

# 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Jay Pandey, Souvik Kundu, & KD, unpublished

Jay Pandey & KD arXiv:2512.11623; unpublished

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## One slide summary

Competition between two different manifestations of spin-orbit 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:

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

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

$$T, \mu \ll J$$

Quantum fluctuations, additional interactions are small  $(J_{\perp}, J' \ll T)$

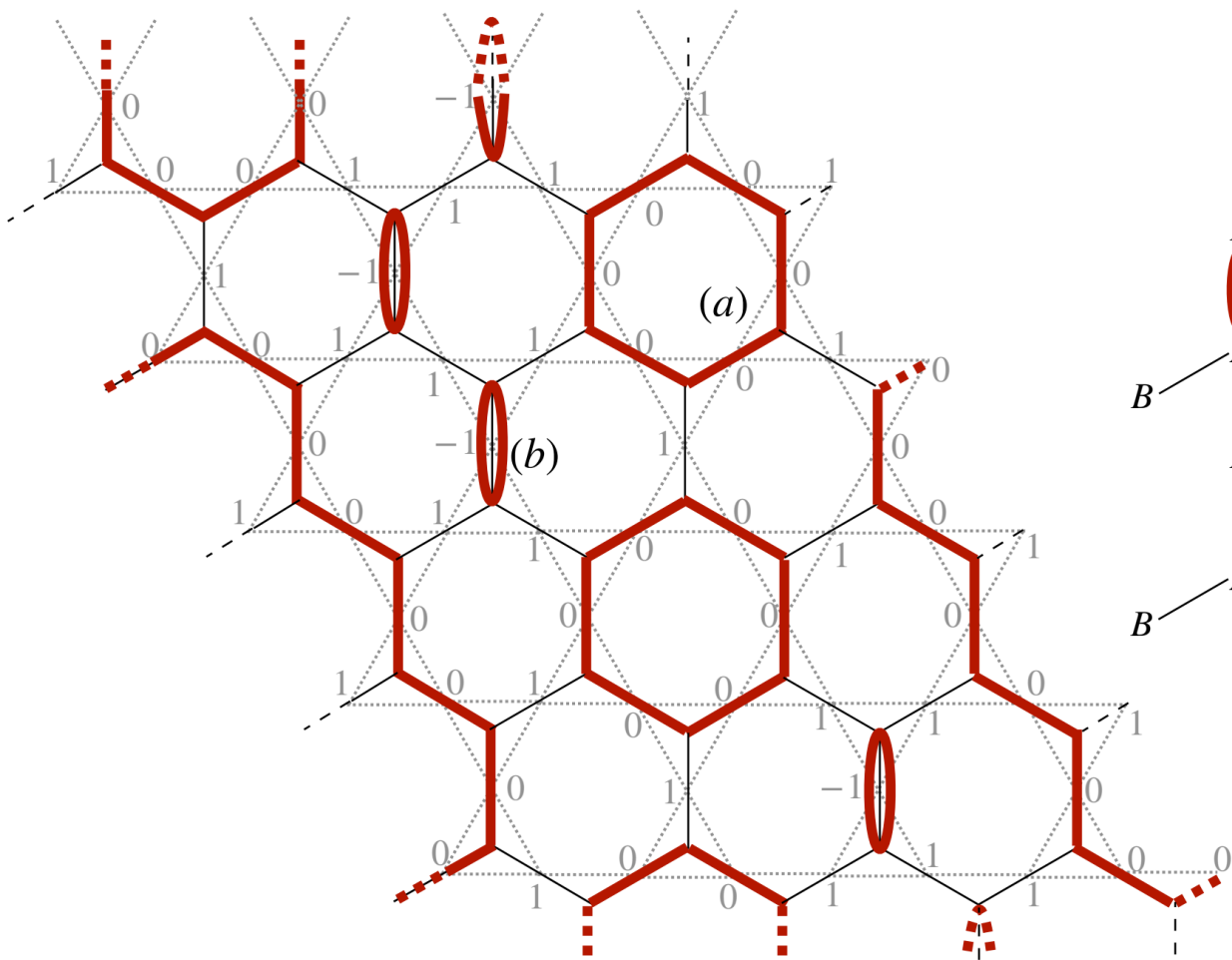
One-third magnetization plateau

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

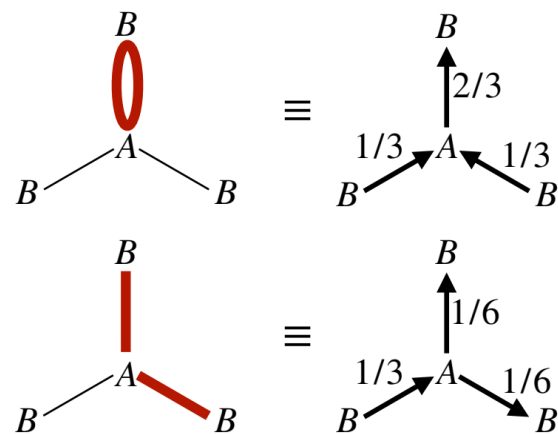
Each kagome triangle has:  $S^z = 1$

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)

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



Divergence-free polarization



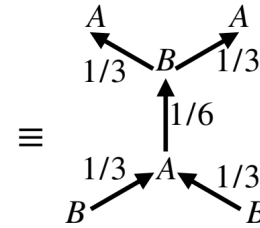
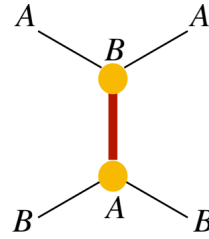
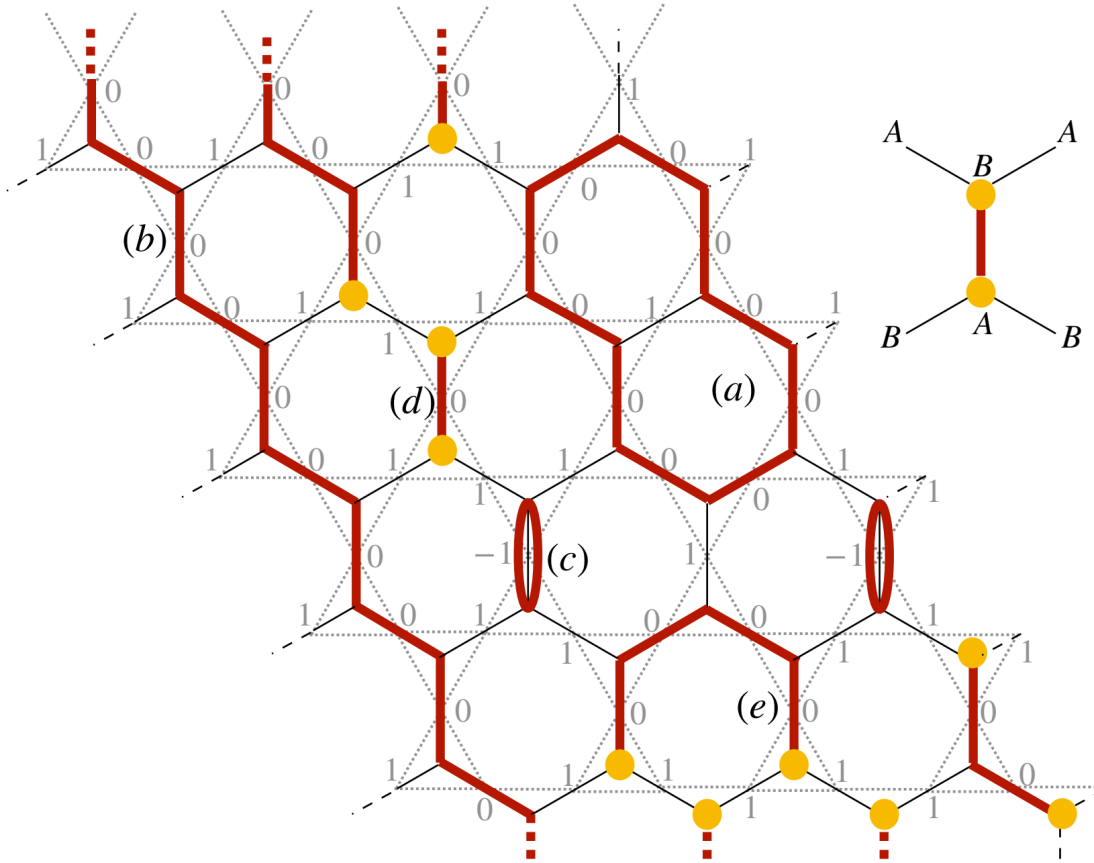
$$\Delta \cdot P = 0$$

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)

## 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

## Coarse-grained height field-theory

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

$h$  is an angle:

$h \rightarrow h+1$  redundancy in pure dimer limit

$h \rightarrow h+1/2$  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  $h \rightarrow h+1/2$  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
- Puts a bound on test unit-vortex correlator
- Periodic boundary conditions: Two independent fluxes of polarization field (winding numbers for height field) are well-defined
- Fluxes are allowed to be half-integer in general except in pure dimer limit.

## Measurements

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

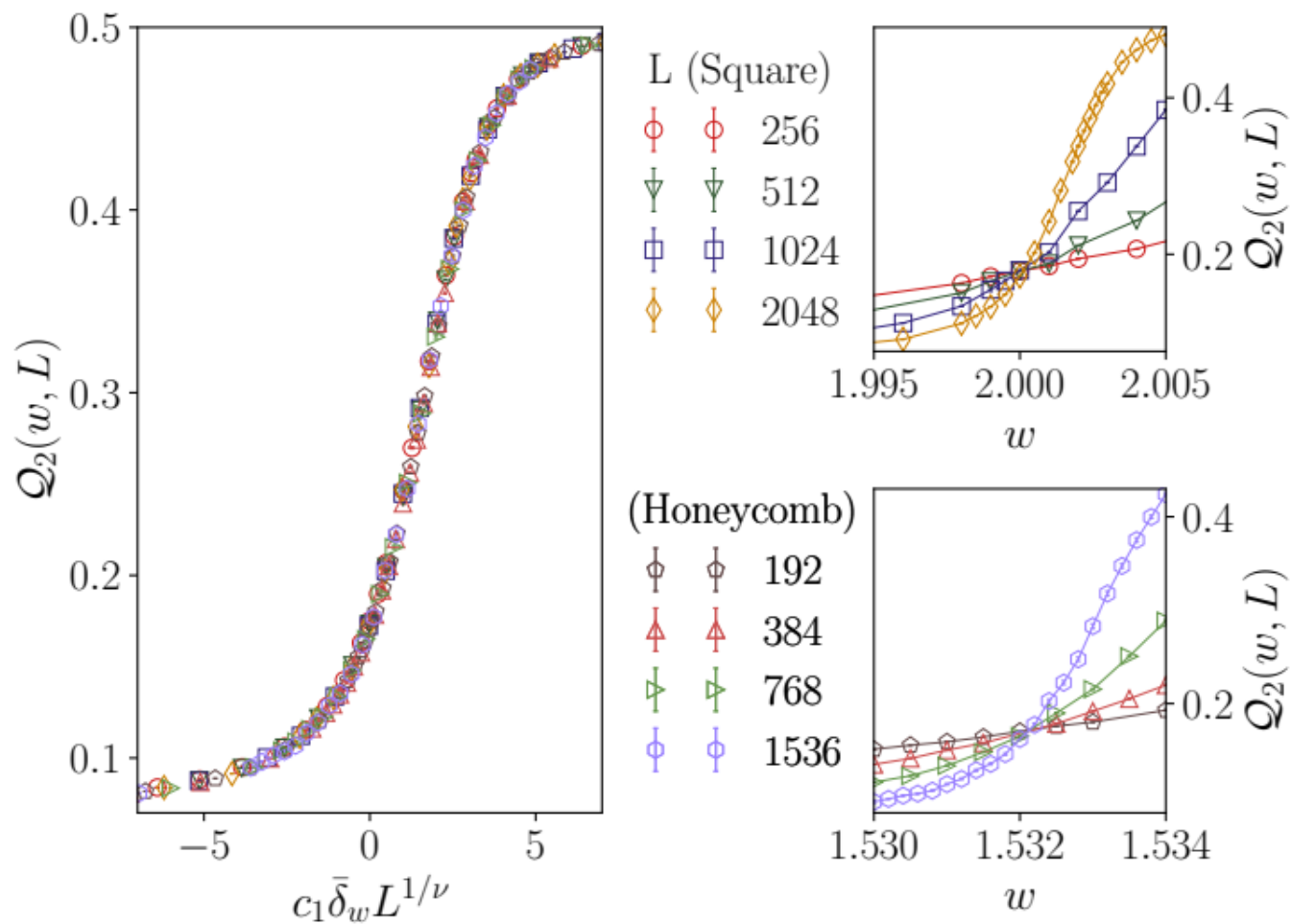
Loop-size Binder ratio  $Q_2 = \langle \sum_{i \neq j} s_i^2 s_j^2 \rangle / S_2^2$

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

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

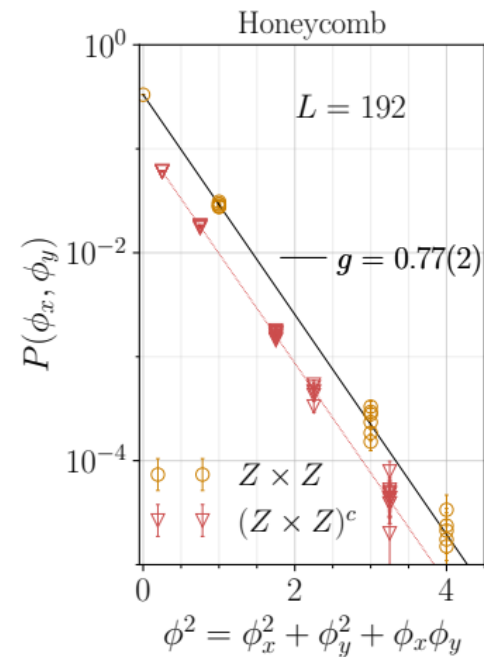
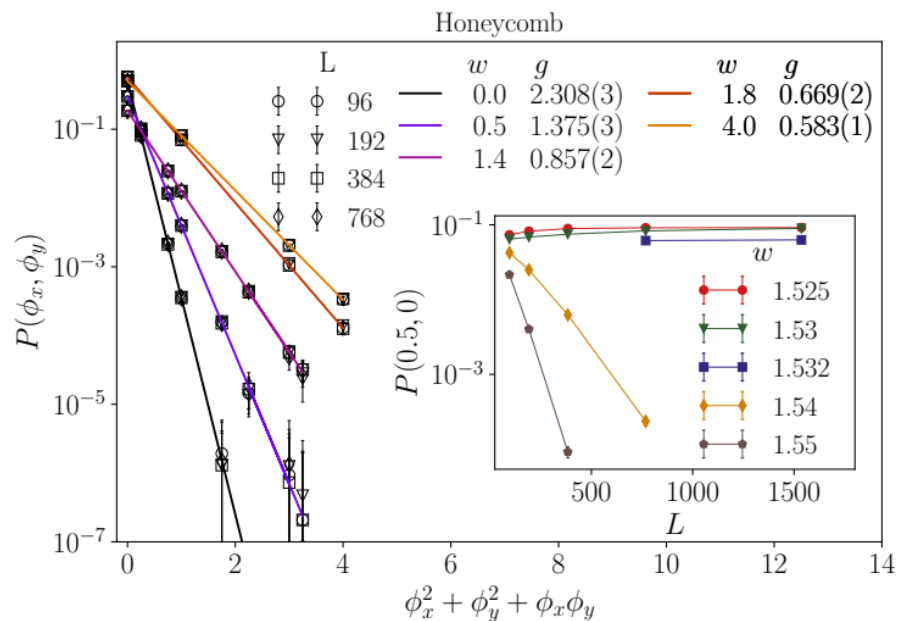
Three-sublattice spin order parameter and half/unit-vortex correlators  $C_\psi(r)$   $C_v^q(r)$  for  $q = 1/2, 1$

## Geometric characterization: short-to-long loop phase transition



$$\nu \approx 1.00(2)$$

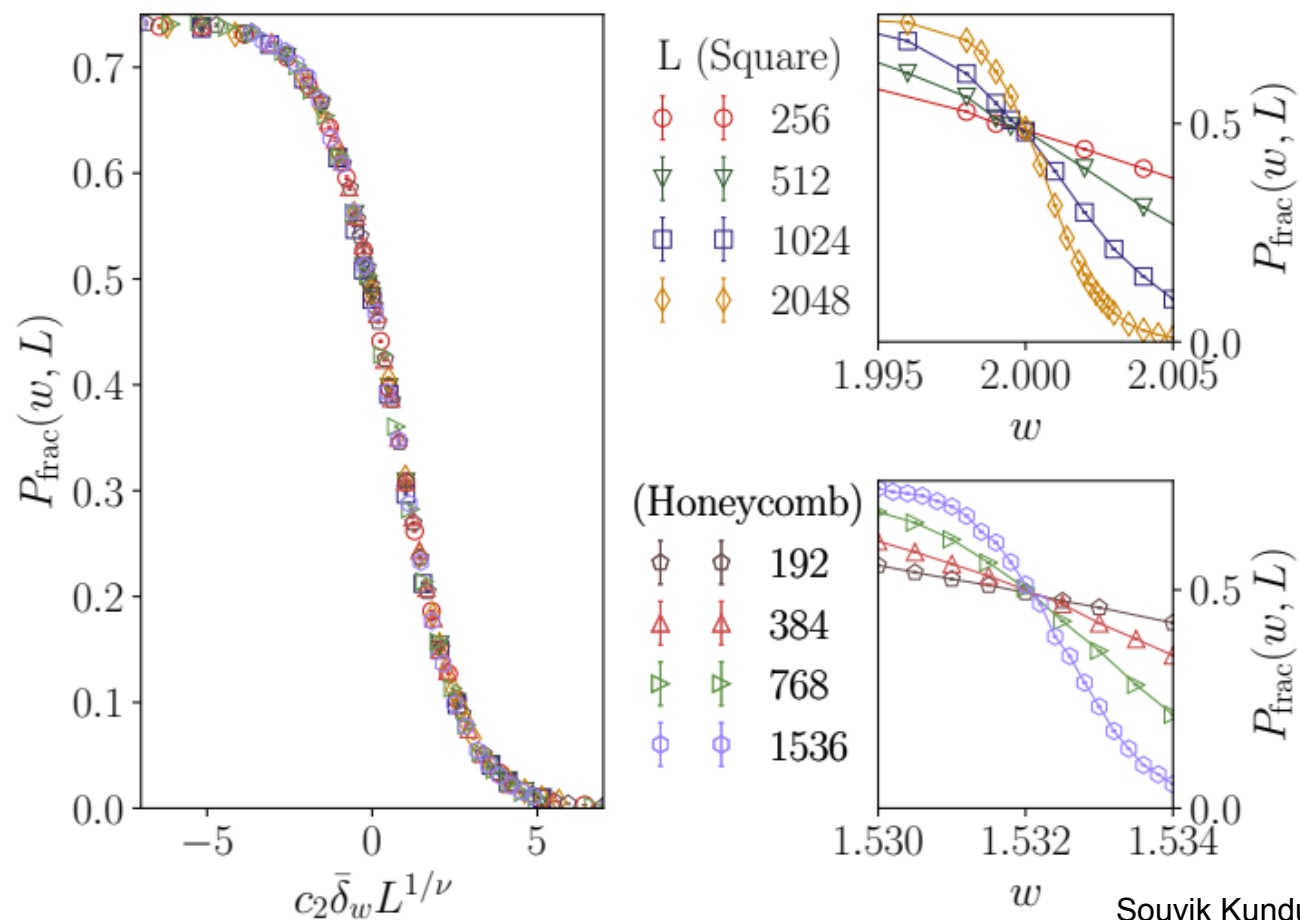
# Topological characterization: Flux confinement-deconfinement transition



$$P(\phi_x, \phi_y) \propto \exp \left[ -\pi g (\phi_x^2 + \phi_y^2 + \phi_x \phi_y) \right]$$

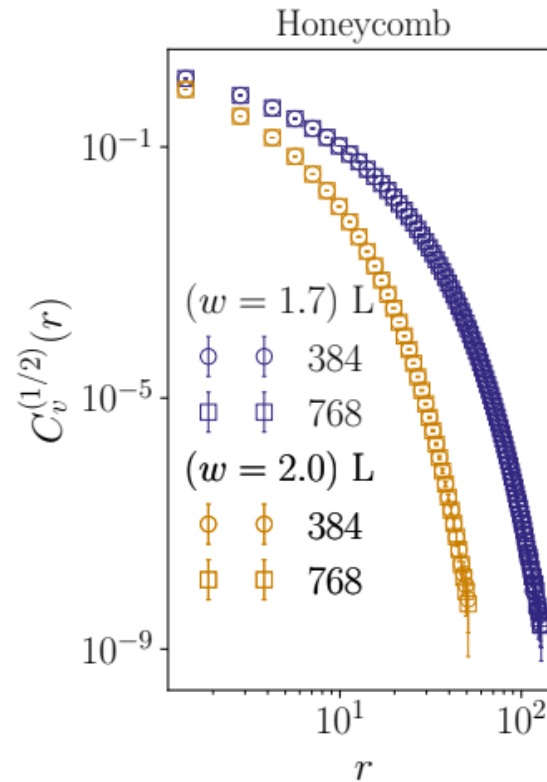
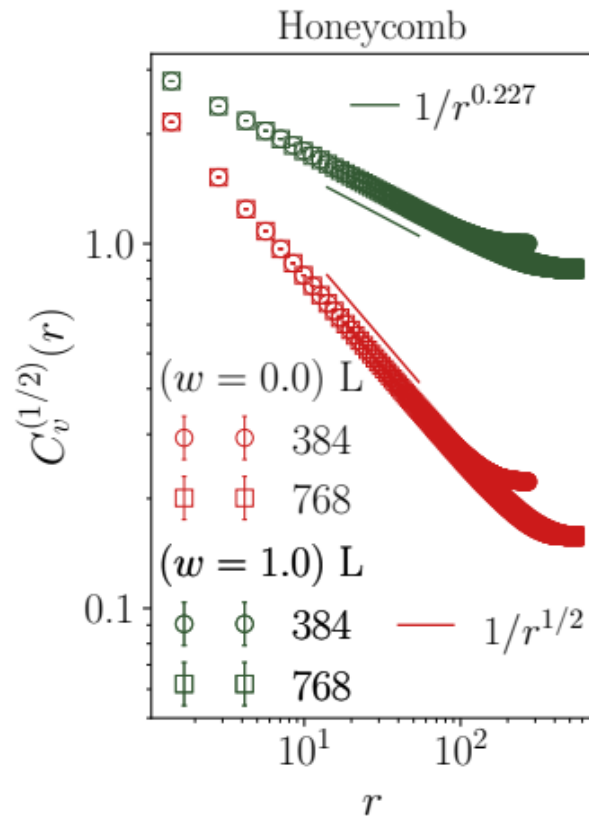


## Topological characterization: Flux confinement-deconfinement transition



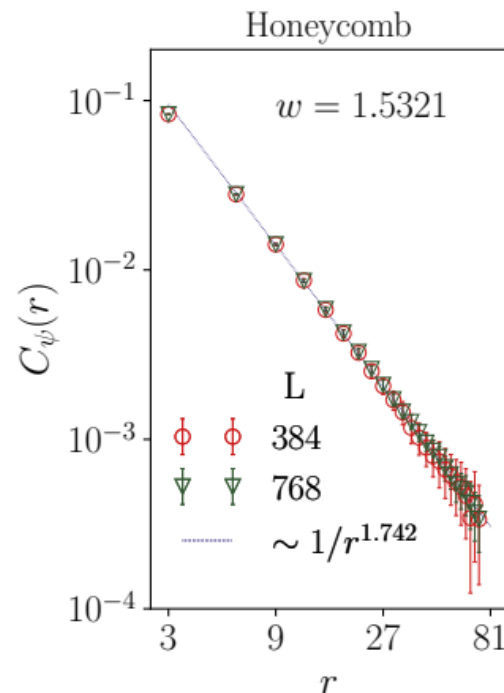
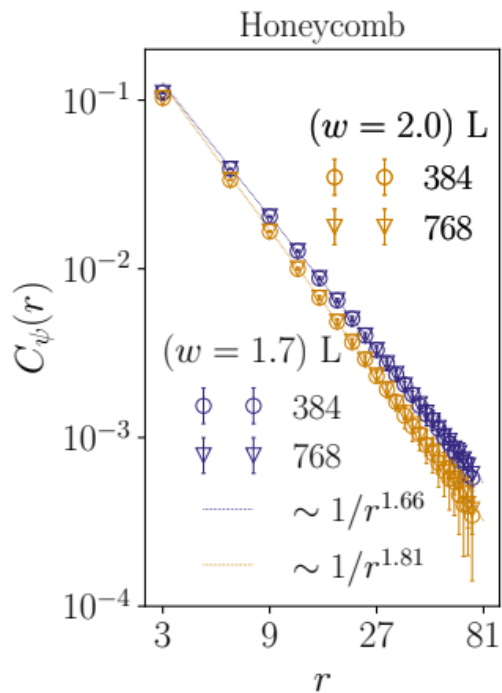
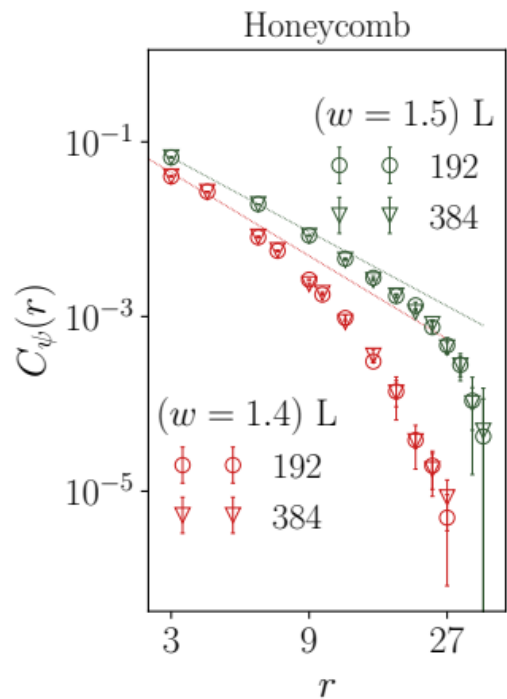
$$\nu \approx 1.00(2)$$

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

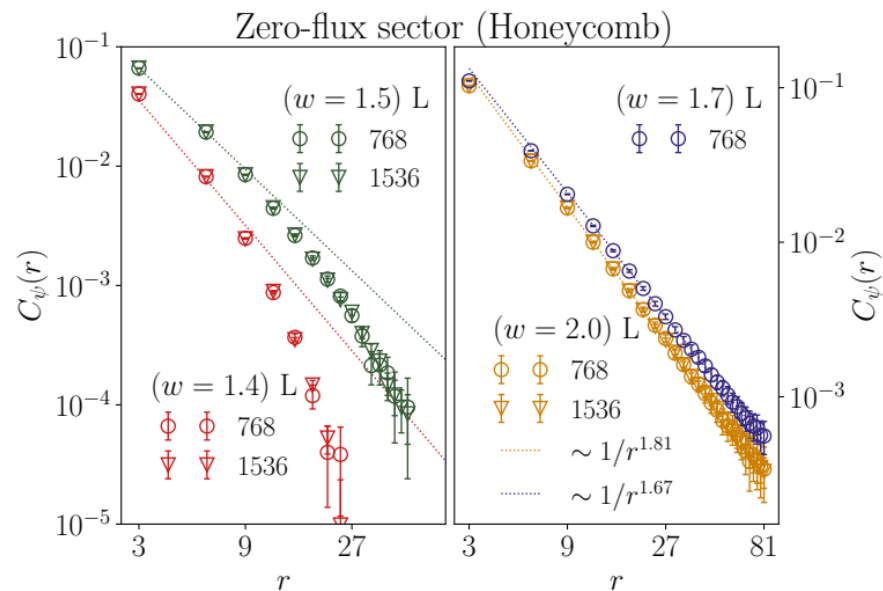
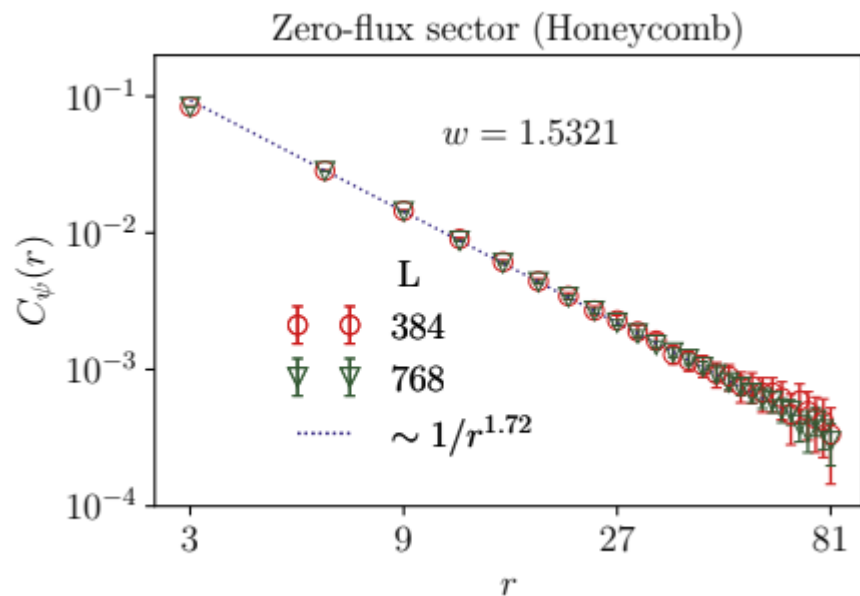


## Transition in kagome spin three-sublattice correlations

$$\langle e^{2\pi i h(r)} e^{-2\pi i h(0)} \rangle \sim \frac{1}{r^{2/\sqrt{3}g}} \quad (\text{but: operator is illegal in flux deconfined phase})$$

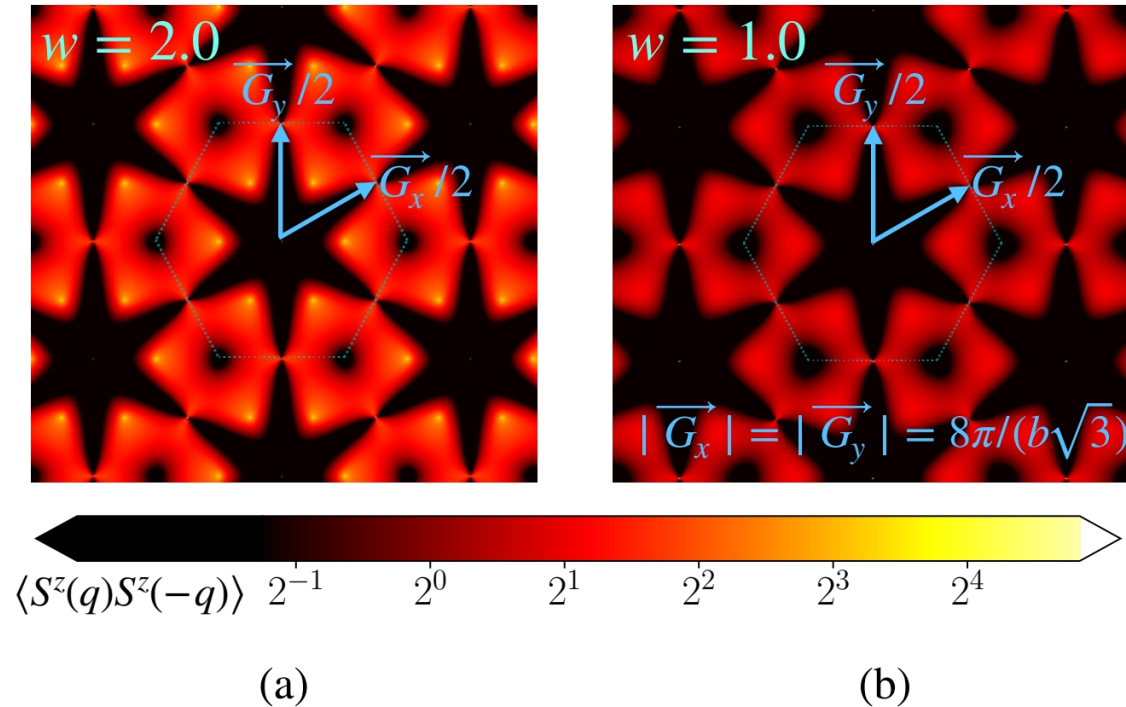


Not an artifact of periodic boundary conditions...



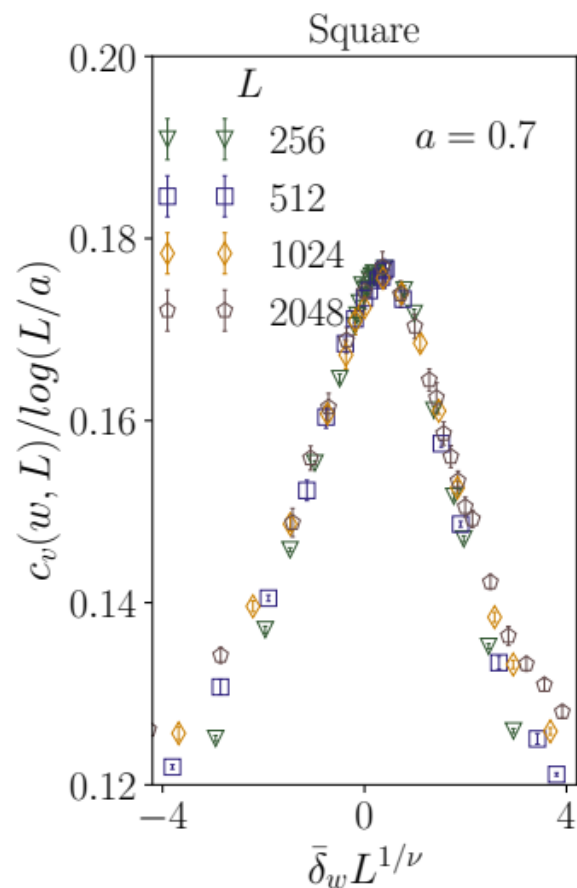
## Transition observable in kagome spin structure factor

$$L = 96$$

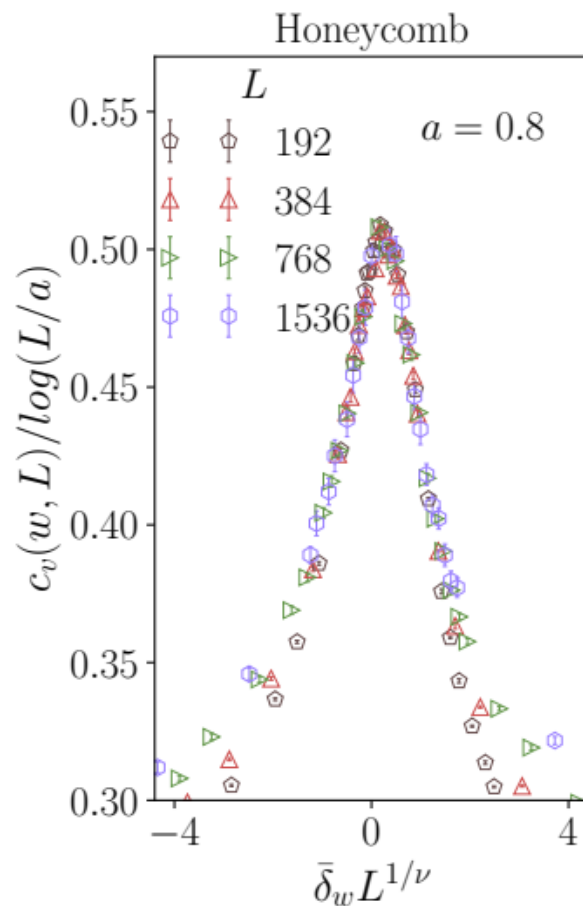


Power-law feature at three sublattice wavevector absent in long-loop phase

## Thermodynamic characterization: Specific heat singularity



Ising-like



## 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 (jump in compactification radius)

**Dynamical:** Half-vortices are deconfined in one phase but not other (unit vortices always deconfined)

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

**Ising transition:** Hidden Ising order parameter

## “Hidden” Ising order parameter

View each non-trivial loop as a domain wall

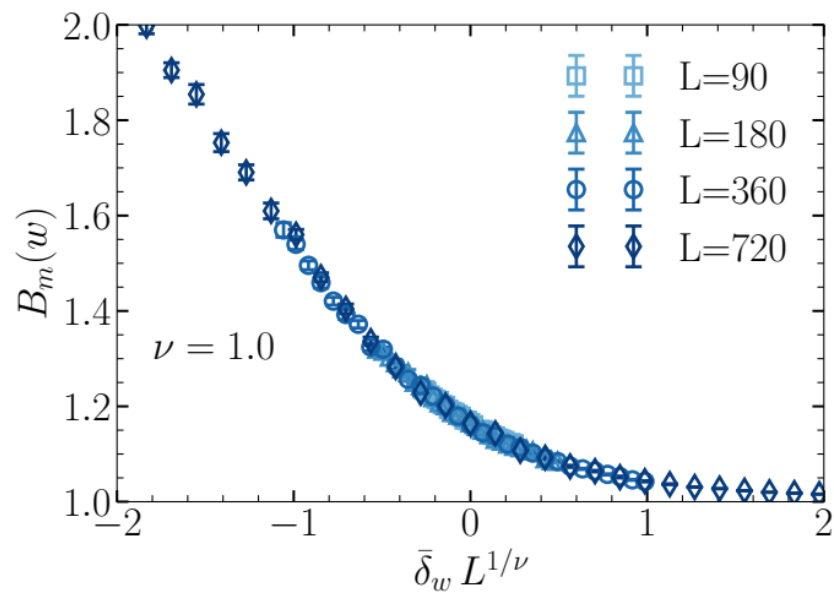
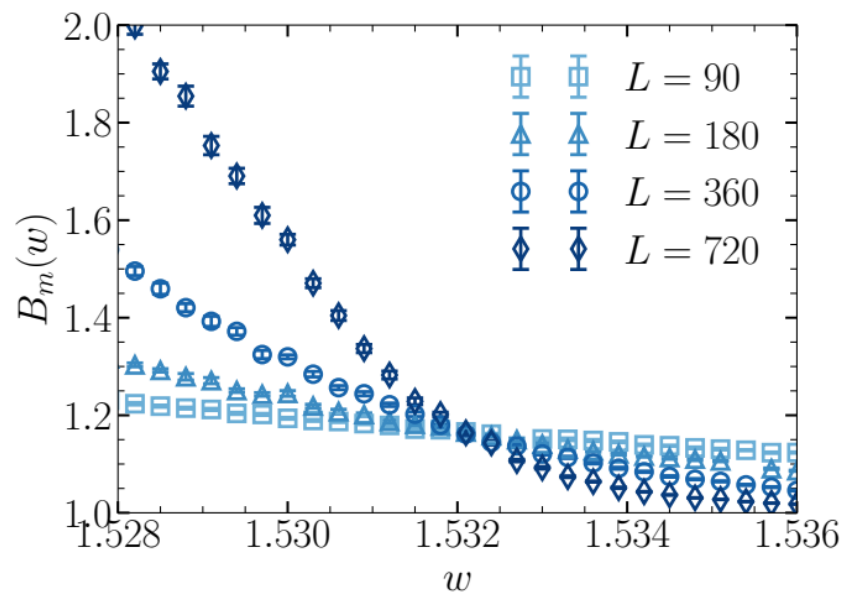
Fine print:

Ising variable only defined for integer flux sectors.

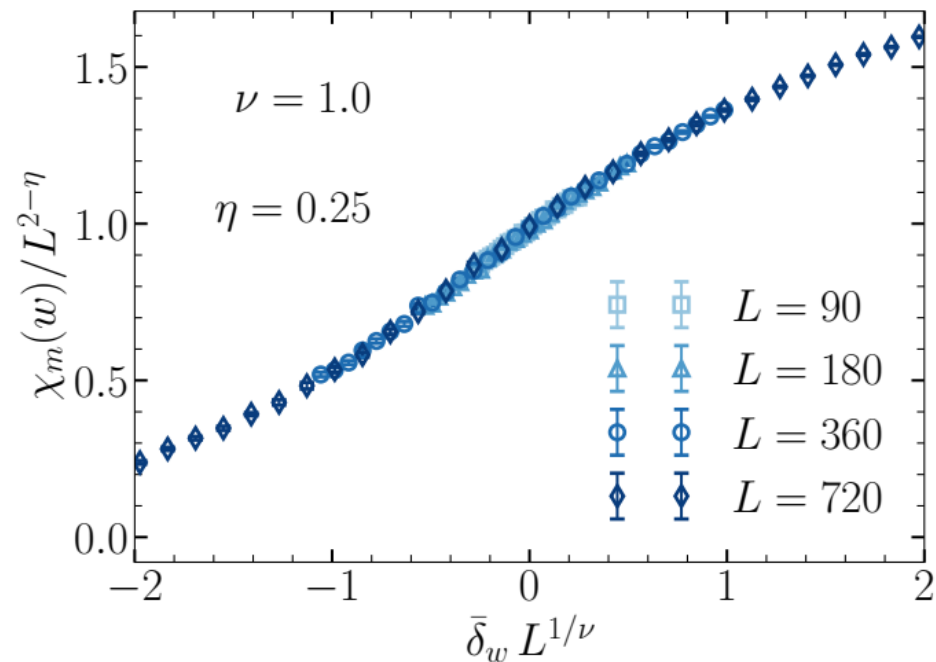
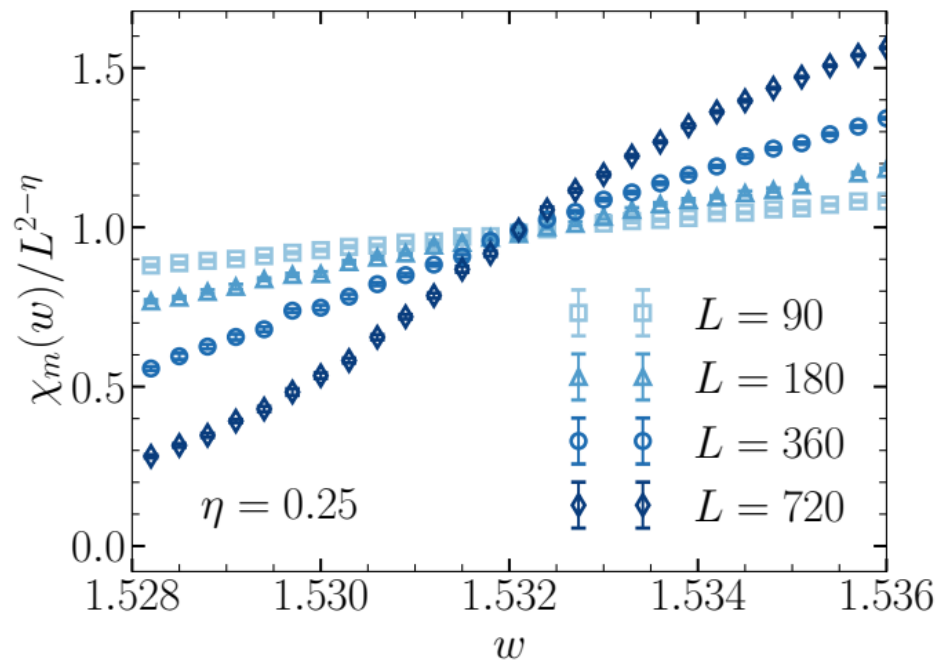
and each dimer-loop state maps to pair of Ising configurations  $\mathcal{C}_I$  and  $\mathcal{C}_I^*$



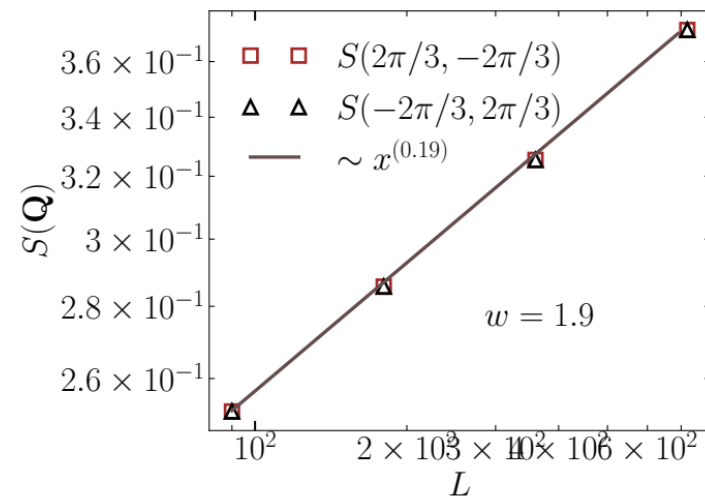
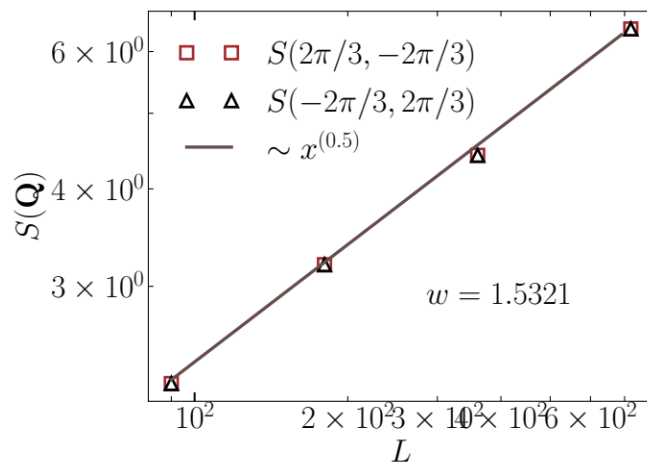
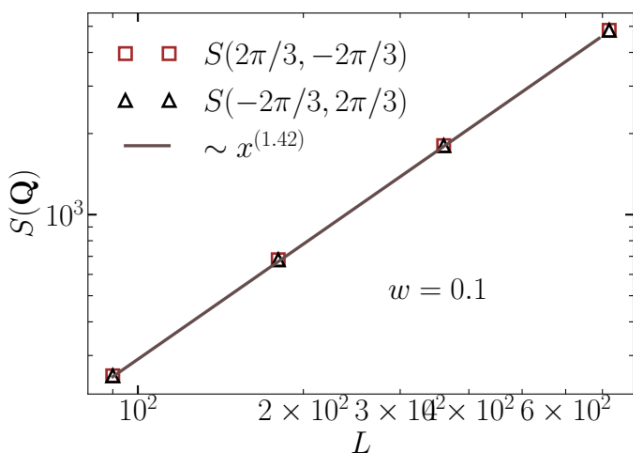
## Ferromagnetic transition seen by Ising Binder ratio



## Ferromagnetic transition seen by Ising susceptibility



Aside: Ising variable has power-law three-sublattice order in both phases



Consistent with:

$$\langle e^{2\pi i h(r)} e^{-2\pi i h(0)} \rangle \sim \frac{1}{r^{2/\sqrt{3}g}}$$

$$S(\mathbf{Q}) \sim L^{2-\eta} \quad \eta = 2/\sqrt{3}g$$

## 2. S=1 kagome in zero field

Representative Hamiltonian:

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

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

$$T, \mu \ll J$$

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

## Description in terms of fluctuating polarization field and heights

Divergence-free polarization on honeycomb links:  $P_{r_{AB}} = S_{r_{AB}}^z \mathbf{e}_{AB}$

$$S_{\Delta}^z = 0 \text{ implies } \Delta \cdot P = 0$$

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:  $h \rightarrow h+1$  redundancy

## Question:

$w=0$  is trivial paramagnet, while infinite  $w$  maps to a  $O(2)$  honeycomb loop model.

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

Viewing polarization field as divergence-free current in current-loop representation of 2dxy model:

Expect an (inverted) KT transition driven by relevance of  $\exp(\pm 2\pi i h)$  (?)

$$\langle e^{2\pi i h(r)} e^{-2\pi i h(0)} \rangle \sim \frac{1}{r^{2/\sqrt{3}g}} \quad \text{would imply transition when } 2/\sqrt{3}g = 4$$

Answering this: Vertex model partition function

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

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

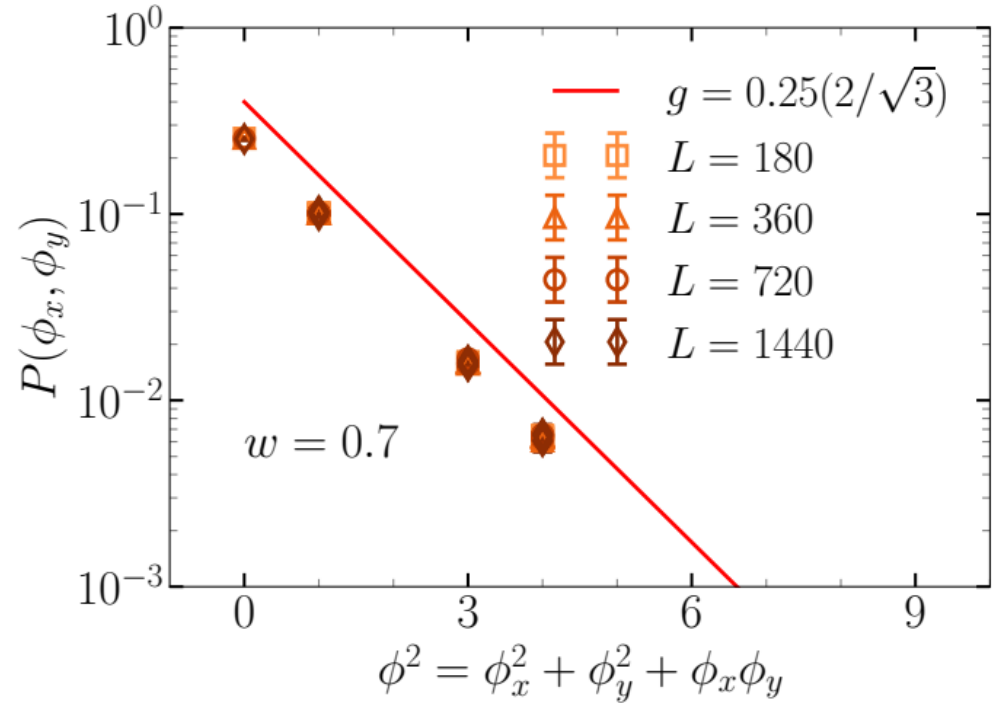
Physics of kagome magnet described in terms of vertex model partition function on honeycomb lattice

Tool: Classical Monte Carlo using a worm algorithm

## Spin 1 kagome in zero field

$$P(\phi_x, \phi_y) \propto \exp \left[ -\pi g (\phi_x^2 + \phi_y^2 + \phi_x \phi_y) \right]$$

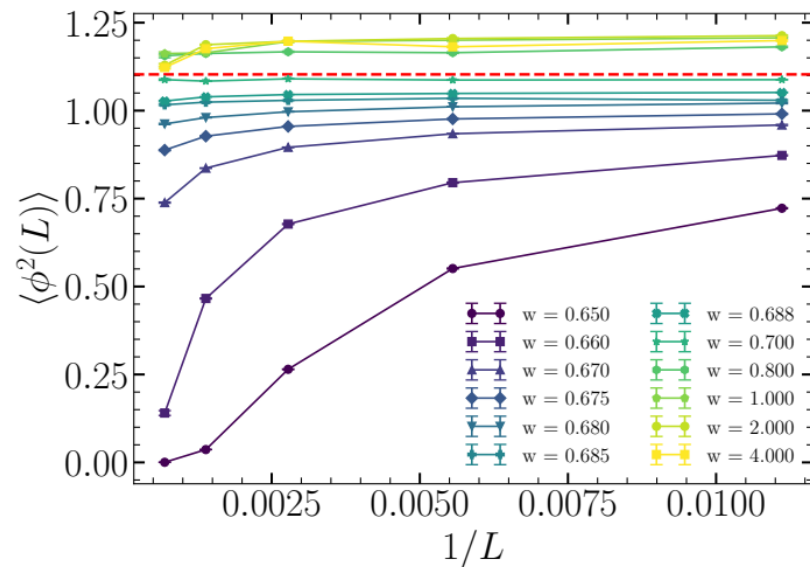
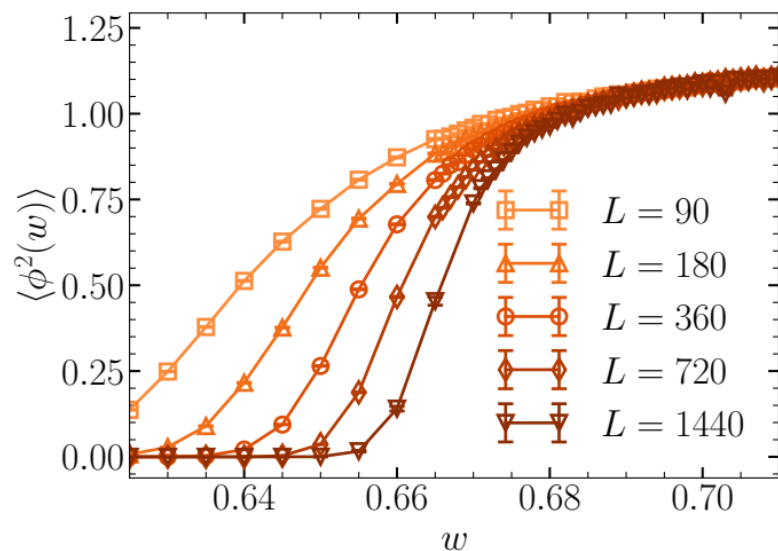
Scaling argument would  
suggest transition at  $w=0.7$





## S=1 kagome in zero field

Analog of superfluid stiffness:  $\langle \phi^2 \rangle$



Dotted line corresponds to expected value at critical  $w$

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

Representative Hamiltonian:

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

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

$$T, \mu \ll J$$

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

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

Representative Hamiltonian:

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

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

$$T, \mu \ll J$$

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

## Description in terms of fluctuating polarization field and vector potential

Divergence-free polarization on diamond links:  $P_{A \rightarrow B} = S_{r_{AB}}^z$

$$S_{\text{tetrahedron}}^z = 0 \quad \text{implies} \quad \Delta \cdot P = 0$$

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

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

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

## Vertex model partition function

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

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

## S=1 case

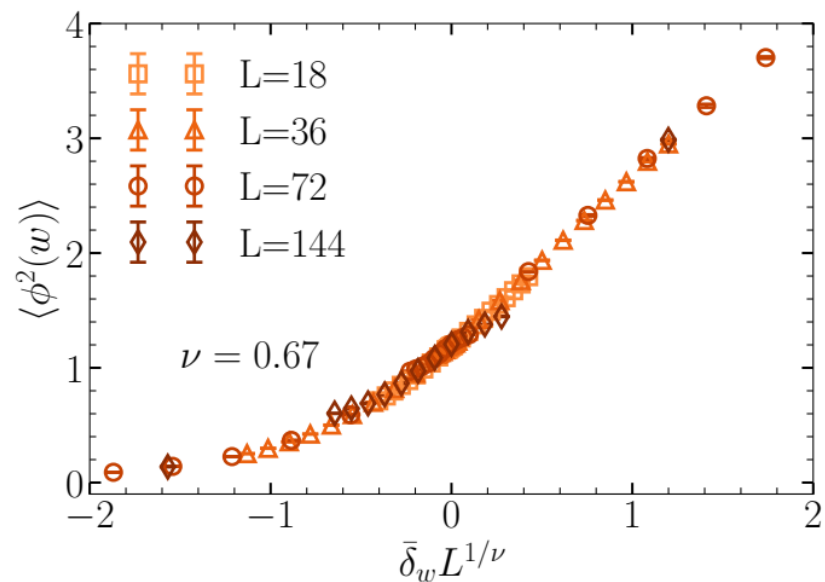
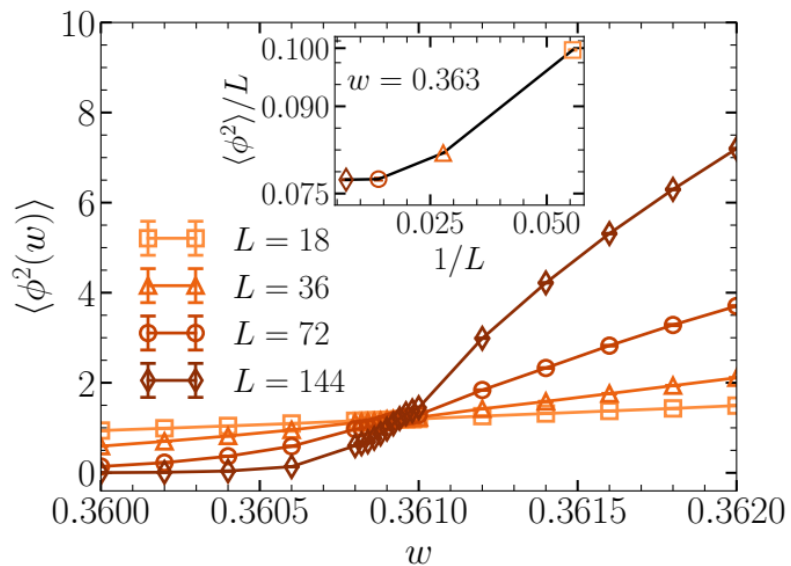
By analogy to kagome:

Viewing the polarization field as a divergence free current of 2+1d bosons

Transition from trivial paramagnet to non-trivial liquid is a 3dxy transition?

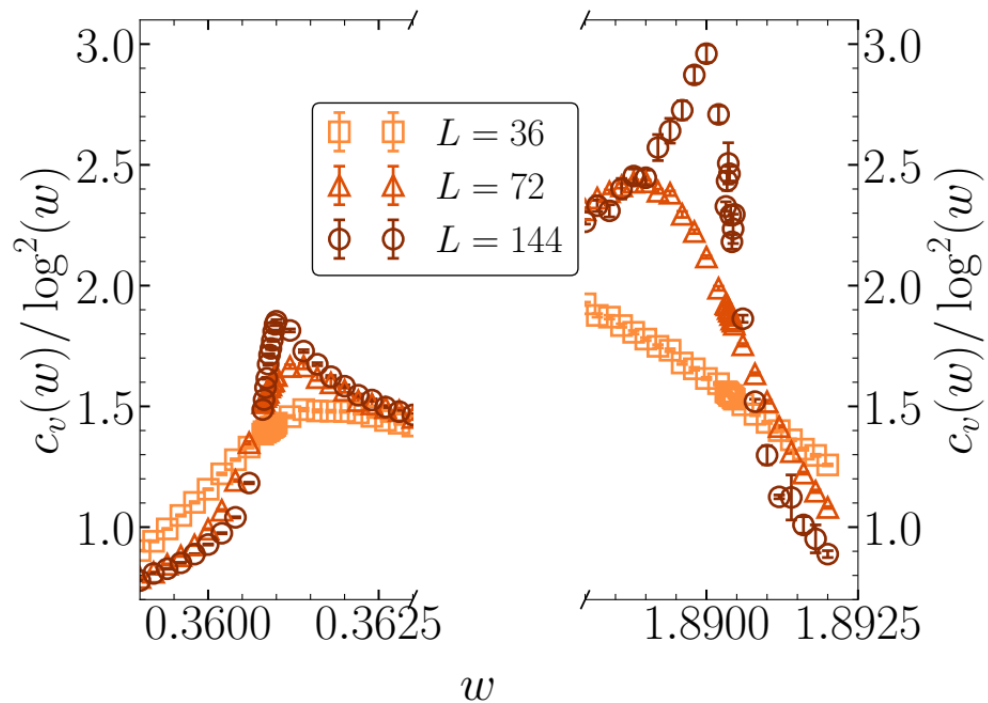
## Superfluid stiffness scales as expected for 3d xy transition

$$\rho_s \sim \langle \phi^2 \rangle / L$$

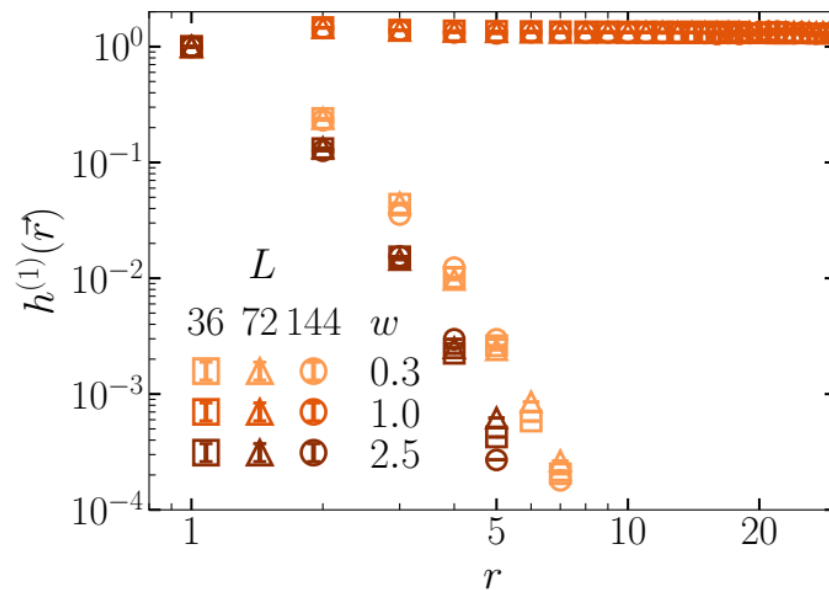


$\rho_s L$  shows expected scaling

## Surprise: second transition



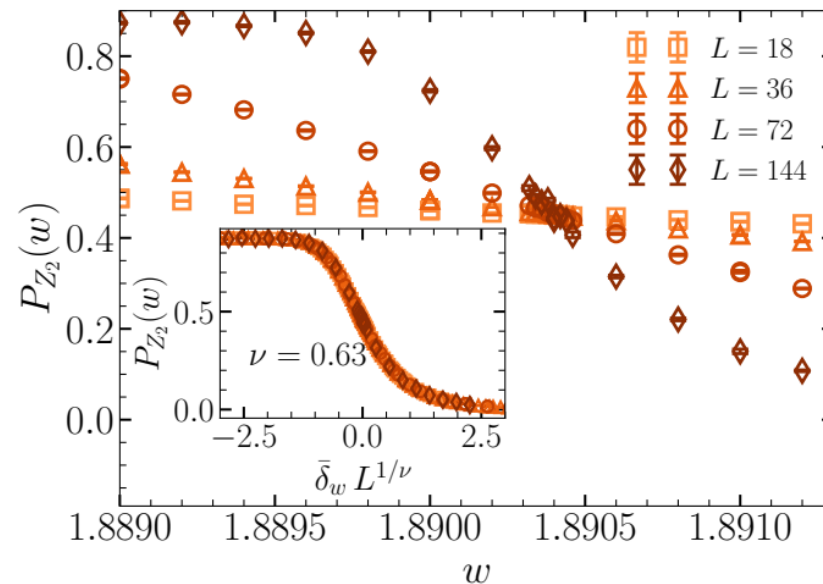
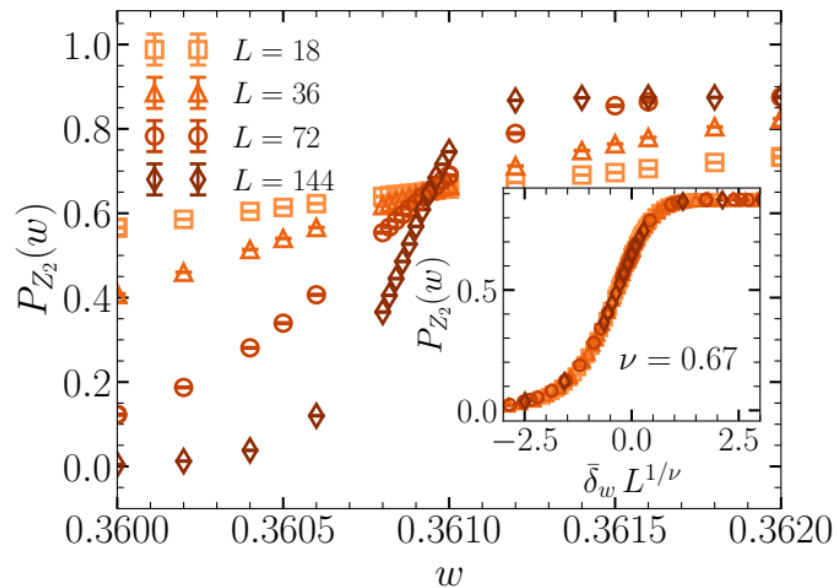
Two transitions seen in specific heat



Three phases seen in unit test charge correlator

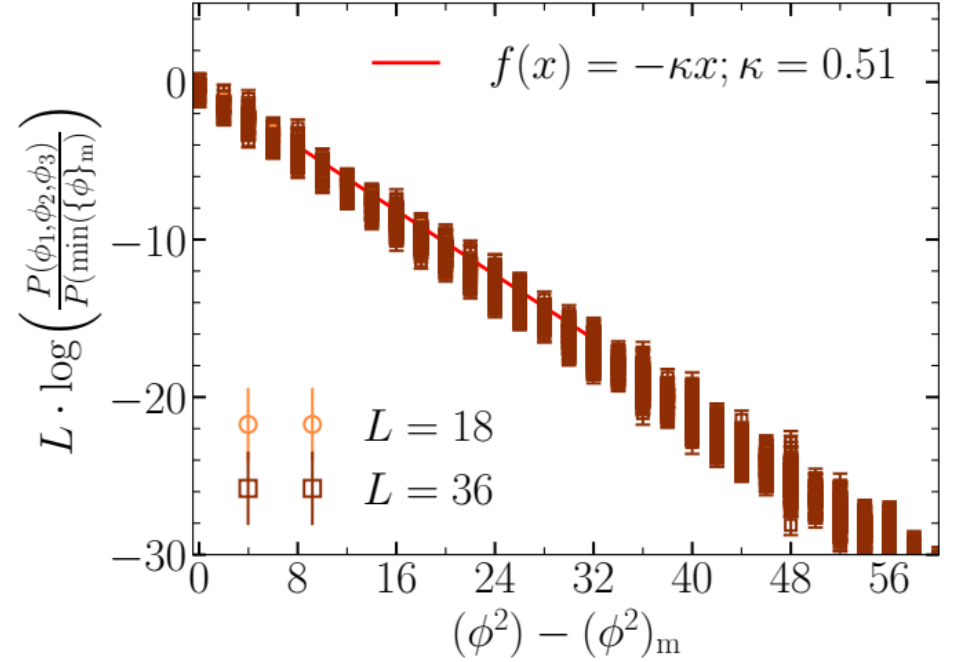
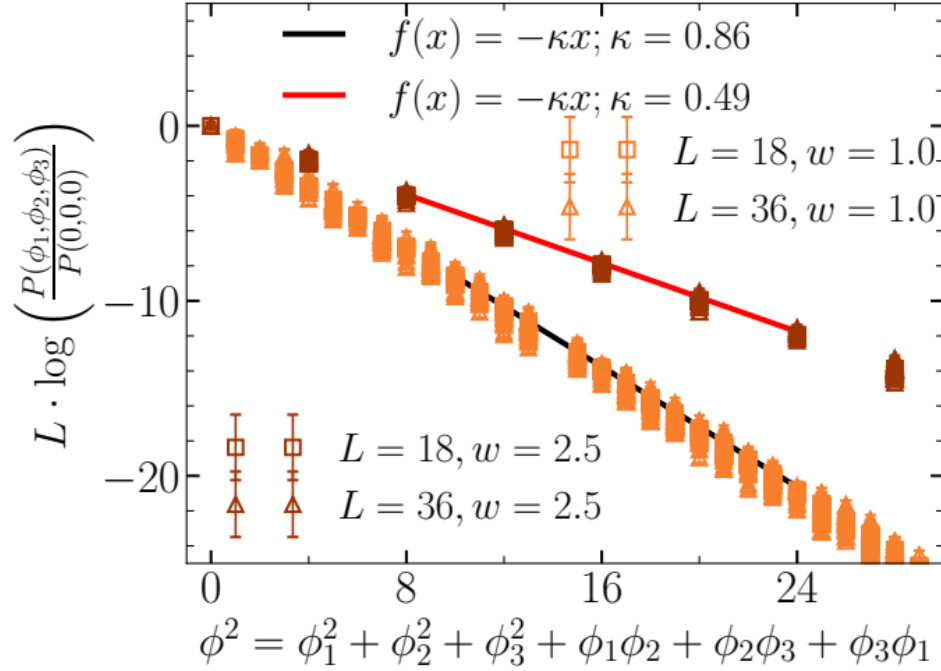


## Understanding the second transition

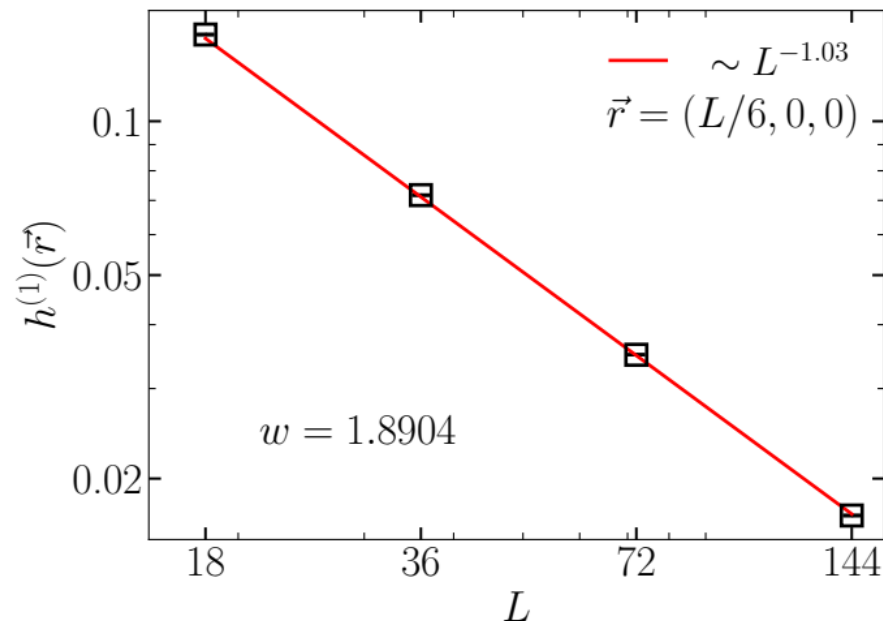
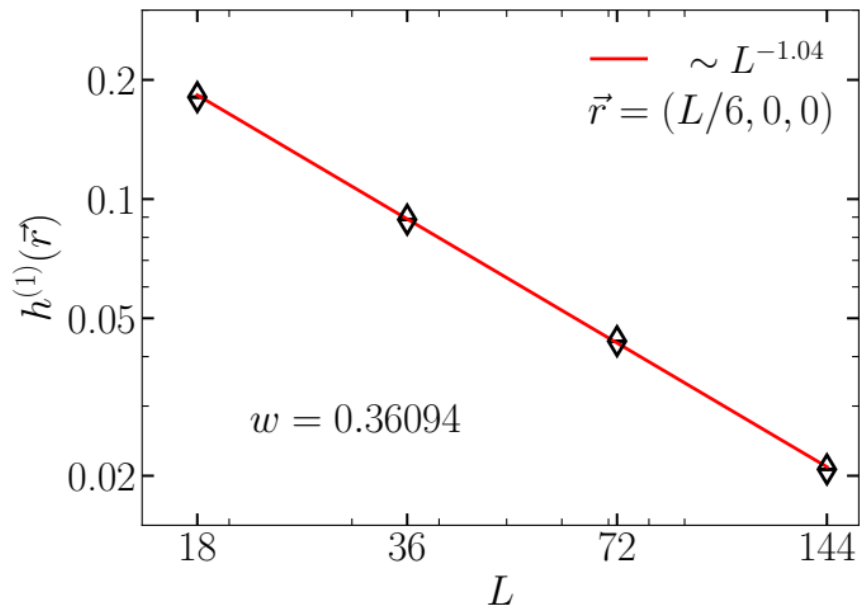


Z2 part of the flux has a confinement transition

## Flux distribution: evidence of Z2 confinement



## Critical test charge correlators



Interpret as correlation function of xy field whose current is the polarization

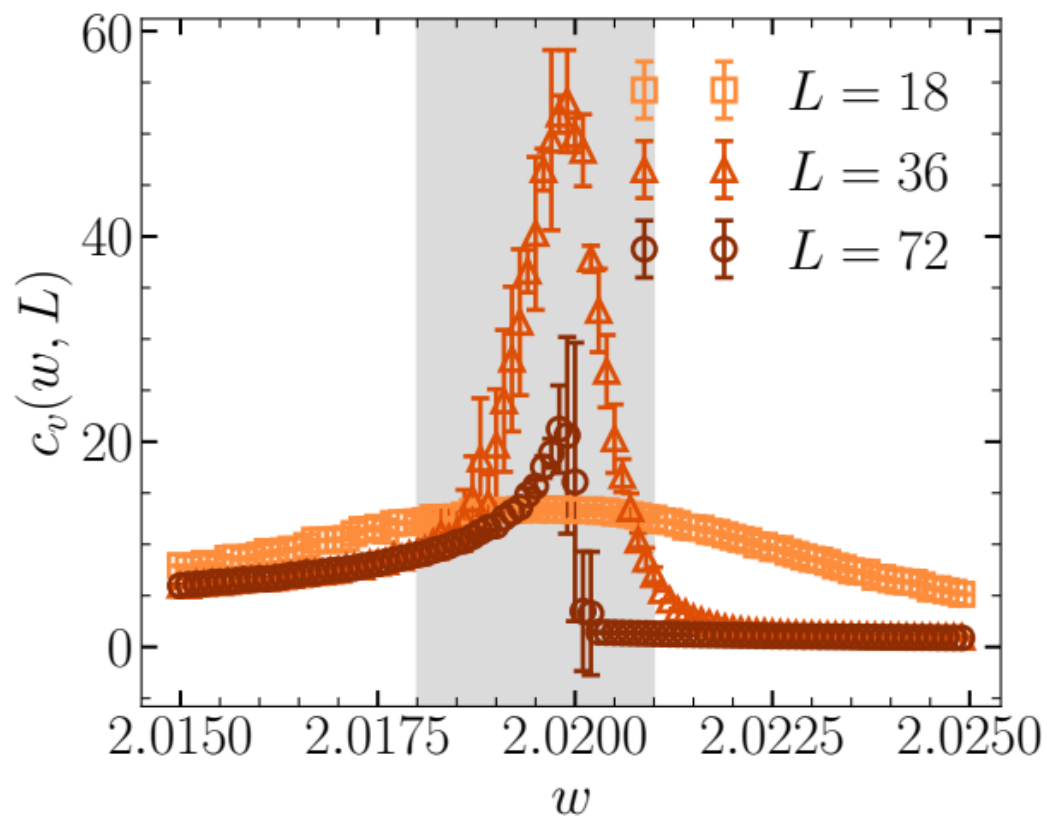
## Summary of spin 1 case:

### 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.)

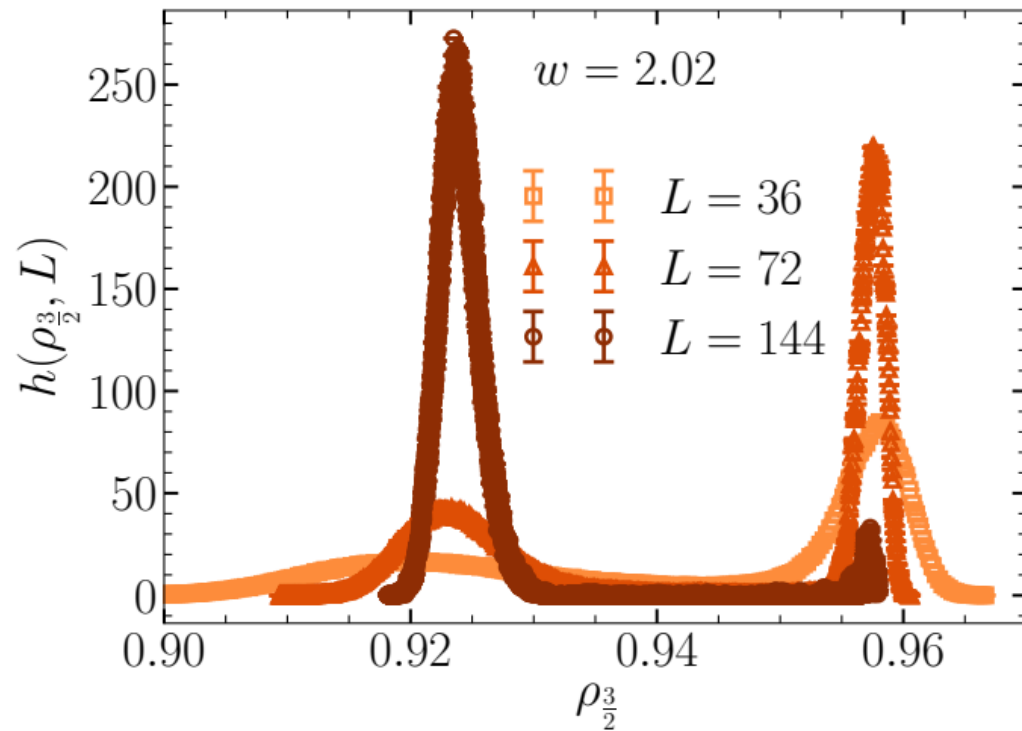
$S=3/2$  case

## First order transition



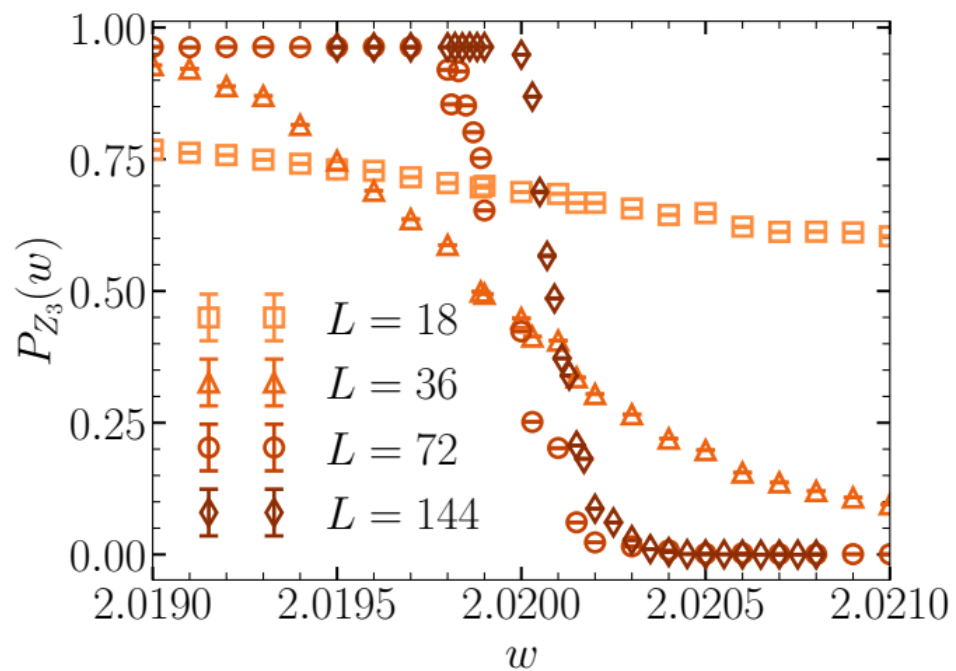
First-order transition between two Coulomb phases

## Clear phase co-existence



First-order transition between two Coulomb phases

## $Z_3$ flux confinement



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



## Summary of spin 3/2 case:

### 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

## Acknowledgements

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