Frustrated transverse field Ising models

Singular ferromagnetic suscetibiilty of the triangular lattice antiferromagnet

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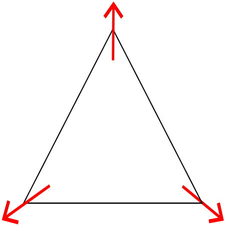
Geometric frustration and spin-orbit coupling

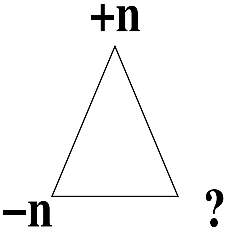
- Insulators with heavy magnetic ions $\rightarrow$ spin-orbit coupling effects matter
- Anisotropic terms in low-energy H for spins
- Anisotropies can amplify effects of geometric frustration

Classical picture

- Isotropic spins on a triangle



- Easy-axis anisotropy of moments: Simplest example: $-D(\mathbf{n} \cdot \vec{S})^2$

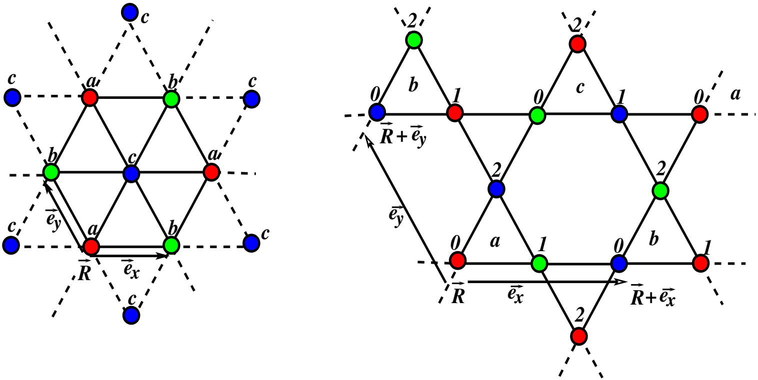


Easy-axis "amplifies" frustration of triangular motifs (?)

Quantum effects

- Simplest example: Perturbative (J/D expansion) effects of exchange J
  Interesting quantum dynamics if $\mathbf{n}$ non-uniform in space
  e.g. Quantum spin ice compounds (details different)
- Transverse field: tunable quantum fluctuations

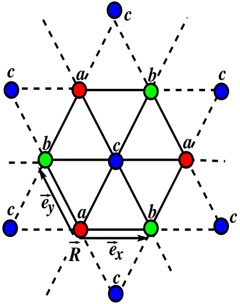
Example: Easy-axis antiferromagnets with triangular lattice symmetry



Natural tripartite structure of lattice

Macroscopic degeneracy (honeycomb dimer model) of classical ground states

Three-sublattice order relieves frustration



θ			
0	–S	+S	+S
$\frac{\pi}{6}$	–S	0	+S

Order parameter: $\psi = |\psi| e^{i\theta} = -\sum_{\vec{R}} e^{i\mathbf{Q}\cdot\vec{R}} S^z_{\vec{R}}$

Two states at same $\mathbf{Q}$

Ferrimagnetic: $\theta = 2\pi m/6$, Antiferromagnetic: $\theta = (2m+1)\pi/6$

$(m = 0, 1, 2 \ldots 5)$

Several realizations of this physics

- Transverse-field Ising antiferromagnet on the triangular lattice
  Quantum order-by-disorder effect
  (Isakov & Moessner 2003)
- $S = 1$ triangular antiferromagnet with moderately strong single-ion anisotropy $\rightarrow$ hard-core bosons with repulsion V ($\gg t$)
  (KD & Senthil 2006)
  Bosons form three-sublattice ordered “supersolid”
  (Melko *et al.*; Heidarian & KD; Wessel & Troyer 2005)
- Aside: “Artificial Kagome Ice” systems
  (Moller & Moessner 2009; Chern *et al.* 2012).

In this talk...

- Warm-up: Melting of three-sublattice order in easy-axis systems: Prediction: Singular uniform susceptibility along easy axis upon partial melting of three-sublattice order
- Numerical test for transverse field Ising model (TFIM): Failure of standard stochastic series expansion (SSE) algorithm
- Solution: plaquette percolation based quantum cluster algorithm
- Generalizations to other cases

Review: Landau theory for ψ

- Bravais lattice symmetries: Translations, rotations and reflection
  $\psi \to \psi^*$, $\psi \to e^{2\pi i/3}\psi$
- In zero easy-axis field, Z_2 spin symmetry of easy-axis spin-flip:
  $S_r^z \to -S_r^z$
  $\psi \to -\psi$
- Landau potential: $r|\psi|^2 + u|\psi|^4 + \lambda_6 \mathrm{Re}(\psi^6) + \ldots$

Symmetries of the six-state clock model universality class

Review: Coarse-grained effective model

- (Classical) effective model for finite-temperature melting transitions: $H_{\text{clock}} = -\sum_{\langle ij \rangle} V(\theta_i - \theta_j) - \lambda_6 \sum_j \cos(\theta_j)$
  $V(x) = K_1 \cos(x) + K_2 \cos(2x) + K_3 \cos(3x)$
  (classic reference: Cardy 1980)

Melting scenarios from Cardy's analysis

- $\rightarrow$ Three generic possibilities:
  Two-step melting, with power-law ordered intermediate phase for $T \in (T_1, T_2)$
  OR
  3-state Potts transition to ferromagnetic state
  OR
  First-order transition (always possible!)

depends on details of domain-wall energetics $\rightarrow$ different in each physical realization

Melting of three-sublattice order in various examples

- Antiferro three-sublattice order in triangular lattice transverse field Ising model
  Two-step melting (Isakov & Moessner 2003)
- Ferrimag. three-sublattice order in S=1 easy axis antiferromagnet on triangular lattice
  Two-step melting (Heidarian & KD 2018)
- Aside: Ferrimagn. three-sublattice order in Kagome Ising antiferromagnets
  With ferro. J' (second-neighbour) : Two step melting (Wolf & Schotte 1988)
  With long-range dipolar couplings: Three-state Potts transition (Moller & Moessner 2009; Chern *et. al.* 2012)

New physics: Uniform magnetization mode m

- Symmetries allow term $\lambda_3 m Re(\psi^3)$ in Landau theory
- For $T \in (T_1, T_2)$ (in power-law phase of two-step melting), λ_6 irrelevant $\rightarrow$ θ fluctuates uniformly over $(0, 2\pi)$
  Contrast: $\lambda_6 \cos(6\theta)$ locks θ to $2\pi m/6$ ($(2m+1)\pi/6$) in ferri (antiferro) ordered state ($T < T_1$)
- Distinction between ferri and antiferro three-sublattice order lost for $T \in (T_1, T_2)$
  $\rightarrow$
  Thermodynamic signature of order-parameter fluctuations in *uniform* easy-axis susceptibility
  (KD 2015)

RG analysis—I

- Fixed point free-energy density: $\frac{\mathcal{F}_{\mathrm{KT}}}{k_B T} = \frac{1}{4\pi g}(\nabla\theta)^2$
  with $g(T) \in (\frac{1}{9}, \frac{1}{4})$ corresponding to $T \in (T_{c1}, T_{c2})$
- $\lambda_6 \cos(6\theta)$ *irrelevant* along fixed line
- $\langle\psi^*(r)\psi(0)\rangle \sim \frac{1}{r^{\eta(T)}}$
  with $\eta(T) = g(T)$

(Jose *et. al.* 1977)

RG analysis—II

- λ_3 formally irrelevant along fixed line $\mathcal{F}_{\mathrm{KT}}$
  $\rightarrow$
  Correlators of ψ unaffected.
- But m "inherits" power-law correlations of $\cos(3\theta)$:
  $C_m(r) = \langle m(r)m(0)\rangle \sim \frac{1}{r^{9\eta(T)}}$
- Uniform $\chi_L(B_z = 0) \sim \int^L d^2 r C_m(r)$ in a finite-size system at $B = 0$
- Uniform $\chi_L(B_z = 0) \sim L^{2-9\eta(T)}$ for $\eta(T) \in (\frac{1}{9}, \frac{2}{9})$

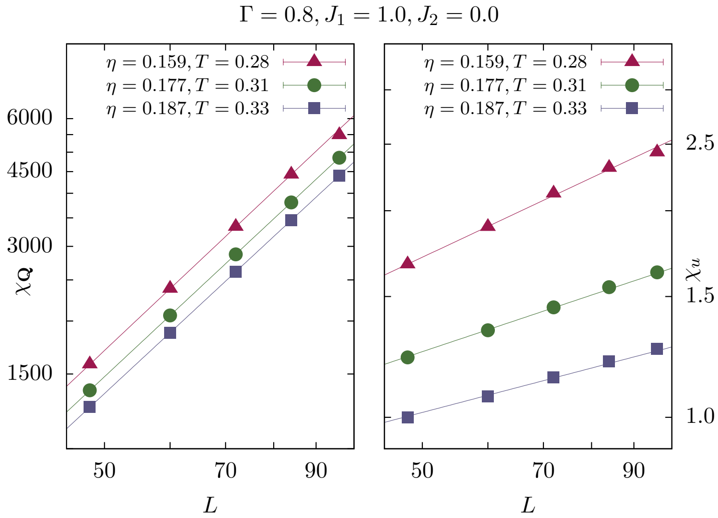
RG analysis—III

- Uniform easy-axis field $B_z > 0 \to$ additional term $h_3 \cos(3\theta)$ in $\mathcal{F}_{\mathrm{KT}}$
- Strongly relevant along fixed line, with RG eigenvalue $2 - 9g/2$
- Implies finite correlation length $\xi(B_z) \sim |B_z|^{-\frac{2}{4-9\eta}}$
- $\chi_{\mathrm{easy-axis}}(B_z) \sim |B_z|^{-\frac{4-18\eta}{4-9\eta}}$ for $\eta(T) \in (\frac{1}{9}, \frac{2}{9})$
  Thermodynamic signature of power-law three-sublatttice order (KD 2015)
  Order parameter fluctuations at nonzero $\mathbf{Q}$ picked up in the uniform susceptibility!

Implication: “Ferromagnetism” of transverse field Ising antiferromagnet

- Perhaps most dramatic manifestation:
  Heat up antiferromagnetically ordered triangular lattice transverse field Ising antiferromagnet to enter phase with divergent *ferromagnetic* susceptibility
- Real effect? Verification?
- first step: Numerical verification—-yes
- second step: Experimental realization—none known (?)

QMC evidence for effect:



Left panel fit: $L^{2-\eta(T)}$. Right panel fit: $L^{2-9\eta(T)}$

(Biswas & KD 2018)

SSE review—I

- $$H_{\text{TFIM}} = -\sum_l H_{\mathbf{e},l} - \sum_i H_{\mathbf{1},i} - \sum_i H_{\sigma^x,i}$$
$$H_{\mathbf{e},l} = |J_1| - J_1 \sigma^z_{1(l)} \sigma^z_{2(l))} \tag{1}$$
$$H_{\mathbf{1},i} = \Gamma \mathbf{1}_i$$
$$H_{\sigma^x,i} = \Gamma \sigma^x_i$$

- non-branching property of decomposition (in $|\alpha\rangle = \prod |\sigma^z\rangle$ basis)
- Simplifies high-temp expansion:

$$Z = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{S_n, |\alpha_1\rangle} \prod_{k=1}^{n} \langle \alpha_{k+1} | H_{a(k),i(k)} | \alpha_k \rangle \ . \tag{2}$$

(Sandvik)

SSE review—II

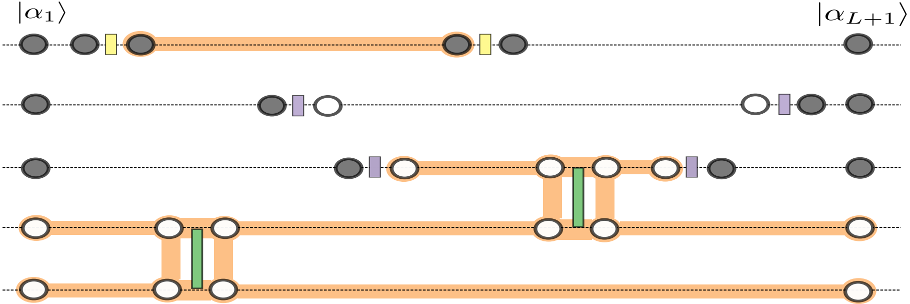
- fixed string length version:

$$Z = \frac{1}{\mathcal{L}!} \sum_{S_{\mathcal{L}}} \beta^n (\mathcal{L} - n)! \prod_{k=1}^{\mathcal{L}} \langle \alpha_{k+1} | H_{a(k),i(k)} | \alpha_k \rangle \tag{3}$$

introduce dummy identity operators $H_{0,0}$ ($\mathcal{L}$ fixed $\gg E\beta$)

SSE review—III

graphically (for ferromagnet):



SSE review—IV

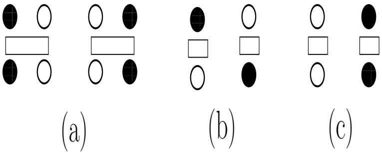
- Update I: Replace dummy $H_{0,0}$ with diagonal operator

$$P(H_{0,0} \to \text{diag. operator}) = \text{Min}\left(1, \frac{\beta(N\Gamma + 2|J|N_{links})}{\mathcal{L} - n}\right),$$
$$P(\text{diag. operator} \to H_{0,0}) = \text{Min}\left(1, \frac{\mathcal{L} - n + 1}{\beta(N\Gamma + 2N_{\text{links}}|J|)}\right), \tag{4}$$

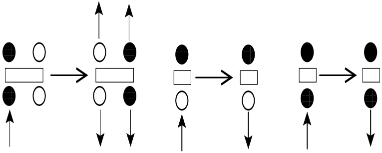
If identity operator $H_{0,0}$ to be replaced:
each $H_{\mathbf{1},i}$ operator is chosen with prob. $\Gamma/(N\Gamma + 2|J|N_{links})$
each $H_{\mathbf{e},l}$ is chosen with prob. $2|J|/(N\Gamma + 2|J|N_{links})$

SSE review—V

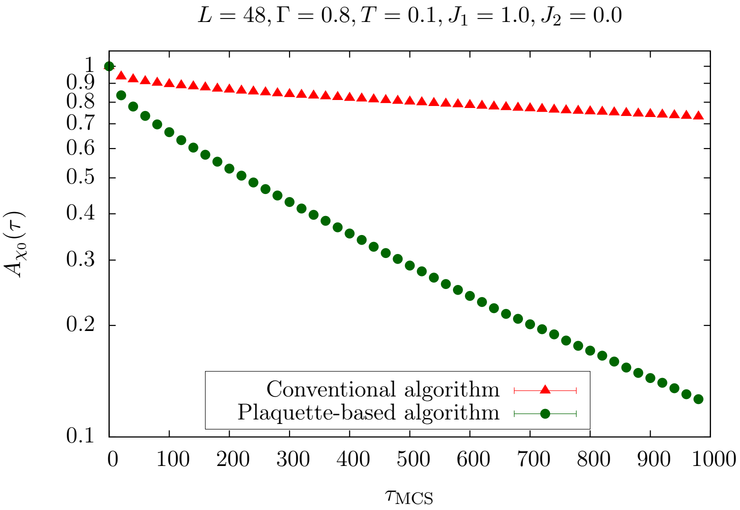
Vertices for antiferromagnet:



Link-percolation to build cluster:



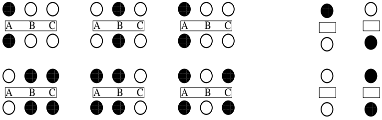
Problem



$L = 48, \Gamma = 0.8, T = 0.1, J_1 = 1.0, J_2 = 0.0$
Conventional algorithm
Plaquette-based algorithm
$A_{\chi 0}(\tau)$
τ_{MCS}
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
100
200
300
400
500
600
700
800
900
1000

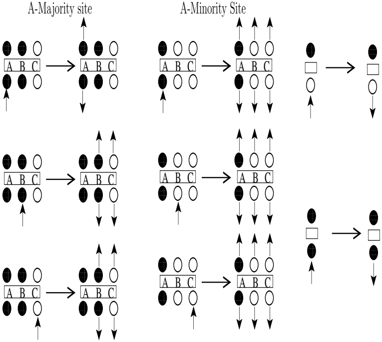
New algorithm—I

Vertices:



(a) (b)

plaquette-percolation to build cluster:

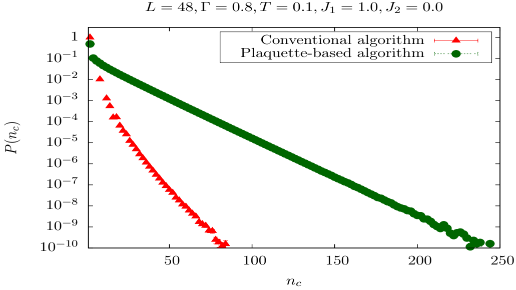


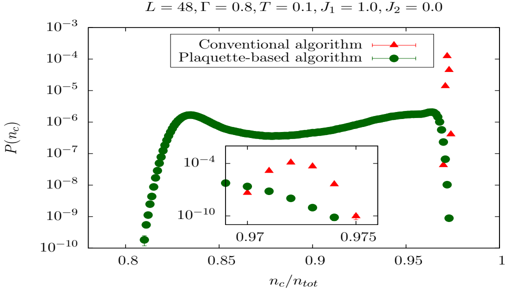
'A' Update

Two key inputs:

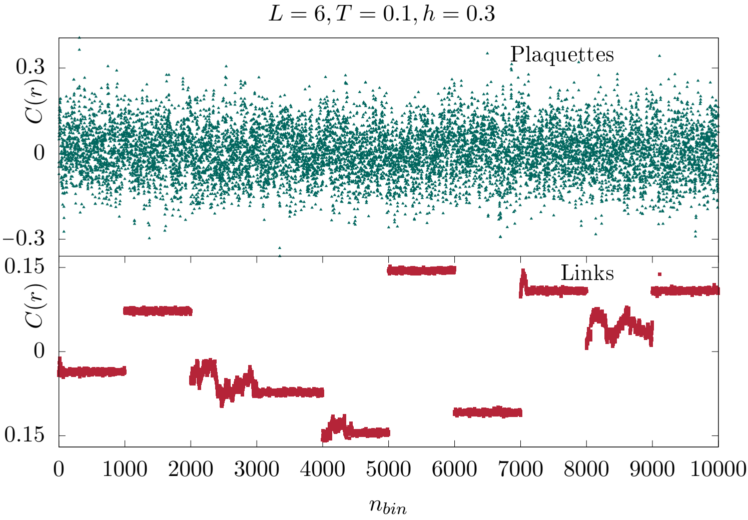
- Plaquette decomposition of Ising exchange energy into terms living on triangular plaquettes
- Premarking of motif (in example: A site of each triangle) that guides plaquette percolation process for building cluster
  Crucial details: Choice of motif & premarking strategy

Origin of performance advantage





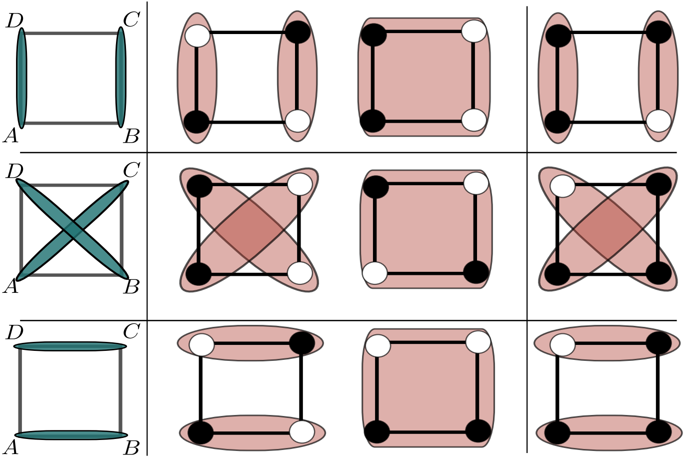
Pyrochlore antiferromagnet: σ^z correlator bin trace



Ideas generalize—I

$$
\begin{aligned}
H_{\text{TFIM}} &= -\sum_i H_{\square,p} - \sum_i H_{\mathbf{1},i} - \sum_i H_{\sigma^x,i} \\
H_{\square,p} &= 16J - J(\sigma^z_A + \sigma^z_B + \sigma^z_C + \sigma^z_D)^2_p
\end{aligned} \tag{5}
$$

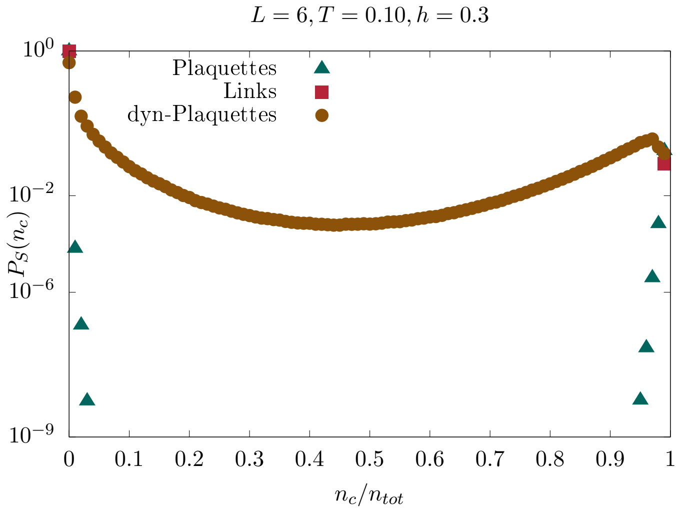
Ideas generalize—II



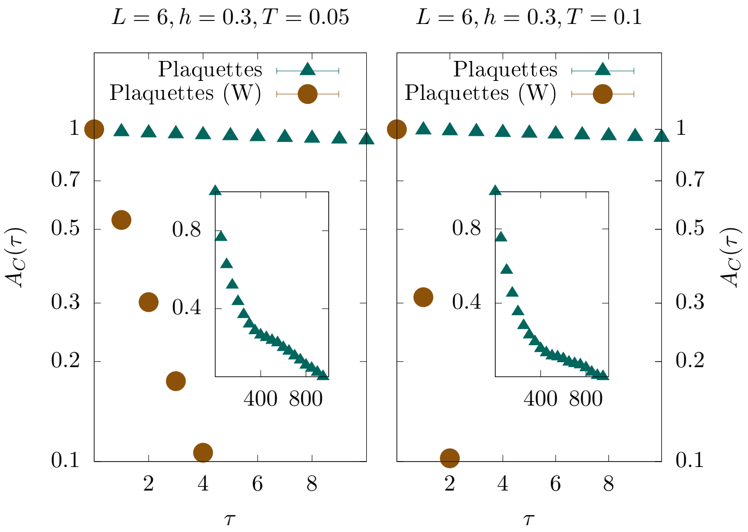
Motifs decomposition rules

Wrinkle: Two different premarking strategies + additional canonical update

Performance—I



Performance—II



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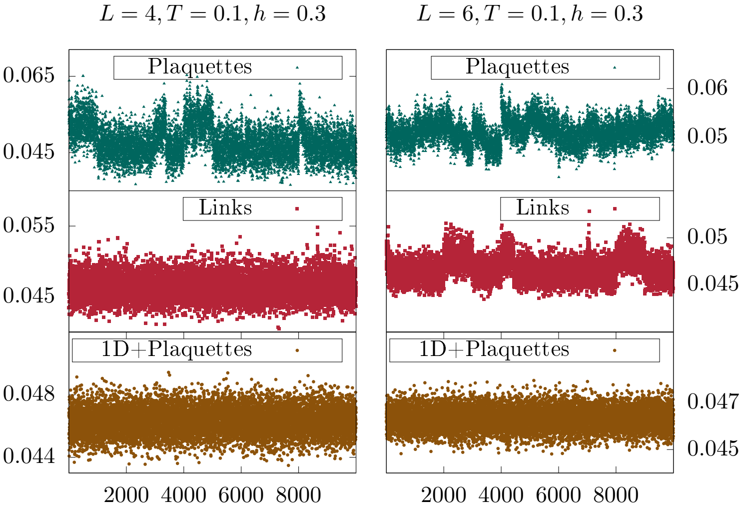
Problem: σ^x estimator bin trace



Performance—σ^x estimator