Competing anisotropies and flux confinement-deconfinement transitions in frustrated kagome and pyrochlore magnets

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Souvik Kundu & KD, Phys. Rev. X 15, 011018 (2025)

Jay Pandey, Souvik Kundu, & KD, unpublished

Jay Pandey & KD unpublished

Funding: DAE-India, SERB-India, Infosys-Chandrasekharan Random Geometry Center

One slide summary

Competition between two different manifestations of SO coupling:

Easy-axis anisotropy of the exchange couplings

Easy-plane anisotropy in the single-ion energetics

Tight-binding descriptions for SO coupled Mott insulators suggest such regimes can exist

Lee, Bhattacharjee, Kim, PRB 87, 214416 (2013)

Rau, Lee, Kee, PRL 112, 077204 (2014)

Our message-

Interplay of geometric frustration and this competition drives interesting physics

However-

Caveat emptor: No candidate materials known to us...

1. Competing anisotropies and the S=1 kagome 1/3-magnetization plateau

Representative Hamiltonian:

$$H_{eff} = J^z \sum_{rr'} S^z_r S^z_{r'} + \Delta \sum_r (S^z_r)^2 - B \sum_r S^z_r + \cdots$$

$J^z = J \; , \quad \Delta = J + \mu$

$T, \; \mu \ll J$

Quantum fluctuations, additional interactions negligible $(J_\perp \, , \; J' \ll T)$

One-third magnetization plateau

($\mathcal{O}(J)$ width around $B \simeq 2J$)

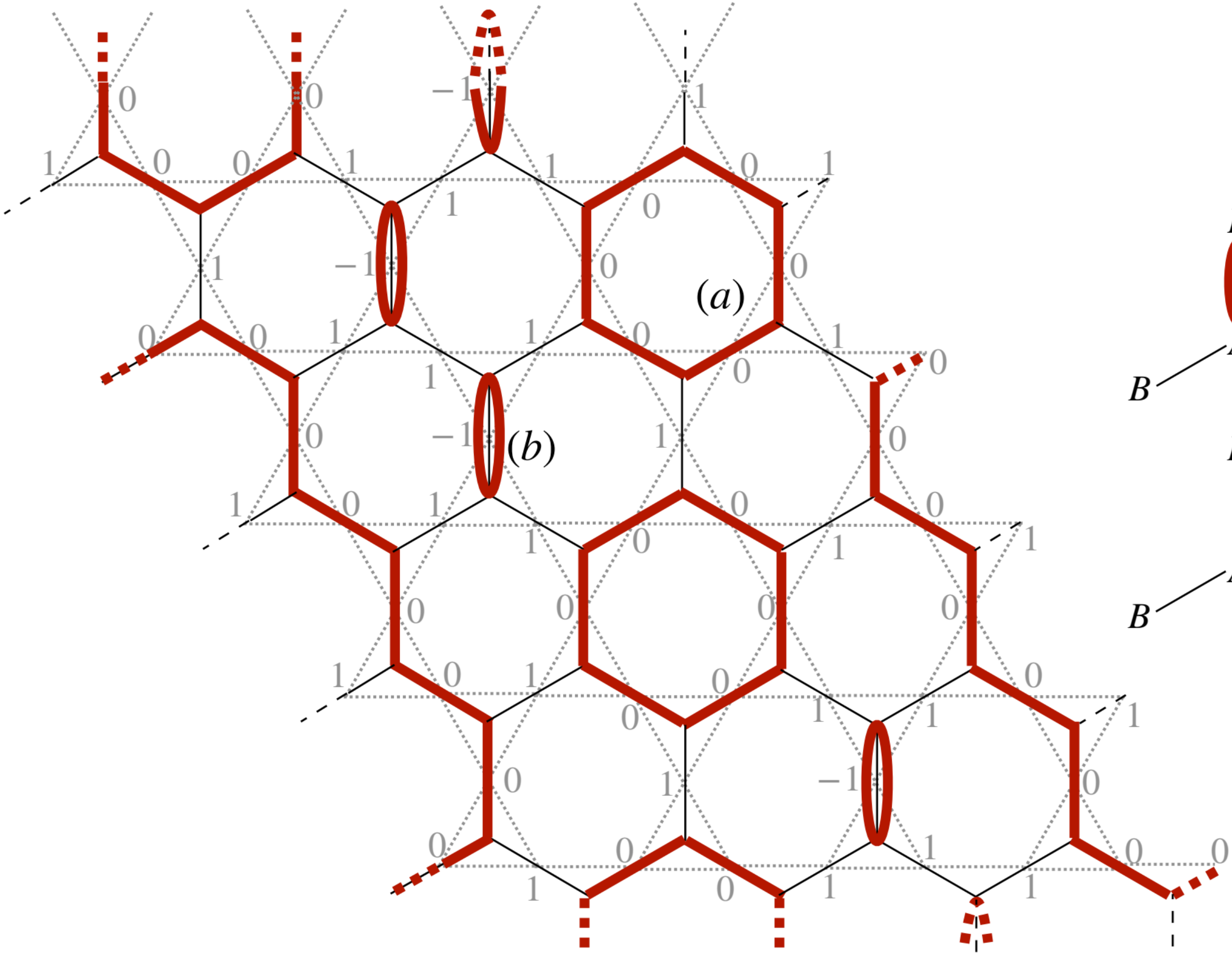
Each kagome triangle has: $S^z = 1$

Two ways to add up to $S^z = 1$ (1,0,0) or (1,1, -1) (Large $\mathcal{O}(J)$ energy gap to other values)

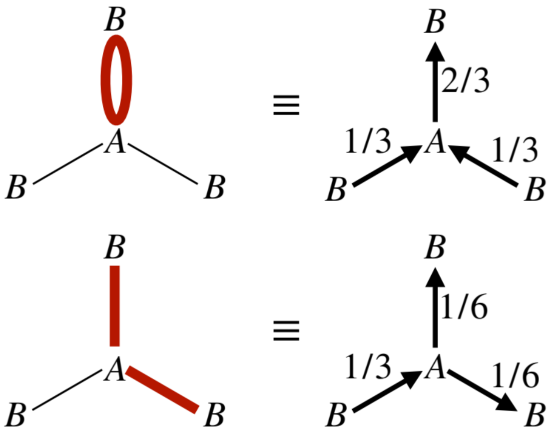
(with slightly different energies)

Souvik Kundu & KD, Phys. Rev. X 15, 011018 (2025)

Fully-packed configurations of loops + trivial loops (dimers)



Divergence-free polarization

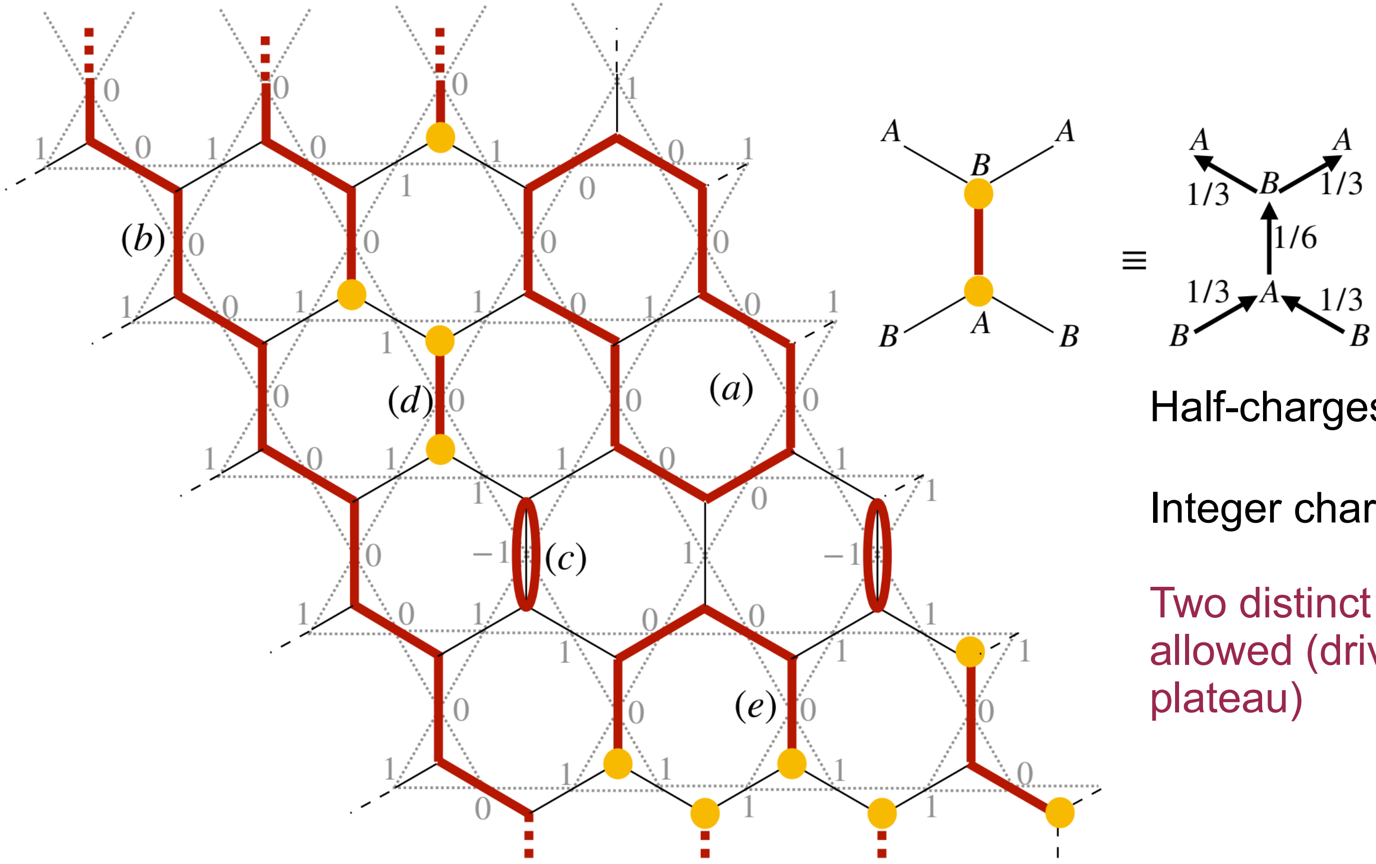


$$\Delta \cdot P = 0$$

Microscopic height construction

$$P = \Delta \times H$$

All open strings disallowed



Half-charges (half-vortices) forbidden

Integer charges (unit-vortices) also forbidden

Two distinct length-1 objects if half vortices allowed (drive transition to 2/3 magnetization plateau)

Souvik Kundu & KD, Phys. Rev. X 15, 011018 (2025)

Dimer-loop partition function

$$Z = \sum_{\mathcal{C}} w^{n_d(\mathcal{C})}$$

$$w = \exp(-2\mu/T)$$

Physics of kagome magnet described in terms of dimer-loop partition function on honeycomb lattice

Tool: Classical Monte Carlo using a worm algorithm

Also useful to study square lattice dimer loop model (to check universality of honeycomb model transitions)

Some theoretical perspective

w=0 is fully-packed O(1) honeycomb loops (loop fugacity is unity). Configurations in one-to-one correspondence with fully-packed dimers (empty links form loops)

Limit of infinite w is usual fully-packed dimer model.

Warning: no obvious duality between w and 1/w for general w

Expect:

At w=0: Power-law loop size distribution, dipolar correlations.

At infinite w: dipolar correlations

(Baxter, Moessner-Tchernyshyov-Sondhi 2004, Jaubert-Haque-Moessner 2011, Jacobsen-Kondev 1998, Saleur-Duplantier 1987)

Coarse-grained height field-theory

$$S = \pi g \int (\nabla h)^2$$

h is an angle: h-->h+1 redundancy in pure dimer limit, h-->h+1/2 redundancy in pure loop limit

(Youngblood 1980, Henley, Fradkin et al 2004, Vishwanath et al 2004, Alet et al 2005, Moessner et al 2004 ...)

Since loops exist at any finite w, expect h-->h+1/2 redundancy for all finite w?
Smooth crossover as a function of w as we go from 0 to infinity?

Numerics:

- Classical Monte Carlo using two worm updates
- One uses a unit-vortex antivortex pair, the other does the same with half-vortices
- Allows measurement of test half-vortex correlator
- Periodic boundary conditions: Two independent fluxes of polarization field (winding numbers) well-defined
- Fluxes are allowed to be half-integer in general except in pure dimer limit.

Measurements

Loop-size distribution and moments $P_l(s, L)$ $S_m = \langle \sum_j s_j^m \rangle$

Loop-size Binder ratio $Q_2 = \langle \sum_{i \neq j} s_i^2 s_j^2 \rangle / S_2^2$

Flux (winding number) distribution $P(\phi_x, \phi_y)$

Probability of having fractional fluxes $P_{\text{frac}} = 1 - \sum_{\phi_x \in Z, \phi_y \in Z} P(\phi_x, \phi_y)$

Three-sublattice spin order parameter and half/unit-vortex correlators $C_\psi(r)$ $C_v^q(r)$ for $q = 1/2, 1$

Preview: Conclusion from numerics

Two distinct Coulomb liquids separated by continuous transition

Multiple characterizations of the two Coulomb liquids and transition between them:

Geometric: Long-loop phase vs short-loop phase

Topological: Flux confinement-deconfinement transition

Dynamical: Half-vortices are deconfined in one phase but not other

Long-wavelength correlations: Power-law three-sublattice order in one but not other phase

Ising transition: Hidden Ising order parameter

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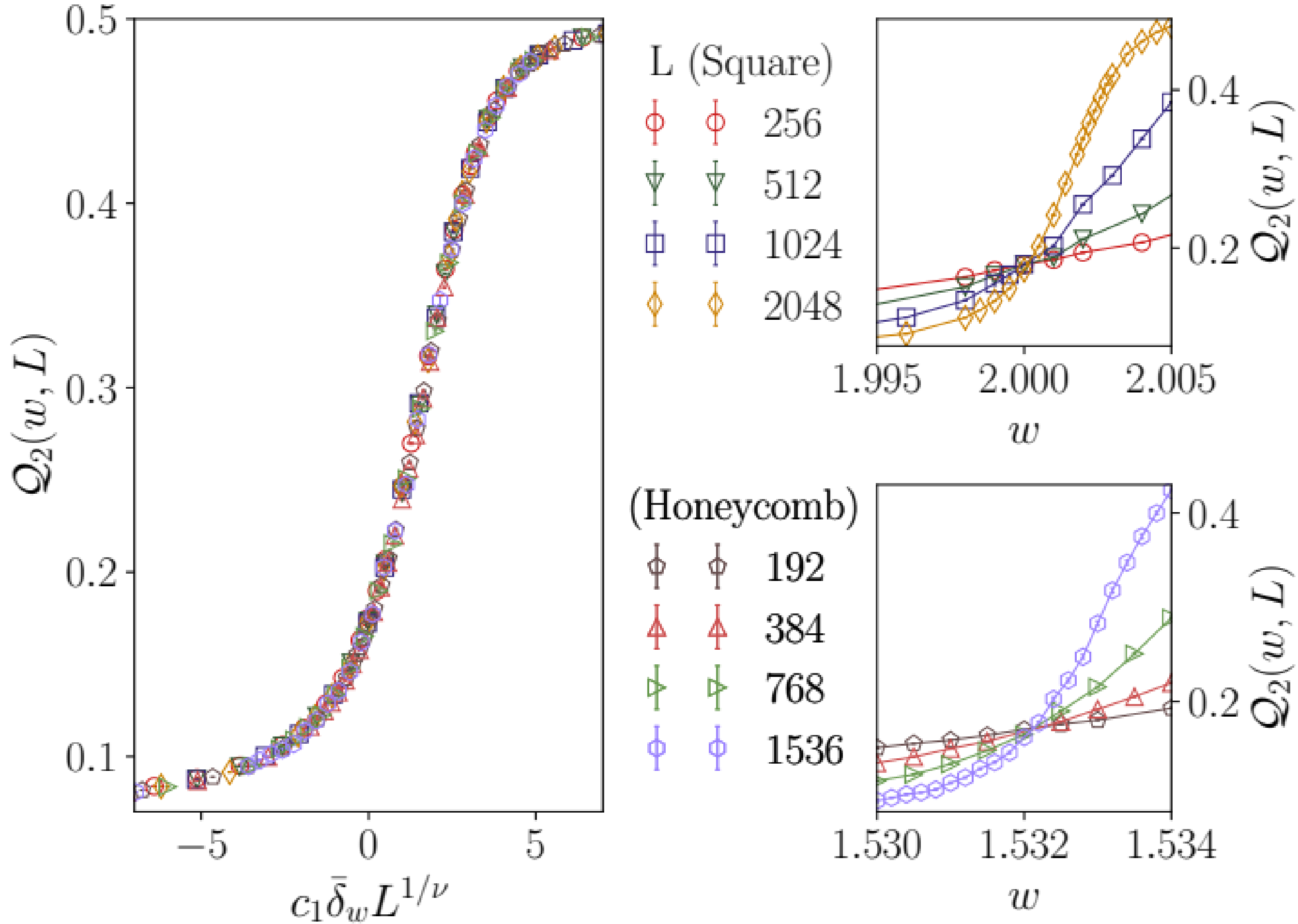
Jay Pandey & KD, unpublished

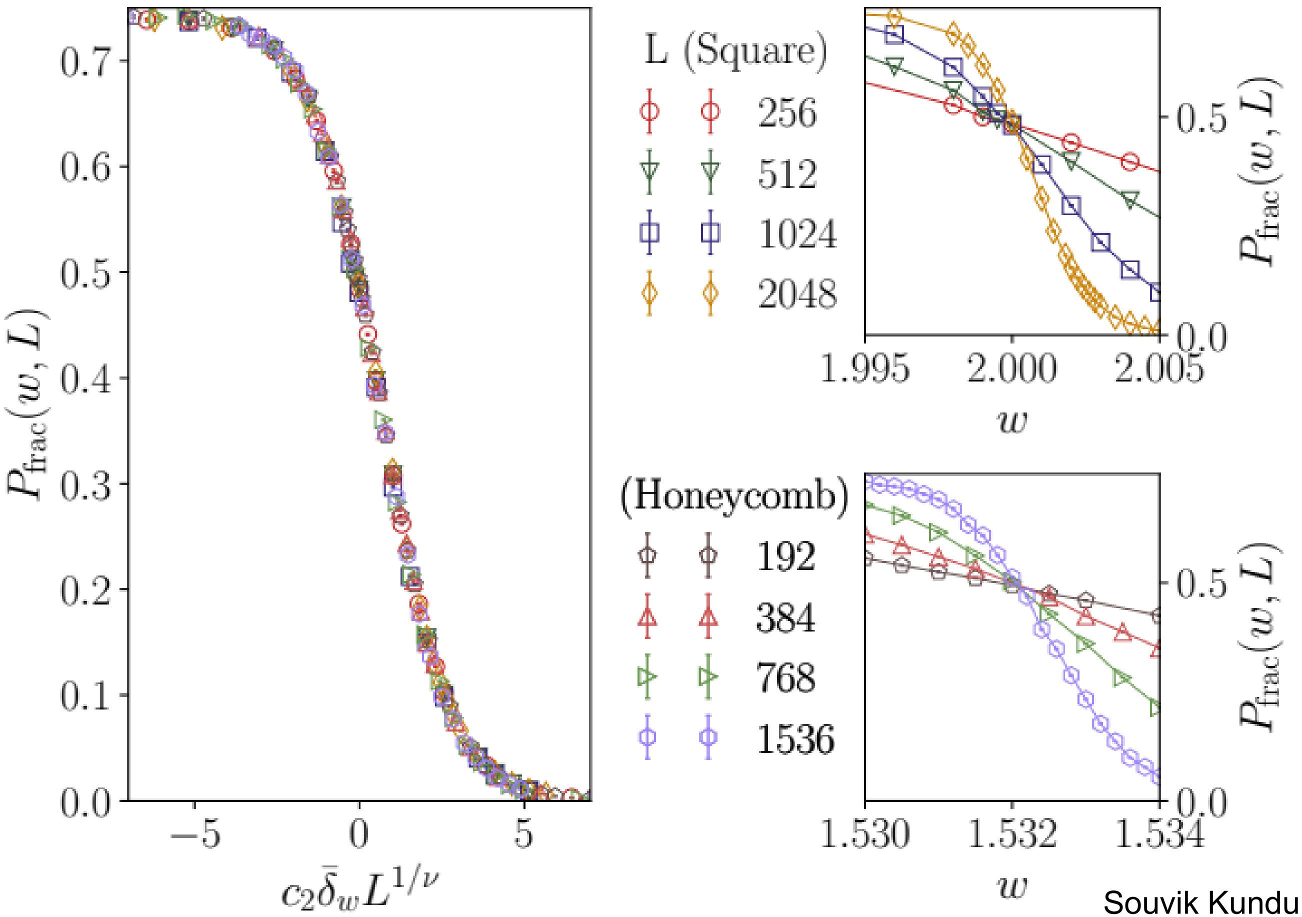
Geometric characterization: short-to-long loop phase transition



$\nu \approx 1.00(2)$

Souvik Kundu & KD, Phys. Rev. X 15, 011018 (2025)

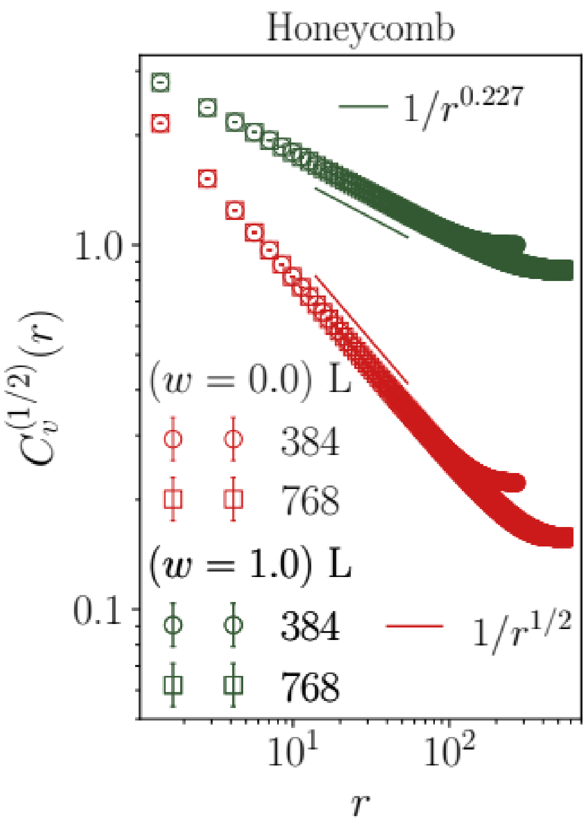
Topological characterization: Flux confinement-deconfinement transition

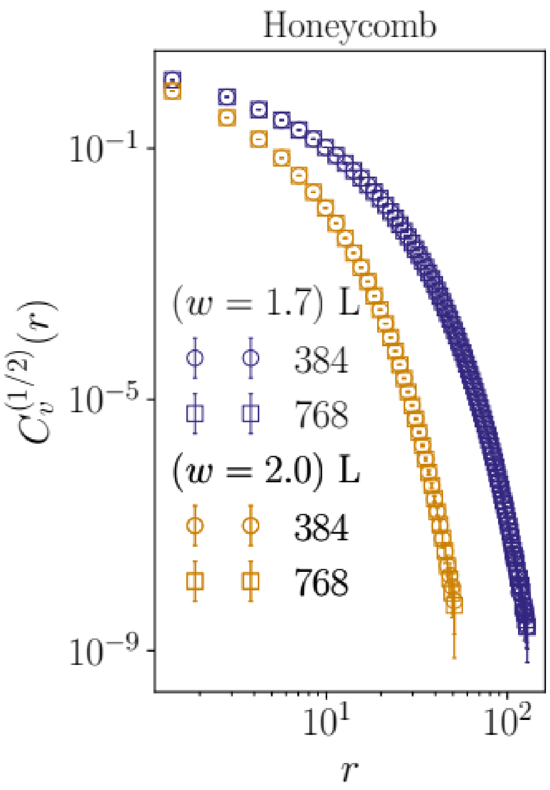


$\nu \approx 1.00(2)$

Souvik Kundu & KD, Phys. Rev. X 15, 011018 (2025)

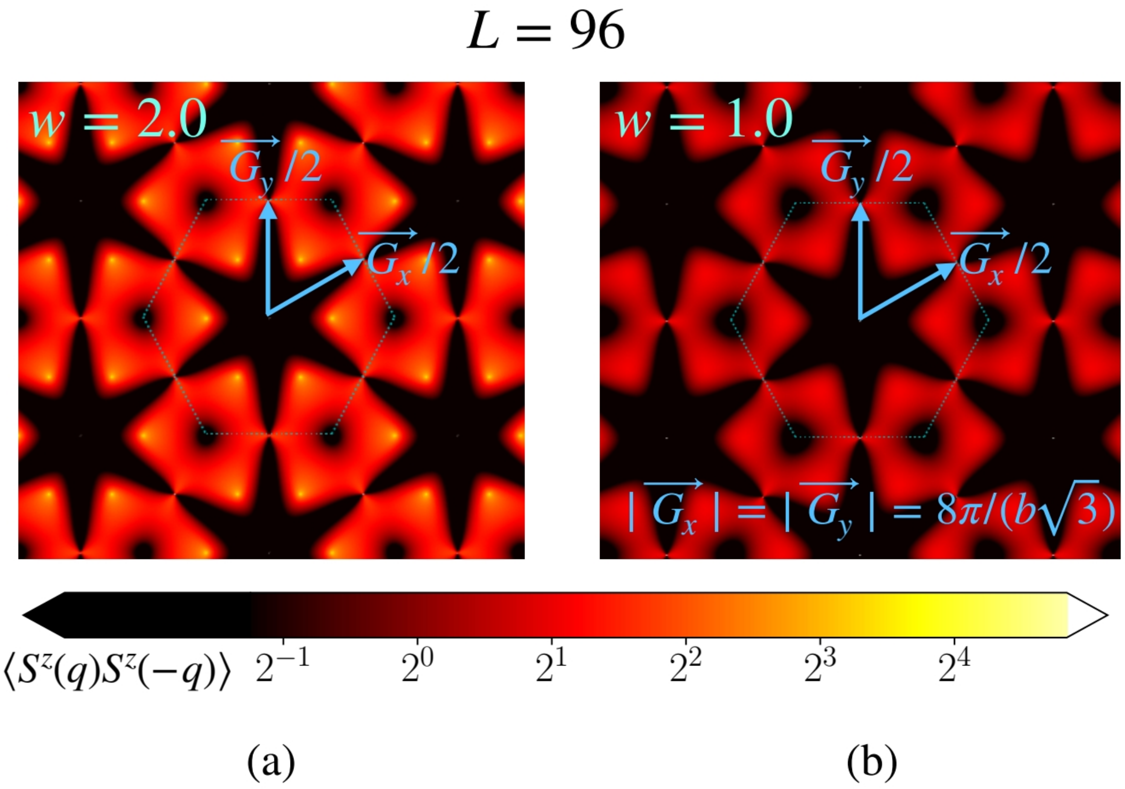
Dynamical characterization: Half-vortex (charge) correlators in two phases





Souvik Kundu & KD, Phys. Rev. X 15, 011018 (2025)

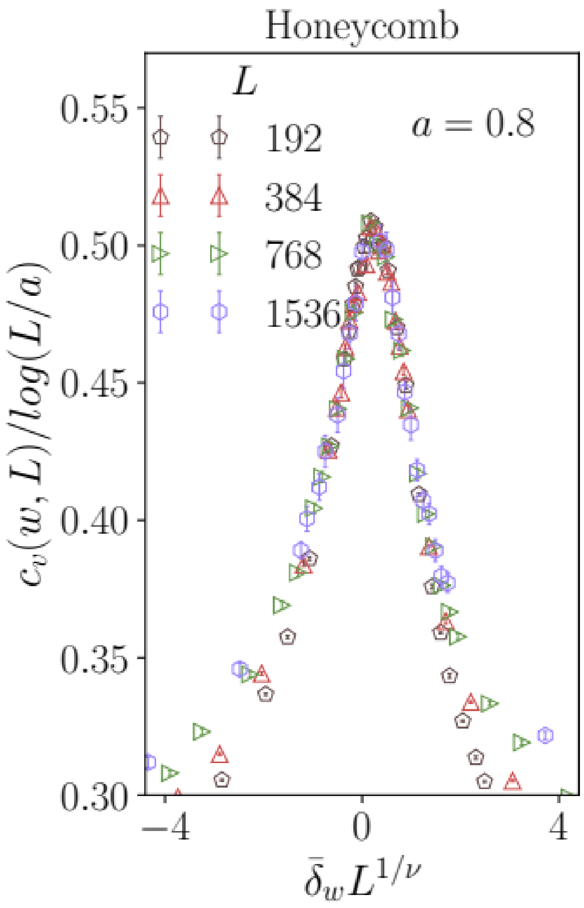
Transition observable in kagome spin structure factor



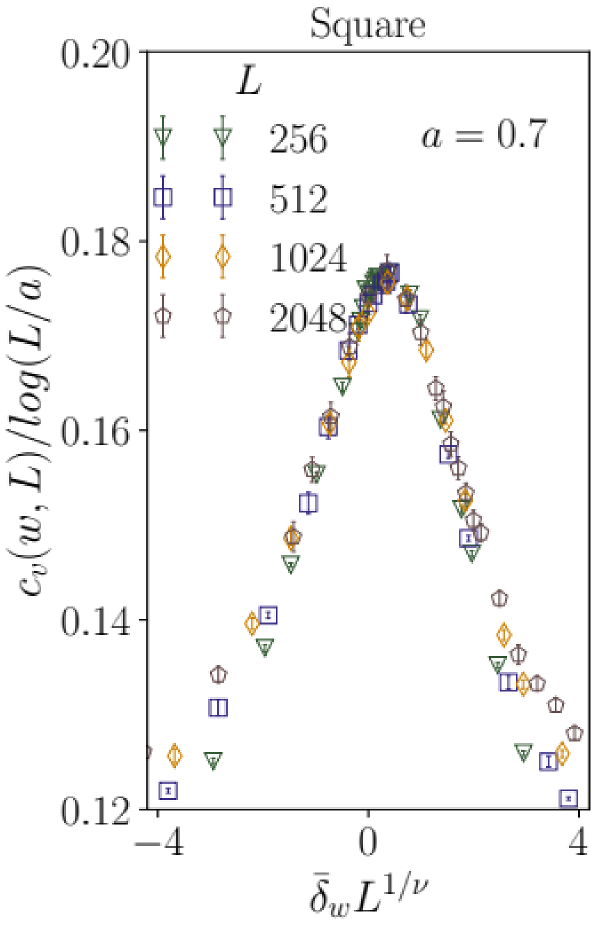
Power-law feature at three sublattice wavevector absent in long-loop phase

Souvik Kundu & KD, Phys. Rev. X 15, 011018 (2025)

Thermodynamic characterization: Specific heat singularity



Ising-like



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“Hidden” Ising order parameter

$$\tau(x,y) = +1 \;\text{ if }\; 3H(x,y) \bmod (3) = 0,1,2 \text{ for } (x,y) \in \text{ sublattice } 0,1,2 \text{ respectively}$$

$$\tau(x,y) = -1 \text{ otherwise}$$

for the kagome magnet (honeycomb dimer-loop model)

Strictly speaking: Each dimer-loop state maps to pair of Ising configurations $\mathcal{C}_I$ and $\mathcal{C}^*{}_I$

$$\tau(x,y) = +1 \;\text{ if }\; 4H(x,y) \bmod (4) = 0,1,2,3 \text{ for } (x,y) \in \text{ sublattice } 0,1,2,3 \text{ respectively}$$

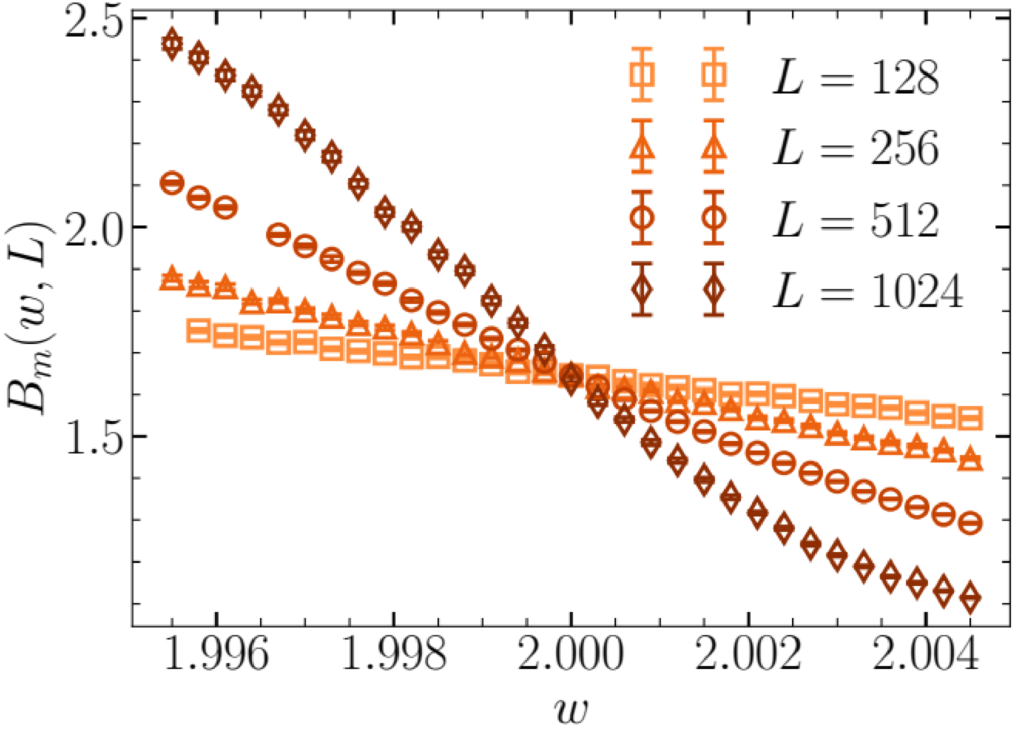
$$\tau(x,y) = -1 \text{ otherwise}$$

for the square lattice dimer-loop model (planar-pyrochlore spin model)

Jay Pandey & KD, unpublished

Transition seen by Ising Binder ratio

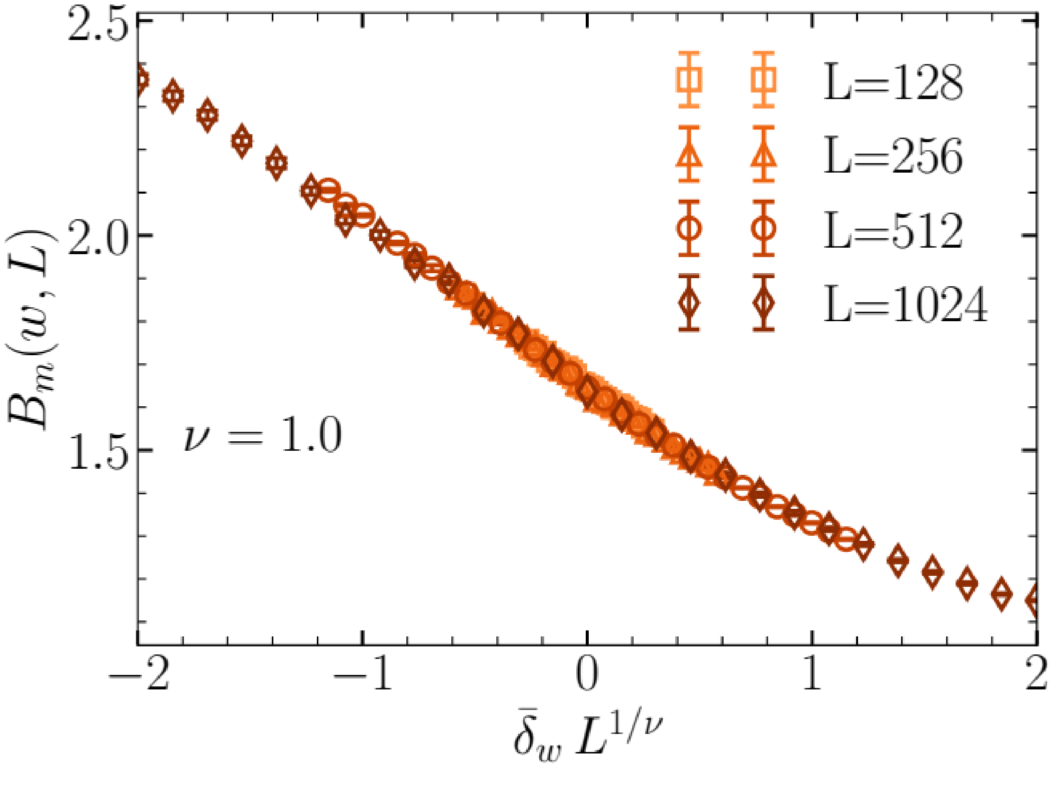
illustrated here for the square-lattice dimer-loop model



Jay Pandey & KD, unpublished

Scaling of Ising Binder

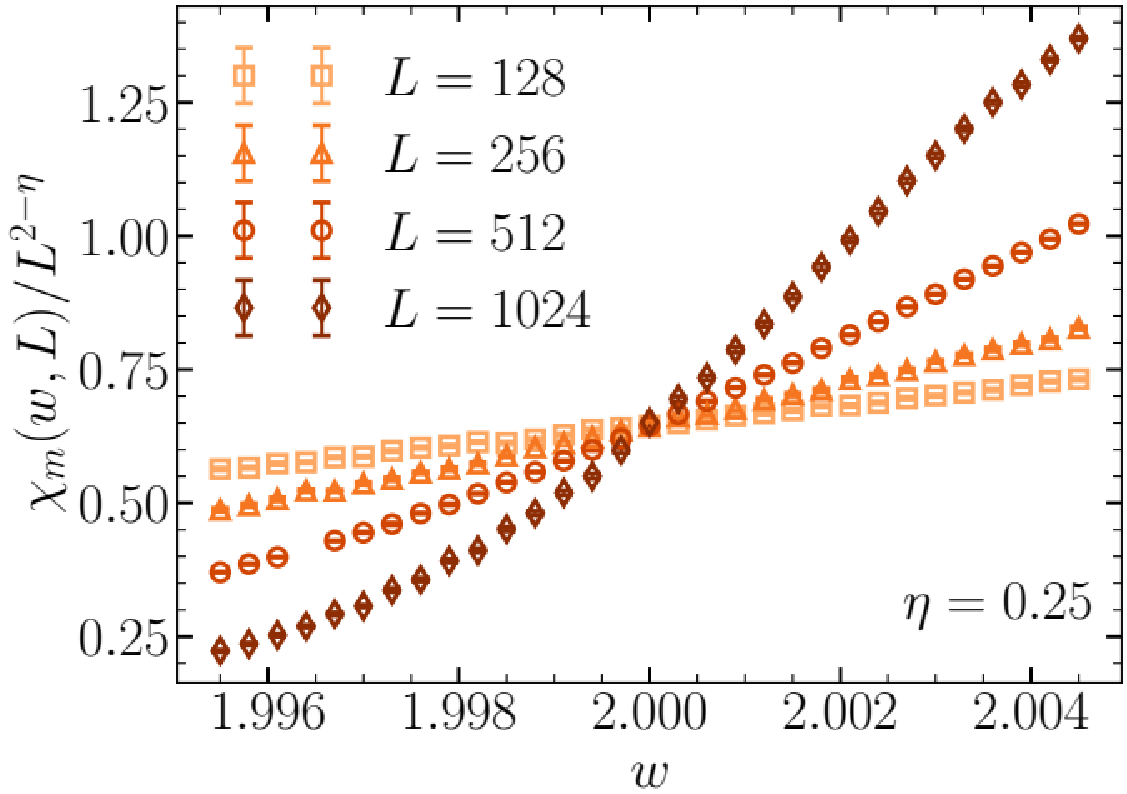
illustrated here for the square-lattice dimer-loop model



Jay Pandey & KD, unpublished

Transition seen by Ising susceptibility

illustrated here for the square-lattice dimer-loop model



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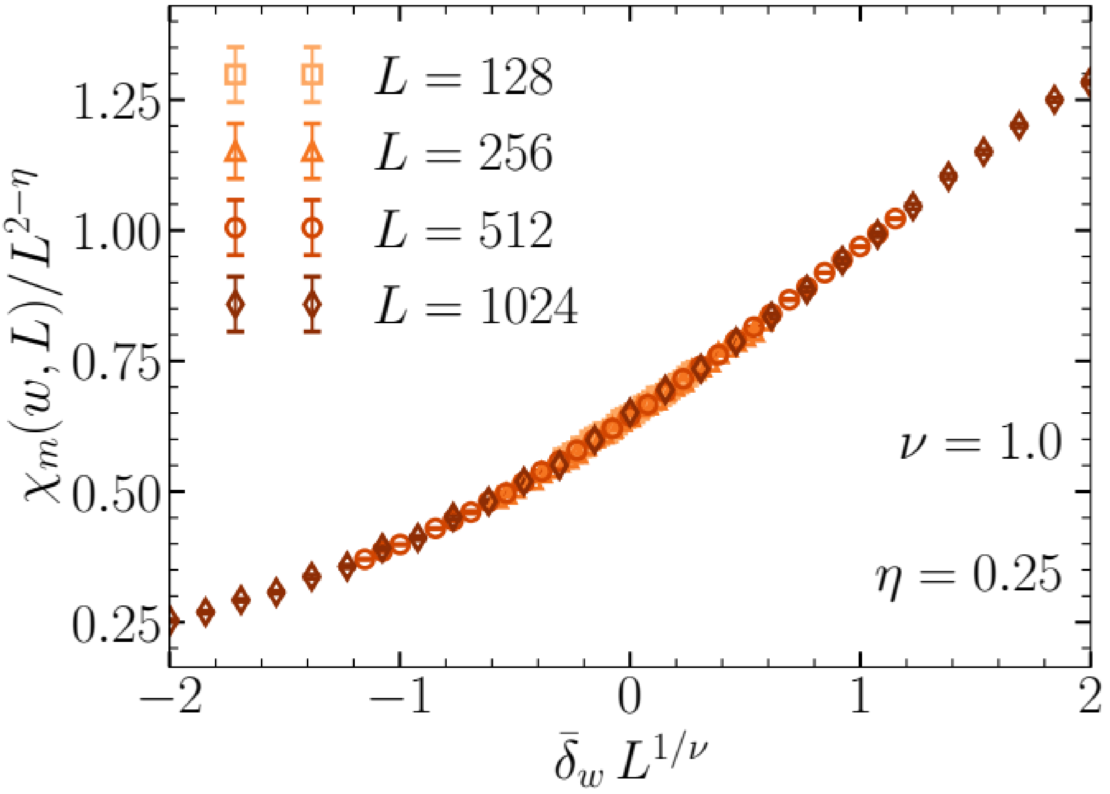
Scaling of Ising susceptibility

illustrated here for the square-lattice dimer-loop model



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2. Competing anisotropies and the S=1 kagome in zero field

Representative Hamiltonian:

$$H_{eff} = J^z \sum_{rr'} S_r^z S_{r'}^z + \Delta \sum_r (S_r^z)^2 + \cdots$$

$J^z = J \;, \quad \Delta = J + \mu$

$T, \; \mu \ll J$

Quantum fluctuations, additional interactions negligible $(J_\perp \;, \; J' \ll T)$

zero field physics: Each kagome triangle has: $S^z = 0$ (Large $\mathcal{O}(J)$ energy gap to other values)

Multiple ways to add up to $S^z = 0$: (with slightly different energies)

(0,0,0), or (1,-1, 0) and permutations (a "vertex model")

Each $S_r^z = \pm 1$ contributes one factor of $w = \exp(-\beta\mu)$ to the Boltzmann weight

Jay Pandey & KD, unpublished

Description in terms of fluctuating polarization field and heights

Divergence-free polarization on honeycomb links: $P_{A \to B} = S^z_{r_{AB}}$

$S^z_\Delta = 0$ implies $\Delta \cdot P = 0$

Periodic boundary conditions: Two independent fluxes of polarization field (winding numbers) well-defined

Microscopic height construction: $P = \Delta \times H$

Expect coarse-grained theory: $$S = \pi g \int (\nabla h)^2$$

h is an angle: h-->h+1 redundancy

Jay Pandey & KD, unpublished

Question:

Is there a smooth crossover from small w to large w, or a thermodynamic phase transition?

By analogy to superfluids, expect a (inverted) KT transition driven by relevance of $\exp(\pm 2\pi i\, h)$ (??)

Answering this: Vertex model partition function

$$Z = \sum_{\mathcal{C}} w^{n_{\pm 1}(\mathcal{C})}$$

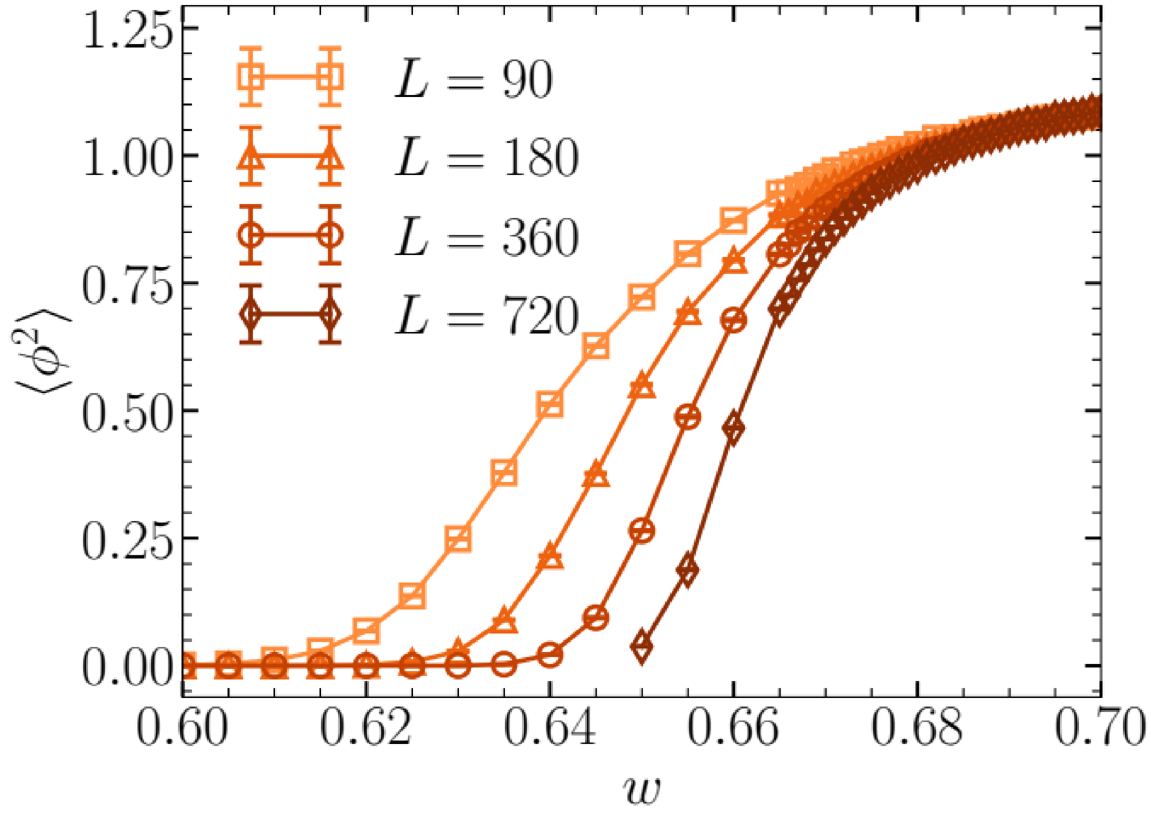
$$w = \exp(-\mu/T)$$

Physics of kagome magnet described in terms of vertex model partition function on honeycomb lattice

Tool: Classical Monte Carlo using a worm algorithm

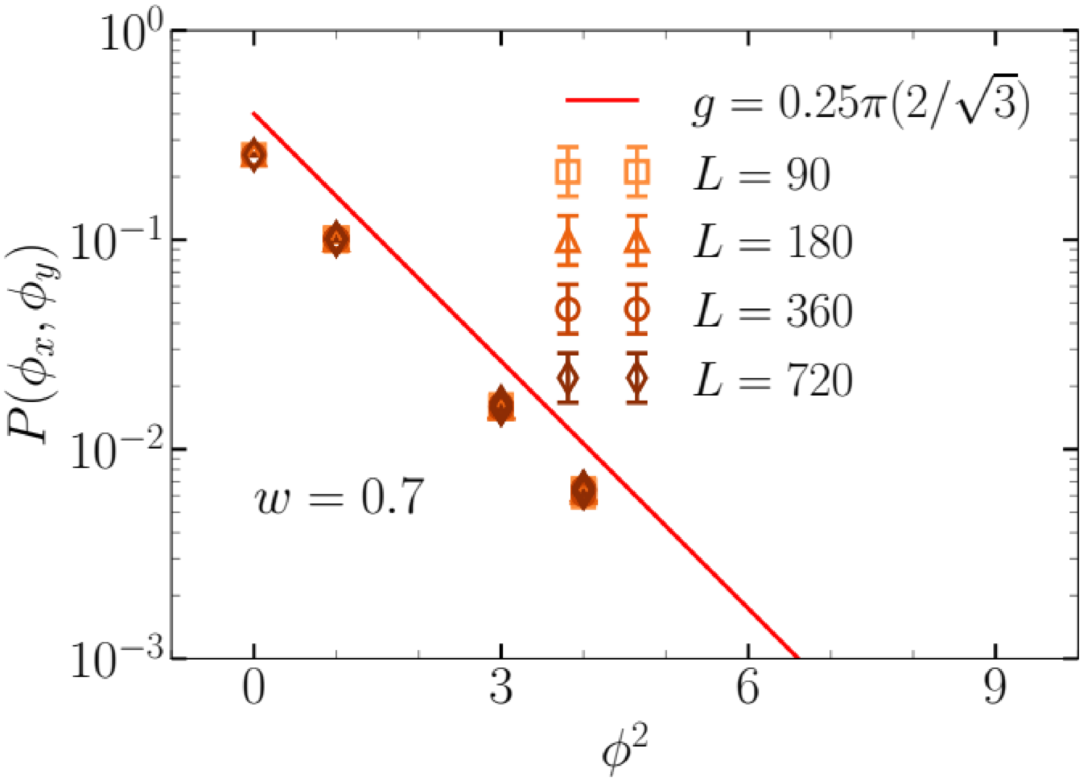
Jay Pandey & KD, unpublished

Answering this...



Jay Pandey & KD, unpublished

Answering this...



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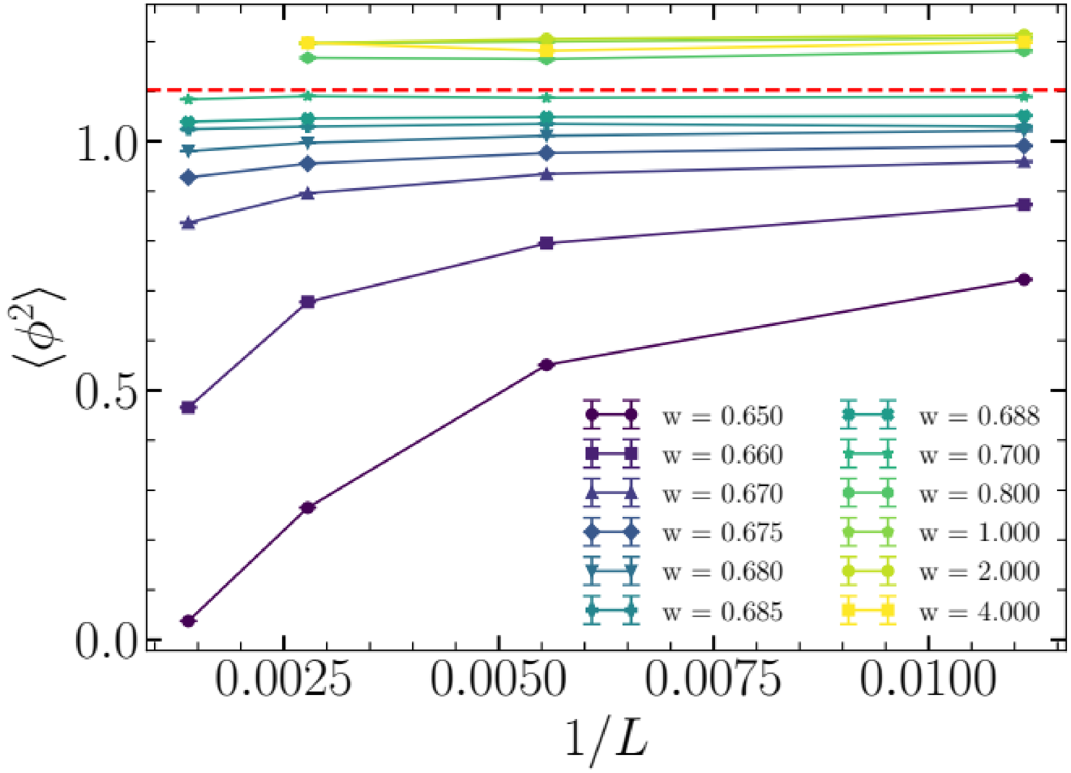
Answering this...



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3. Competing anisotropies and the S=1 pyrochore in zero field

Representative Hamiltonian:

$$H_{eff} = J^z \sum_{rr'} S^z_r S^z_{r'} + \Delta \sum_r (S^z_r)^2 + \cdots$$

$J^z = J \;, \quad \Delta = J + \mu$

$T, \; \mu \ll J$

Quantum fluctuations, additional interactions negligible $(J_\perp \,, \; J' \ll T)$

zero field physics: Each pyrochlore tetrahedron has: $S^z = 0$ (Large $\mathcal{O}(J)$ energy gap to other values)

Multiple ways to add up to $S^z = 0$: (with slightly different energies)

(a “vertex model” on the diamond lattice)

Each $S^z_r = \pm 1$ contributes one factor of $w = \exp(-\beta\mu)$ to the Boltzmann weight

Jay Pandey & KD, unpublished

4. Competing anisotropies and the S=3/2 pyrochore in zero field

Representative Hamiltonian:

$$H_{eff} = J^z \sum_{rr'} S^z_r S^z_{r'} + \Delta \sum_r (S^z_r)^2 + \cdots$$

$J^z = J \;, \quad \Delta = J + \mu$

$T,\ \mu \ll J$

Quantum fluctuations, additional interactions negligible $(J_\perp \,,\ J' \ll T)$

zero field physics: Each pyrochlore tetrahedron has: $S^z = 0$ (Large $\mathcal{O}(J)$ energy gap to other values)

Multiple ways to add up to $S^z = 0$: (with slightly different energies)

(a "vertex model" on the diamond lattice)

Each $S^z_r = \pm 3/2$ contributes one factor of $w = \exp(-2\beta\mu)$ to the Boltzmann weight

Jay Pandey, Souvik Kundu, & KD, unpublished

Description in terms of fluctuating polarization field and vector potential

Divergence-free polarization on diamond links: $P_{A\to B} = S^z_{r_{AB}}$

$S^z_{\mathrm{tetrahedron}} = 0$ implies $\Delta \cdot P = 0$

Periodic boundary conditions: Three independent integer-valued fluxes of polarization field well-defined

Microscopic height construction: $P = \Delta \times A$

Expect coarse-grained theory: $S = \frac{K}{2} \int (\nabla \times a)^2$

Question(s):

Is there a smooth crossover from small w to large w, or thermodynamic phase transitions?

Our answers-

Three phases in the S=1 case:
small-w paramagnet, intermediate-w flux-deconfined Coulomb, & large-w flux-confined Coulomb phases. (with intervening 3dxy transition followed by flux confinement-deconfinement transition with Z_2 character.

Jay Pandey & KD, unpublished

Two phases in the S=3/2 case:
Small-w flux-deconfined Coulomb phase separated from large-w flux-confined Coulomb phase by a first order flux confinement-deconfinement transition with Z_3 character

Jay Pandey, Souvik Kundu, & KD, unpublished

Answering these questions in both cases: Vertex model partition function

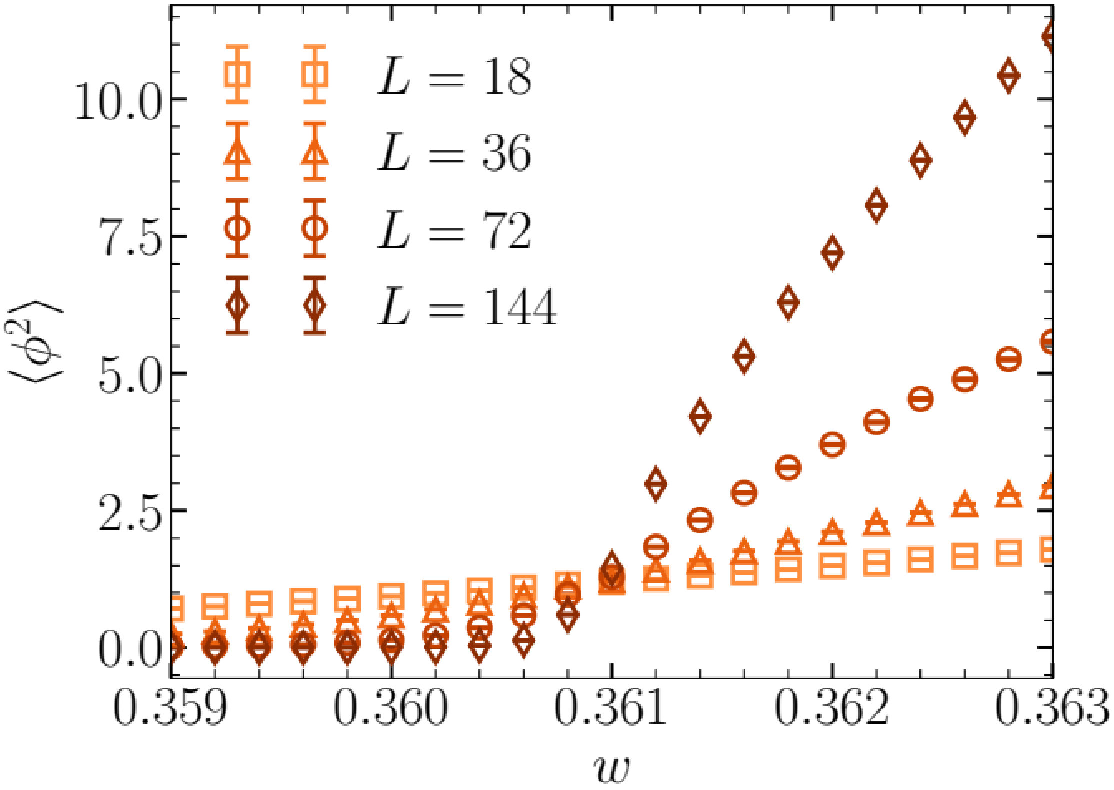
$$Z = \sum_{\mathcal{C}} w^{n(\mathcal{C})}$$

$$w = \exp(-c\mu/T)$$

Physics of S=1 and S=$3/2$ pyrochlore magnets described by respective vertex models on diamond lattice

Tool: Classical Monte Carlo using a worm algorithm

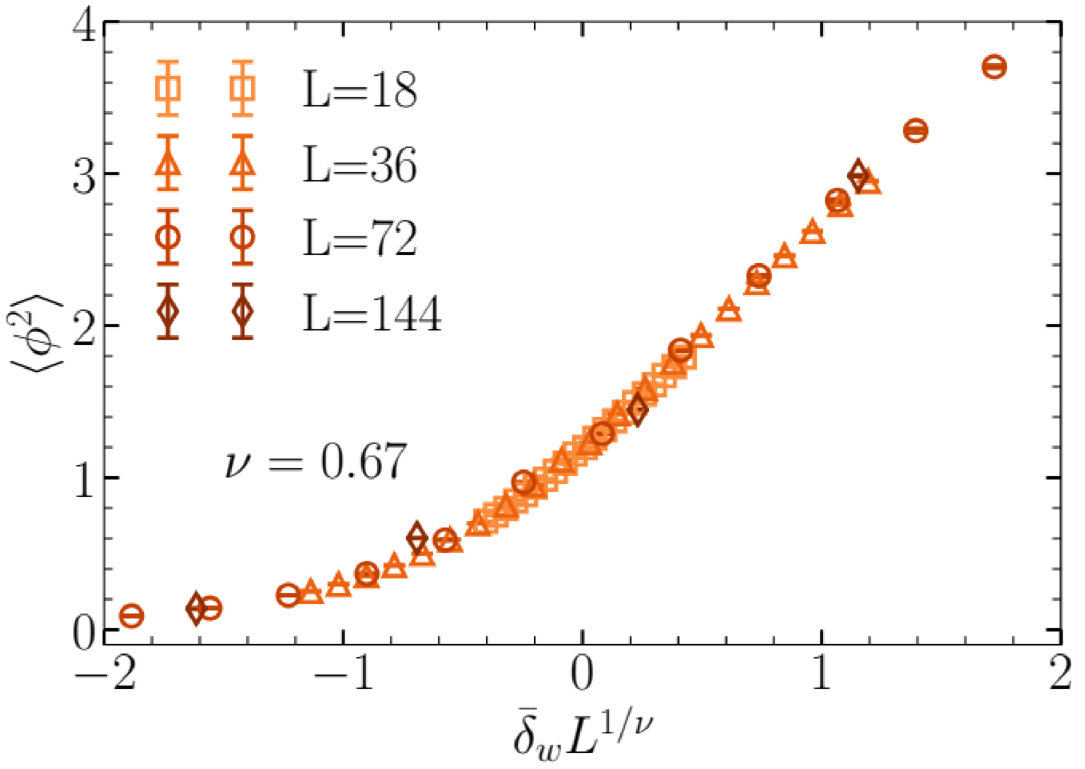
Answering this question for S=1 case...



“Insulator-Superfluid” transition from paramagnet to flux-deconfined Coulomb phase

Jay Pandey & KD, unpublished

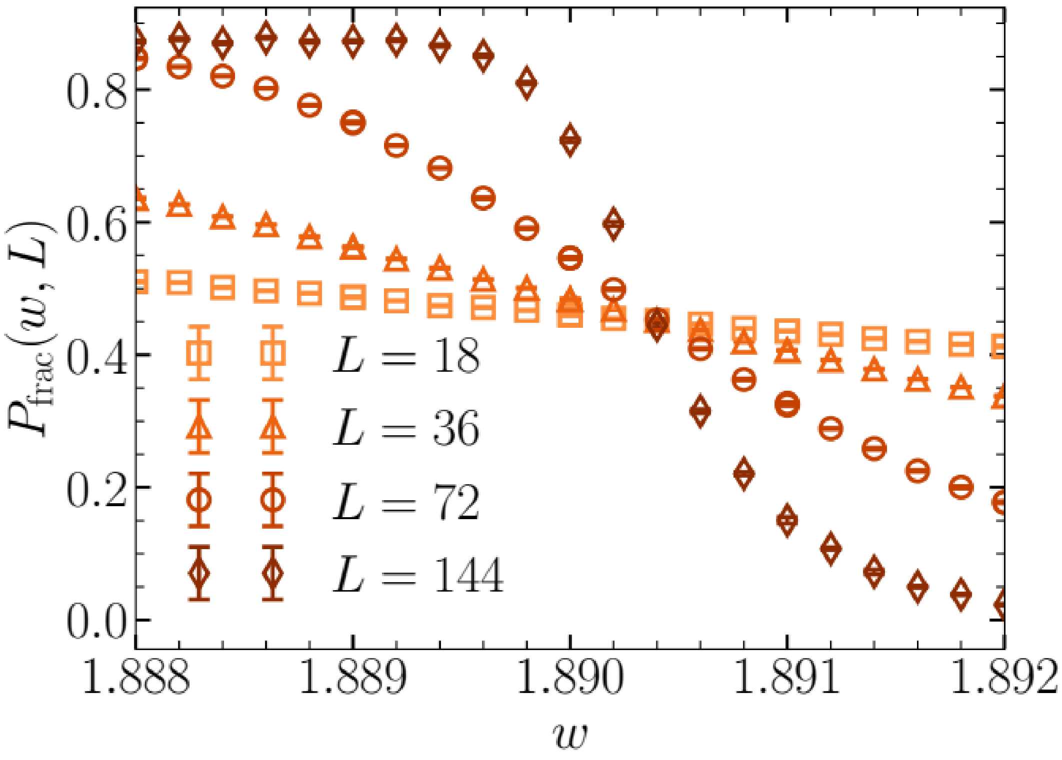
Answering this question for S=1 case...



"Insulator-Superfluid" transition from paramagnet to flux-deconfined Coulomb phase

Jay Pandey & KD, unpublished

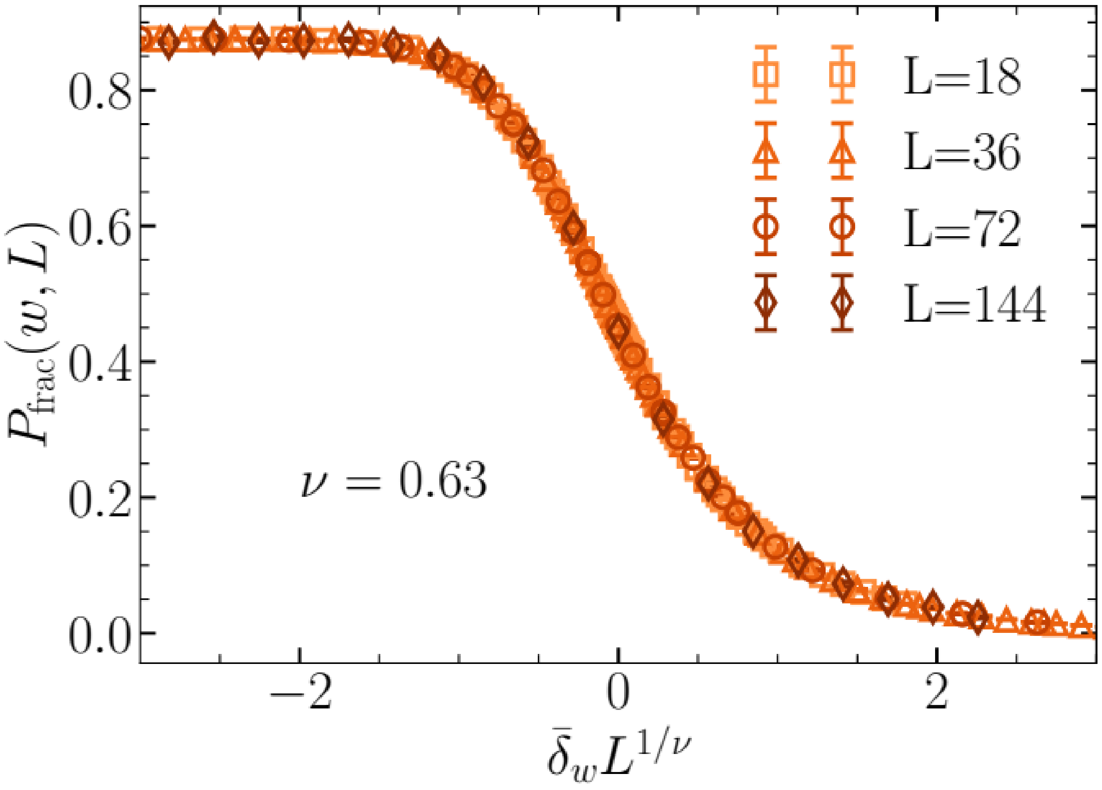
Answering this question for S=1 case...



Z_2 Flux confinement-deconfinement transition between two Coulomb phases

Jay Pandey & KD, unpublished

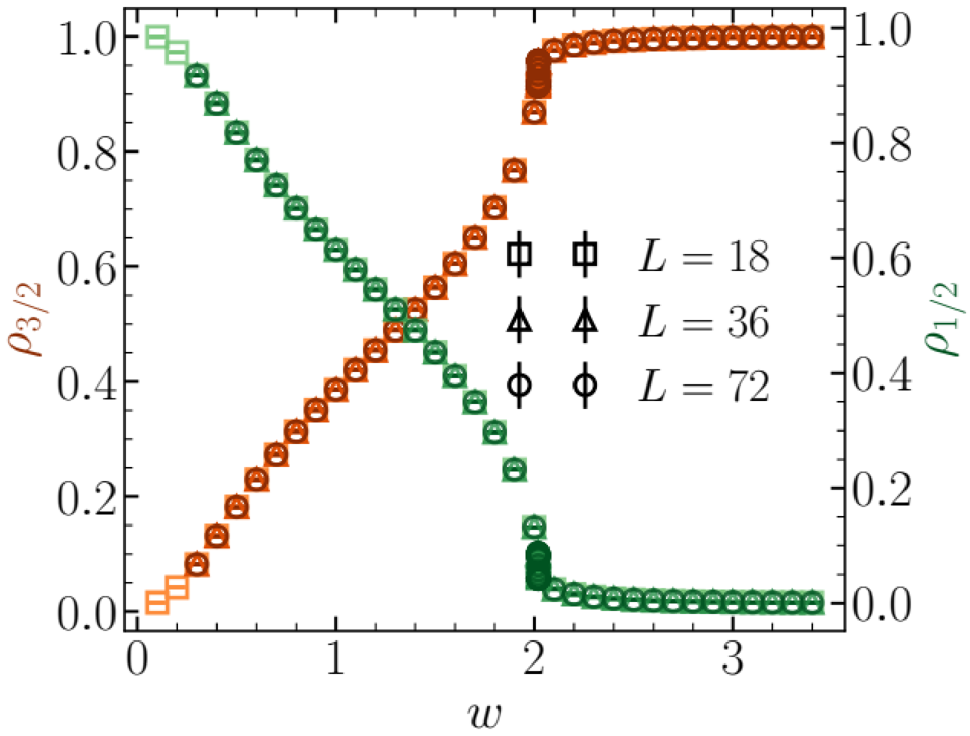
Answering this question for S=1 case...



Z_2 Flux confinement-deconfinement transition between two Coulomb phases

Jay Pandey & KD, unpublished

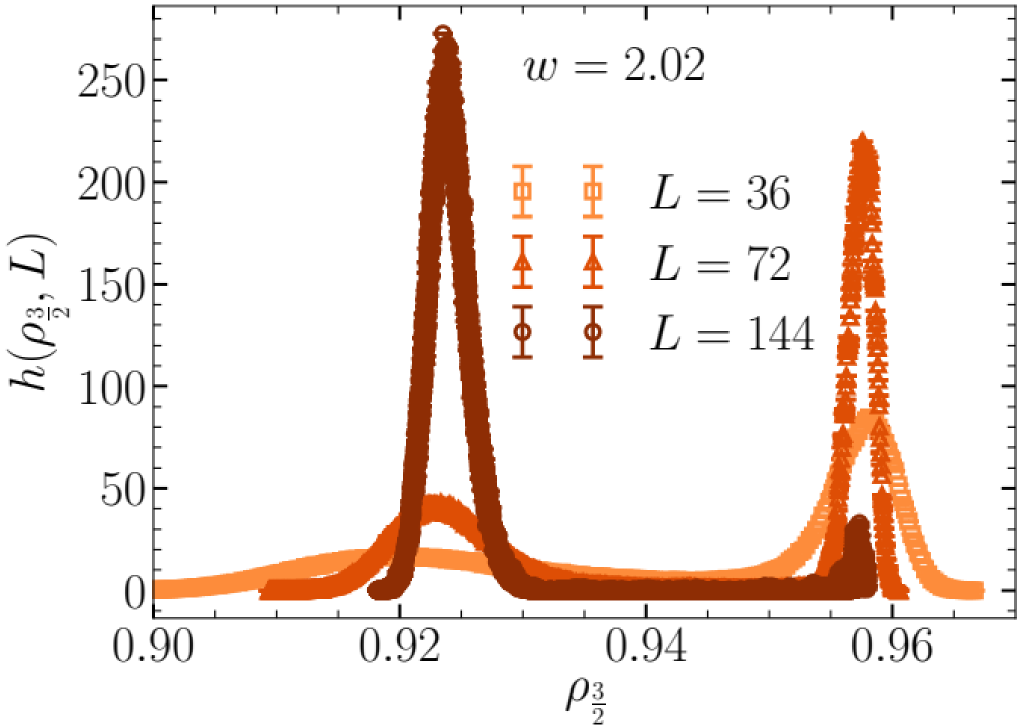
Answering this in the S=3/2 case...



First-order transition between two Coulomb phases

Jay Pandey, Souvik Kundu, & KD, unpublished

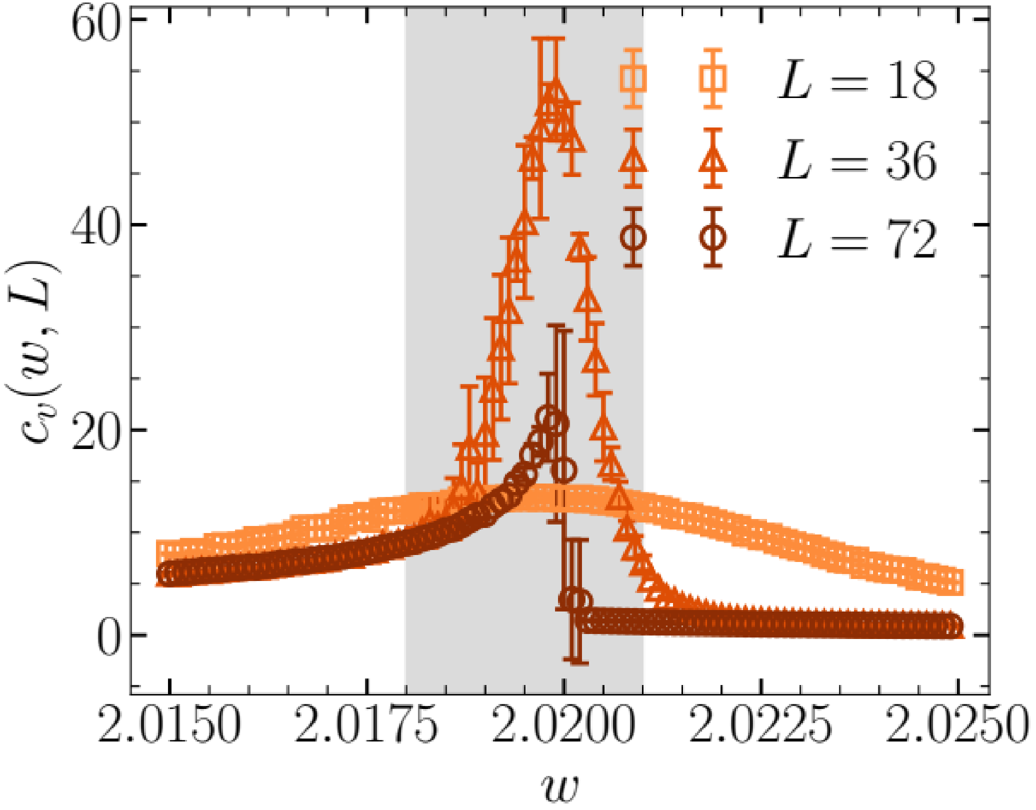
Answering this in the S=3/2 case...



First-order transition between two Coulomb phases

Jay Pandey, Souvik Kundu, & KD, unpublished

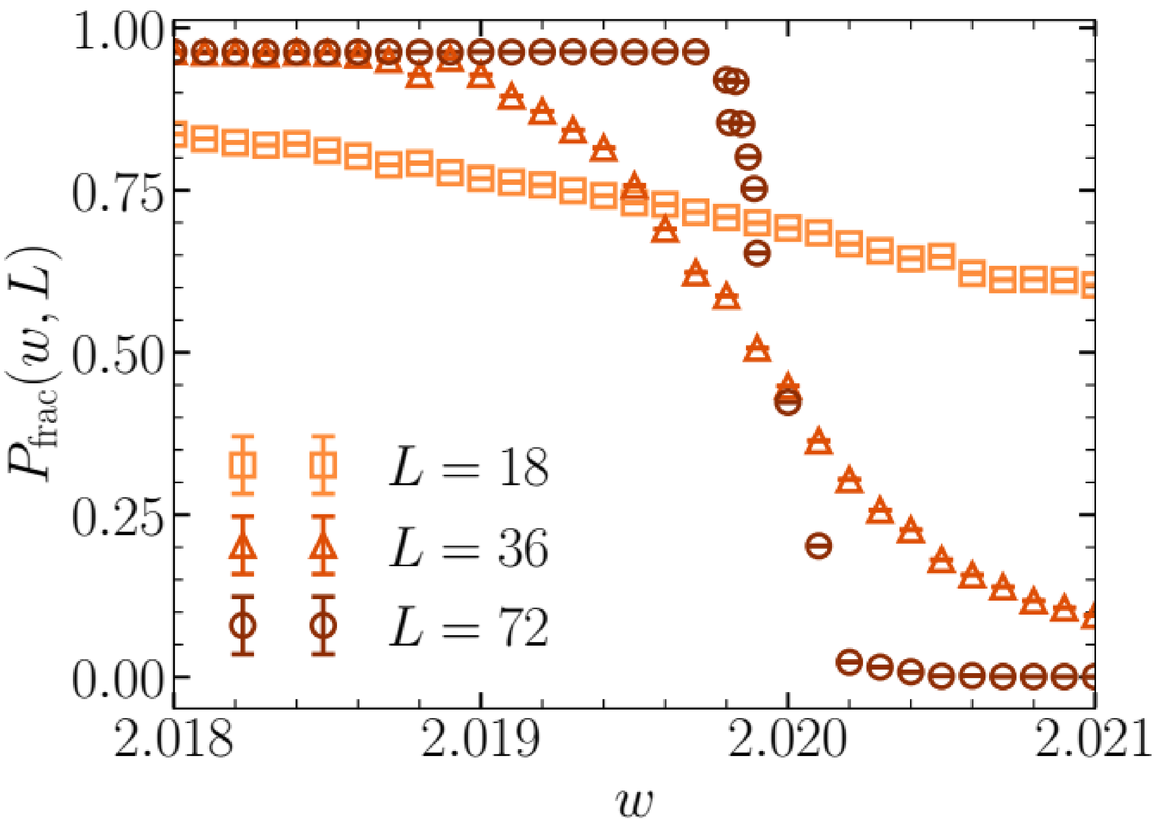
Answering this in the S=3/2 case...



First-order transition between two Coulomb phases

Jay Pandey, Souvik Kundu, & KD, unpublished

Answering this in the S=3/2 case...



Transition is a Z_3 flux confinement-deconfinement transition between two Coulomb liquids

Jay Pandey, Souvik Kundu, & KD, unpublished

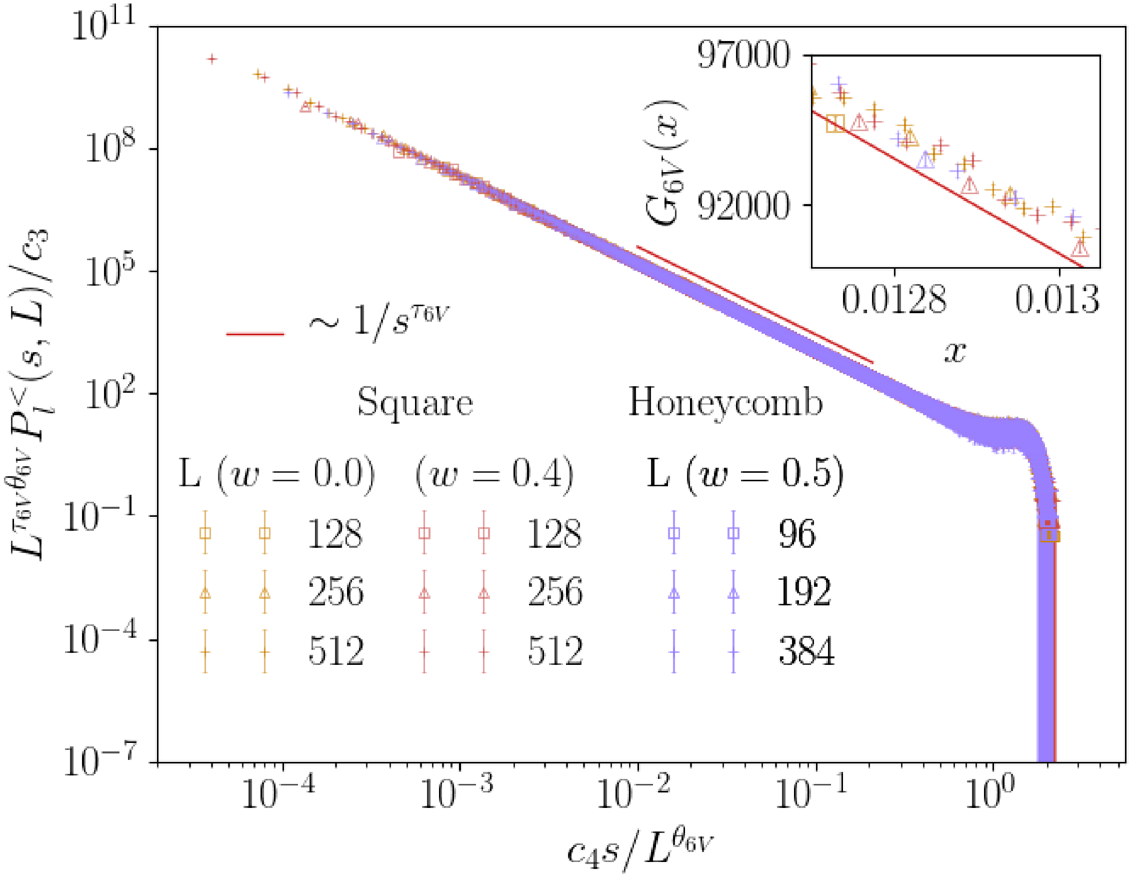
Acknowledgements

Crucial enablers: Computational resources @ TIFR & TIFR sys-ads Kapil Ghadiali and Ajay Salve

Supplementary

Slide(s) used in response to question during talk...

Universal loop size distribution in 2d long-loop phase



$$\tau_{6\mathrm{V}} = \frac{15}{7} \quad \theta_{6\mathrm{V}} = \frac{7}{4}$$

Note scaling relation:

$$\tau_{6\mathrm{V}}\theta_{6\mathrm{V}} = \theta_{6\mathrm{V}} + 2$$

O(1) loops with

$$s \sim L^{\theta_{6\mathrm{V}}}$$