Melting of three-sublattice order in easy-axis antiferromagnets

Singular thermodynamics, multicriticality, and algorithms

Kedar Damle, LDQM Lausanne 2016
Tata Institute, Bombay

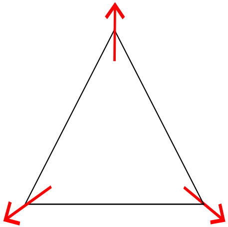
Sounak Biswas Geet Rakala Deepak Dhar

Geometric frustration and spin-orbit coupling

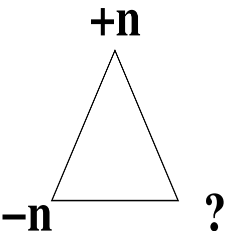
- Insulators with heavy magnetic ions $\rightarrow$ spin-orbit coupling effects matter
- Anisotropic terms in low-energy H for spins
- Anisotropies can amplify effects of geometric frustration

Classical picture

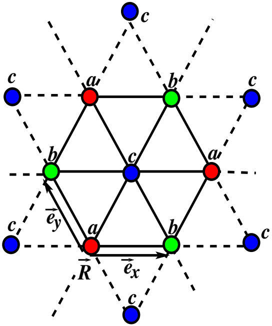
- Isotropic spins on a triangle

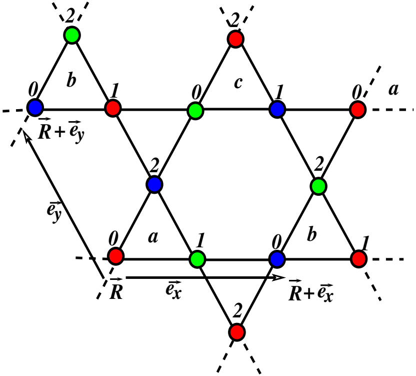


- Easy-axis $\mathbf{n}$ and triangular motifs...



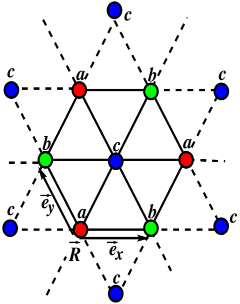
Focus: Easy-axis antiferromagnets with triangular lattice symmetry





Natural tripartite structure of lattice

Three-sublattice order minimizes frustration



θ	●	●	●
0	−S	+S	+S
$\frac{\pi}{6}$	−S	0	+S

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

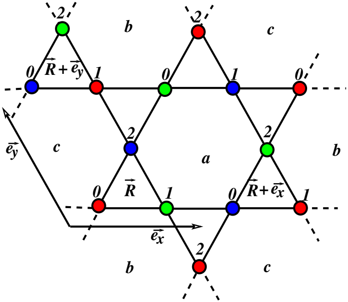
Two states at same $\mathbf{Q}$

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

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

Three-sublattice order on the Kagome lattice

θ	🔴	🟢	🔵
0	−S	+S	+S
$\frac{\pi}{6}$	−S	0	+S



Order parameter: $\psi = |\psi| e^{i\theta} = -\sum_{\vec{R}} \sum_{\alpha=0,1,2} e^{i\mathbf{Q}\cdot\vec{R} - 2\pi i \frac{\alpha}{3}} S^z_{\vec{R},\alpha}$

Again: 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 PRB **68** 104409)
- $S = 1$ triangular antiferromagnet with moderately strong single-ion anisotropy $\rightarrow$ hard-core bosons with repulsion V ($\gg t$)
  (KD & Senthil PRL **97** 067202)
  Bosons form three-sublattice ordered "supersolid"
  (Melko *et. al.* PRL **95** 127207; Heidarian & KD PRL **95** 127206; Wessel & Troyer PRL **95** 127205)
- "Artificial Kagome Ice" systems
  (Moller & Moessner PRB **80** 140409(R); Chern *et. al.* PRL **106** 207202).
- Classical Ising models of adsorbed noble-gases on graphite substrates
  (DP Landau PRB **27** 5604).

In this talk...

- Review of well-known melting scenarios: Two-step melting (intermediate phase with power-law three-sublattice order) *or* 2d Three-state Potts criticality
- Results:
  Physics:
  - Thermodynamic signature of two-step melting: $\chi^{zz}_{\text{uniform}}(B) \sim 1/|B|^{p(T)}$ with $p(T) \in (\frac{2}{3}, 0)$ for $T \in (T_{c1}, T_{c2})$.
  - Intervening multicritical point $\mathcal{M}$ with $c_{\mathcal{M}} \in (1, 3/2)$ (subleading) further-neighbour couplings could drive melting to multicritical point $\mathcal{M}$ (?)

  Algorithms:
  - Efficient quantum cluster algorithm for frustrated transverse field Ising models.
  - Efficient dual-worm construction(s) of clusters for frustrated classical models.
  - *Analytical* theory for continuously varying persistence exponent of worms.

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:
  $S^z_r \to -S^z_r$
  $\psi \to -\psi$
- Landau potential: $r|\psi|^2 + u|\psi|^4 + \lambda_6 \mathrm{R}e(\psi^6) + \ldots$

Symmetries of the six-state clock model universality class

Review: Coarse-grained effective model

- (Classical) effective model for finite-temperature melting transitions: $H_{\text{clock}} = -\sum_{\langle ij \rangle} V(\theta_i - \theta_j) - \lambda_6 \sum_j \cos(\theta_j)$
  $V(x) = K_1 \cos(x) + K_2 \cos(2x) + K_3 \cos(3x)$
  (Cardy J. Phys. A **13** 1507)

Review: Melting scenarios

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

Multiplicity of possibilities related to details of domain-wall energetics
$\rightarrow$ each realization needs separate analysis

Review: A closer look at various systems

$H_{\text{easy-axis}} = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j - D\sum_i (S_i^z)^2 + J' \ldots$ with $S > 1/2$ and $D > J$

- When $D \gg J$: Ising antiferromagnet at low energies
  $H_{\text{Ising}} = JS^2 \sum_{\langle ij\rangle} \sigma_i^z \sigma_j^z + J' \cdots + \text{negligible}$
  Small ferromagnetic J' induces three-sublattice order (DP Landau)
  Transverse field $-\vec{B}_\perp \cdot \sum_j \vec{S}_j^\perp \to -\Gamma \sum_j \sigma_j$ with $\Gamma \sim SB_\perp \times (B_\perp/D)^{2S}$
  Small transverse field induces three-sublattice order on triangular lattice (Isakov & Moessner)
- When D dominates over J, but J/D non-negligible: Low energy theory depends on S
  $S = 1$: hard-core bosons with repulsive $V \gg t$ (KD & Senthil)
  $H_b = -\frac{J^2}{D} \sum_{\langle ij\rangle} (b_i^\dagger b_j + h.c.) + J\sum_{\langle ij\rangle} (n_i - \frac{1}{2})(n_j - \frac{1}{2}) + \ldots$
  Three-sublattice ordered on triangular lattice (Wessel & Troyer; Melko *et. al.*; Heidarian & KD)
  $S > 1$: Classical Ising antiferromagnet with additional multi-spin interaction (Sen *et. al.* PRL **102**, 227001)
  Not three-sublattice ordered (lattice nematic state)

Melting of three-sublattice order in various examples

- Antiferro three-sublattice order in triangular lattice transverse field Ising model
  Two-step melting (Isakov & Moessner)
- Ferrimagn. three-sublattice order in triangular lattice Ising models with ferro. J'
  Two-step melting (D.P. Landau)
- Ferrimagn. three-sublattice order in Kagome Ising antiferromagnets
  With ferro. J' (second-neighbour) : Two step melting (Wolf & Schotte J. Phys. A **21** 2195)
  With long-range dipolar couplings: Three-state Potts transition (Moller & Moessner; Chern *et. al.*)

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

RG analysis—I

- Fixed point free-energy density: $\frac{\mathcal{F}_{\rm KT}}{k_B T} = \frac{1}{4\pi g}(\nabla\theta)^2$
  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.* Phys. Rev. B **16** 1217)

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 $\eta(T) \in (\frac{1}{9}, \frac{2}{9})$

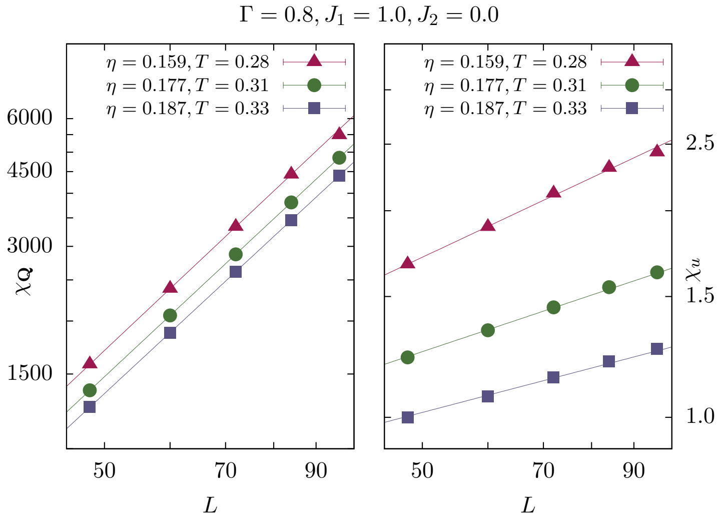
RG analysis—III

- 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 PRL **115** 127204)
  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

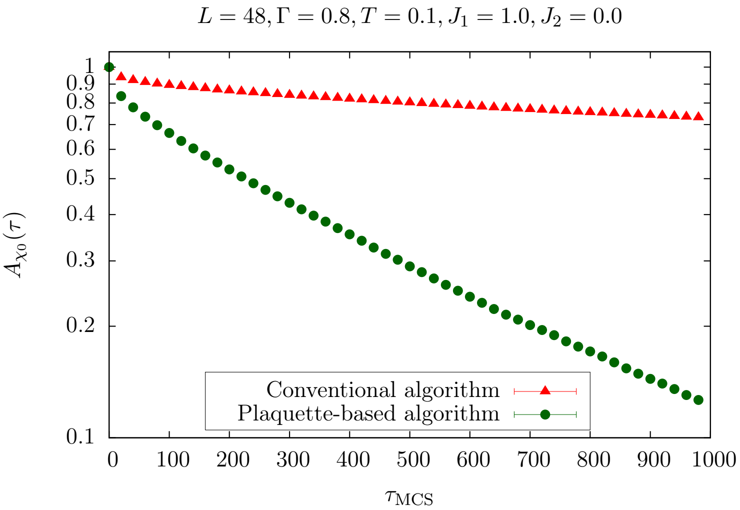
QMC evidence:



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

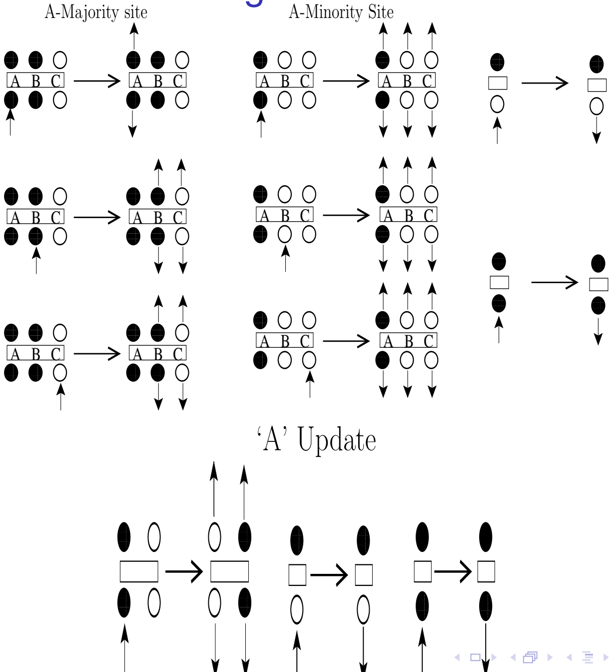
(Biswas & KD arXiv:1603.06473)

Needed new quantum cluster algorithm to probe effect

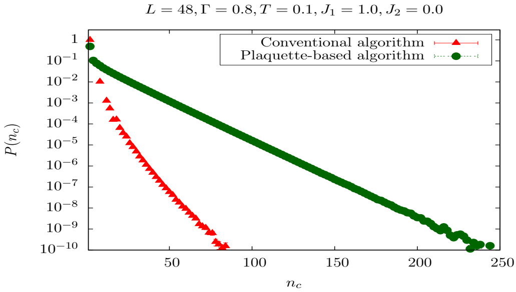


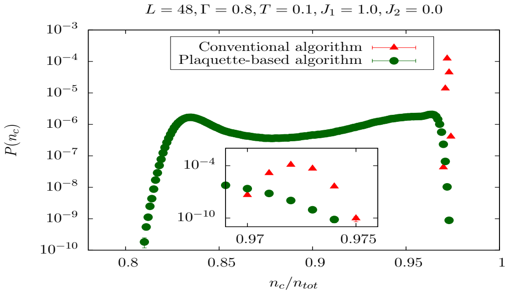
(Biswas Rakala & KD Phys. Rev. B **93** 235103)

New quantum cluster algorithm: Basic idea



Performance advantage





Relevance for $S = 1$ on triangular lattice with moderately strong $D > J$?

Maps to hard-core bosons with n.n. repulsion $\rightarrow$ ferimagnetic three-sublattice order

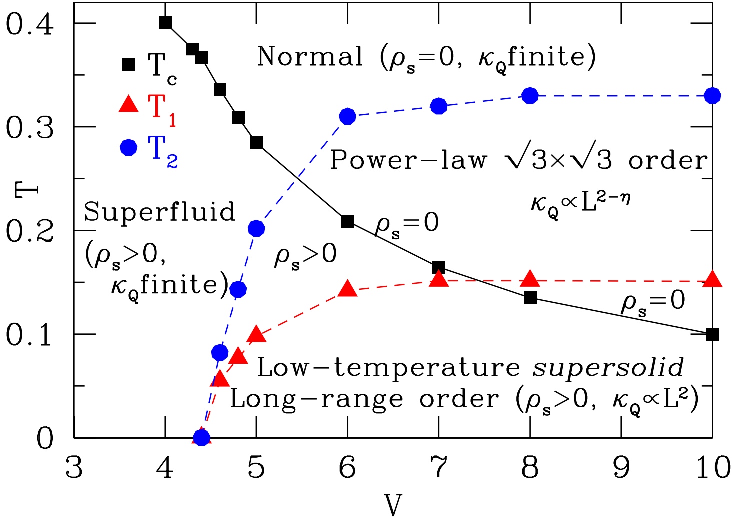
But: Conflicting predictions about nature of melting transition

- Three-state Potts (Boninsegni &Prokof'ev PRL **95** 237204)
- Two-step melting (Heidarian & KD)

Educated guesswork

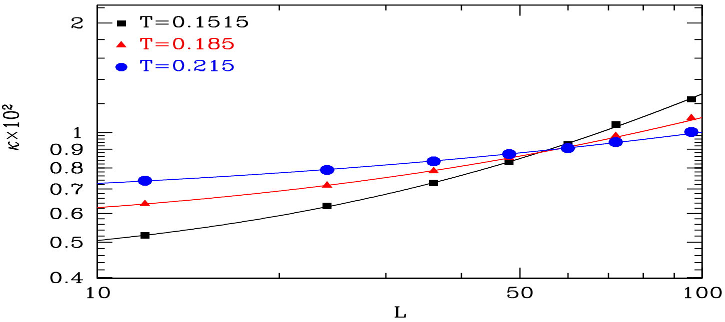
Hard to get right without high-precision QMC mapping of phase diagram

Recent QMC verdict: Two-step melting



$V = 4D/J$ and T measured in units of J^2/D (Heidarian & KD arXiv:1512.01346)

Singular ferromagnetic susceptibility in power-law phase



$\chi_{\text{easy}-\text{axis}} = 4\kappa$ (Heidarian & KD arXiv:1512.01346)

Effective model incorporating new physics

$$
\begin{aligned}
H_{\text{eff}} &= H_{\text{xy}} + H_{\text{Ising}} - J_{\theta\tau} \sum_{\vec{r}} \tau_{\vec{r}} \cos(3\theta_{\vec{r}}) \ , \\
\text{where} \quad H_{\text{Ising}} &= -J_{\text{Ising}} \sum_{\langle \vec{r}\vec{r}' \rangle} \tau_{\vec{r}} \tau_{\vec{r}'} - h \sum_{\vec{r}} \tau_{\vec{r}} \ , \\
H_{\text{xy}} &= -J_{\text{xy}} \sum_{\langle \vec{r}\vec{r}' \rangle} \cos(\theta_{\vec{r}} - \theta_{\vec{r}'}) - h_6 \sum_{\vec{r}} \cos(6\theta_{\vec{r}}) \ ,
\end{aligned}
$$

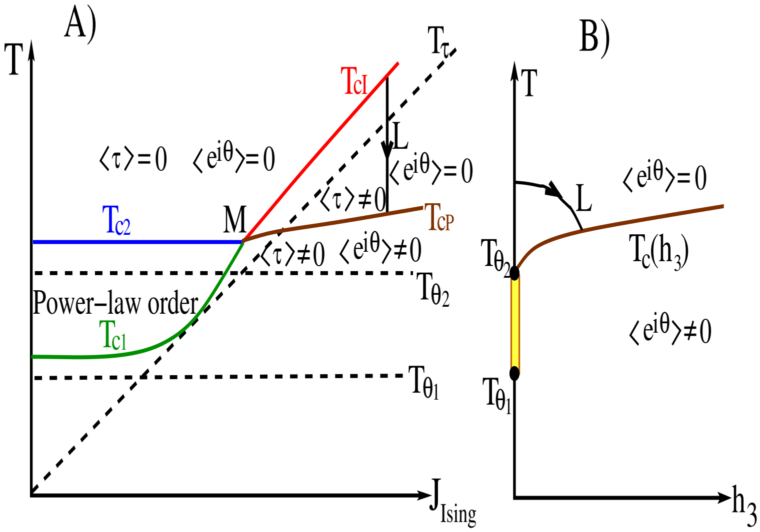
with $h \propto B$.

(KD PRL **115** 127204)

Effect of further neighbour couplings on effective coupling strengths

- J_τ expected to increase if further-neighbour ferromagnetic couplings present.

Phase diagram of effective model



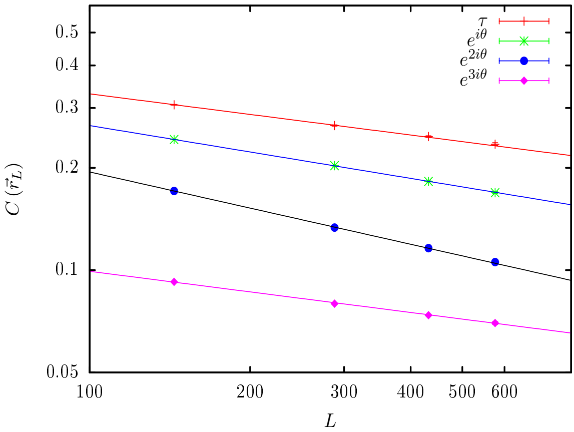
The argument...

- Start with known phase diagrams of $H_{\rm xy}$ and $H_{\rm Ising}$ and build in effects of $J_{\theta\tau}$
- When τ orders, $H_{\rm xy}$ sees effective three-fold symmetric perturbation $h_{\rm 3eff}\cos(3\theta_{\vec{r}})$ with $h_{\rm 3eff} \sim \langle\tau\rangle$
- When $e^{i\theta}$ orders, $H_{\rm Ising}$ sees effective field $h_{\rm eff}\tau_{\vec{r}}$ with $h_{\rm eff} \sim \langle\cos(3\theta)\rangle$

The multicritical point

- c-theorem argument: $1 \leq c \leq \frac{3}{2}$
- To search:
  $J_{\mathrm{xy}} = h_6 = 1.0$, $J_{\theta\tau} = 0.25$
  Parametrize: $J_{\mathrm{Ising}} = f_{xy} T_{\theta_1} / T_\tau$ and $T = f_I f_{xy} T_{\theta 1}$ [with $T_{\theta 1} = 1.04$ and $T_\tau = 3.6409$]

Multicritical melting



$[f_{\rm xy}^{\mathcal{M}}, f_I^{\mathcal{M}}] \approx [1.5570(8), 1.0061(5)]$

$C_{2\theta}$ [$C_{3\theta}$] rescaled by a factor of 7 [factor of 10]

$\eta_{3\theta} = \eta_\tau = 0.201(20)$, $\eta_\theta = 0.258(5)$, and $\eta_{2\theta} = 0.353(6)$.

(KD PRL **115** 127204)

Scenario for realizing $\mathcal{M}$?

- Start with system undergoing three-state Potts transition
- Turn on transverse field to combat further-neighbour ferromagnetic couplings
- Drive system back to two-step melting via $\mathcal{M}$???

Not entirely fanciful?

- Artificial Kagome Ice
- Classical triangular lattice Ising models with further neighbour ferromagnetic couplings
  Caveat: Extreme $D \gg J$ limit associated with strongly one-dimensional geometries.
  New systems with more two-dimensional character?

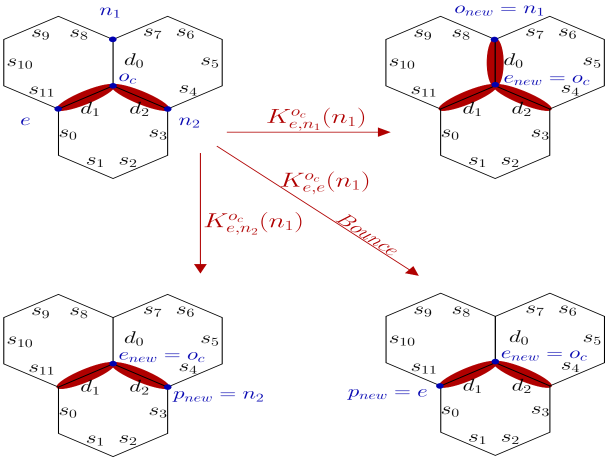
Acknowledgements

- Sounak Biswas and Geet Rakala (Quantum cluster algorithm)
- Geet Rakala (Dual worm algorithms for frustrated Ising models)
- Deepak Dhar (Statistical mechanics of worms)

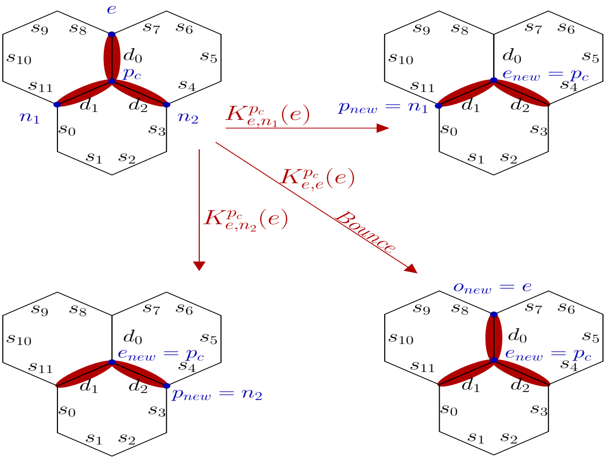
Dual worm algorithm for frustrated Ising models

- Represent system in terms of dual bond variables $\rightarrow$ generalized dimer interacting model
- Design efficient worm update for dimer variables
- Precursor: For $T \rightarrow 0$, used previously in multiple contexts. $S > 3/2$ Kagome and triangular lattice easy-axis antiferromagnets in $T = 0$ limit (Sen *et. al.* PRL **102**, 227001) (More recently: $T = 0$ limit of frustrated triangular lattice Ising models (Smerald, Korshunov, Mila PRL **116** 197201)) (For $T > 0$ unfrustrated systems: original work of Alet *et. al.* (2003))

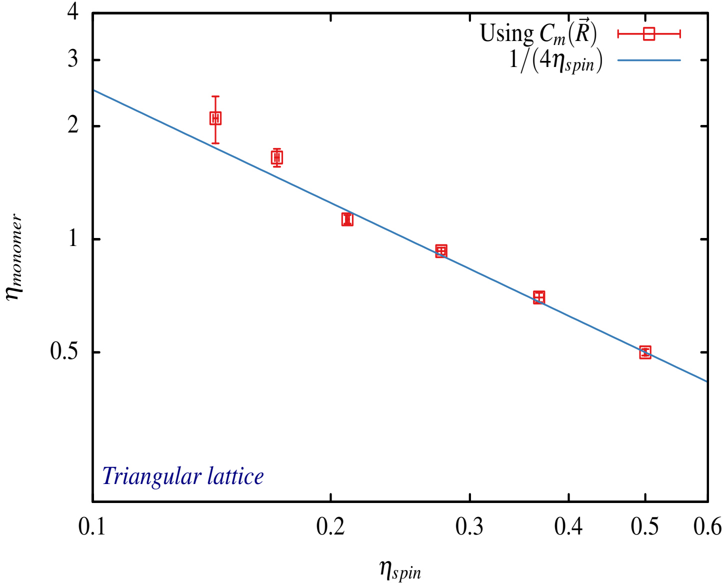
New ingredient—I



New ingredient—II



Analytical theory of worm statistics—I



Analytical theory for worm statistics—III