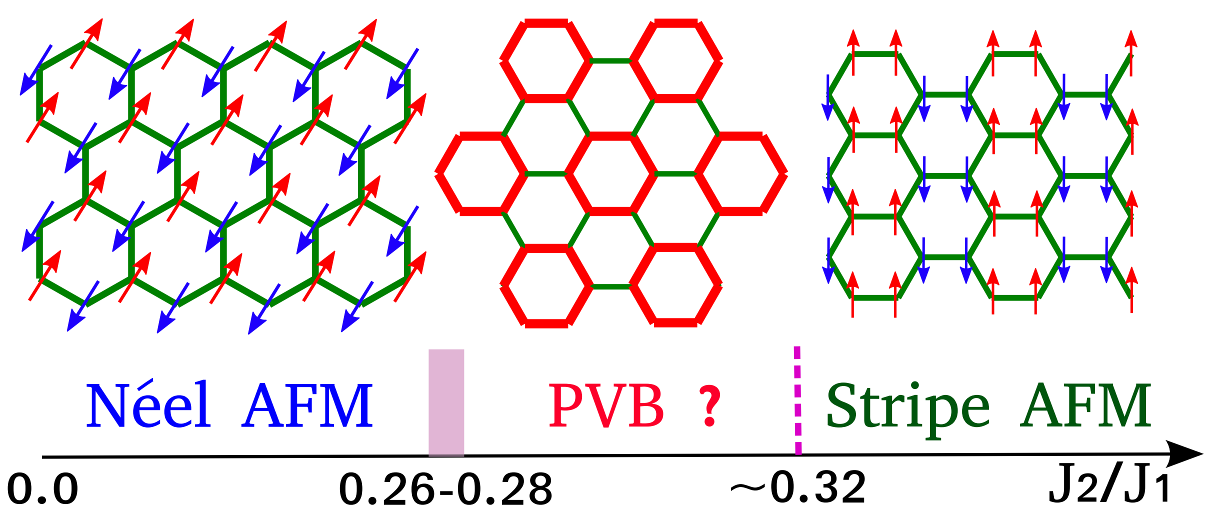
$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

- Phase diagram S = 1/2:



(Ganesh, van den Brink, Nishimoto, PRL 2013)

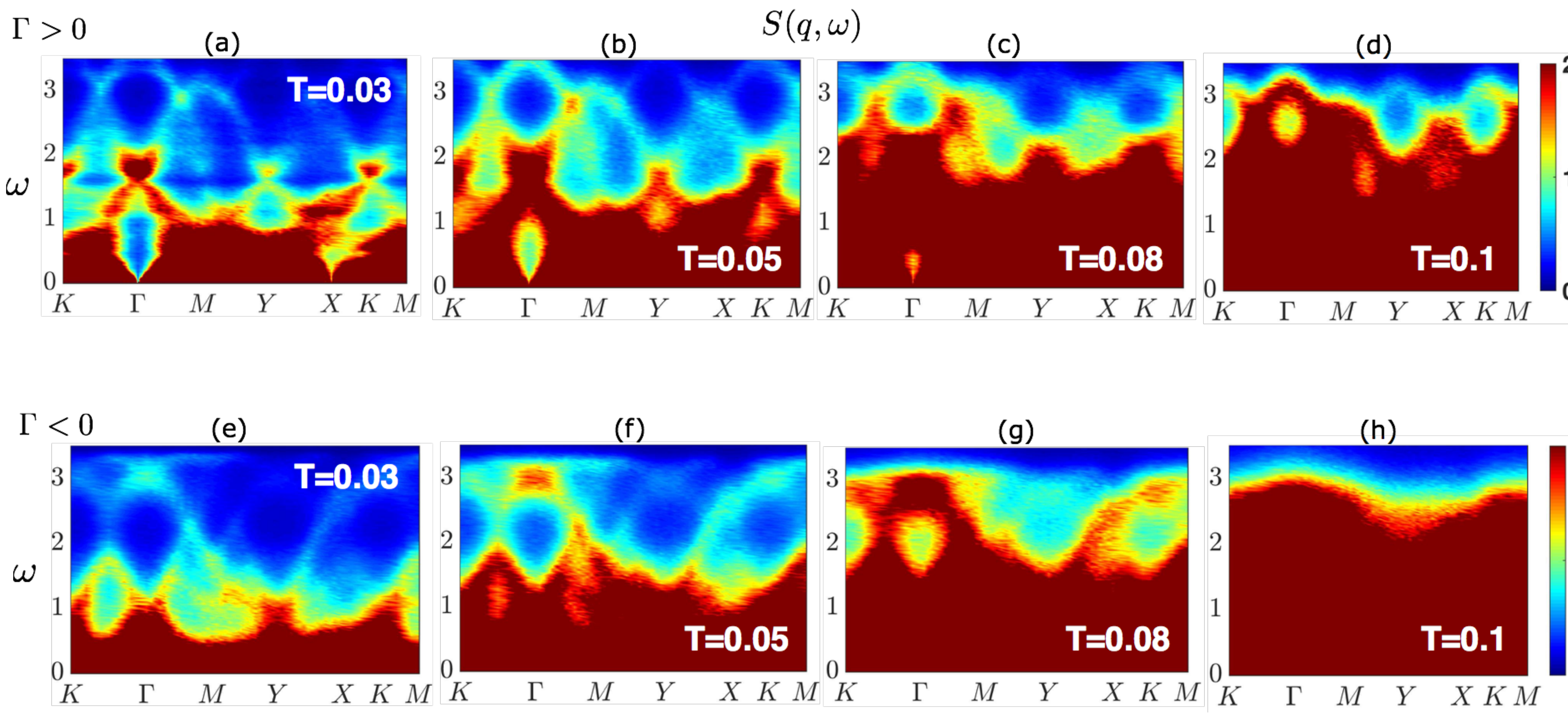
- Phase diagram S = 1:



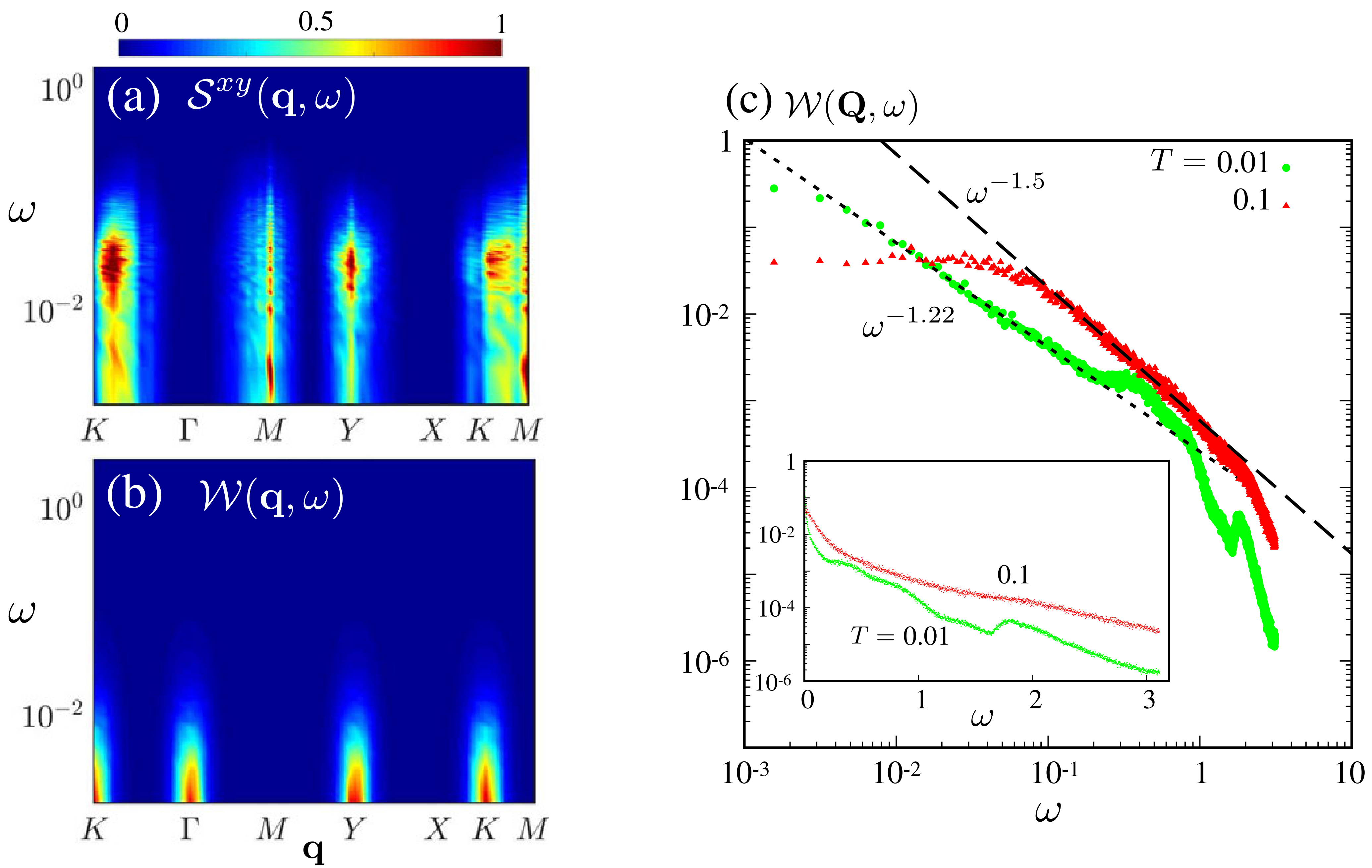
(S-S Gong, Wei Zhu, and D. N. Sheng, PRB 2015)

Dynamical Structure Factor:

- Landau-Lifshitz dynamics: $\frac{d\mathbf{S}_i}{dt} = -\mathbf{S}_i \times \frac{\partial \mathcal{H}}{\partial \mathbf{S}_i},$
- Dynamical Structure factor: $S(\mathbf{q},\omega) = \int \langle \mathbf{S}(\mathbf{q},t)\cdot\mathbf{S}(-q,0)\rangle e^{-i\omega t}\,dt$



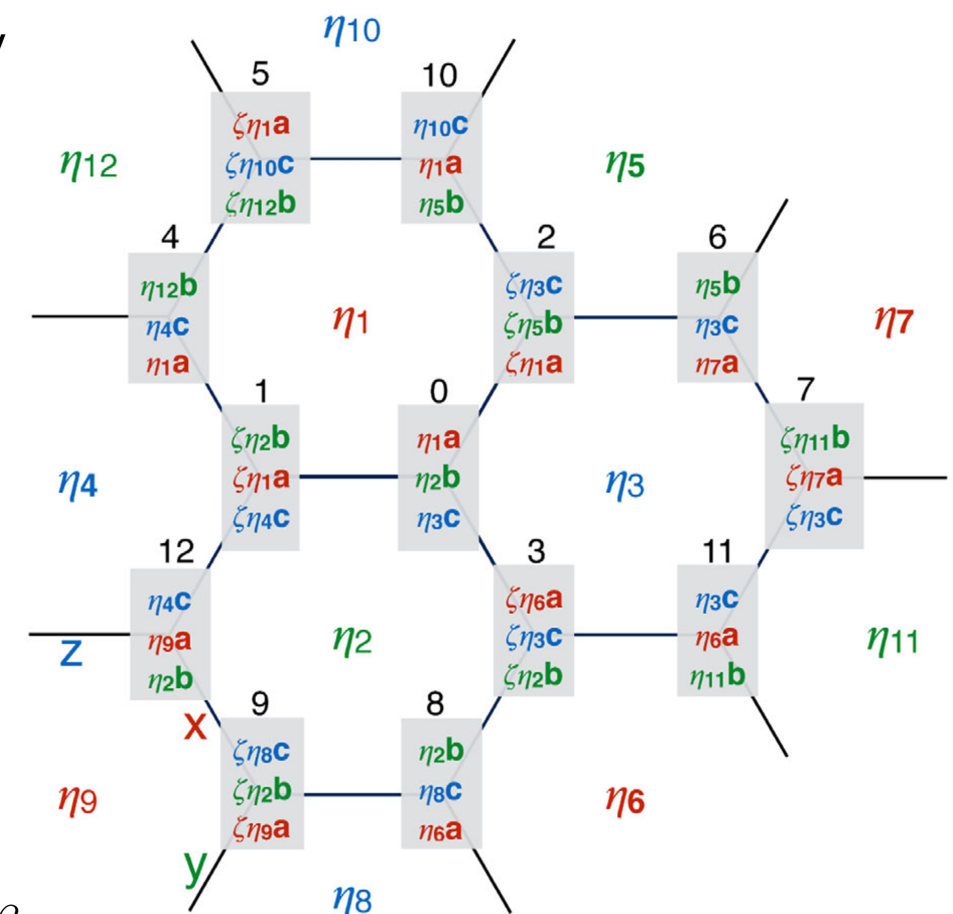
Dynamical Structure Factor: Off-diagonal



Quantum order by disorder

(Rousochatzakis & Perkins, PRL 2017)

- The degenerate ground states are characterized by continuous variables $\hat{\mathbf{n}} = (a, b, c)$ and a set of discrete Ising variables $\{\eta_i\}$



- Real-space perturbation calculation:

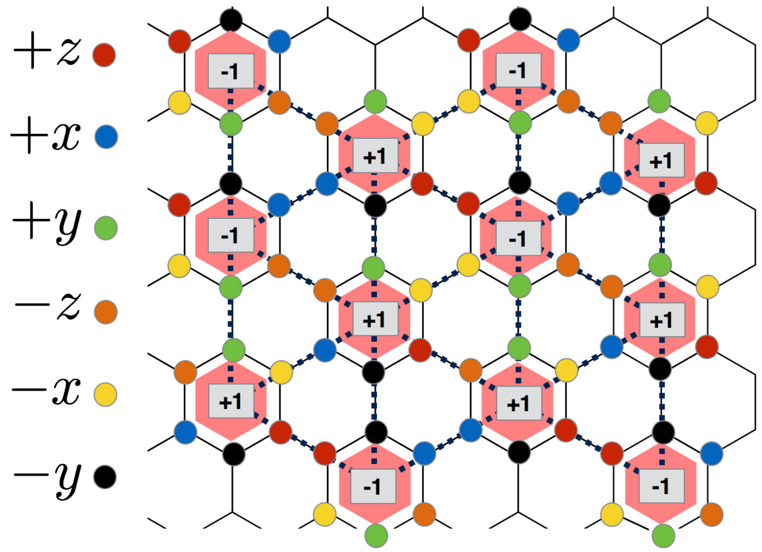
$$E_{\text{eff}} = -\frac{|\Gamma| S}{32}(a^4 + b^4 + c^4)$$

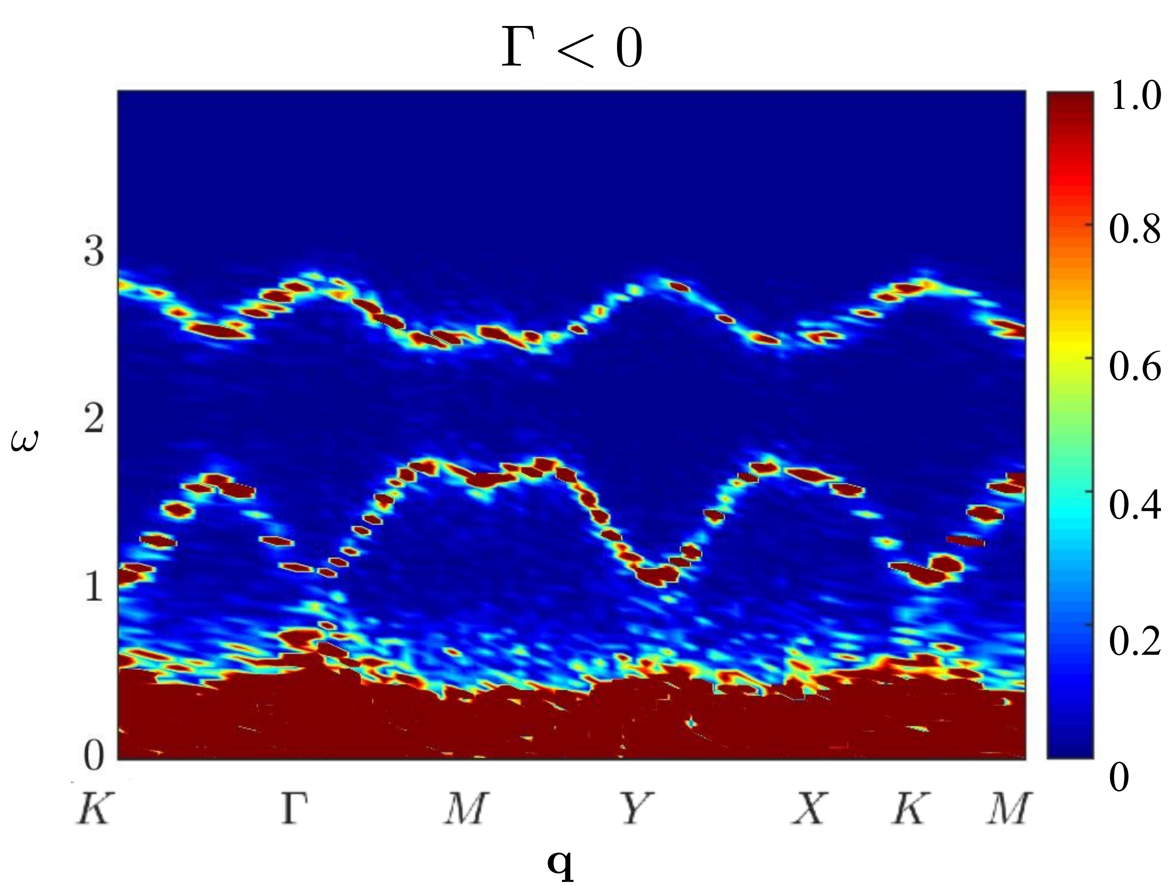
$$+\frac{\Gamma S a^2}{8} \sum_{\langle\alpha\beta\rangle}^{\text{red}} \eta_\alpha \eta_\beta \quad + \frac{\Gamma S b^2}{8} \sum_{\langle\alpha\beta\rangle}^{\text{green}} \eta_\alpha \eta_\beta \quad + \frac{\Gamma S c^2}{8} \sum_{\langle\alpha\beta\rangle}^{\text{blue}} \eta_\alpha \eta_\beta$$

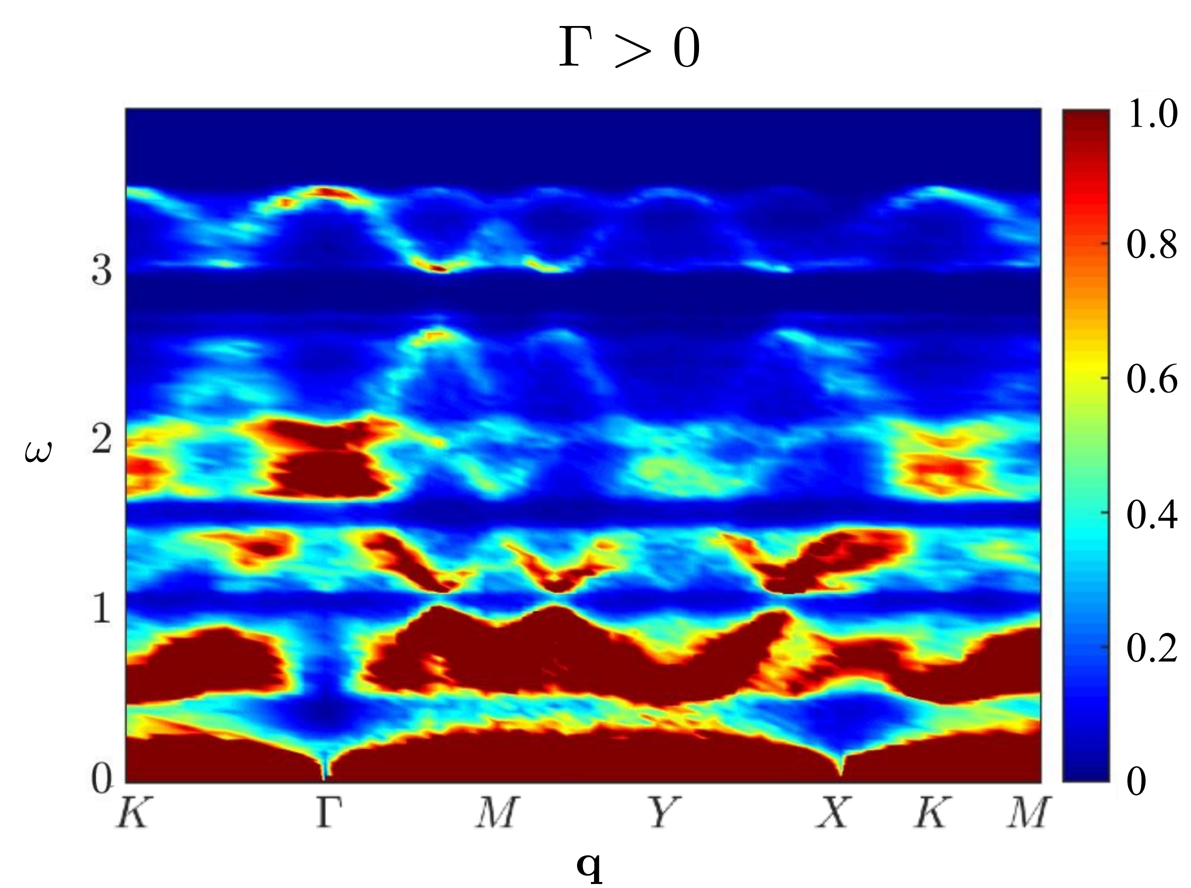
- (a, b, c) favors cubic direction.

Quantum Order by disorder

$$\mathcal{H}_{\text{Ising}} = \epsilon\,\Gamma \sum_{\langle\alpha\beta\rangle}{}' \eta_\alpha\,\eta_\beta$$







Quantum spin-1/2 Gamma model?

Title: Ground State of the Spin-1/2 Honeycomb Γ Model: Zigzag Magnetic Order

Authors: Liao, Hai-Jun; Huang, Ruizhen; Guo, Yi-Bin; Xie, Zhi-Yuan; Normand, Bruce; Xiang, Tao

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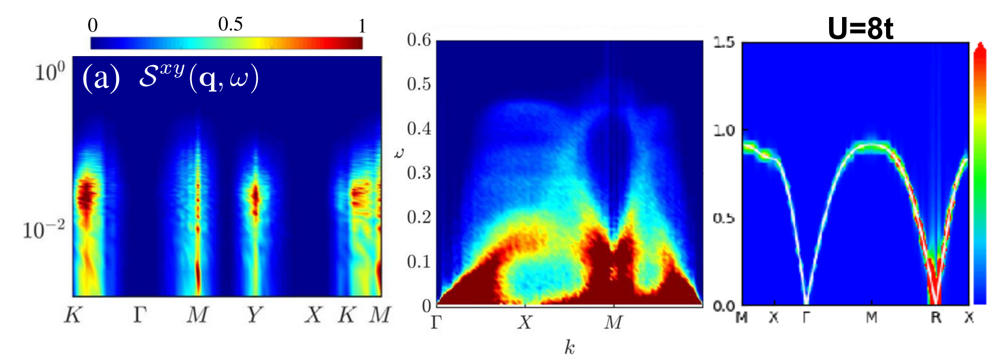
Abstract

The off-diagonal symmetric interaction, Γ ($S_i\alpha S\beta i_{+\gamma} + S_i\beta\ S\alpha i_{+\gamma}$), has sprung to prominence as a competing term in the spin Hamiltonians of candidate Kitaev materials. We investigate the quantum (S = 1/2) Γ model on the honeycomb lattice using the tensor-network method of infinite projected entangled pair states (iPEPS). We demonstrate that the ground state is a zigzag magnetically ordered state, rather than the spin liquid reported on the basis of density-matrix renormalization-group (DMRG) studies. By applying two quasi-one-dimensional numerical treatments, the infinite matrix-product-state (iMPS) and DMRG methods, we show that this contrast is a consequence of the system size considered. Thus the quantum Γ model is quite different from its classical counterpart, which is a classical spin liquid due to its macroscopic ground-state degeneracy.

Summary

- Numerical methods for dynamical structure factors based on equation-of-motion approach



- Hidden plaquette order and thermal order by disorder in the honeycomb Gamma model

THANK YOU