Quantum Monte-Carlo study of deconfined bosonic spinons, a Higgs-confining transition, and two crossovers in quantum spin ice

Yasuyuki Kato[1], Shigeki Onoda[1,2]

[1]RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan

[2]Condensed Matter Theory Laboratory, RIKEN, Wako, Japan

RIKEN CEMS

Motivation

J.B. Kogut,
“*An introduction to lattice gauge theory and spin systems*”
Rev. Mod. Phys. **51,** 659 (1979).

M. Hermele, M.P.A. Fisher, and L. Balents,
“*Pyrochlore photons: The U(1) spin liquid in a S=1/2 three-dimensional frustrated magnet*”
Phys. Rev. B **69**, 064404 (2004).

Frustrated quantum magnets ↔ **Lattice gauge theory (Maxwell action on lattice)**

Hot topics:

- Spin liquids
- (Ferro)magnetic transition

- Deconfinement of magnetic and electric charges
- etc…

Study of this connection with an unbiased numerical method

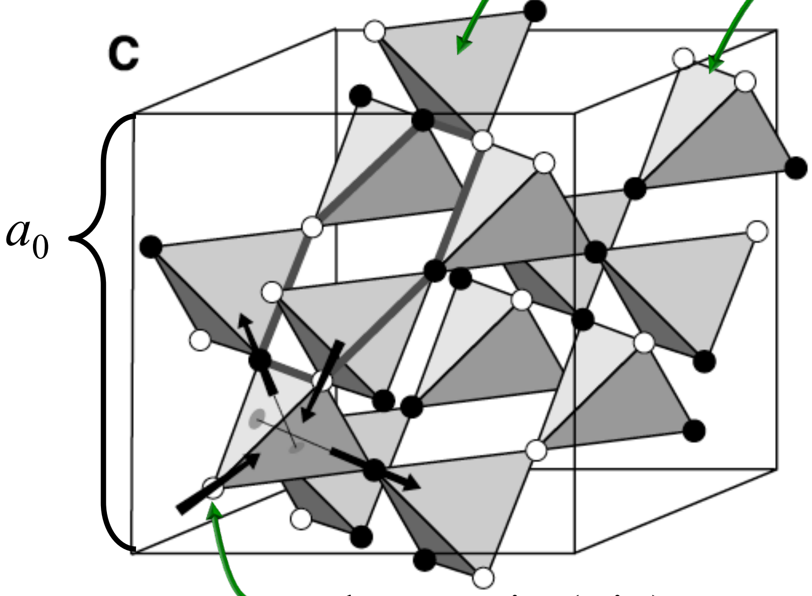
Contents

- Introduction – Spin ice compounds
- Model – XXZ model on a Pyrochlore lattice
- Method – Worldline Monte-Carlo Method
- Results – Finite temperature phase diagram
  - – Spin structure factors
  - – Wilson loop
- Summary

Introduction: Spin Ice compounds $Dy_2Ti_2O_7$, $Ho_2Ti_2O_7$

Pyrochlore Ising magnets

$$\mathcal{H}_C = J \sum_{\langle r,r' \rangle} s_r^z s_{r'}^z, \left[s = \frac{1}{2},\ J > 0 \right]$$

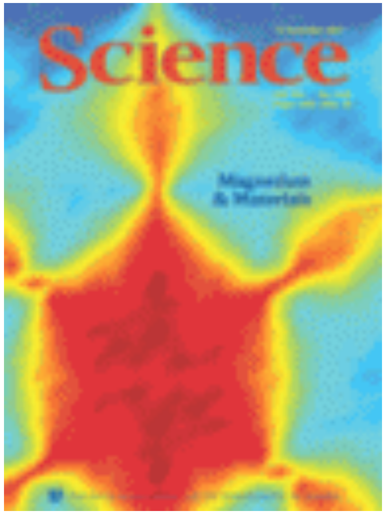


B-type

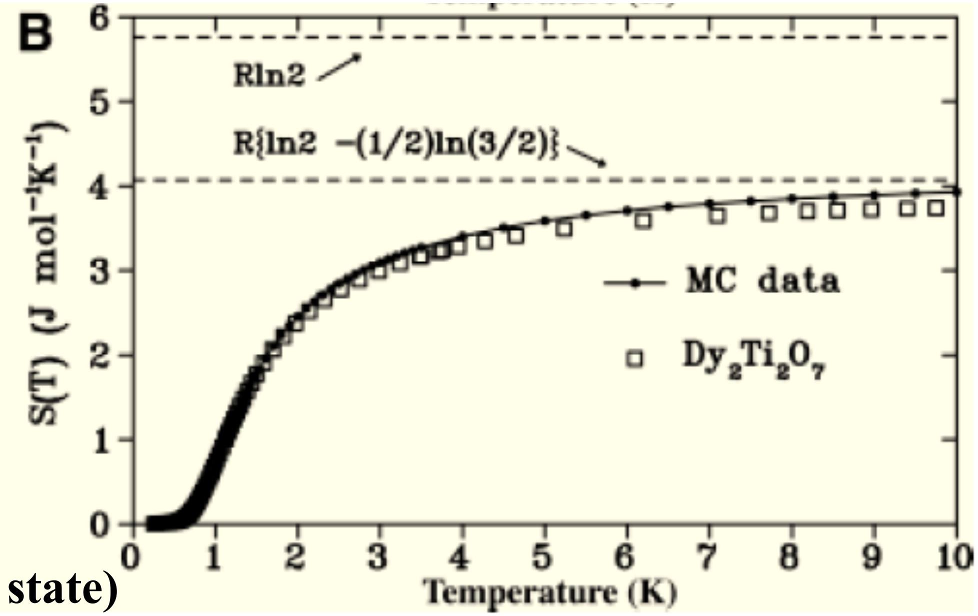
A-type

down spin (=in)

Ramirez *et al*., Nature **399**, 333 (1999)
Bramwell & Gingras, Science **294**, 1495 (2001).



Neutron scattering (Pinch point)



Ground state (= all tetrahedra are 2in-2out state)
Residual entropy = [Pauling entropy for water ice] = (1/2) ln(3/2).

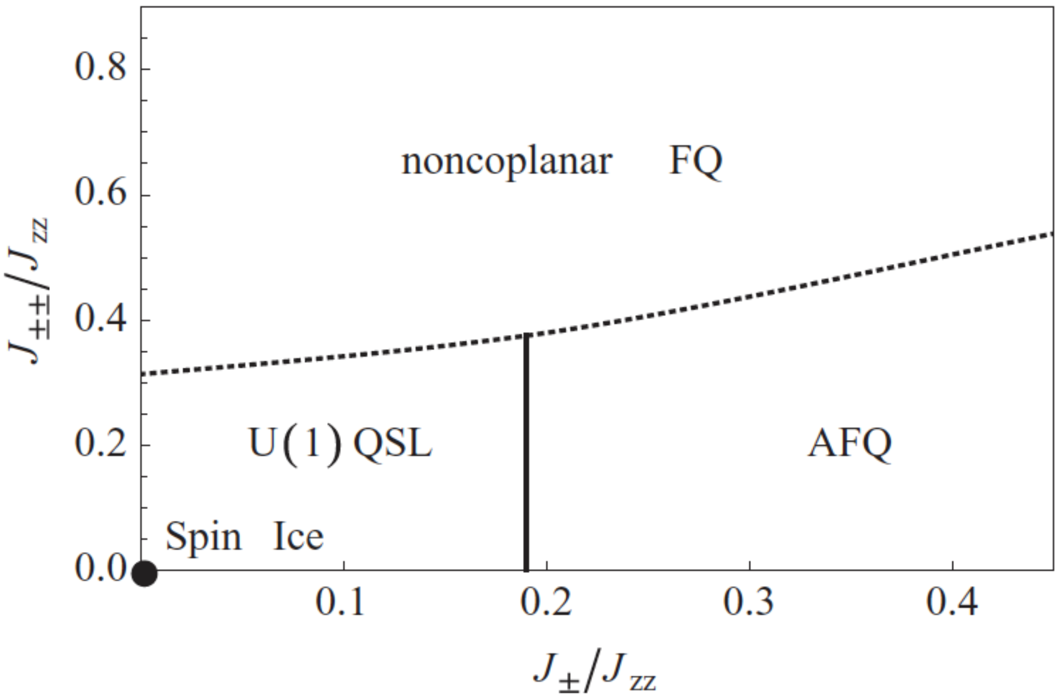
Introduction: Quantum effects ($Yb_2Ti_2O_7$, $Pr_2Zr_2O_7$)

$$\mathcal{H}_Q = \sum_{<r,r'>}\Big[J s_r^z s_{r'}^z - 2J_\pm\left(s_r^x s_{r'}^x + s_r^y s_{r'}^y\right)$$

Onoda & Tanaka, Phys. Rev. Lett. **105**, 047201 (2010).
Lee, Onoda & Balents, Phys. Rev. B **86**, 104412 (2012).

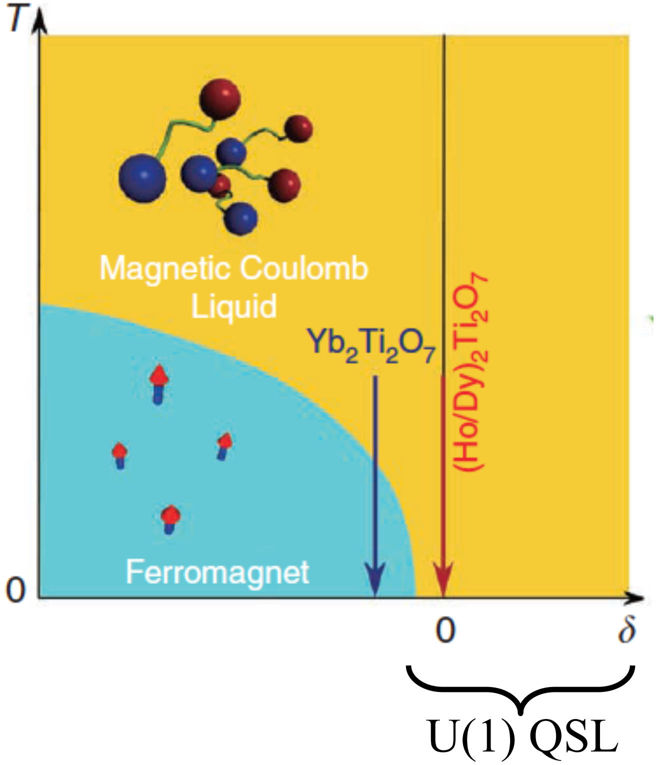
$$+\left(J_{\pm\pm}\gamma_{rr'} s_r^+ s_{r'}^+ + J_{z\pm} s_r^z\left(\zeta_{rr'} s_{r'}^+ + \zeta_{rr'}^* s_{r'}^-\right) + \mathrm{H.c.}\right)\Big].$$

Gauge mean-field theory phase diagram (*T*=0)



Higgs transition in $Yb_2Ti_2O_7$

Chang et al., Nat. Commun. **3**, 992 (2012).



U(1) quantum spin liquid is stabilized at small quantum fluctuation.

Model:

Hamiltonian: XXZ model on a pyrochlore lattice with PBC

$$\mathcal{H} = \sum_{<\boldsymbol{r},\boldsymbol{r}'>} \left[J s_{\boldsymbol{r}}^{z} s_{\boldsymbol{r}'}^{z} + J_{\perp} \left(s_{\boldsymbol{r}}^{x} s_{\boldsymbol{r}'}^{x} + s_{\boldsymbol{r}}^{y} s_{\boldsymbol{r}'}^{y} \right) \right].$$

$$s = \frac{1}{2},\ J_{\perp} < 0,\ \ J >> |J_{\perp}| > 0.$$

No negative sign problem!

Mapping to Maxwell’s action

Hermele, Fisher, & Balents, Phys. Rev. B **69**, 064404 (2004).

Quantum Monte-Carlo simulation

Banerjee, *et al*., Phys. Rev. Lett. **100**, 047208 (2008).

Detailed analysis of an effective model

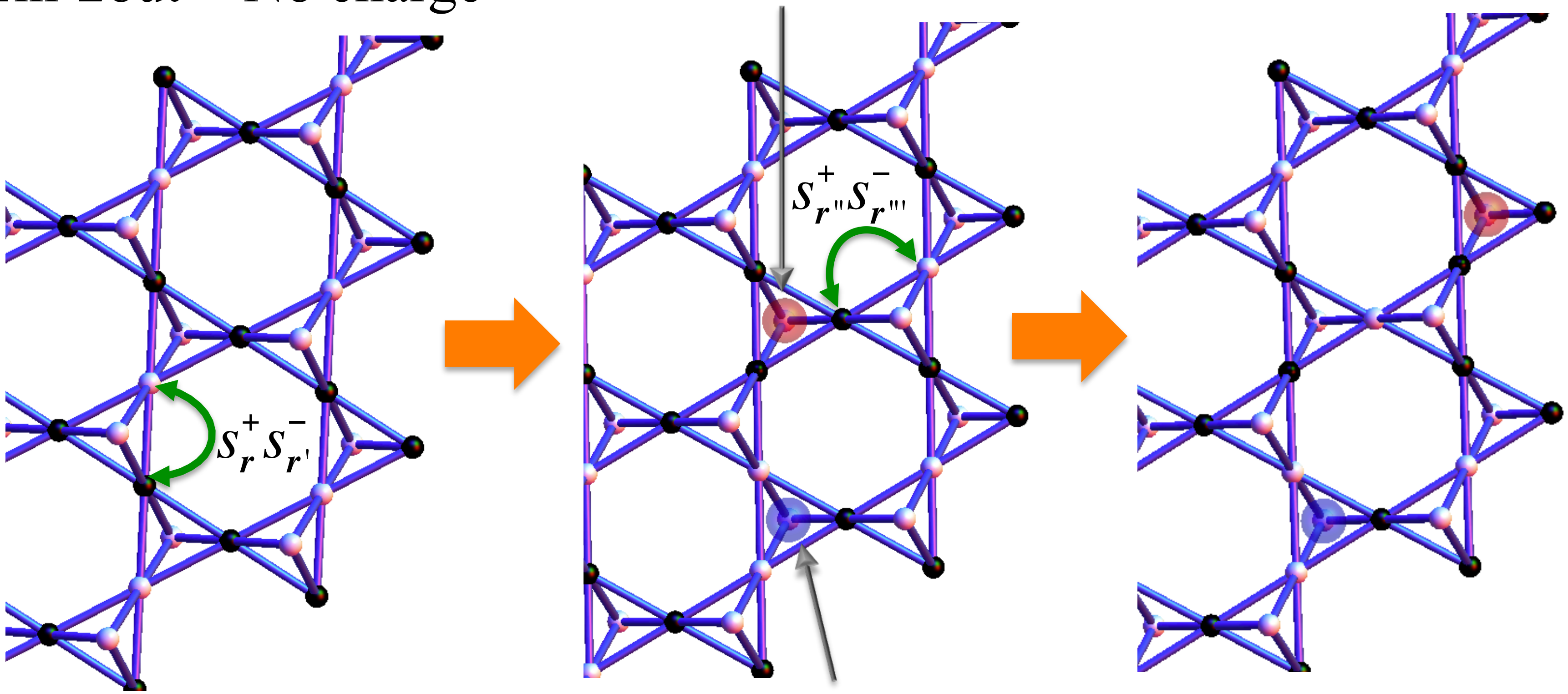
Shannon, *et al*., Phys. Rev. Lett. **108**, 067204 (2012).

Model: What is "Electric charge"?

Hermele, Fisher, & Balents, Phys. Rev. B (2004).

2in-2out = No charge

1in-3out = ⊕ charge



Vacuum

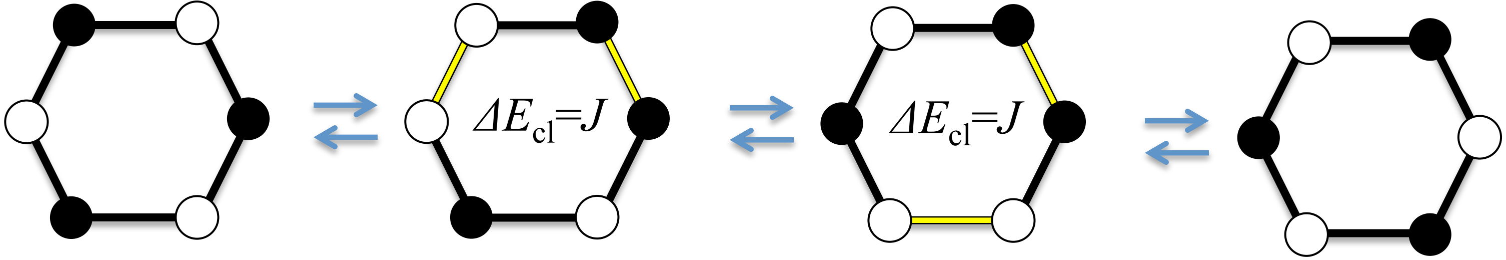
3in-1out = ⊖ charge

$$s^{z}_{r} \rightarrow E_{r}$$ electric field

$$s^{\pm}_{r} \rightarrow \exp\left[\pm iA_{r}\right]$$ vector potential

Model: Effective model at $J >> J_\perp$.

Third order perturbation process



Hermele, Fisher, & Balents, PRB (2004).

$$\mathcal{H}_{eff} = -g \sum_{\text{All Hexagon}} \left[s_1^+ s_2^- s_3^+ s_4^- s_5^+ s_6^- + \text{H.c.} \right], \quad g = \frac{3}{2}\left|\frac{J_\perp^3}{J^2}\right|.$$

$s_r^z \rightarrow E_r$ electric field

$s_r^\pm \rightarrow \exp\left[\pm i A_r\right]$ vector potential

Maxwell hamiltonian

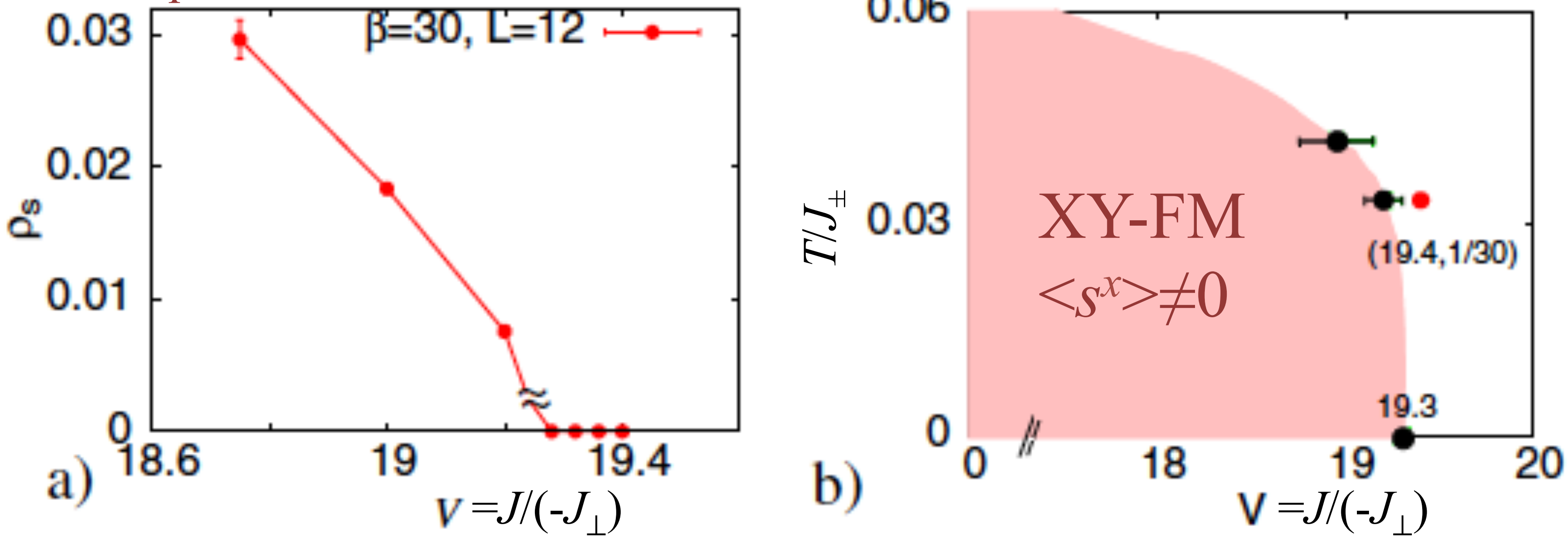
$$\mathcal{H}_{ML} = \frac{U}{2}\sum_r E_r^2 - K \sum_{\hexagon} \cos\left[\sum\nolimits_{r\subset\hexagon} A_r\right].$$

Force carrier = photon
(k-linear dispersion)

Detailed analysis of this effective model
Benton, Sikora, & Shannon, PRB (2012).

Model: Quantum Monte-Carlo simulation of quantum spin ice

A. Banerjee, et al., Phys. Rev. Lett. **100**, 047208 (2008).



Spin stiffness

XY-FM transition has been confirmed.
XY-FM is corresponding to the Higgs confined phase
(the condensates of “electric charges”) in mean-field level.

They confirmed that

s^z-s^z correlation functions fits the electrodynamics very well.

Method: World-line Monte-Carlo method

Review paper: Kawashima & Harada, J. Phys. Soc. Jpn. (2004).

World-line configurations drawn in *d*+1 dimension based on Feynmann path integral are sampled in this method.

Advantage:

- Exact results within the statistical error
- Large systems relative to exact diagonalization
- Finite temperature

Disability:

- Negative sign problem

Global updating method by two discontinuities:

Worm algorithm:

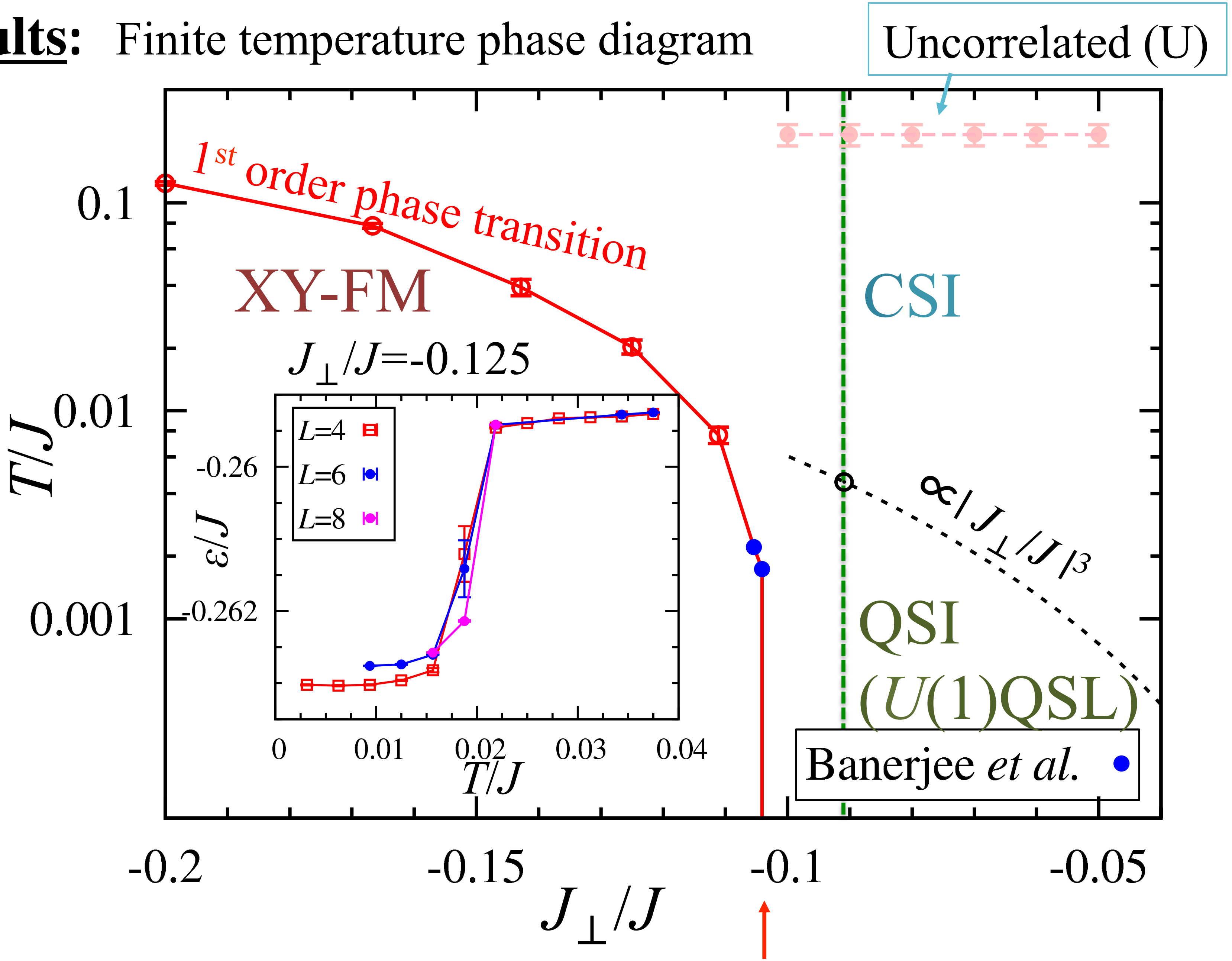
Prokof'ev, Svistunov, and Tupitsyn, Phys. Lett. A **238**, 253 (1998).

Directed-loop algorithm:

Syljuåsen and Sandvik, Phys. Rev. E **66**, 046701 (2002).

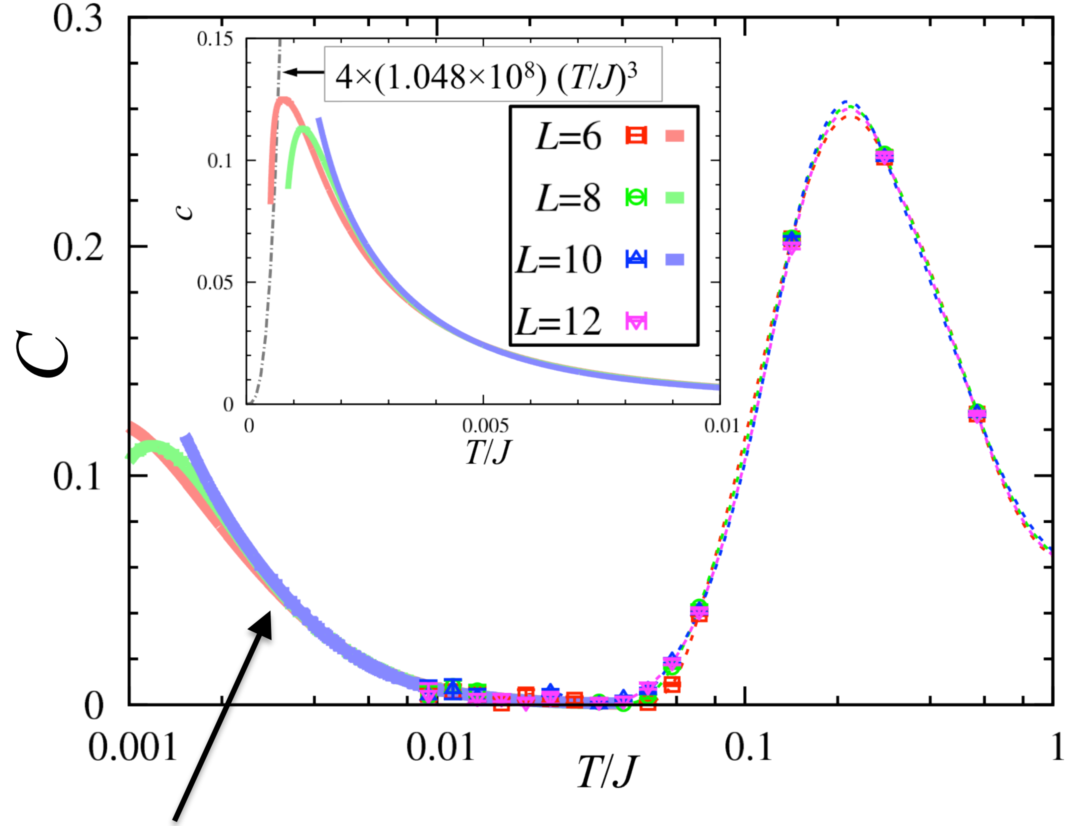
We used a modified directed-loop algorithm
Kato, Suzuki & Kawashima, Phys. Rev. E **75**, 066703 (2007)
with a thermal annealing method.

Results: Finite temperature phase diagram



$(J_\perp/J)_c \approx -0.103$ [Banerjee et al., PRL(2008)]

<u>Results</u>: Specific heat and entropy at $|J_\perp/J| < |(J_\perp/J)_c|$.



D. Pomaranski *et al.*,
Nat. Phys. **9**, 353 (2013).

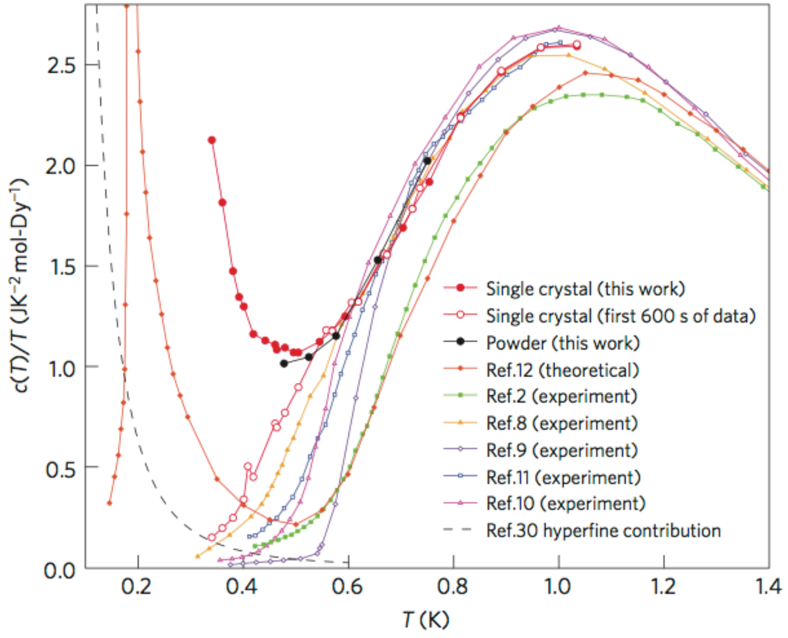


Figure 3 | Specific heat versus temperature of $Dy_2Ti_2O_7$ in zero field. Previous experimental results had no signature of an upturn below 0.6 K (refs 2,8–11). The Dy nuclear hyperfine contribution (dashed line) is insignificant at these temperatures[30].

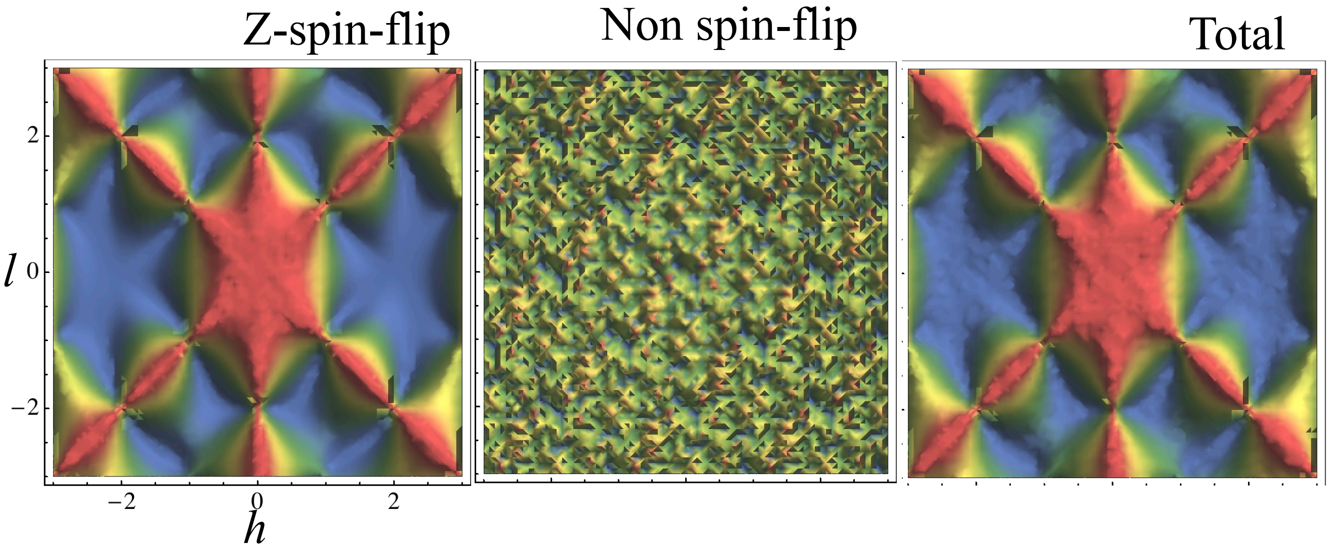
Numerical derivative of B-spline interpolation of energy

Possibility of the crossover to the U(1) spin liquid in $Dy_2Ti_2O_7$

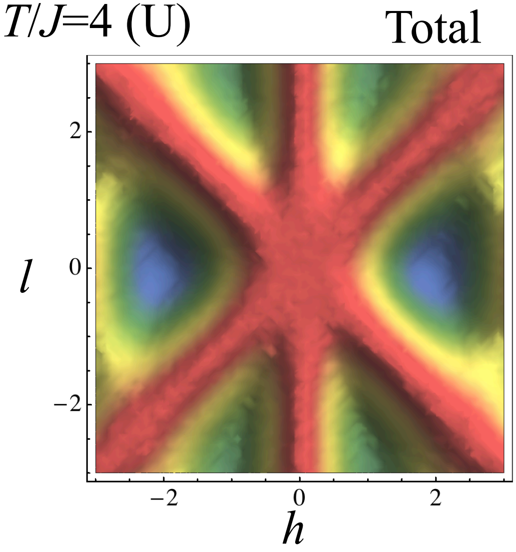
Results: Spin structure factors at $|J_\perp/J| < |(J_\perp/J)_c|$.

$$\boldsymbol{q} = \frac{4\pi}{a_0}(h,h,l)$$

T/J=0.1 (CSI)

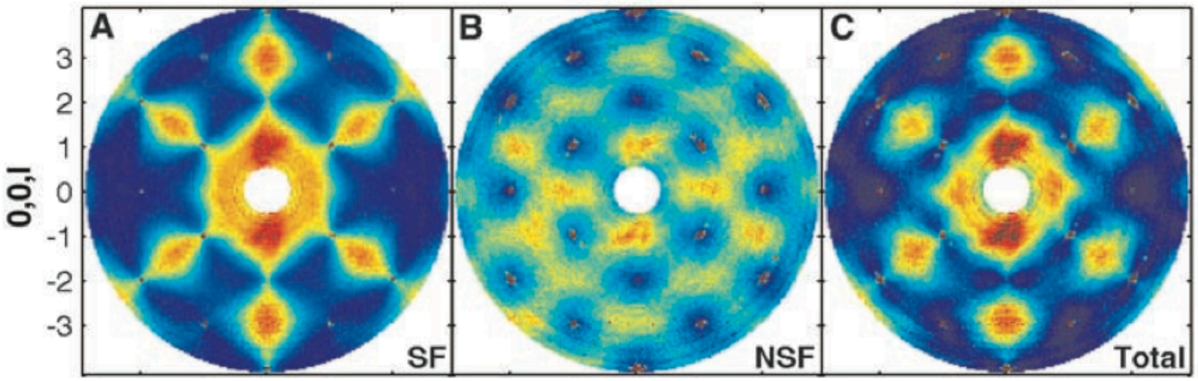


T/J=4 (U)



Pinch point!

Fennell et al., Science (2009) :$Ho_2Ti_2O_7$



Neutron scattering data (QSI)

$Pr_2Zr_2O_7$

Kimura *et al*., Nat. Commun. (2013).

$Yb_2Ti_2O_7$

Chang et al., Nat. Commun. (2012).

Ross et al., Phys. Rev. Lett. (2009).

Results: Wilson loop

$$W = \left\langle \exp\left[i \oint \vec{A} \bullet d\vec{x} \right] \right\rangle$$

Line integral of a closed path

In the pure gauge theory (No charge),
Confinement → (+) and (-) charges are confined.

$$\log W \sim \left[\text{Area of the closed loop} \right]$$

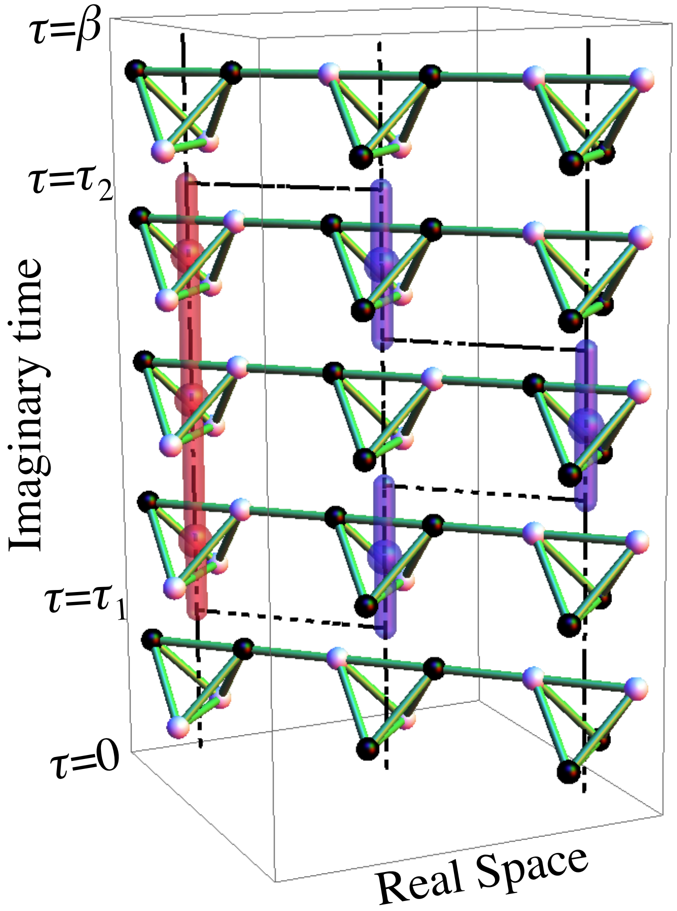
Deconfinement → (+) and (-) charges are deconfined.

$$\log W \sim \left[\text{Perimeter of the closed loop} \right]$$

QMC simulation:

Example in the QMC simulation

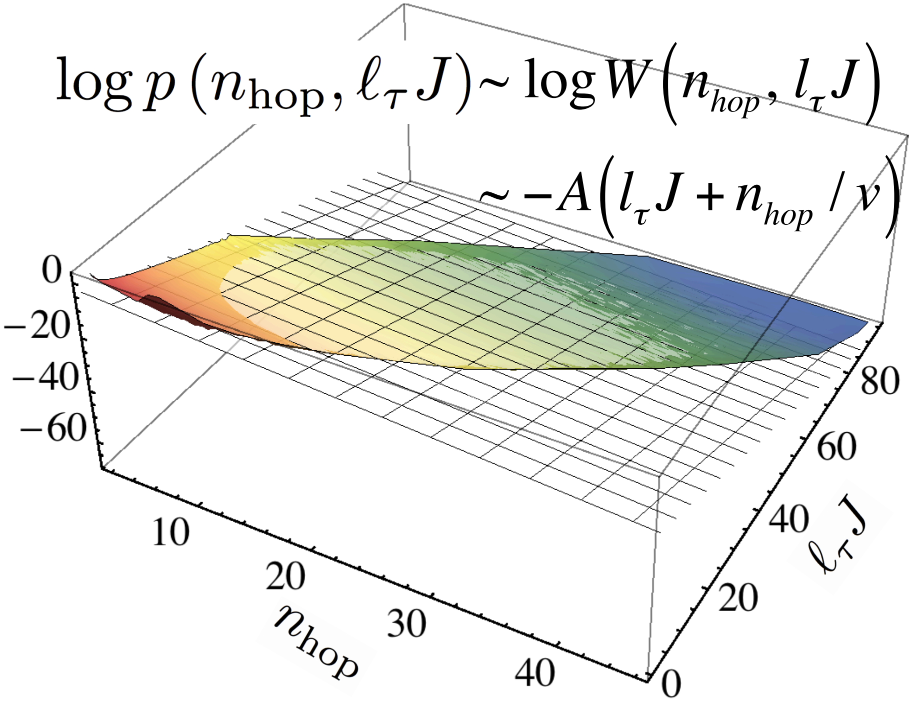
$l_\tau = 2\times(\tau_2 - \tau_1)$
$n_{\text{hop}}=4$



$$W = [\text{Probability of existence of corresponding loop of charges}]$$
$$\rightarrow \text{Distribution of loops}$$

Results: Wilson loop at $|J_\perp/J| < |(J_\perp/J)_c|$.

n_{hop}: Number of hopping, $l_\tau J$: temporal length

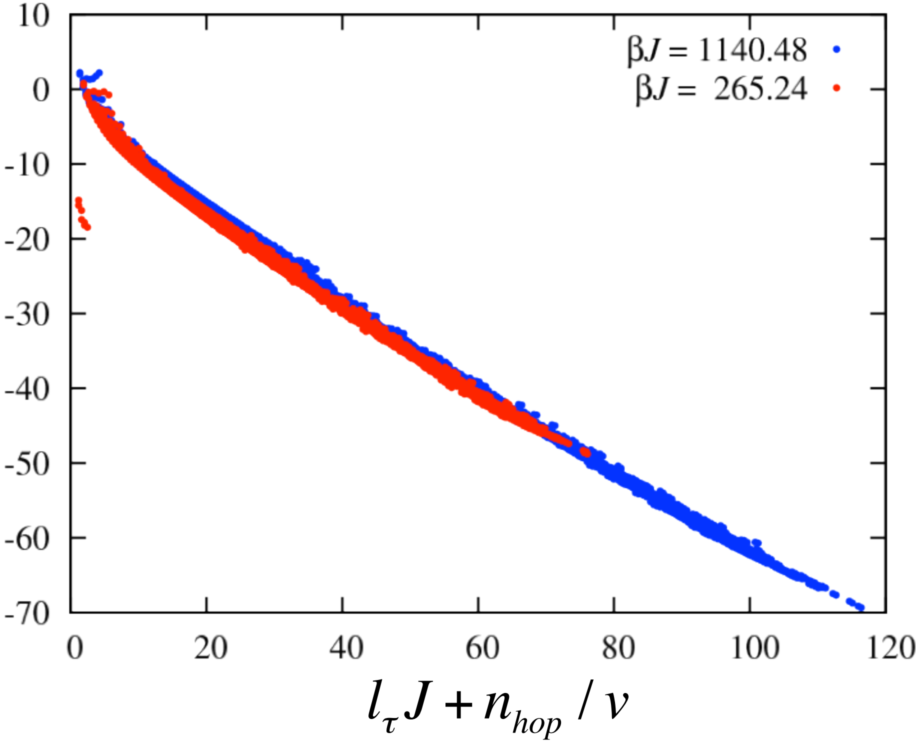


$$\log p\,(n_{\text{hop}}, \ell_\tau J) \sim \log W\left(n_{hop}, l_\tau J\right)$$

$$\sim -A\left(l_\tau J + n_{hop}/v\right)$$

Perimeter law

Exponential decay



Gapped → Deconfinement of electric charges

Summery

We confirmed

- The successive crossover at $|J_{\perp}/J| < |(J_{\perp}/J)_{\mathrm{c}}|$
- The pinch point in the spin structure factors
- The Wilson loop shows the perimeter law and it is consistent with the deconfinement of the “electric charges”.

Future work

‘t Hooft loop (Deconfinement of “magnetic charges”)

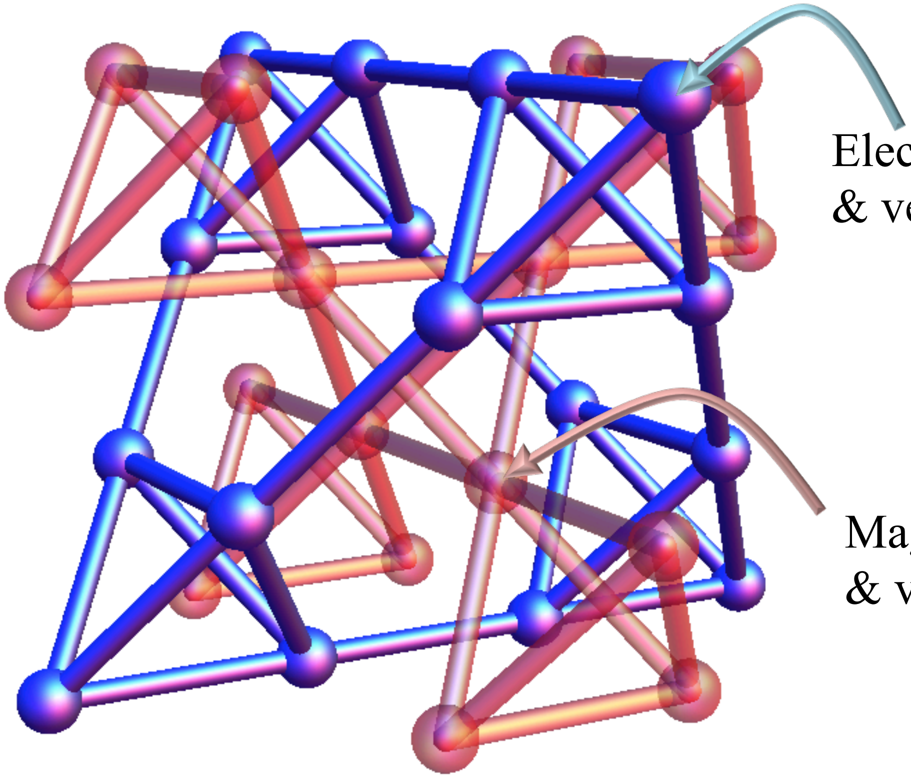
$$T = \left\langle \exp\left[i \oint \vec{\alpha} \bullet d\vec{x} \right] \right\rangle$$

Model: What is "Magnetic charge"?

Hermele, Fisher, & Balents, Phys. Rev. B **69**, 064404 (2004).

Blue: original lattice

Red: center of pyrochlore hexagon



Electric field

& vector potential for magnetic field

$$E_r^z \ \& \ A_r \qquad \vec{B} = \mathrm{curl}\vec{A}.$$

⇕ duality exists.

Magnetic field

& vector potential for electric field

$$B_x^z \ \& \ \alpha_x$$

We can define the vector potential for electric field as $\vec{E} = \mathrm{curl}\vec{\alpha}.$

➡ Magnetic charges can be located at the center of red tetrahedra while electric charges can be located at the center of blue tetrahedra.