Melting of three-sublattice order

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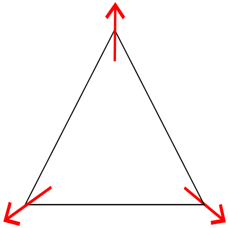
Geometric frustration and spin-orbit coupling

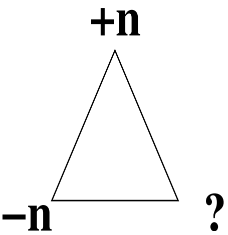
- Insulators with heavy magnetic ions $\rightarrow$ spin-orbit coupling effects matter
- Anisotropic terms in low-energy H for spins
- Anisotropies can amplify effects of geometric frustration

Classical picture

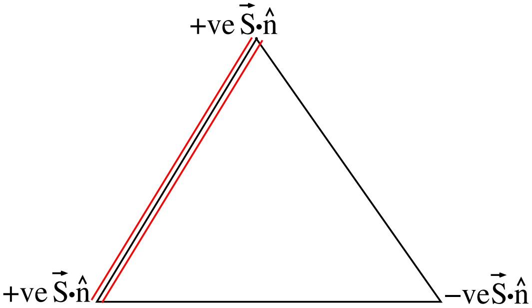
- Isotropic spins on a triangle



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

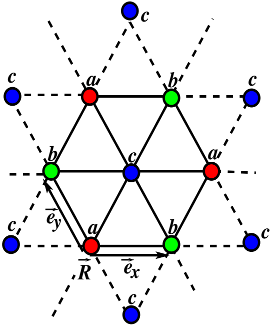


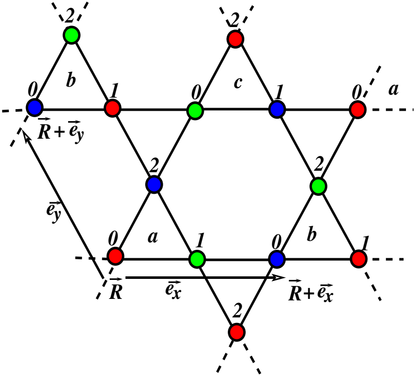
Huge degeneracy of minimally frustrated configurations



- On planar lattices—parametrization in terms of (generalized) dimer models

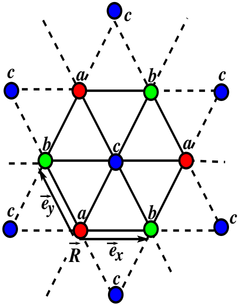
Easy-axis antiferromagnets on Kagome and triangular lattices





Natural tripartite structure

Three-sublattice order on the triangular lattice



θ	● (red)	● (green)	● (blue)
0	−S	+S	+S
$\frac{\pi}{6}$	−S	0	+S

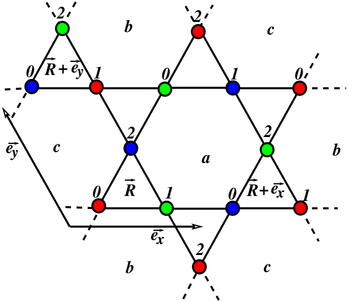
$\psi = |\psi| e^{i\theta} = -\sum_{\vec{R}} e^{i\mathbf{Q}\cdot\vec{R}} S^z_{\vec{R}}$

Ferri vs antiferro order distinguished by the choice of phase θ

Ferri: $\theta = 2\pi m/6$, Antiferro: $\theta = (2m+1)\pi/6$ $(m = 0, 1, 2 \ldots 5)$

Three-sublattice order on the Kagome lattice

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



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

Again: Ferri vs antiferro distinguished by the choice of phase θ

Ferri: $\theta = 2\pi m/6$, Antiferro: $\theta = (2m+1)\pi/6$ ($m = 0, 1, 2 \ldots 5$)

In this talk...

- Two well-known ways in which this order melts on heating
  Two-step melting (intermediate phase with power-law order for $T \in (T_{c1}, T_{c2})$)
  OR
  Three-state Potts criticality
- Main message(s) of talk—
  - Thermodynamic signature of two-step melting: $\chi_{\hat{n}}(B) \sim 1/|B|^{p(T)}$ with $p(T) \in (\frac{2}{3}, 0)$ for $T \in (T_{c1}, T_{c2})$.
  - Intervening multicritical point $\mathcal{M}$
    Central charge $c_{\mathcal{M}} \in (1, 3/2)$
  - (speculation: $\mathcal{M}$ accessible in "artificial Kagome-ice" systems...)

Wannier's triangular lattice Ising antiferromagnet

- $H_{\text{Ising}} = J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z$ on the triangular lattice
  (Wannier 1950)
- $T \to 0$ limit characterized by power-law correlations:
  $\langle \sigma_r^z \sigma_0^z \rangle \sim \frac{\cos(\mathbf{Q} \cdot \mathbf{r})}{r^{1/2}}$
  Incipient order at three-sublattice wavevector $\mathbf{Q} = (2\pi/3, 2\pi/3)$
  Stephenson (1964)
  Power-law spin-liquid in the $T \to 0$ limit

Lattice-gas models for monolayer films on graphite

- Three-sublattice long-range order of noble-gas monolayers on graphite
  Birgeneau, Bretz, Chan, Vilches, Wiechert...(1970—1990)
  $H_{\mathrm{J_1J_2}} = J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - J_1 \sum_{\langle\langle ij \rangle\rangle} \sigma_i^z \sigma_j^z - J_2 \cdots - B \sum_i \sigma_i^z$
  Long-range three-sublattice ordering (wavevector $\mathbf{Q}$) at low temperature
  D. P. Landau (1983)

Prototypical example of order-by-(quantum) disorder

- $H_{\text{TFIM}} = J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$ on the triangular lattice
  Long-range order at three-sublattice wavevector $\mathbf{Q}$
- Ordering of "antiferro" type $\rightarrow (+, -, 0)$
  antiferro order provides maximum "room" for quantum fluctuations
  Moessner, Sondhi, Chandra (2001), Isakov & Moessner (2003)

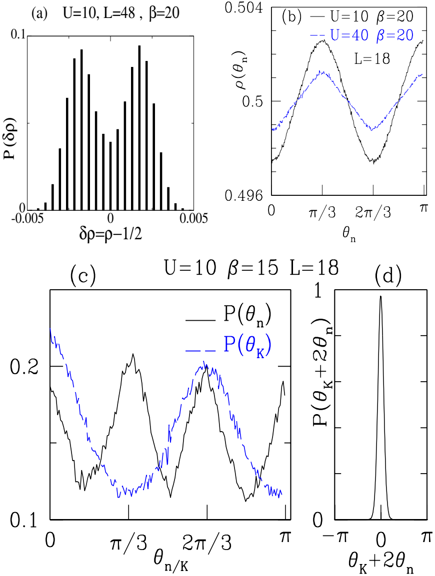
$S = 1$ antiferromagnets with single-ion anisotropy

- $H_{\mathrm{AF}} = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j - D\sum_i (S_i^z)^2$ on triangular lattice
- Low-energy physics for $D \gg J$:
  $H_b = -\frac{J^2}{D}\sum_{\langle ij\rangle}(b_i^\dagger b_j + h.c.) + J\sum_{\langle ij\rangle}(n_i - \frac{1}{2})(n_j - \frac{1}{2}) + \ldots$
  KD & Senthil (06)
- Low-temperature state for $D \gg J$: "supersolid" state of hard-core bosons at half-filling.
  Auerbach & Murthy (97), Heidarian, Melko, Wessel...(05)
- Implies: Three-sublattice order in S^z + "ferro-nematic" order in $\vec{S}_\perp^2$
  (Simple easy-axis version of Chandra-Coleman (1991) "spin-nematic" ideas)

Is three-sublattice ordering of S^z in $H_{\rm AF}$ ferri or antiferro?

- Natural expectation: Quantum fluctuations induce antiferro order (like in the transverse field Ising model)
  $\rightarrow$
  Prediction: Ordering will be antiferro three-sublattice order
  e. g. Melko *et. al.* (2005)

QMC evidence: Ferri three-sublattice order of S^z



Heidarian & KD (2005)

Ising models for “Artificial Kagome-ice”

- $H_{\text{Kagome}} = J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - J_1 \sum_{\langle\langle ij \rangle\rangle} \sigma_i^z \sigma_j^z - J_2 \ldots$
- Only nearest-neighbour couplings $\rightarrow$ classical short-range spin liquid (Kano & Naya 1950)
- Second-neighbour ferromag. couplings destabilize spin liquid (Wolf & Schotte 88)
  Ferrimagnetic three-sublattice order at low T.
- “Artificial Kagome-ice: Moments $\mathbf{M}_i = \sigma_i^z \mathbf{n}_i$
  ($\mathbf{n}_i$ at different sites non-collinear)
  Expt: Tanaka *et. al.* (2006), Qi *et. al.* (2008), Ladak *et. al.* (2010,11)
  Theory: Moller, Moessner (2009), Chern *et. al.* (2011)

Symmetry breaking transitions: Generalities

- Symmetry-breaking state characterized by long-range correlations of "order-parameter" $\hat{O}$
- phenomenological Landau free energy density $\mathcal{F}[\hat{O}]$
  Expanding $\mathcal{F}$ in powers of $\hat{O}$ (symmetry allowed terms)
- Neglecting derivatives (fluctuations):
  phase transition $\rightarrow$ change in minimum of $\mathcal{F}$

Fluctuation effects at continuous transitions:

- More complete description of long-wavelength physics: Include (symmetry allowed) gradient terms in $\mathcal{F}$
- In most cases: Corrections to mean-field exponents
- In rare cases: Fluctuation-induced first-order behaviour

Symmetries are (usually) decisive:

- Transformation properties of $\hat{O}$ determine nature of continuous transition

Landau-theory for melting of three-sublattice order

- $\mathcal{F} = K|\nabla\psi|^2 + r|\psi|^2 + u|\psi|^4 + \lambda_6(\psi^6 + \psi^{*6}) + \ldots$
  Connection to physics of six-state clock models
  $Z = \sum_{\{p_i\}} \exp[\sum_{\langle ij\rangle} V(\frac{2\pi}{6}(p_i - p_j))]$
  Each $p_i = 0, 1, 2, \ldots 5$
  $V(x) = K_1 \cos(x) + K_2 \cos(2x) + K_3 \cos(3x)$
  Cardy (1980)

Coarse-grained lattice model

$$H_{\mathrm{xy}} = -J_{\mathrm{xy}} \sum_{\langle \vec{r}\vec{r}' \rangle} \cos(\theta_{\vec{r}} - \theta_{\vec{r}'}) - h_6 \sum_{\vec{r}} \cos(6\theta_{\vec{r}}) \ .$$

where $\langle \vec{r}\vec{r}' \rangle$ are nearest-neighbour links of our coarse-grained triangular lattice, and higher harmonics $J^{(p)}$ $(p = 2, 3)$ left out of H_{xy} displayed here

Melting scenarios for three-sublattice order

- Analysis (Cardy 1980) of generalized six-state clock models
  $\rightarrow$ Three generic possibilities of relevance here:
  Two-step melting, with power-law ordered intermediate phase
  OR
  3-state Potts transition to ferromagnetic phase followed by loss of ferromagnetism via Ising transition at higher temperature..
  OR
  First-order transition (always possible!)

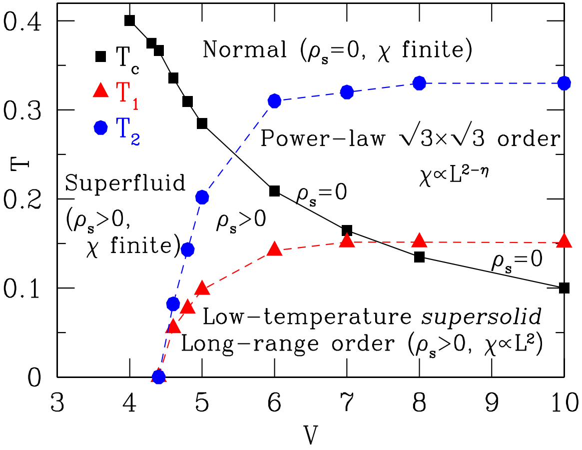
Melting of three-sublattice order in various examples

- Antiferro three-sublattice order in transverse field Ising model
  Two-step melting
  Isakov & Moessner (2001)
- Ferrimagn. three-sublattice order in lattice gas models of monolayer films
  Two-step melting
  D.P. Landau (83)
- Ferri three-sublattice order in Kagome Ising antiferromagnets
  With second-neighbour ferro couplings: Two step melting
  Wolf & Schotte (88)
  With long-range dipolar couplings: Three-state Potts transition
  Moller & Moessner (09), Chern, Mellado, Tchernyshyov (11)

Nature of melting transition in $S = 1$ H_{AF}?

- Prediction of Boninsegni & Prokofiev (2005)
  Three-state Potts transition
  Prediction based on argument about relative energies of different kinds of domain walls
  hard to get right at quantitative level

Our answer from large-scale QMC simulations



KD & Heidarian ((*unpublished*))

Detecting power-law order?

Need scattering experiment to detect power-law version of Bragg peaks
Or
Real-space data by scanning some local probe $+$ Lots of image-processing

Alternate thermodynamic signature(!)

- Singular thermodynamic susceptibility to *uniform* easy-axis field B:
  $\chi_u(B) \sim \frac{1}{|B|^{p(T)}}$
- $p(T) = \frac{4-18\eta(T)}{4-9\eta(T)}$ for $\eta(T) \in (\frac{1}{9}, \frac{2}{9})$
  So $p(T)$ varies from $1/3$ to 0 as T increases from T_{c1} to just below T_{c2}

(KD *arXiv:1507.08393*)

Review: picture for power-law ordered phase

- In state with long-range three-sublattice order, θ feels $\lambda_6 \cos(6\theta)$ potential.
  Locks into values $2\pi m/6$ (resp. $(2m+1)\pi/6$) in ferri (resp. antiferro) three-sublattice ordered state for $T < T_{c1}$
- In power-law three-sublattice ordered state for $T \in (T_{c1}, T_{c2})$, λ_6 does not pin phase θ
  θ spread uniformly $(0, 2\pi)$
- But vortices continue to be irrelevant
  Distinction between ferri and antiferro three-sublattice order lost for $T \in (T_{c1}, T_{c2})$

Review: more formal RG description

- 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 $T \in (T_1, T_2)$
- $\lambda_6 \cos(6\theta)$ *irrelevant* along fixed line
- $\langle \psi^*(r)\psi(0)\rangle \sim \frac{1}{r^{\eta(T)}}$
  with $\eta(T) = g(T)$

Jose, Kadanoff, Kirkpatrick, Nelson (1977)

General argument for result—I

- Landau theory admits term $\lambda_3 m(\psi^3 + \psi^{*3})$
  m is uniform magnetization mode
- Formally irrelevant along fixed line $\mathcal{F}_{\mathrm{KT}}$
  $\rightarrow$
  Physics of two-step melting unaffected—m “goes for a ride...”

But ...

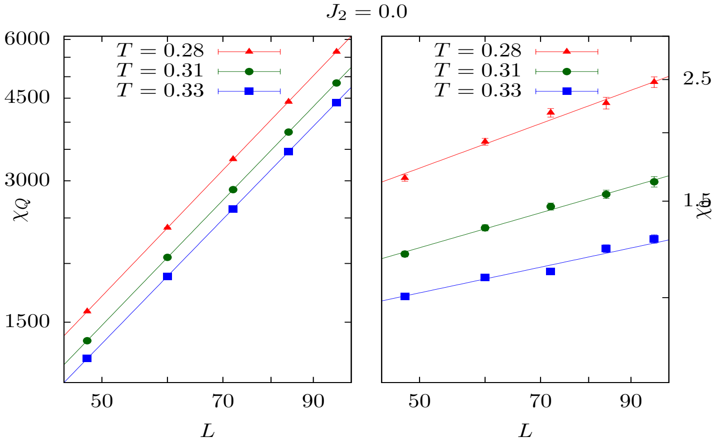
General argument for result—II

- m "inherits" power-law correlations of $\cos(3\theta)$:
  $C_m(r) = \langle m(r)m(0)\rangle \sim \frac{1}{r^{9\eta(T)}}$
- $\chi_L \sim \int^L d^2 r C_m(r)$ in a finite-size system at $B = 0$
- $\chi_L = \chi_{\text{reg}} + bL^{2-9\eta(T)}$ for $\eta(T) \in (\frac{1}{9}, \frac{2}{9})$
  Diverges with system size at $B = 0$

General argument for result—III

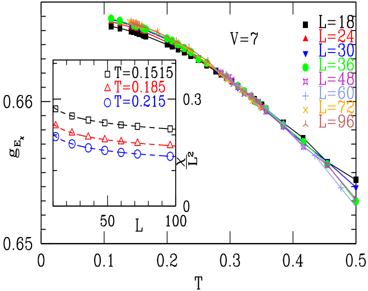
- Uniform field $B > 0 \rightarrow$ additional term $h_3 \cos(3\theta)$ in $\mathcal{F}_{\text{KT}}$
- Strongly relevant along fixed line, with RG eigenvalue $2 - 9g/2$
- Implies finite correlation length $\xi(B) \sim |B|^{-\frac{2}{4-9\eta}}$
- $\chi_u(B) \sim |B|^{-\frac{4-18\eta}{4-9\eta}}$ for $\eta(T) \in (\frac{1}{9}, \frac{2}{9})$

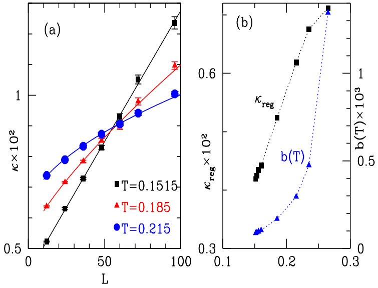
The proof of the pudding...I



In power-law ordered phase of H_{TFIM} (Biswas, KD (*unpublished*))

The proof of the pudding...II





In power-law ordered phase of H_b (KD, Heidarian (*unpublished*))

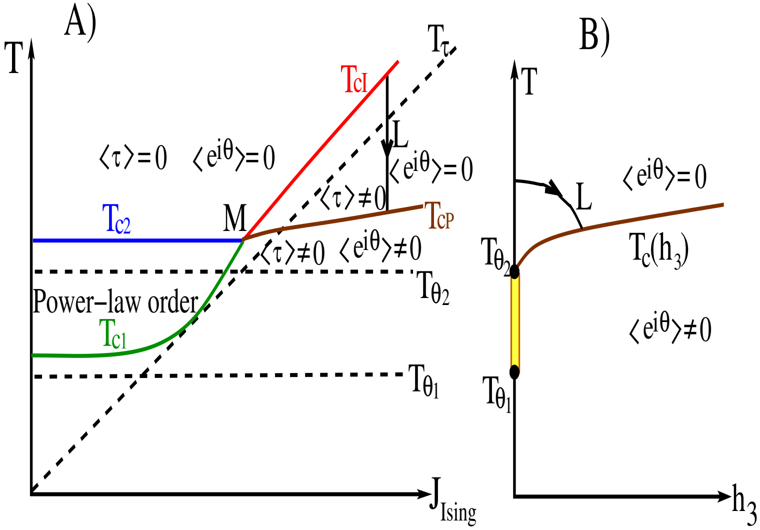
More complete coarse-grained description

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

with $h \propto B$.

(KD *arXiv:1507.08393*)

Phase diagram of H_{eff}



(KD *arXiv:1507.08393*)

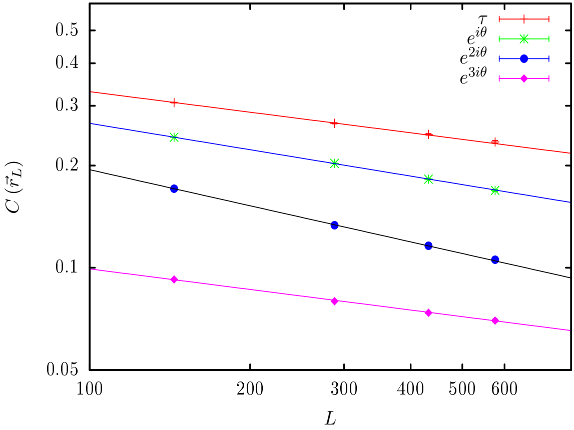
The argument...

- 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:
  $J_{\rm xy} = h_6 = 1.0$, $J_{\theta\tau} = 0.25$
  Parametrize: $J_{\rm Ising} = f_{xy} T_{\theta_1} / T_\tau$ and $T = f_I f_{xy} T_{\theta 1}$ [with $T_{\theta 1} = 1.04$ and $T_\tau = 3.6409$]

Multicritical melting



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

$C_{2\theta}$ [$C_{3\theta}$] 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 *arXiv:1507.08393*)

Any guesses about CFT description?...

Speculation (aka wishful thinking?)

- If relative strength of first/second neighbour exchange tunable relative to long-range dipolar part in artificial kagome-ice: Could tune melting to multicritical point...

Acknowledgements

- Collaborators:
  QMC on H_{b}: Dariush Heidarian (Toronto)
  QMC on H_{TFIM}: Geet Ghanshyam and Sounak Biswas (TIFR)
  Classical MC of $H_{\mathrm{J_1J_2}}$: Geet Ghanshyam (TIFR)
- Computational resources at TIFR