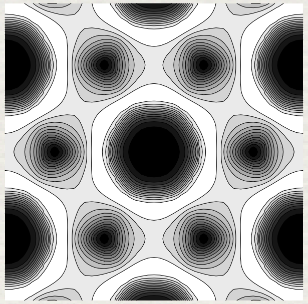
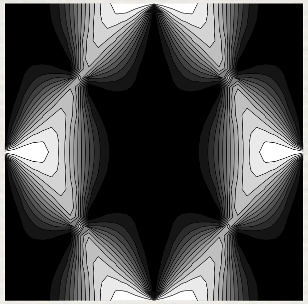
Unusual liquid states in hard-core boson models on the kagome and pyrochlore lattices

Sergei Isakov (University of Toronto)

Collaborators:

Argha Banerjee, Kedar Damle, Yong Baek Kim, Arun Paramekanti

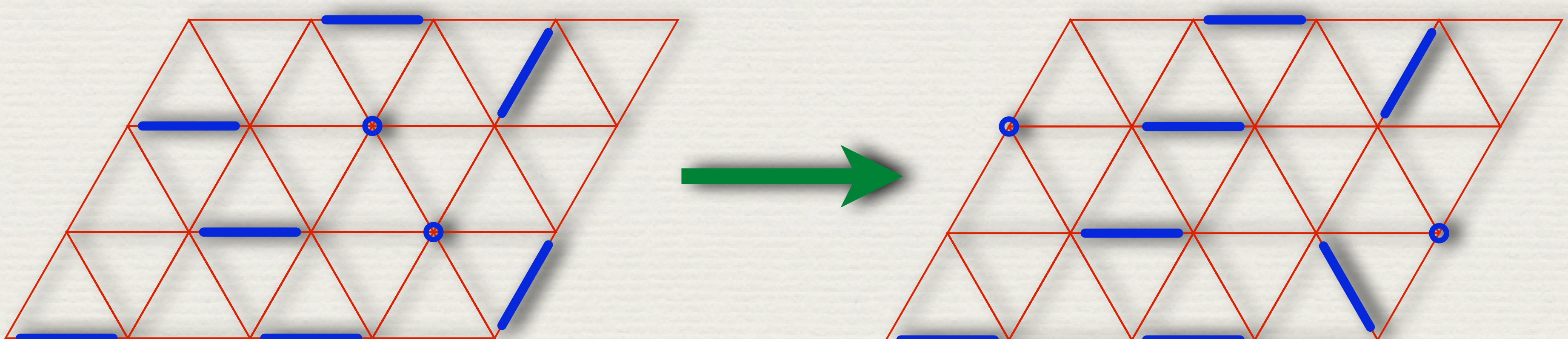




Fractionalized phases

- Fractionalized phases or spin liquids — no symmetry breaking, fractionalized excitations, and topological order
- Experimental situation is not clear — a few candidates

- Effective field theories and properties of such spin liquids phases are quite well understood theoretically, many people
- Excitations carry fractional quantum numbers and interact with emergent gauge fields



$$\frac{1}{\sqrt{2}}[|+-\rangle - |-+\rangle]$$

Electron fractionalization

Fractionalized phases

- Microscopic models that have been identified to have a spin liquid ground state — unusual interactions, restricted Hilbert spaces
  - Moessner and Sondhi — dimer model on the triangular lattice
  - Balents, Fisher, and Girvin — easy axis limit of the AF XXZ model on the kagome lattice (nn, nnn, nnnn interactions)
  - Hermele, Balents, and Fisher — easy axis limit of the AF XXZ model on the pyrochlore lattice

- Show the presence of spin liquid phases in simple models on the kagome and pyrochlore lattices by quantum Monte Carlo method
- Local interactions and no Hilbert space constraints

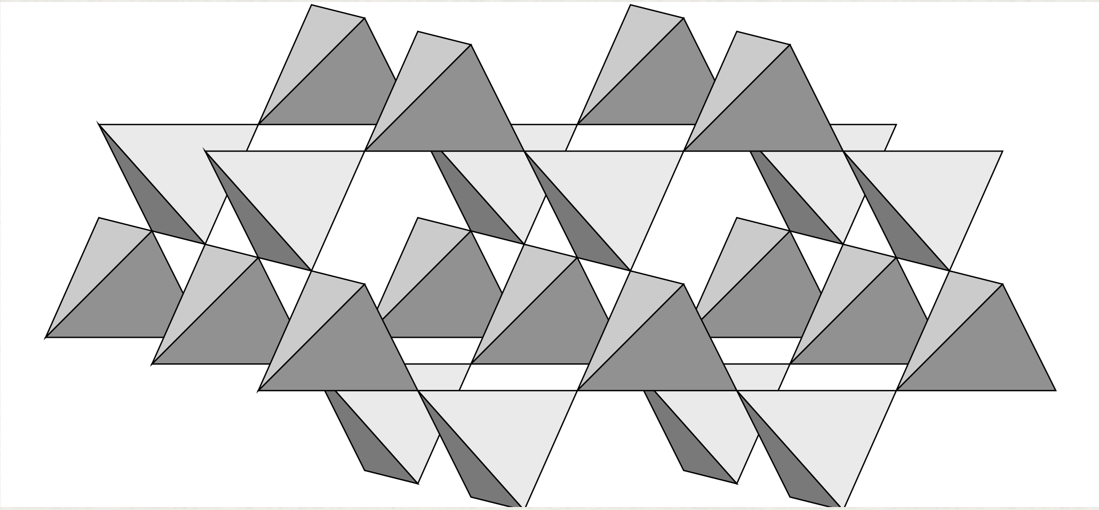
- Stochastic series expansion algorithm Sandvik

Pyrochlore lattice

Hard-core bosons on the pyrochlore lattice

$$H_{\mathrm{b}} = -t \sum_{\langle ij \rangle} \left(b_i^\dagger b_j + \mathrm{H.c.} \right) + V \sum_{\langle ij \rangle} n_i n_j - \mu \sum_i n_i$$

nearest neighbor repulsion



Model

At half filling, maps onto a spin-1/2 model $J_z = V, \; J_\perp = 2t$

$$H = -J_\perp \sum_{\langle ij \rangle} [S_i^x S_j^x + S_i^y S_j^y] + J_z \sum_{\langle ij \rangle} S_i^z S_j^z$$

Effective ring exchange model in the large V/t limit

$$H_{\mathrm{ring}} = -J_{\mathrm{ring}} \sum_{\hexagon} \left(S_1^+ S_2^- S_3^+ S_4^- S_5^+ S_6^- + \mathrm{H.c.} \right)$$

$$J_{\mathrm{ring}} = 3J_\perp^3 / 2J_z^2$$

Ring exchange model

Hermele, Balents, Fisher

$$H_{\rm ring} = -J_{\rm ring} \sum_{\hexagon} \left(S_1^+ S_2^- S_3^+ S_4^- S_5^+ S_6^- + \text{H.c.} \right)$$

Relaxing hard-core constraint — quantum rotor model — effective U(1) gauge theory

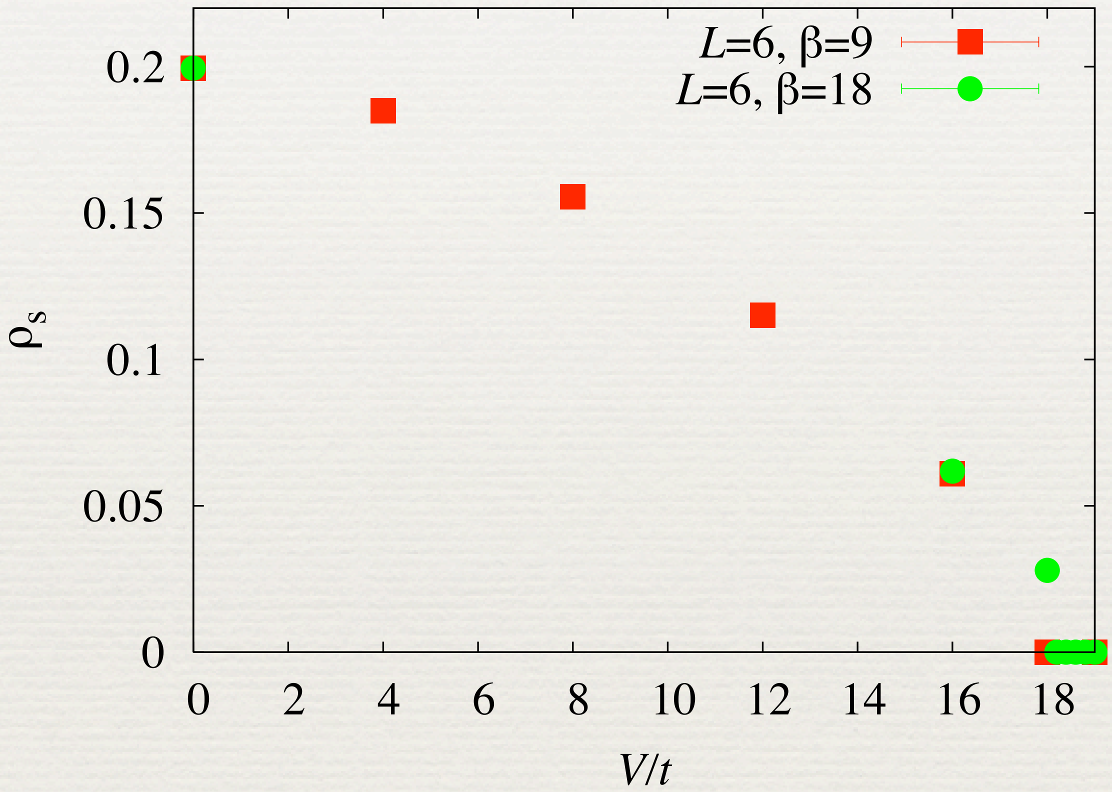
$$\mathcal{H} = \frac{\gamma}{2} \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} e_{\mathbf{r}\mathbf{r}'}^2 + \frac{\kappa}{2} \sum_{\hexagon} (\nabla \times a)^2$$

Ground state is a U(1) spin liquid that is associated with the Coulomb phase of the above gauge theory

Gapless photon excitations — T^3 contribution to the specific heat

Gapped monopole and deconfined spinon excitations

Superfluid density



Insulating phase at large values of V/t

What is the nature of the insulating phase?

Correlation functions

Equal time density correlator

$$C(\tau = 0, \mathbf{q})/N = \langle n^\dagger_{\mathbf{q}\tau} n_{\mathbf{q}\tau} \rangle, \quad n_{\mathbf{q}\tau} = (1/N) \sum_i n_{i\tau} \exp(i\mathbf{q}\mathbf{r}_i)$$

Static density correlator

$$S(\omega = 0, \mathbf{q})/N = \langle \int d\tau \, n^\dagger_{\mathbf{q}\tau} n_{\mathbf{q}0} \rangle$$

Equal time bond-bond correlator

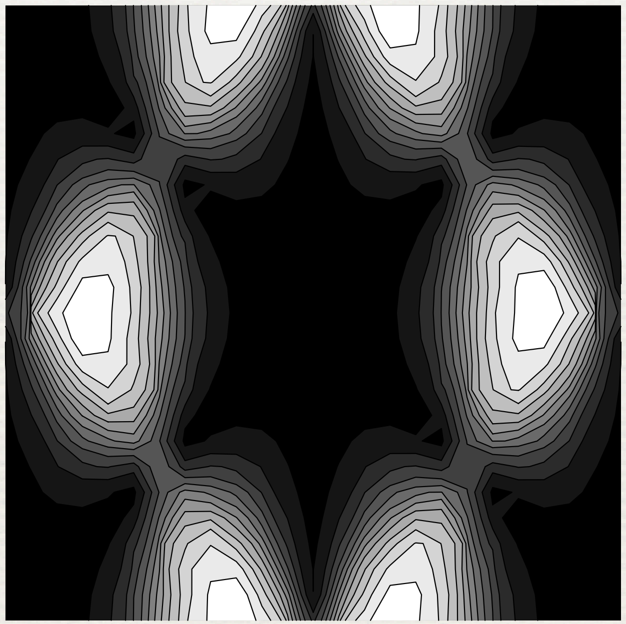
$$C_{\mathrm{b}}(\tau = 0, \mathbf{q})/N = \langle B^\dagger_{\mathbf{q}\tau} B_{\mathbf{q}\tau} \rangle, \quad B_{\mathbf{q}\tau} = (1/N) \sum_\alpha B_{\alpha\tau} \exp(i\mathbf{q}\mathbf{r}_\alpha)$$

$$B_{\alpha(i,j),\tau} = t(b^\dagger_i b_j + b_i b^\dagger_j)$$

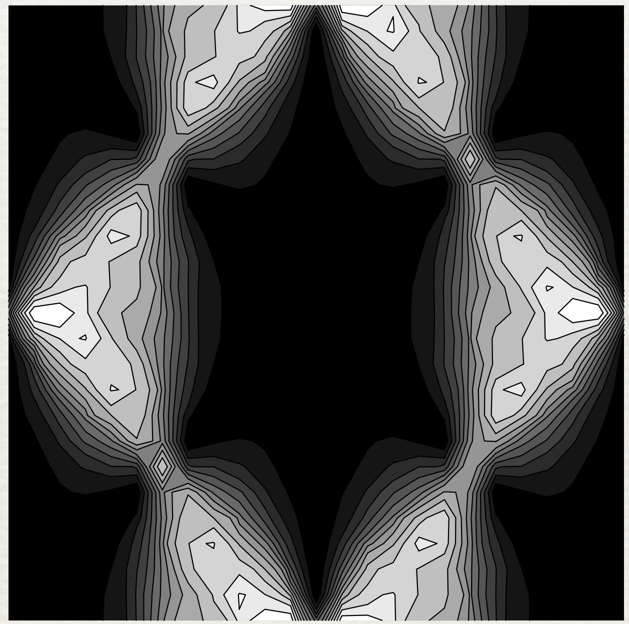
Structure factors in the [hhl] plane

Quantum correlators in the insulating phase

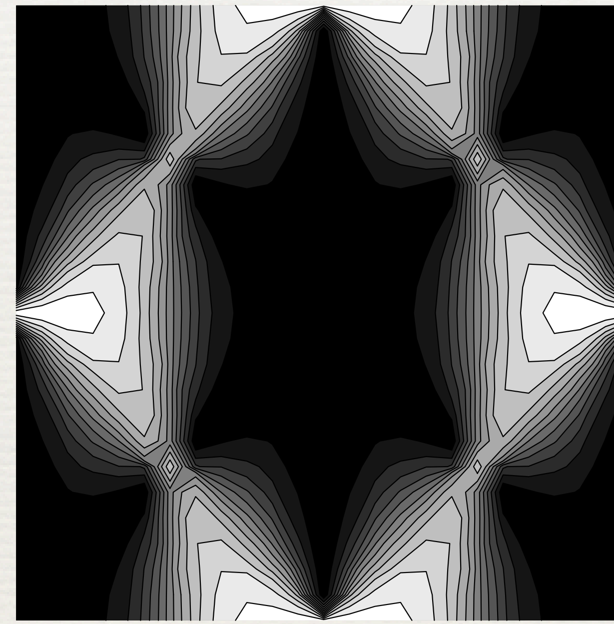
Equal time s.f.



Static s.f.



Ising model s.f.

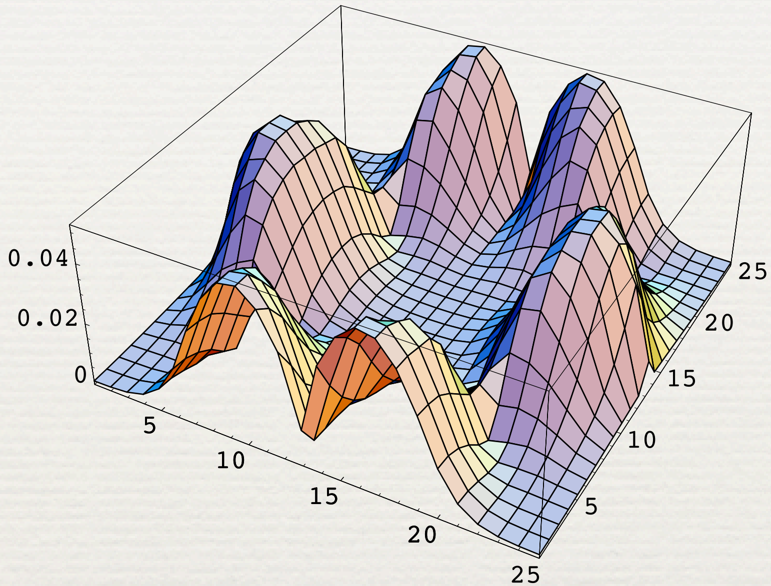


No Bragg peaks — no symmetry breaking

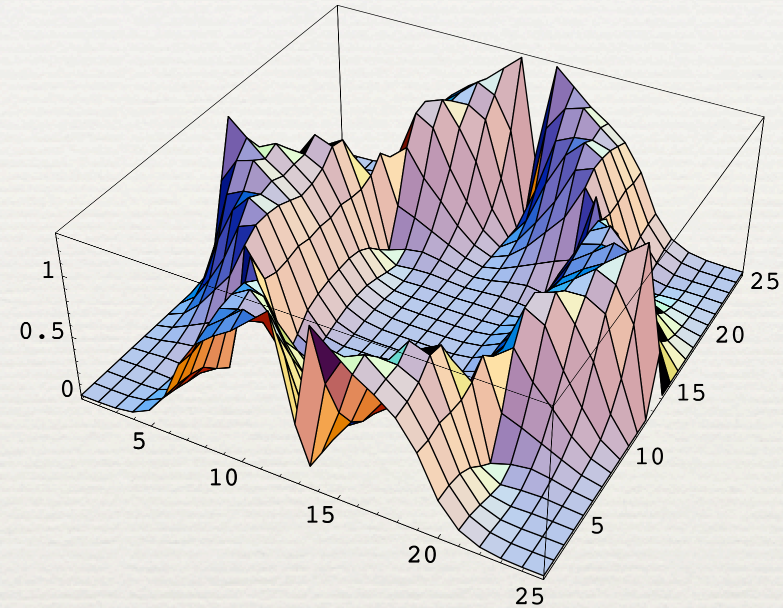
Bond correlators also do not show any Bragg peaks — no bond or plaquette order   spin liquid?

Correlations in the [hhl] plane

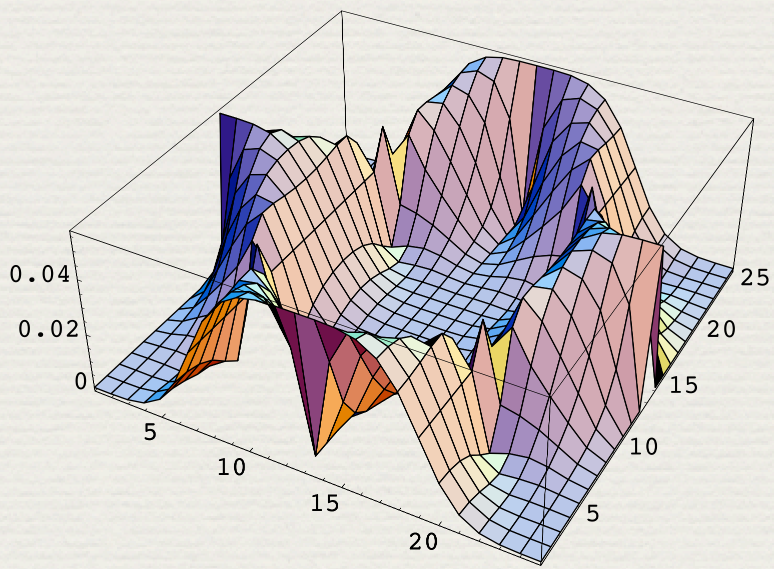
Equal time s.f.



Static s.f.



Ising model s.f.



How to detect a U(1) spin liquid phase

Photon excitations give a T^3 contribution to the specific heat
Might be hard to measure at low temperatures

Look at correlation functions:

Static correlators have a dipolar form $\sim \dfrac{q_\perp^2}{q^2}$

Hermele, Balents, and Fisher

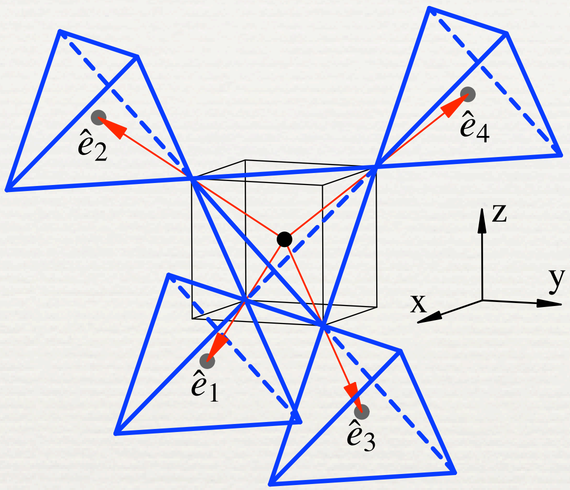
Equal time correlators decay faster (in real space) $\sim \dfrac{q_\perp^2}{q}$

Static and equal time correlation functions have those two distinct forms — U(1) spin liquid phase

Lattice correlators

Non-compact lattice gauge theory

$$\mathcal{H} = \frac{\gamma}{2} \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} e_{\mathbf{r}\mathbf{r}'}^2 + \frac{\kappa}{2} \sum_{\hexagon} (\nabla \times a)^2,$$



where $n_{\mathbf{r}\mathbf{r}'} = \epsilon e_{\mathbf{r}\mathbf{r}'}$

Equal time and static correlators

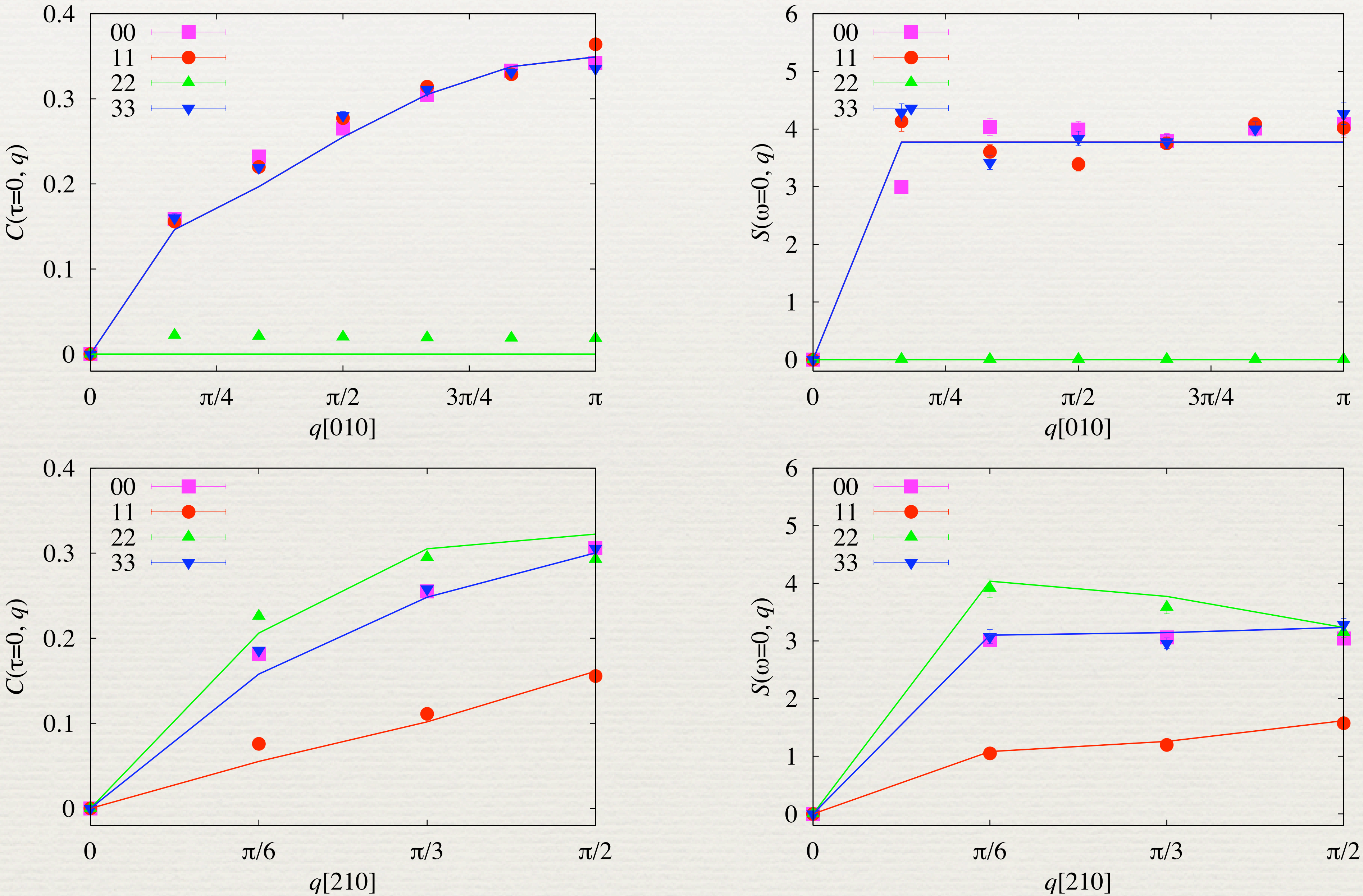
$$C(\tau = 0, \mathbf{q}) = \epsilon^2 \sqrt{\frac{\kappa}{\gamma}} f_{\mathrm{eq}}(\beta\sqrt{\kappa\gamma}, \mathbf{q})$$

$$S(\omega = 0, \mathbf{q}) = \epsilon^2 \sqrt{\frac{\kappa}{\gamma}} \frac{1}{\sqrt{\kappa\gamma}} f_{\mathrm{st}}(\mathbf{q})$$

Fit equal time and static data to those functions — good diagnostic of the U(1) spin liquid

Fitting to electric correlators

$$V/t = 19.4, \beta t = 30 \qquad \epsilon^2\sqrt{\kappa/\gamma} = 0.3, \sqrt{\kappa\gamma} = 0.053$$



Fitting to electric correlators

Data fit the predictions of non-compact electrodynamics extremely well

$$C(\tau = 0, \mathbf{q}) = \epsilon^2 \sqrt{\frac{\kappa}{\gamma}} f_{\text{eq}}(\beta\sqrt{\kappa\gamma}, \mathbf{q})$$

$$S(\omega = 0, \mathbf{q}) = \epsilon^2 \sqrt{\frac{\kappa}{\gamma}} \frac{1}{\sqrt{\kappa\gamma}} f_{\text{st}}(\mathbf{q})$$

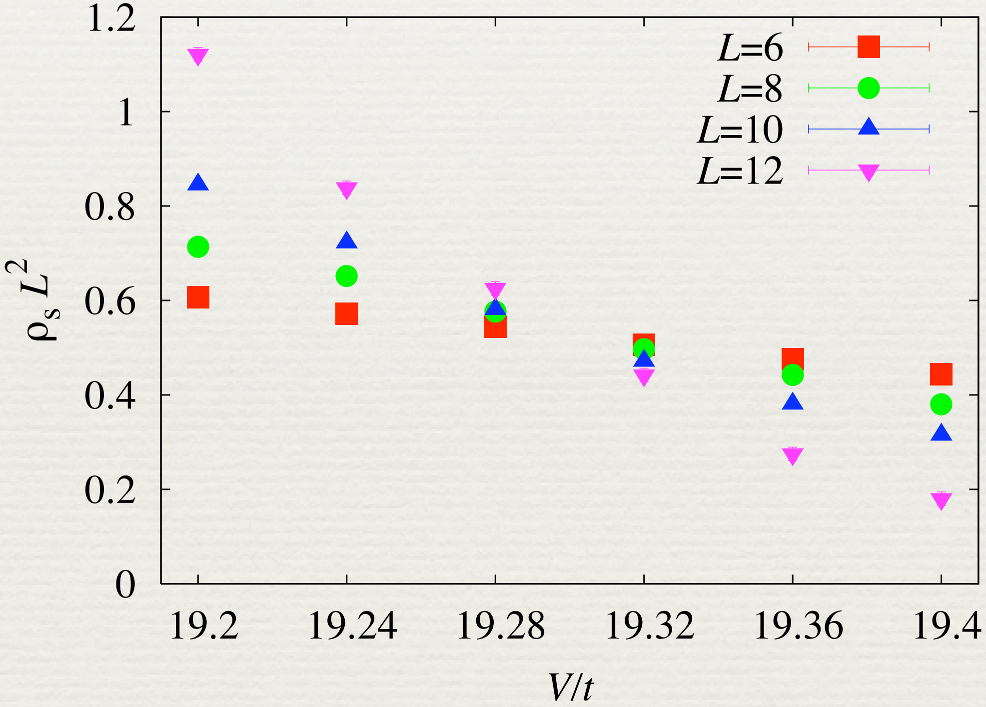
Fits are highly constrained — $\sqrt{\kappa\gamma}$ is overdetermined — it can be obtained both from the best fit value of the first argument of f_{eq} and from the ratio of equal time and static data

Insulator is a U(1) spin liquid phase!

Quantum phase transition: Scaling I

In the vicinity of a continuous quantum phase transition, superfluid density scales as

$$\rho_s = L^{-1-z} F_{\rho_s}(L^{1/\nu}(K_c - K), \beta/L^z)$$



Dynamical critical exponent

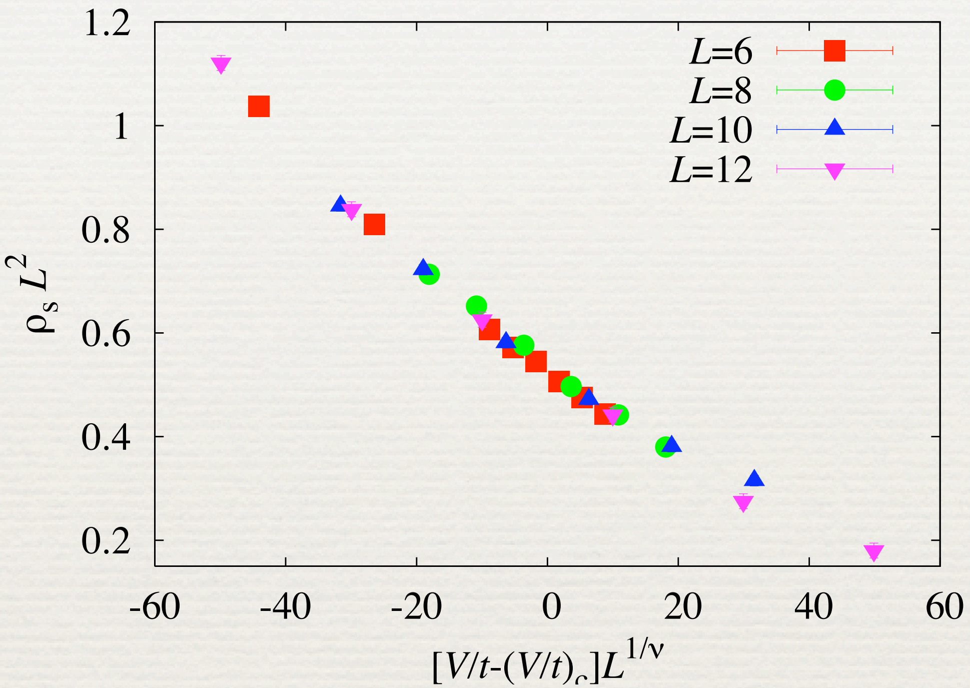
$$z = 1$$

Transition at $(V/t)_c = 19.3$

β/L is fixed

Quantum phase transition: Scaling II

Data collapse



Quantum critical point at

$$(V/t)_c = 19.30(2)$$

Correlation length exponent

$$\nu = 0.40(3)$$

Looks continuous, but ...

Correlation length exponents is too small?
Weakly first order transition?

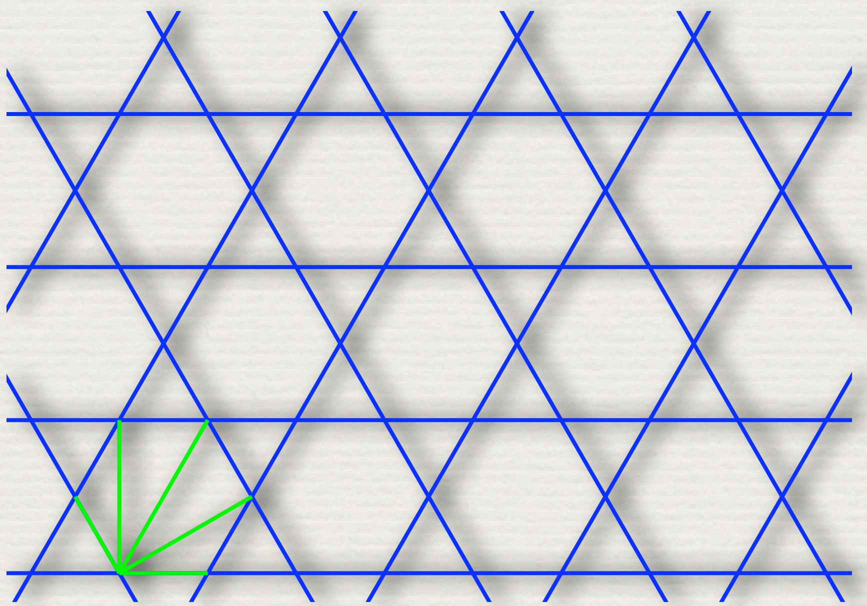
Halperin, Lubensky, Ma

Kagome lattice

Hard-core bosons on the kagome lattice

$$H_{\mathrm{b}} = -t \sum_{(i,j)} \left(b_i^\dagger b_j + \mathrm{H.c.} \right) + V \sum_{\hexagon} (n_{\hexagon})^2 - \mu \sum_i n_i ,$$

Interactions over nearest, next nearest and next next nearest neighbors



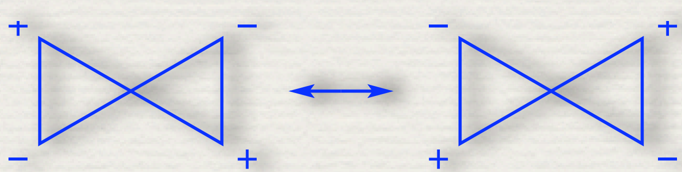
Model, continue

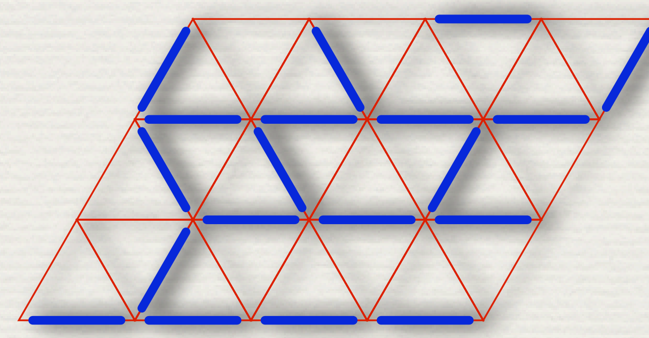
At half filling, maps onto a spin model $J_z = V, \; J_\perp = t$

$$H = -J_\perp \sum_{\hexagon} [(S^x_{\hexagon})^2 + (S^y_{\hexagon})^2 - 3] + J_z \sum_{\hexagon} (S^z_{\hexagon})^2$$

Effective ring exchange model in the large V/t limit

$$H_{ring} = -J_{ring} \sum_{\bowtie} \left(S_i^+ S_j^- S_k^+ S_l^- + \text{H.c.} \right), \quad J_{ring} = J_\perp^2 / J_z$$





Three-dimer model on the triangular lattice in the classical limit $t = 0$

Ring exchange model

Balents, Fisher, and Girvin

$$H_{ring} = -J_{ring} \sum_{\bowtie} \left(S_i^+ S_j^- S_k^+ S_l^- + \mathrm{H.c.} \right)$$

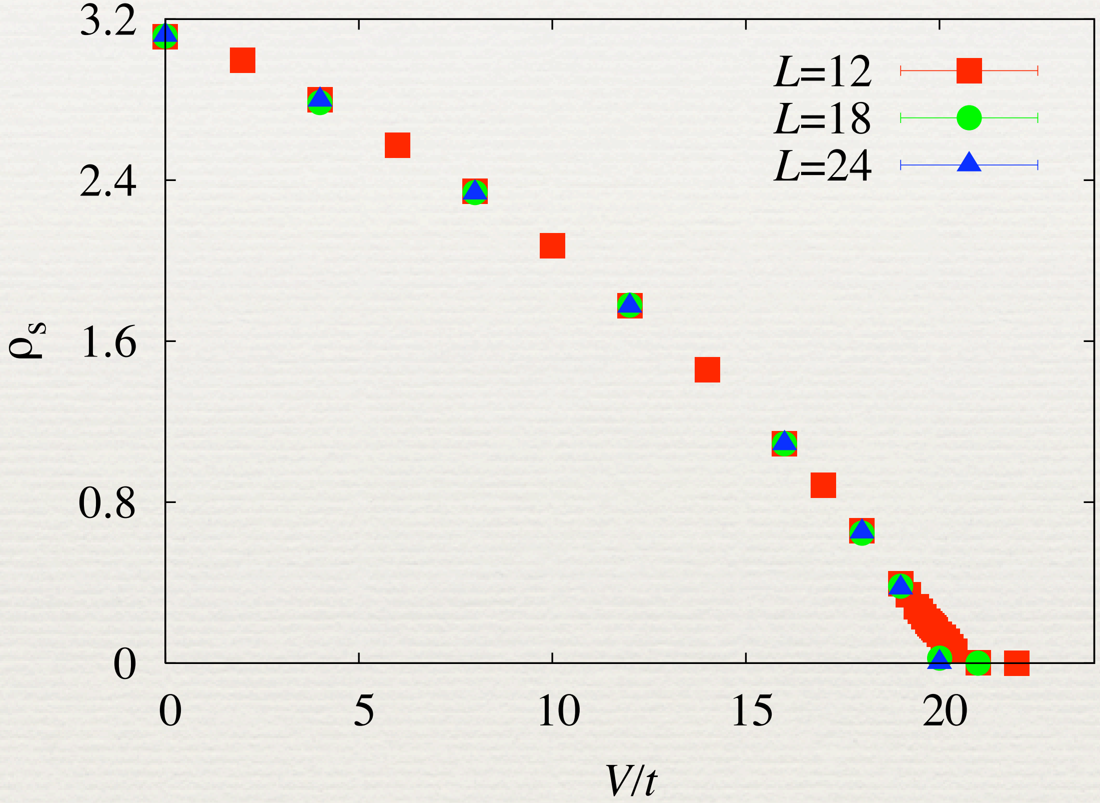
Supplemented the ring-exchange model with the Rokhsar-Kivelson potential energy term

Z_2 spin liquid phase close to the solvable RK point (in the absence of the RK term exact diag. by Sheng and Balents)

Gapped vison excitations
Deconfined spinon excitations

Topological order, e.g., ground state on a torus is four-fold degenerate

Superfluid density

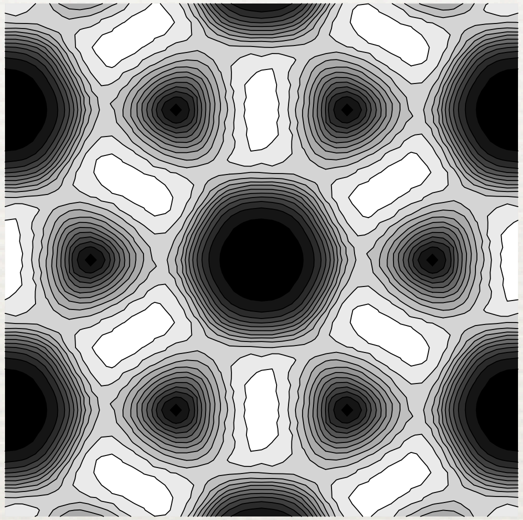


Insulating phase at large values of V/t

What is the nature of the insulating phase?

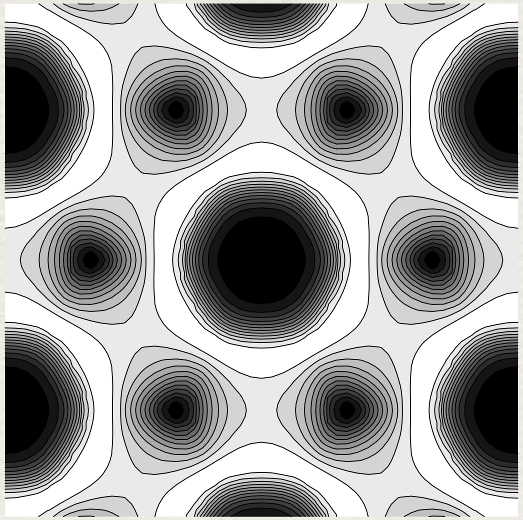
Insulating phase: Correlations

Equal-time density and bond-bond structure factors do not show any Bragg peaks — no symmetry breaking!



Equal-time density structure factor in momentum space in the spin liquid phase for

$$L = 24, V/t = 20, T = t/12$$

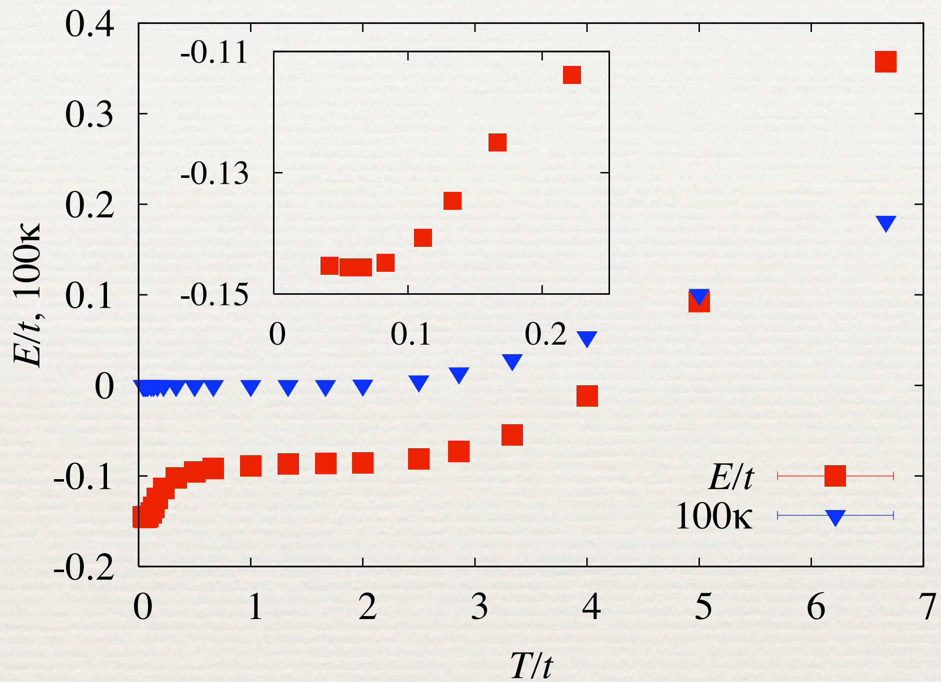


Compare to the structure factor of the classical 3-dimer model on the triangular lattice

Gregor, SI, Moessner, and Sondhi, (unpublished)

Insulating phase: Finite-temperature properties

Energy per site E and compressibility κ as a function of T



$L = 24, V/t = 20.5$

Vison gap $E_v \sim 0.35(15)t \sim t^2/V$

Energy decreases in two steps:
First drop — freezing out of charge excitaions
Second drop — evolving into the spin liquid ground state (vison gap)

Compressibility is zero at low temperatures and finite at temperatures where the energy plateau terminates indicating charge excitations

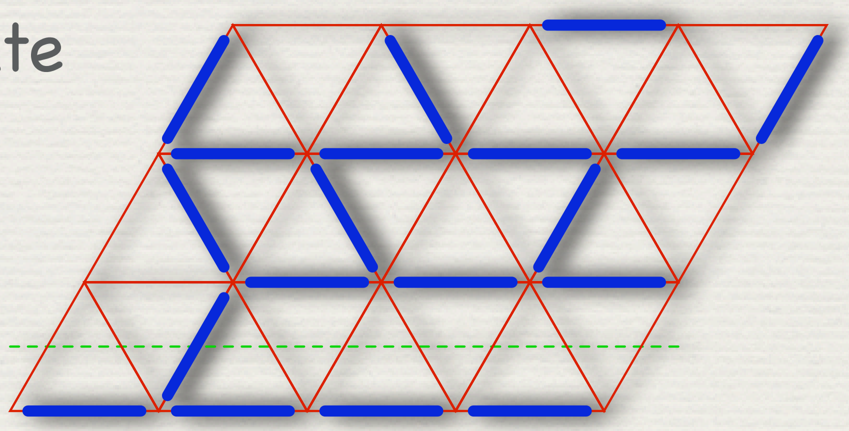
Topological order: ring exchange model

Lattice with periodic boundary conditions in both directions

In the dimer subspace ($n_{\hexagon} = 3$), topological sectors are defined by having odd or even number of bosons on each row/column (parity sectors)

Four topological sectors in the ring exchange model are not changed by local moves

Ground state is four-fold degenerate



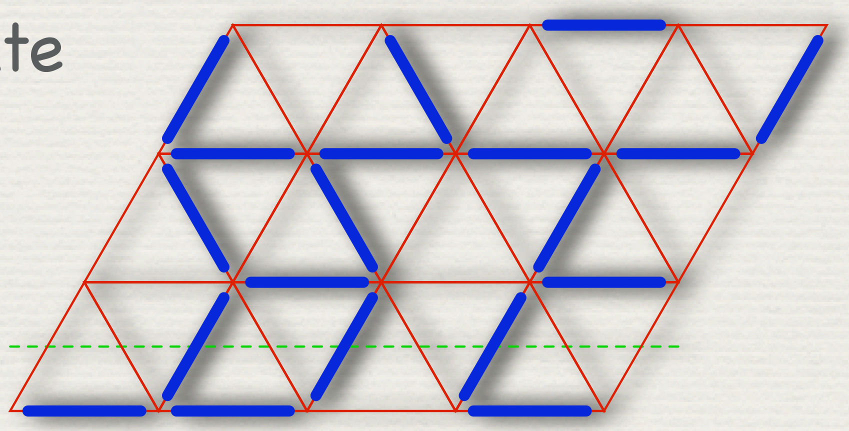
Topological order: ring exchange model

Lattice with periodic boundary conditions in both directions

In the dimer subspace ($n_{\hexagon} = 3$), topological sectors are defined by having odd or even number of bosons on each row/column (parity sectors)

Four topological sectors in the ring exchange model are not changed by local moves

Ground state is four-fold degenerate



Topological order

Parities are not conserved quantities in the boson model

Quantum ground state no longer lies in the dimer subspace — small density of defects ($n_{\hexagon} \neq 3$)

However, we still can define topological sectors

Ground state wave functions, $|\psi_{ab}\rangle$, have nonzero zero overlap with the dimer subspace wave functions $|\psi^d_{ab}\rangle$

$$|\psi_{00}\rangle = |\psi^d_{00}\rangle + |\psi'_{00}\rangle \qquad |\psi_{01}\rangle = |\psi^d_{01}\rangle + |\psi'_{01}\rangle$$
$$|\psi_{10}\rangle = |\psi^d_{10}\rangle + |\psi'_{10}\rangle \qquad |\psi_{11}\rangle = |\psi^d_{11}\rangle + |\psi'_{11}\rangle$$

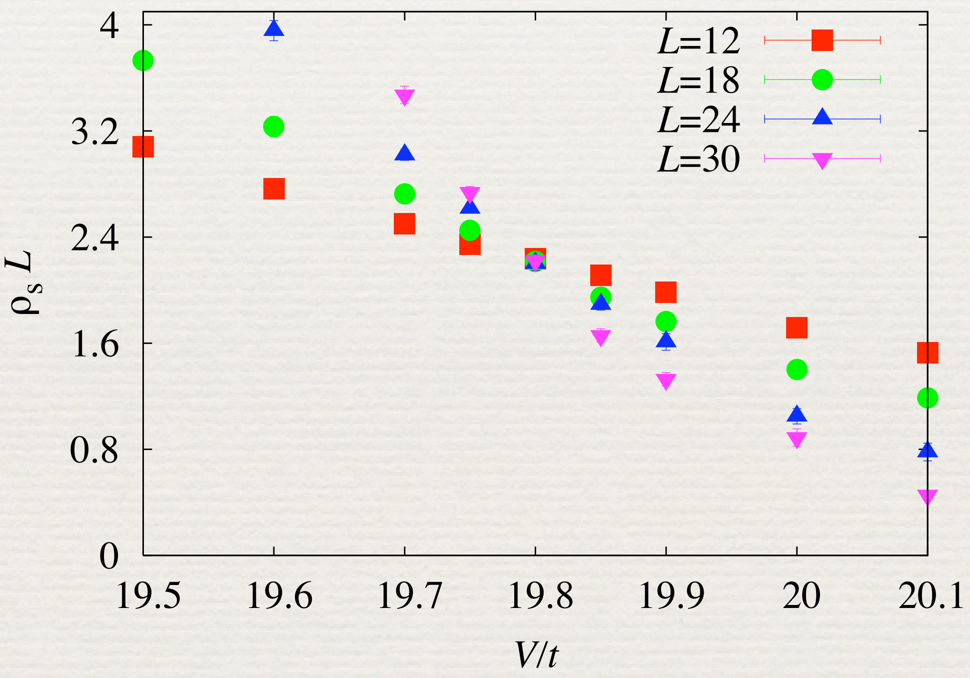
These wave functions are not connected by local moves

Energies are the same within statistical errors — ground state is four-fold degenerate — topological order

Quantum phase transition: Scaling I

In the vicinity of a continuous quantum phase transition, superfluid density scales as

$$\rho_s = L^{-z} F_{\rho_s}(L^{1/\nu}(K_c - K), \beta/L^z)$$



Dynamical critical exponent

$$z = 1$$

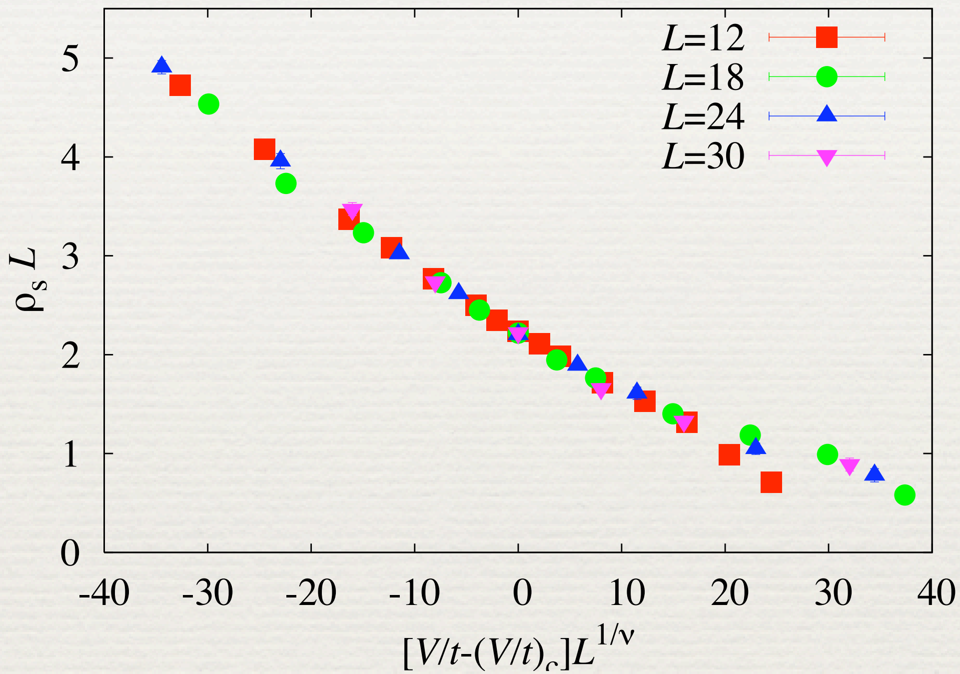
Distinct crossing point

Transition at $(V/t)_c = 19.8$

β/L is fixed

Quantum phase transition: Scaling II

Data collapse



Quantum critical point at

$$(V/t)_c = 19.80(2)$$

Correlation length exponent

$$\nu = 0.67(5)$$

3D XY value

Senthil and Motrunich

Conclusions

- Studied a hard-core model on the kagome lattice by quantum Monte Carlo method
- Z_2 fractionalized phase with topological order, gapped vison and deconfined spinon excitations
- Superfluid-insulator quantum phase transition is continuous

- Studied a hard-core model on the pyrochlore lattice by quantum Monte Carlo method
- $U(1)$ fractionalized phase
- Static and equal time correlators in this phase are well described by electric field correlators in the Coulomb phase of a $U(1)$ lattice gauge theory