Chiral spin liquid phase of the triangular lattice Hubbard model

Evidence from iDMRG in a mixed real- and momentum-space basis

AARON SZASZ

(With Johannes Motruk, Michael P. Zaletel, and Joel E. Moore)

UC BERKELEY

LBNL

TNSAA 2018-2019

Outline

1. Introduction
2. Calculation methods
3. Phase diagram
4. Chiral spin liquid phase
5. Implications/comparisons and summary
6. Future directions

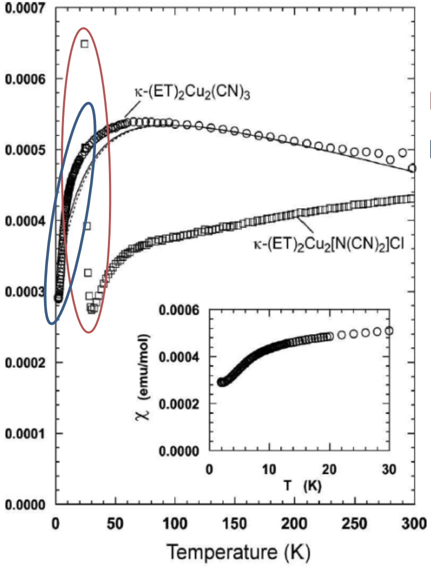
Motivation from experiments

Possible spin liquids in triangular lattice systems!

Eg: $\kappa-(ET)_2(Cu)_2(CN)_3$: approximately isotropic triangular lattice

Nonmagnetic at low T:

Magnetic susceptibility



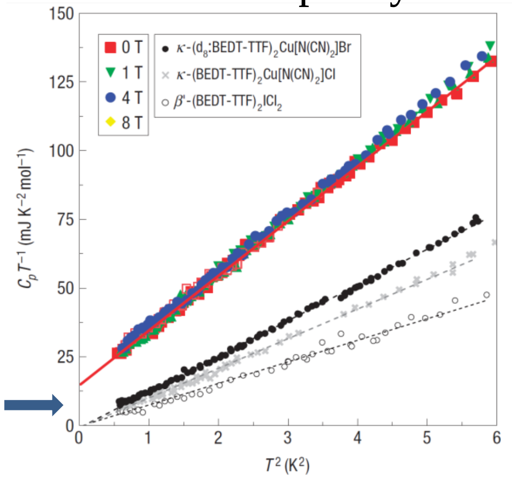
AFM

Spin liquid?

Shimizu et al., PRL 2003

Gapless?

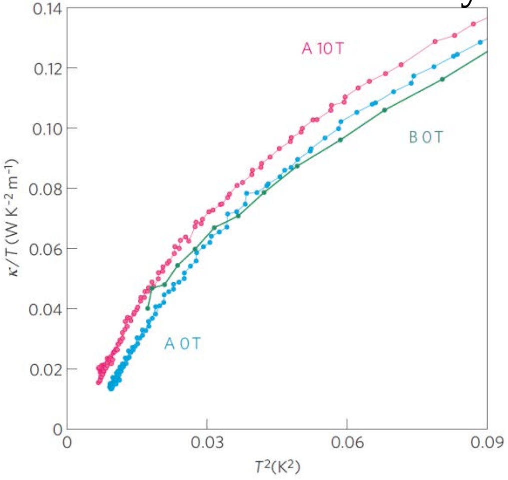
Heat capacity



Yamashita et al., Nat. Phys. 2008

Gapped?

Thermal conductivity

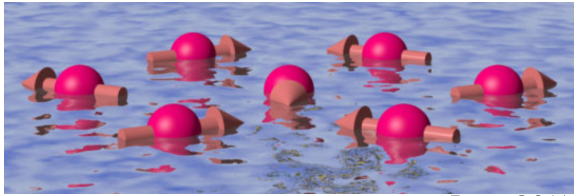


Yamashita et al., Nat. Phys. 2008

Spin liquids


Anderson 1973

Candidate states:


Pratt 2011

Gapless states:

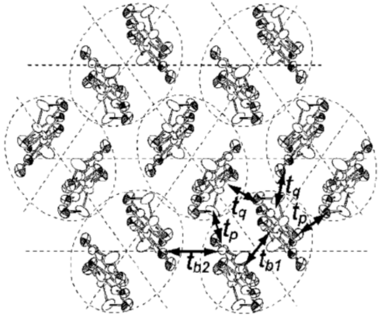
- U(1) spin liquid: spinon Fermi surface
- Dirac spin liquid: gapless Dirac cones at specific points in Brillouin zone
- Quadratic band-touching

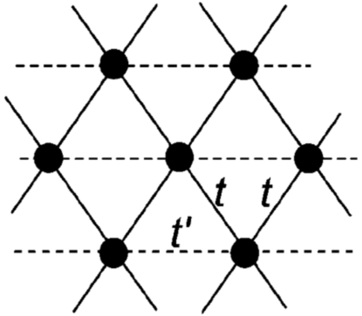
Gapped states:

- Z_2 spin liquid: equivalent to toric code
- Chiral spin liquid:
  - Time-reversal symmetry breaking
  - Gapless edge modes
  - More later!

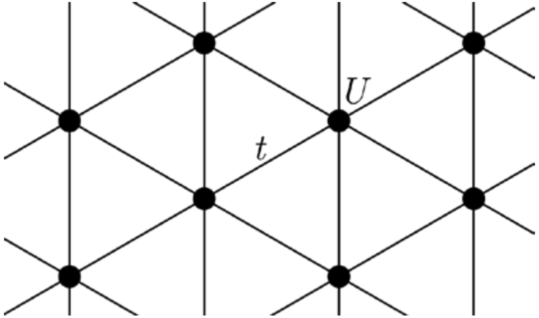
Models for real materials

Crystal structure of $\kappa-(ET)_2(Cu)_2(CN)_3$:





Hubbard model:



Parameter estimates:

- $t'/t = 1.06,\ U/t = 8.2$ [Shimizu et al., PRL 2003]
- $t'/t = 0.8,\ U/t \approx$ 12-15 [Nakamura et al., J. Phys. Soc. Jpn. 2009]

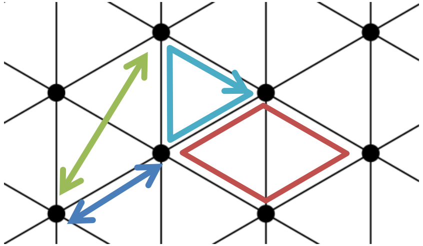
Try to simplify: t/U expansion

½ filling $\rightarrow$ extended Heisenberg model

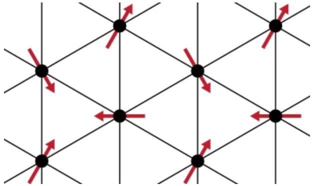
Existing results – theory

Spin models:

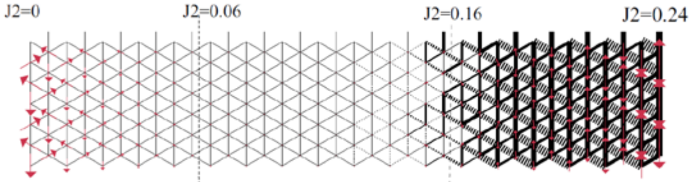
$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + K \sum_{\langle ijkl \rangle} (P_{ijkl} + \text{H.c.}) + \chi \sum_{\triangle} \mathbf{S} \cdot (\mathbf{S} \times \mathbf{S})$$



Heisenberg:



J_1—J_2 :



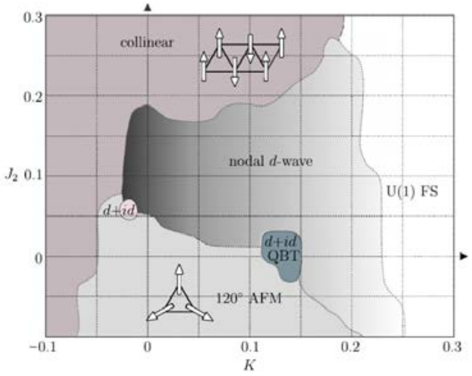
Ordered | Gapped SL | Ordered

Zhu & White, PRB 2015

J_1, J_2, K:

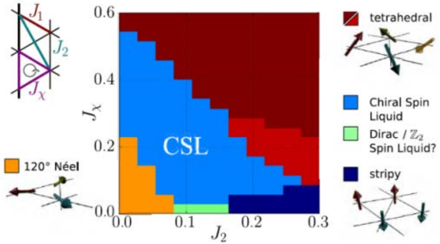
Spinon Fermi surface

- Variational: Motrunich, PRB, 2005
- Ladder DMRG: Sheng, PRB 2009

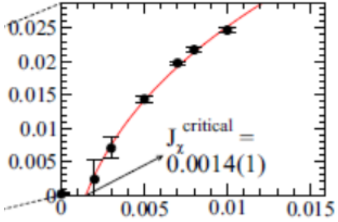


Mishmash et al, PRL 2013

J_1, J_2, χ:



Wietek & Lauchli, PRB 2017

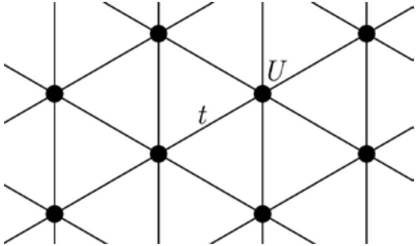


Saadatmand & McCulloch, PRB 2017

Existing results – theory

Hubbard model:

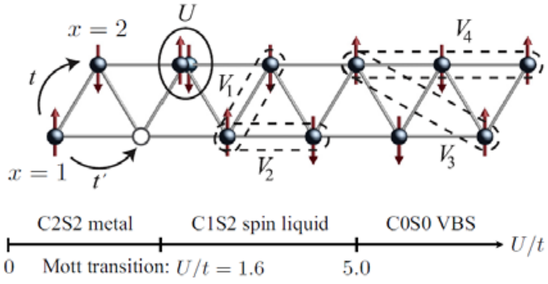
$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



Via spin models:

- Low order expansion: U(1) SL, spinon Fermi surface [Motrunich 2005]
- 12^{th} order: SL nature unclear, maybe U(1) [Yang et al, PRL 2010]

Two leg ladder DMRG + extra terms:

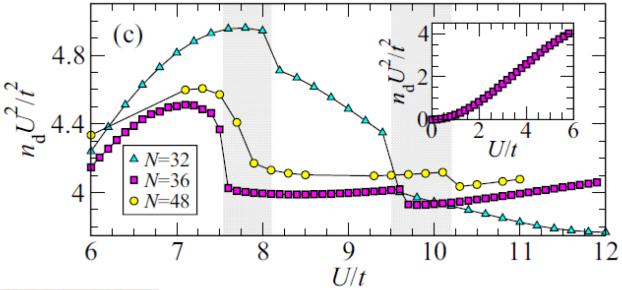


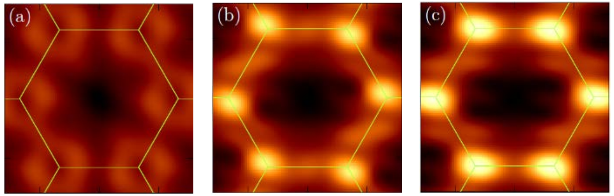
Mishmash et al, PRB 2015

DMRG on finite cylinder [RIKEN group]:

Three phases:

- Metal, SL, ordered
- First order transitions: $\left(\partial E / \partial U\right)(U/t)^2$:





SL spin correlations:

- No Fermi surface
- Nodal gapless unclear

Shirakawa et al, PRB 2017

Partial information on nature of spin liquid

Outline

1. Introduction
2. Calculation methods
3. Phase diagram
4. Chiral spin liquid phase
5. Implications/comparisons and summary
6. Future directions

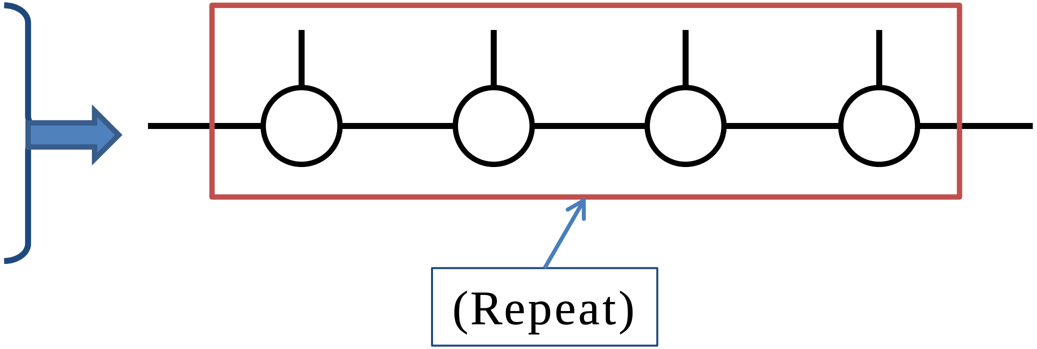
Calculation methods – iDMRG

Find ground state with the **infinite-system density matrix renormalization group (iDMRG)** method

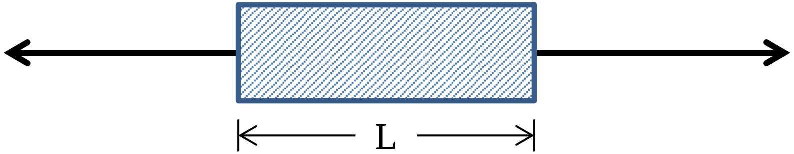
- Variational method within **Matrix Product State (MPS)** ansatz

$$|\psi\rangle = \sum_{\{\sigma_i\}} \dots A_i^{(\sigma_i)} A_{i+1}^{(\sigma_{i+1})} \dots |\dots\sigma_i \sigma_{i+1} \dots\rangle$$

$A_i \rightarrow$ d x χ x χ tensor,
d: physical dimension
χ: MPS bond dimension



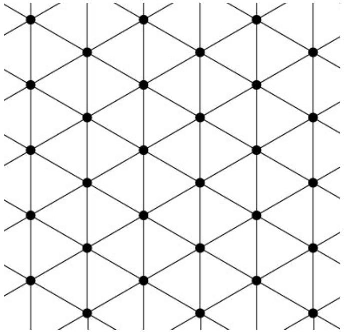
- Max entanglement $\rightarrow$ log(χ)
  - Necessary χ scales with exp(S)
  - MPS is efficient for 1D *area law* states (eg. gapped ground states!)



$$S \propto L^0 = \text{const.}$$

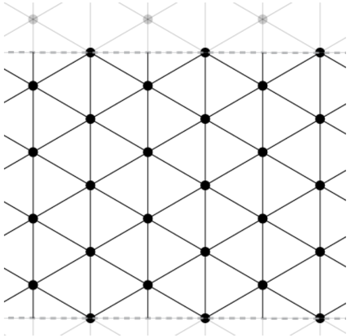
Calculation methods – cylinder DMRG

Apply DMRG to 2D system:

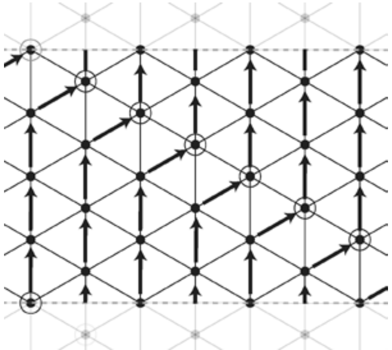


1. Use finite width strip

(YC boundary conditions)

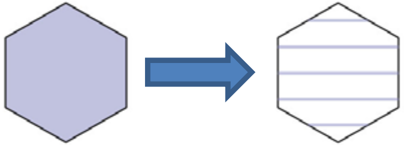


2. Order sites



Consequences & Limitations:

1. Discrete momenta

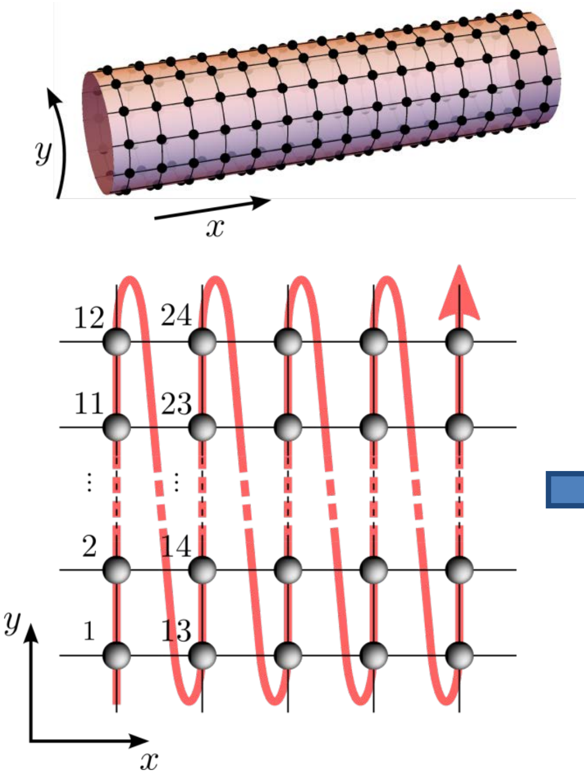


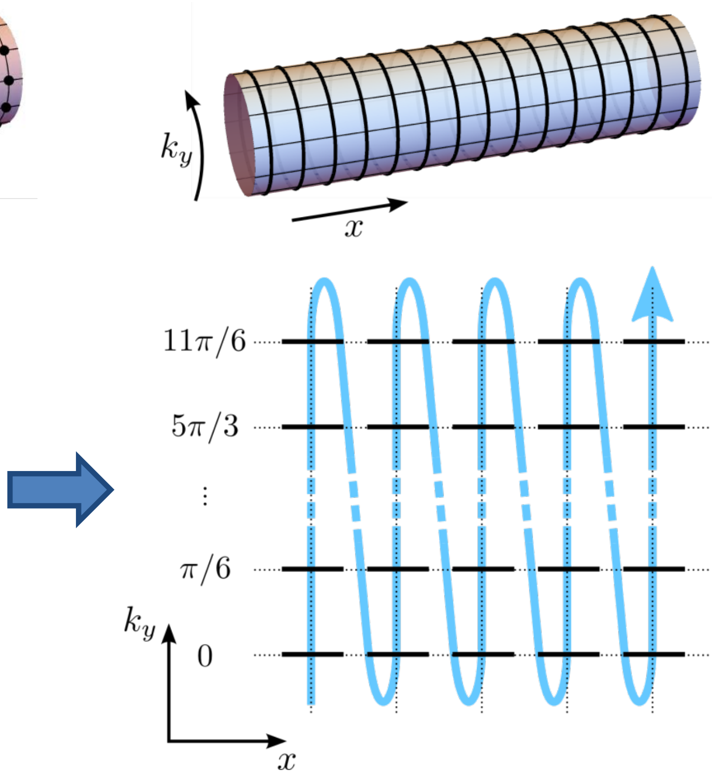
2. Entanglement growth

(Area law)

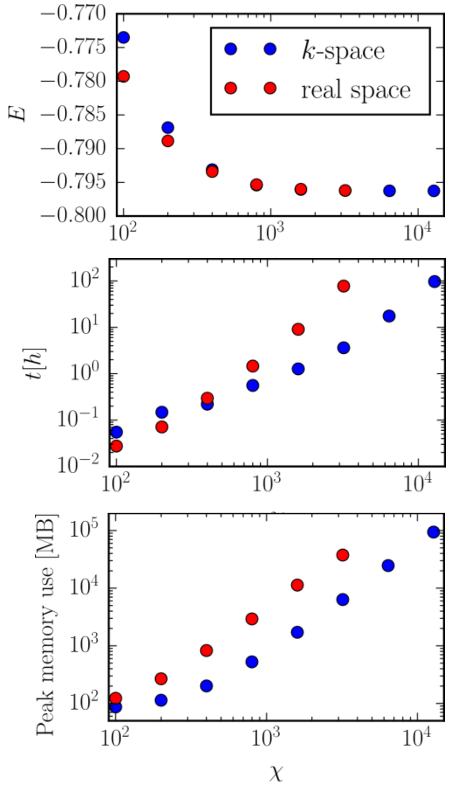
$$S \propto L \longrightarrow \chi \propto \exp(L) \longrightarrow L \lesssim 6$$

Calculation methods – mixed-space DMRG





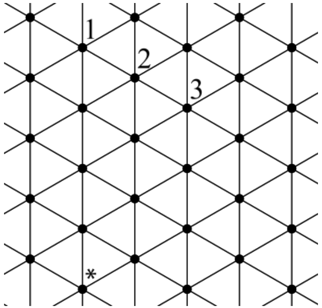
Benchmark:
Hofstadter model



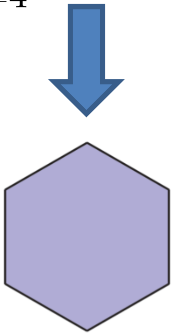
Motruk et al, PRB 2016

Calculation methods – mixed-space DMRG

On triangular lattice

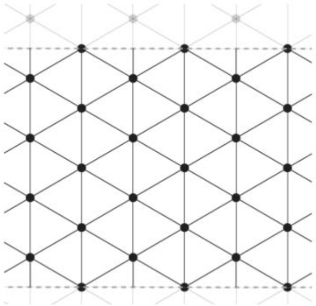


$\boldsymbol{L}=4$

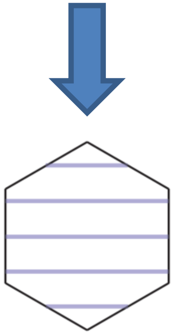


Number of $\boldsymbol{k_y}$ quantum numbers:

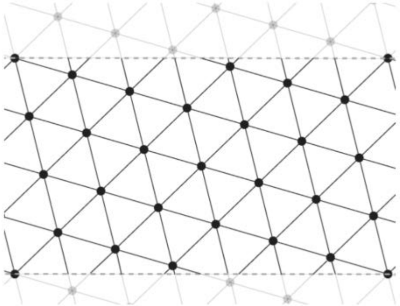
Number of k quantum numbers depends on boundary conditions:

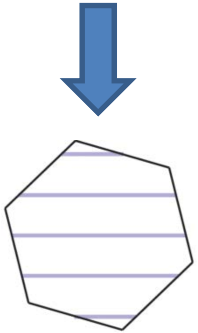


YC

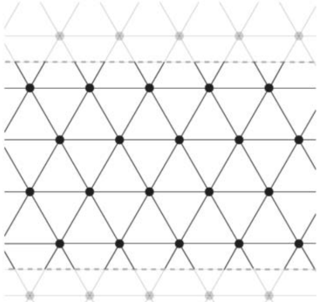


4
($\boldsymbol{L}$)

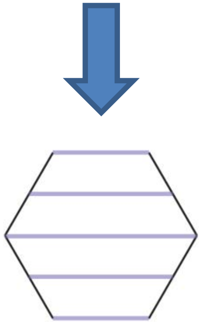




1



XC



2
($\boldsymbol{L}/2$)

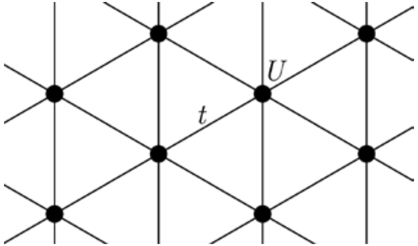
Outline

1. Introduction
2. Calculation methods
3. Phase diagram
4. Chiral spin liquid phase
5. Implications/comparisons and summary
6. Future directions

Phase diagram: expected

Hubbard model:

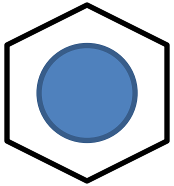
$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



Phase diagram (expected):

Metal — × — Nonmagnetic insulator — × — Spin-ordered → U/t

Exact solution:



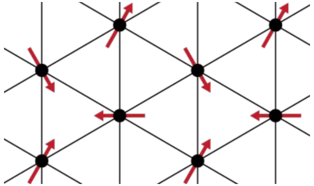
Candidates:

- U(1) spin liquid with spinon Fermi surface
- Gapped Z_2 spin liquid
- Nodal gapless spin liquid
- Chiral spin liquid
- Others ...

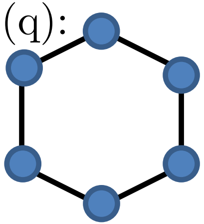
Reduces to Heisenberg:

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

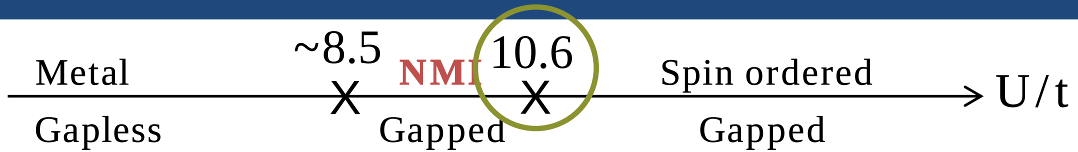
120° order:



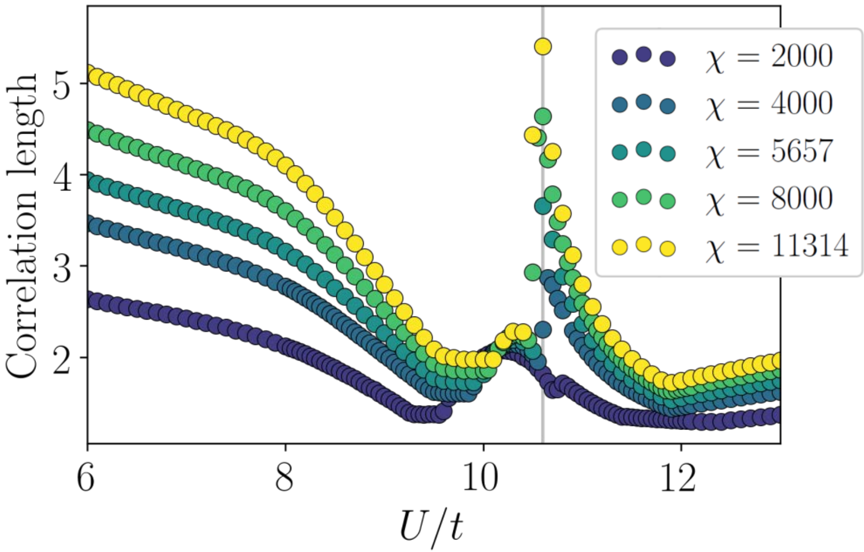
S(q):



Phase diagram: L=4 cylinder



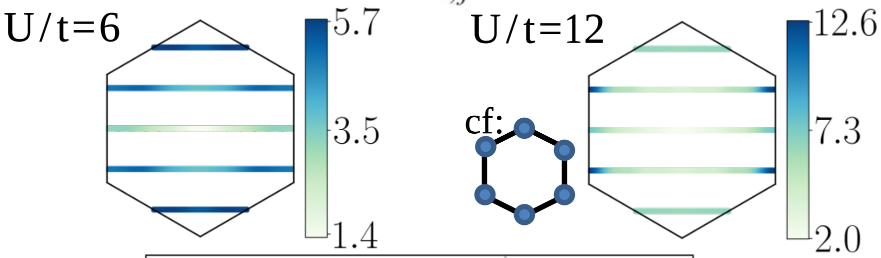
Correlation length

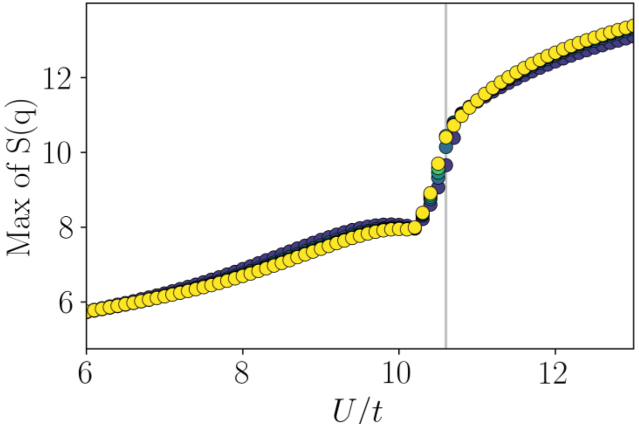


χ: MPS bond dimension

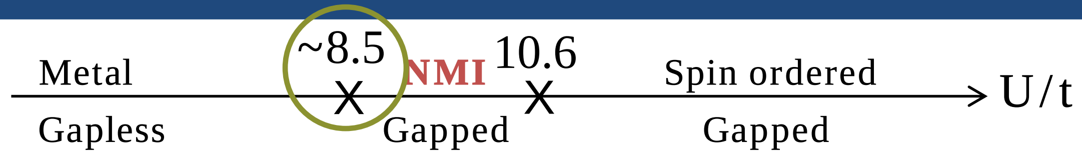
- Controls precision of DMRG

Spin order: $S(\boldsymbol{q}) = \frac{1}{N_s} \sum_{i,j} e^{i\boldsymbol{q}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)} \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle$



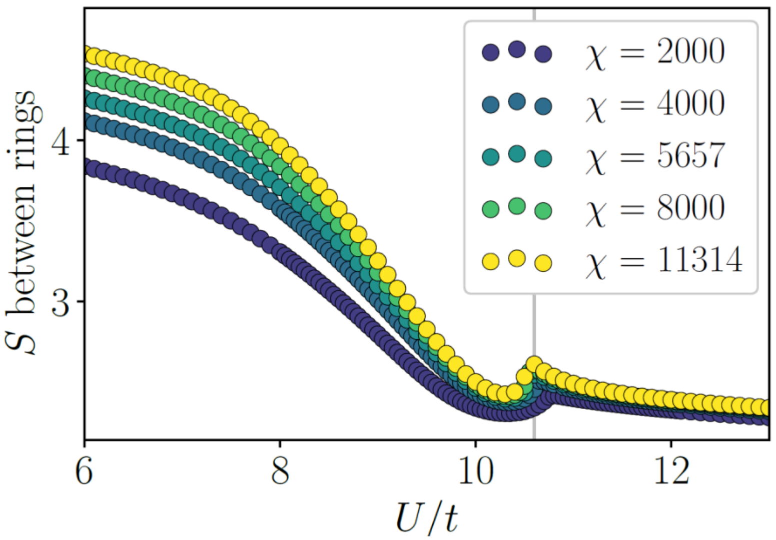


Phase diagram: L=4 cylinder



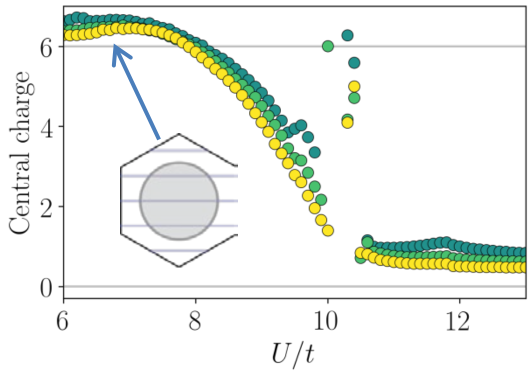
Entanglement:

$$|\psi\rangle = \sum_{i=1}^{\cancel{\infty}\ \chi} \lambda_i |\psi_i^A\rangle |\psi_i^B\rangle \quad \Rightarrow \quad S = \sum_{i=1}^{\cancel{\infty}\ \chi} -\lambda_i^2 \log(\lambda_i^2)$$

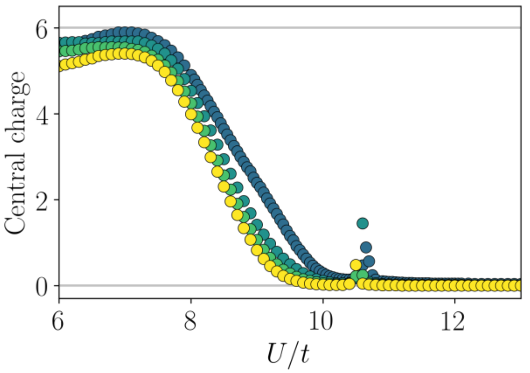


Finite entanglement scaling:

$$S = \frac{c}{6}\log(\xi)$$

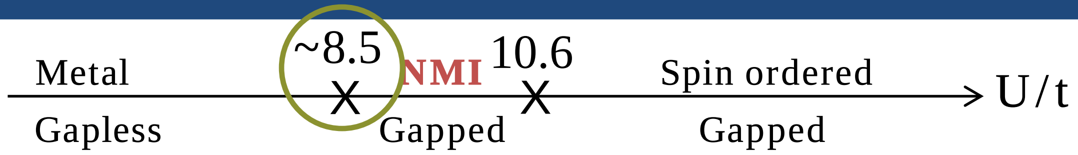


$$S \approx \left(1 + \sqrt{12/c}\right)^{-1} \log(\chi)$$



Calabrese & Cardy, J. Stat. Mech. 2004
Pollmann et al, PRL 2009

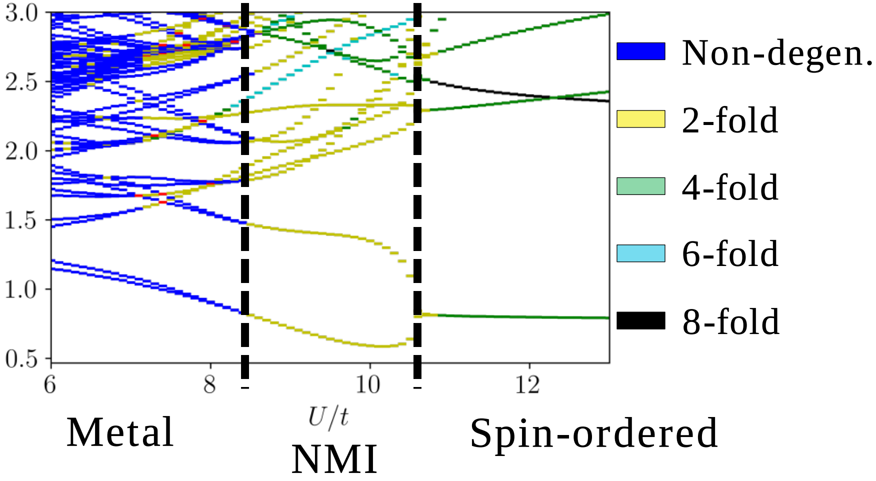
Phase diagram: L=4 cylinder



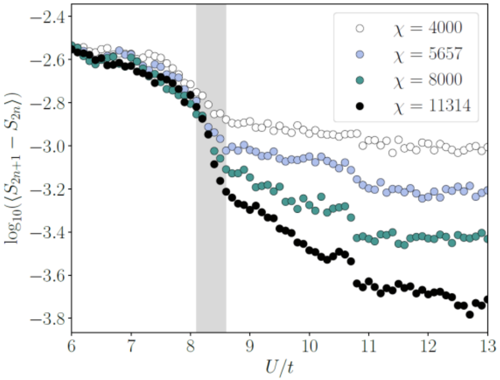
Entanglement:

$$|\psi\rangle = \sum_{i=1}^{\cancel{\infty}\ \chi} \lambda_i |\psi_i^A\rangle |\psi_i^B\rangle \quad \rightarrow \quad S = \sum_{i=1}^{\cancel{\infty}\ \chi} -\lambda_i^2 \log(\lambda_i^2)$$

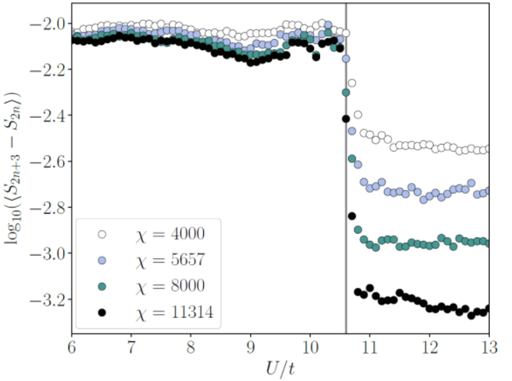
Entanglement spectrum: $\{-\log(\lambda_i)\}$



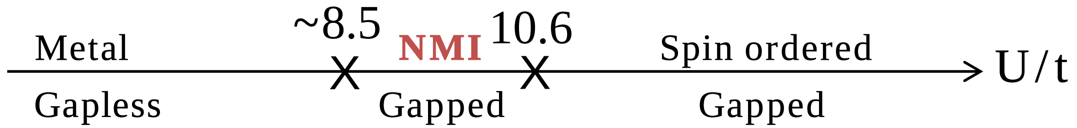
Separation of pairs



Separation of "quads"

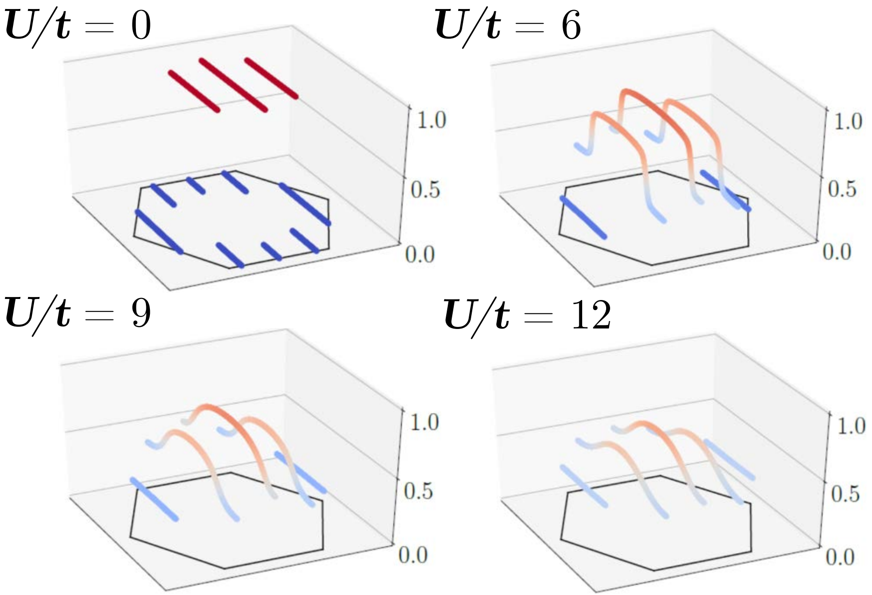


Phase diagram: L=4 cylinder

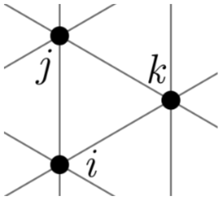


Occupation and Fermi surface:

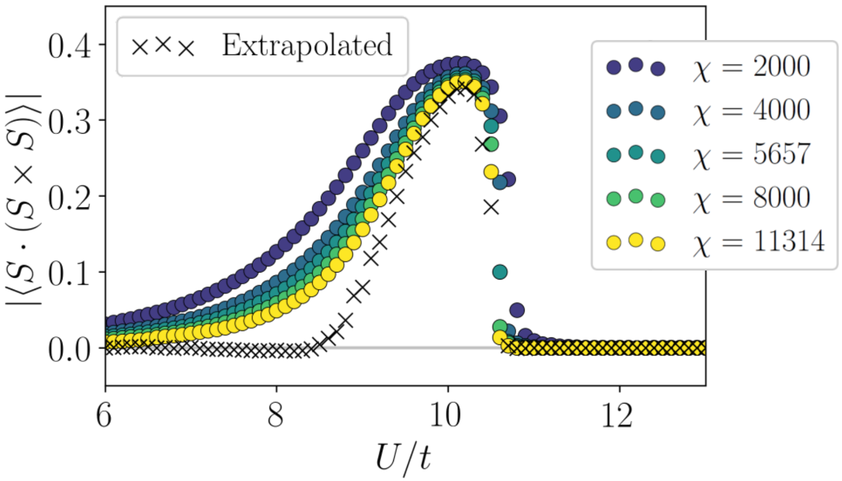
$$\langle n_{k_x,k_y,\uparrow}\rangle = \sum_{x=-50}^{50} e^{ik_x x}\langle c^\dagger_{0,k_y,\uparrow} c_{x,k_y,\uparrow}\rangle$$



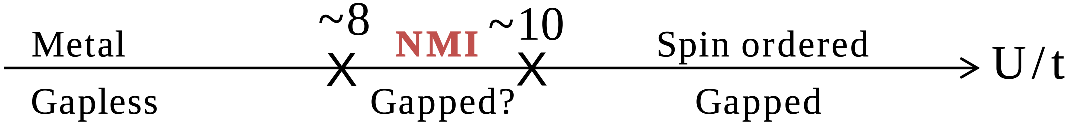
Scalar chiral order parameter:



$$\langle \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k) \rangle$$

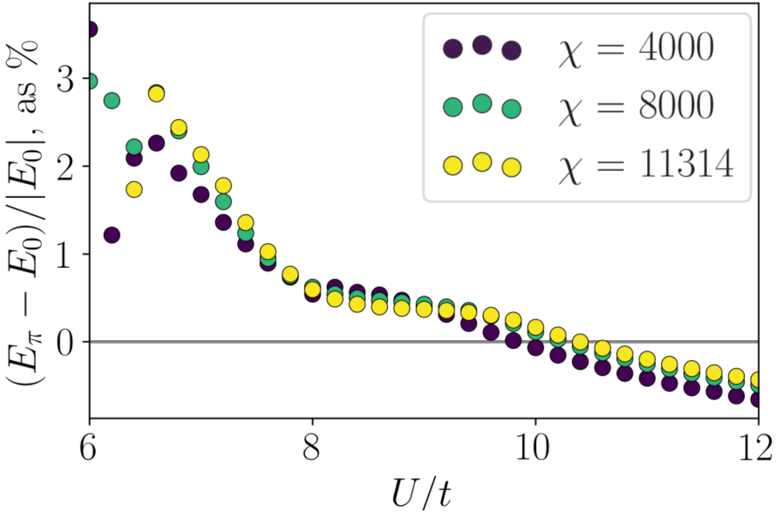


Phase diagram: L=6 cylinder

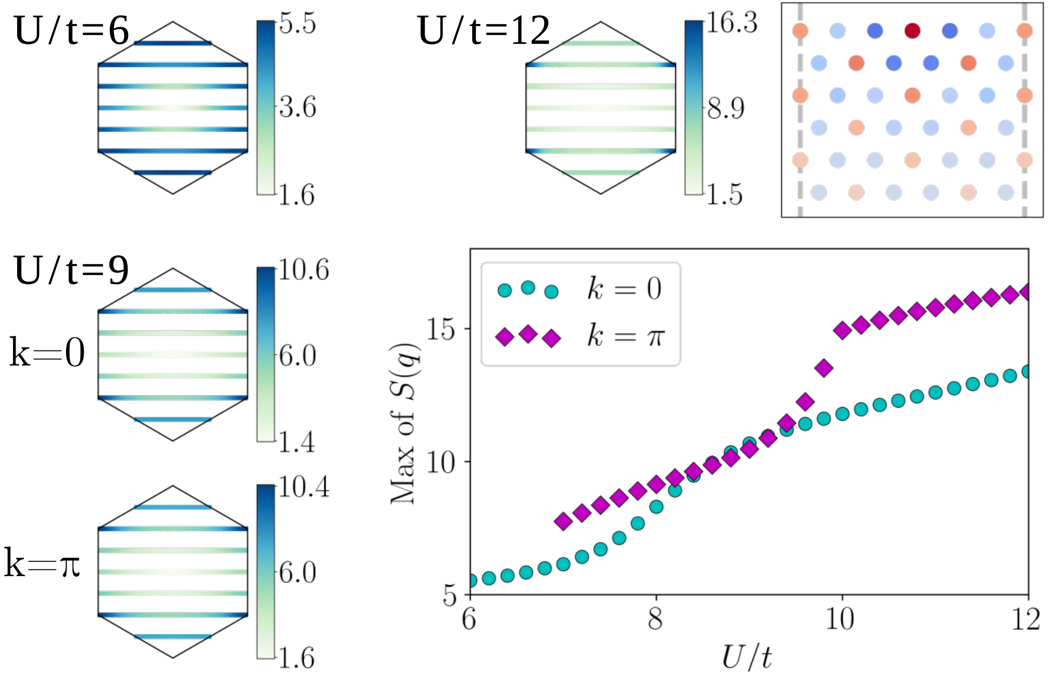


Two low-energy states:

k=0, k=π
per ring



Spin order:

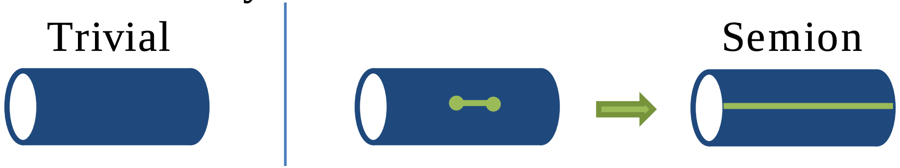


Outline

1. Introduction
2. Calculation methods
3. Phase diagram
4. Chiral spin liquid phase
5. Implications/comparisons and summary
6. Future directions

What is a chiral spin liquid?

- ν=1/2 fractional quantum Hall effect state for spins
- Signatures:
  - Time-reversal symmetry breaking
    - eg: scalar chiral order parameter
    - 2 chiralities → 2x ground state degeneracy
  - Topological ground state degeneracy and fractionalized quasiparticles (semions)
    - 2x on infinite cylinder

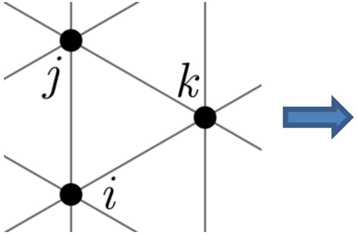


  - Chiral edge modes in 2D → entanglement spectrum on cylinder
    - Characteristic level counting vs momentum: 1, 1, 2, 3, 5, …
    - 2x degeneracy for semion sector
  - Quantized spin Hall effect: 2π flux insertion → spin ½ pumping

Kalmeyer & Laughlin, PRL 1987
Wen et al., PRB 1989

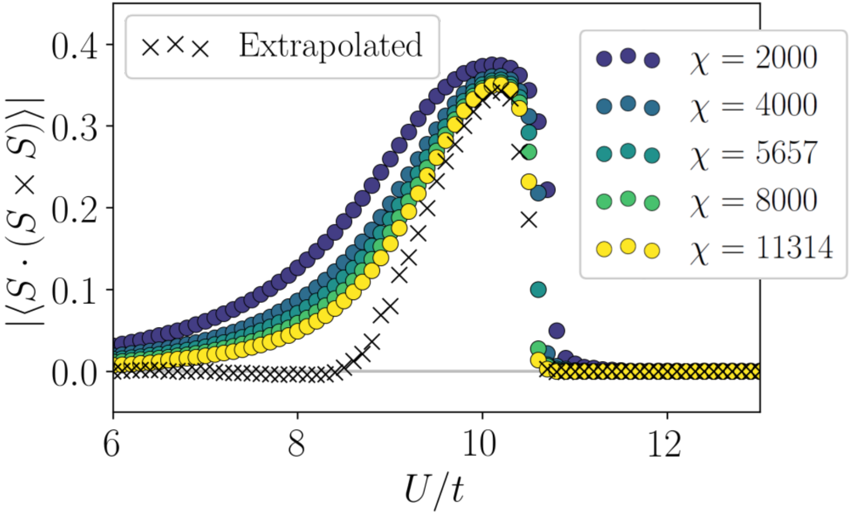
Identification as a CSL

Chiral order parameter:



$$\langle \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k) \rangle$$

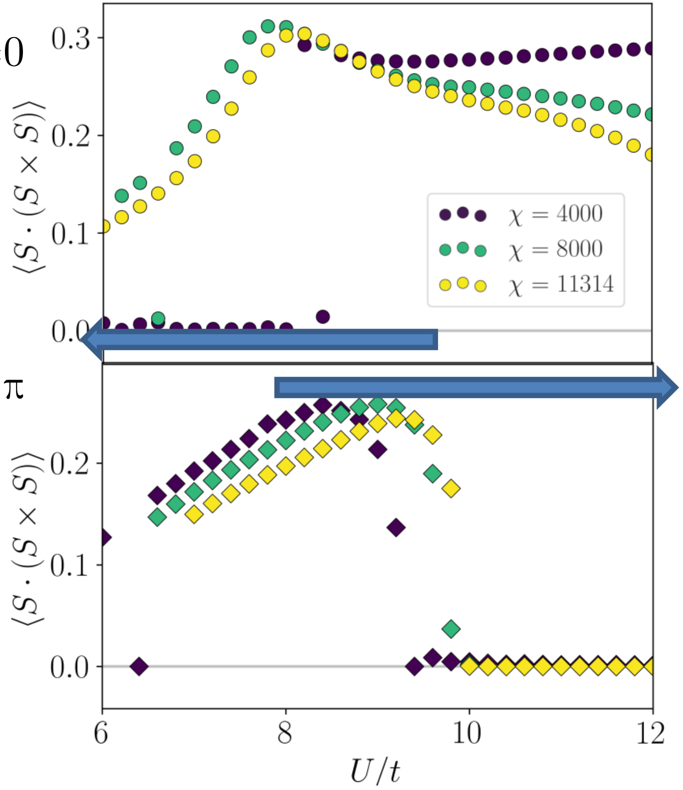
L=4



L=6

k=0

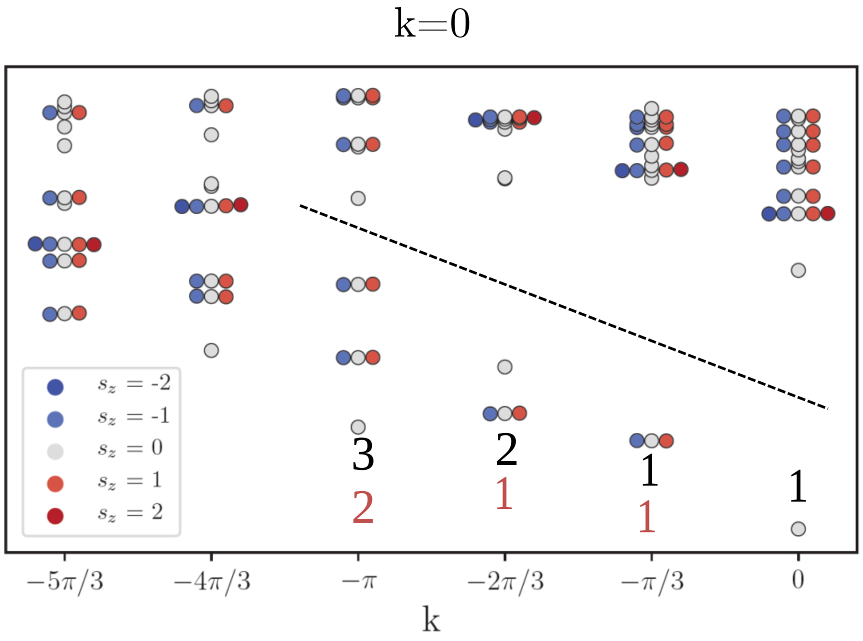
k=π



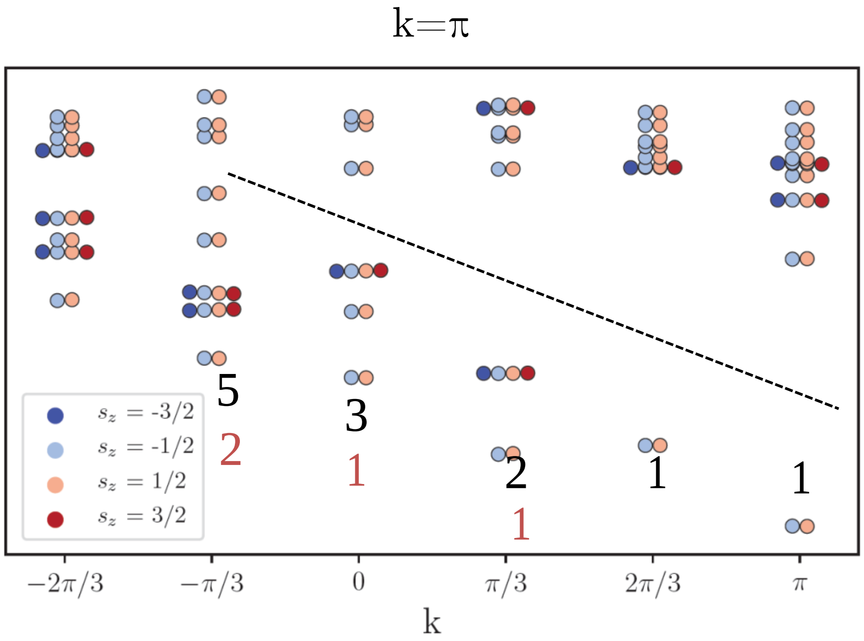
Ground state

Identification as a CSL

Spin- and momentum-resolved entanglement spectrum, L=6, U/t = 9:



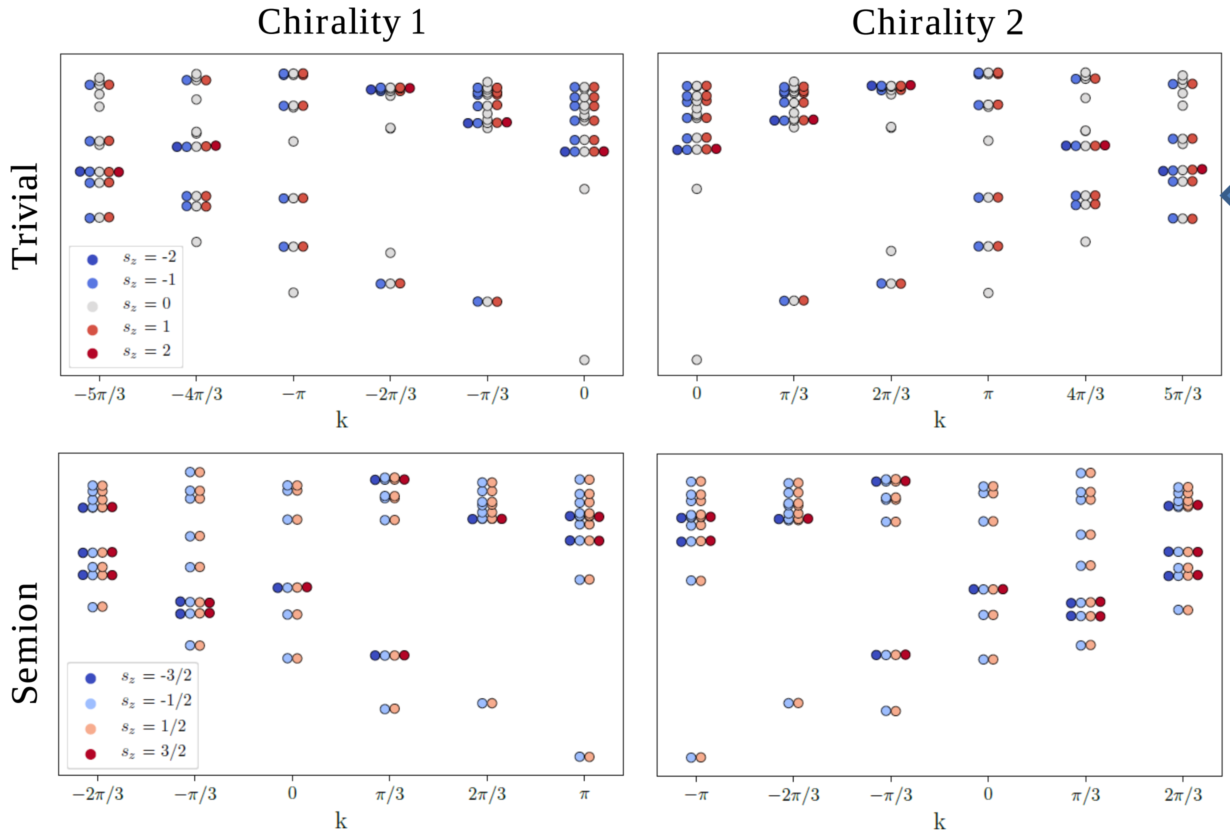
Trivial sector



Semion sector

Identification as a CSL

Ground state degeneracy, L=6, U/t = 9:



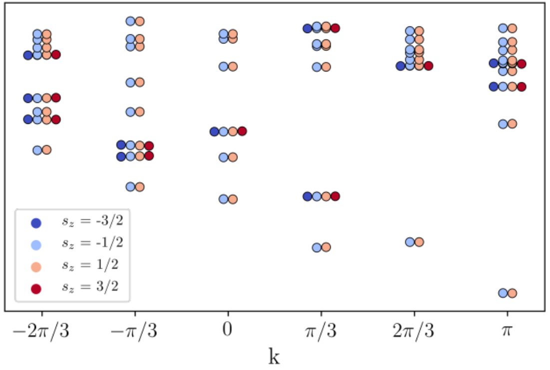
Initialize: 10 random product states

Identification as a CSL

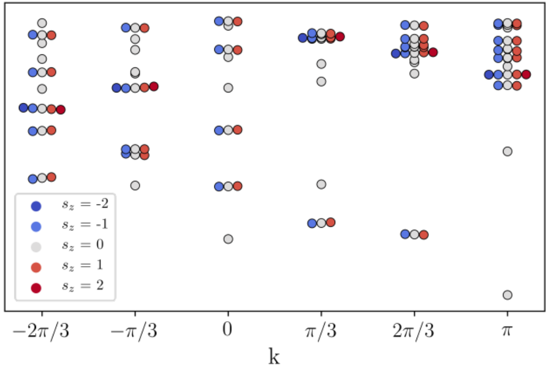
Flux insertion and spin Hall effect:

$$H \rightarrow -t \sum_{\langle ij\sigma \rangle} \left(e^{i(i_y - j_y)\sigma\theta/2} c^{\dagger}_{i\sigma} c_{j\sigma} + \text{H.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

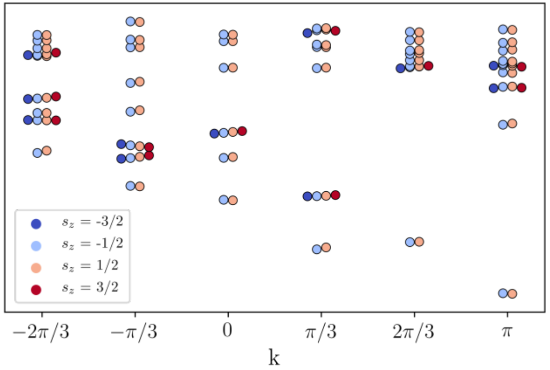
0 flux



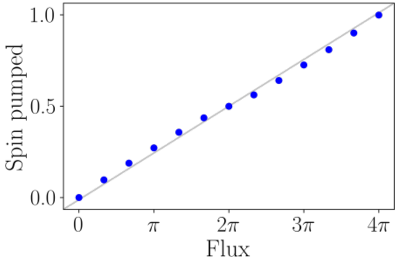
2π flux



4π flux



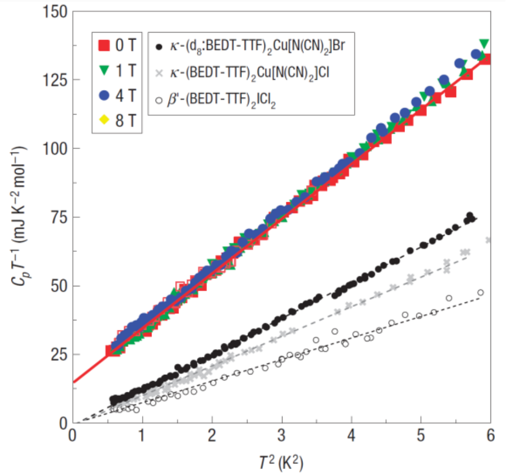
Spin Hall effect:

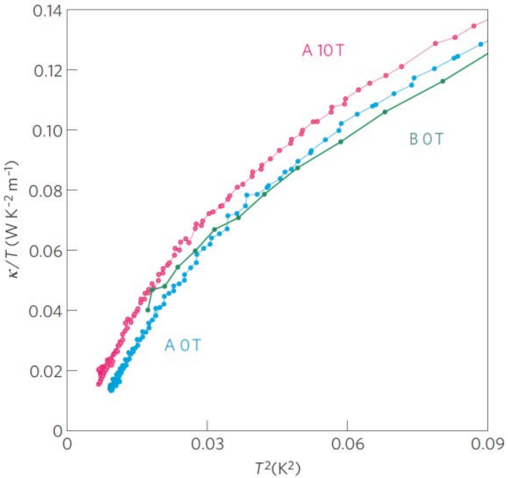


Outline

1. Introduction
2. Calculation methods
3. Phase diagram
4. Chiral spin liquid phase
5. Implications/comparisons and summary
6. Future directions

Comparison with experiments



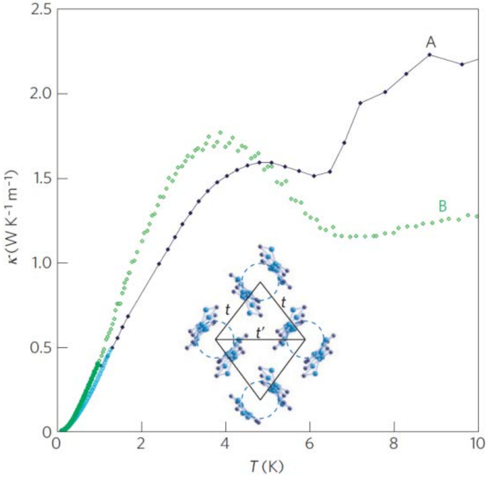


Gapless heat capacity

Gapped conductivity

Gapless chiral edge modes?

Peak in thermal conductivity

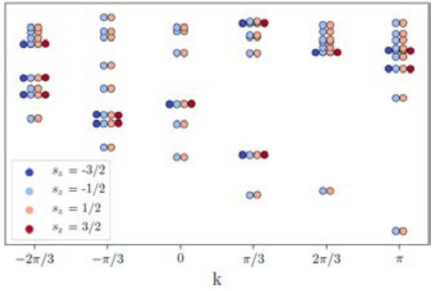


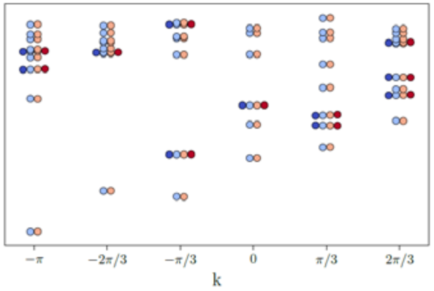
Maybe a finite T phase transition?

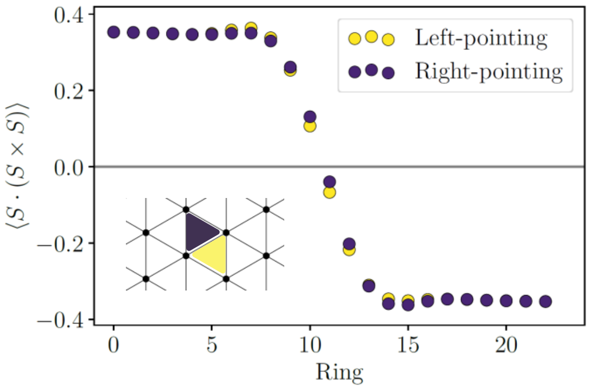
Ising-like ordering transition for two chiralities?

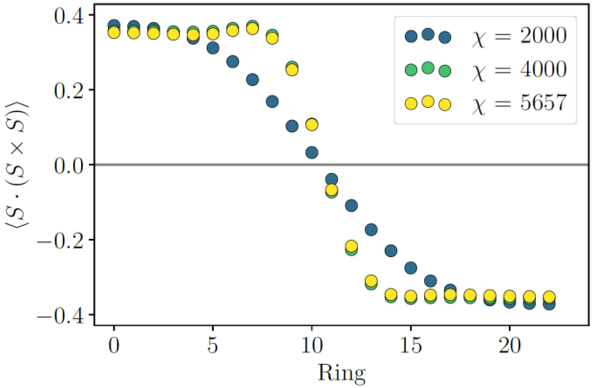
Look at chiral domain wall tension

Chiral domain wall







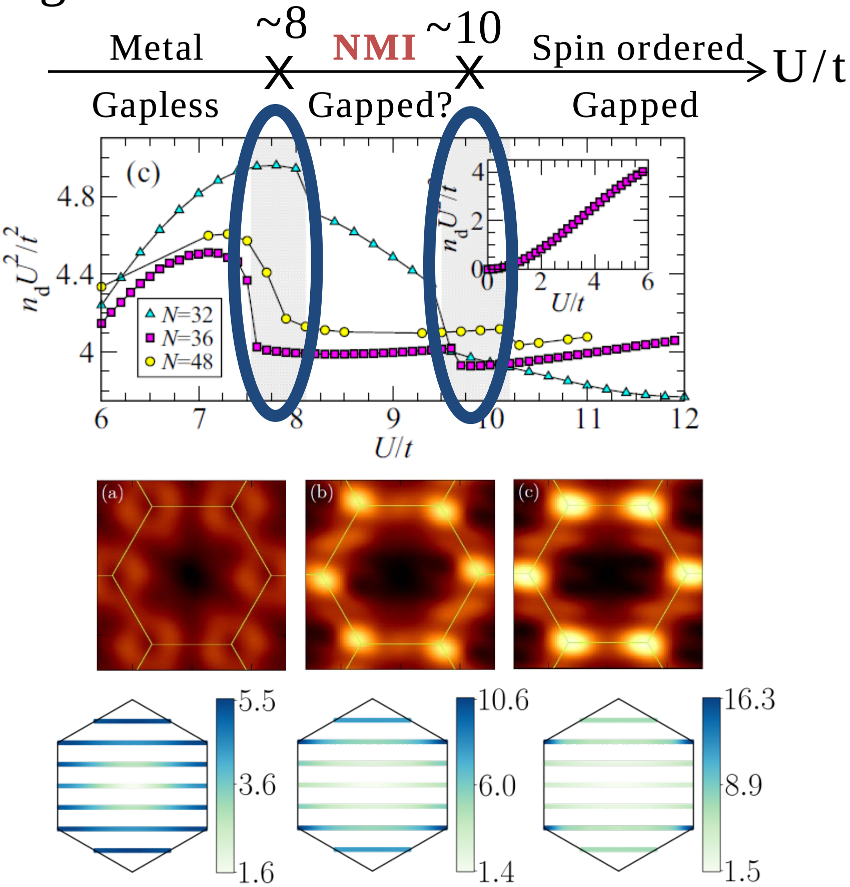


Domain wall tension:
$0.0065\ \boldsymbol{t/a} \approx 4\ \boldsymbol{K}$

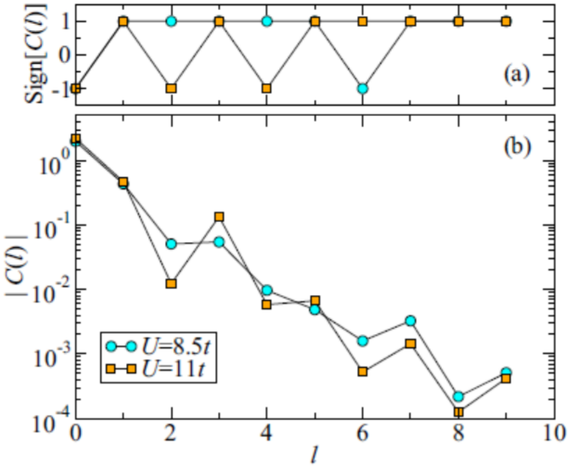
Same order of magnitude:
may explain transition

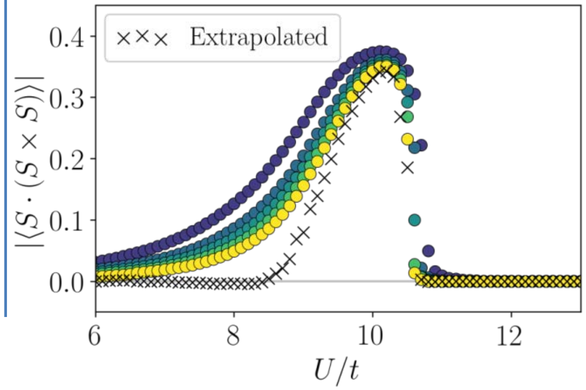
Comparison with RIKEN group results

Agreement:



Disagreement:

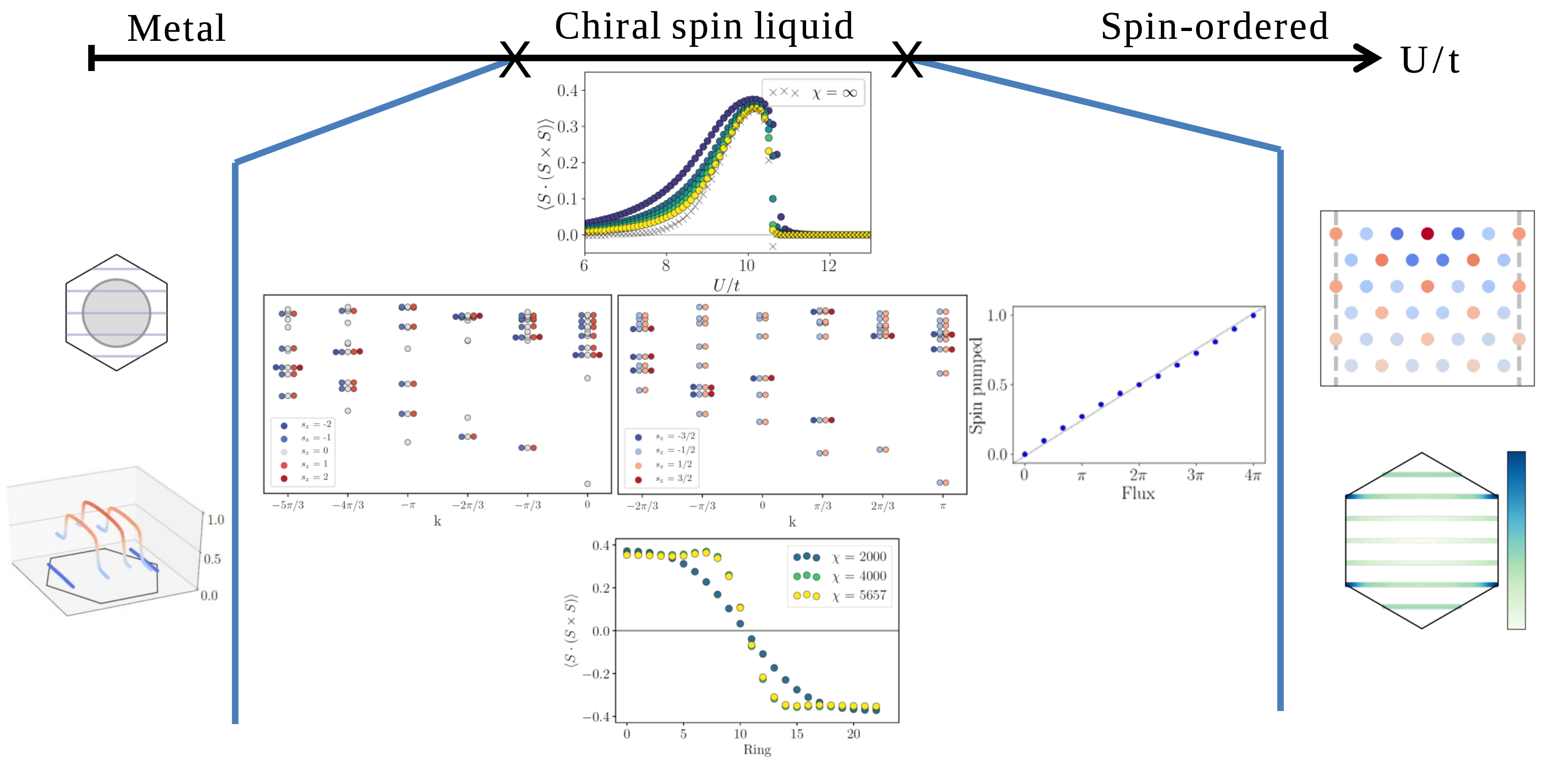




Why?

- Different bcs?
- k-space?
- Finite vs infinite?

Summary



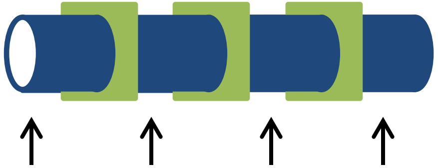
Metal
Chiral spin liquid
Spin-ordered
U/t
$\chi = \infty$
$\langle S \cdot (S \times S) \rangle$
U/t
k
k
Spin pumped
Flux
$\chi = 2000$
$\chi = 4000$
$\chi = 5657$
Ring

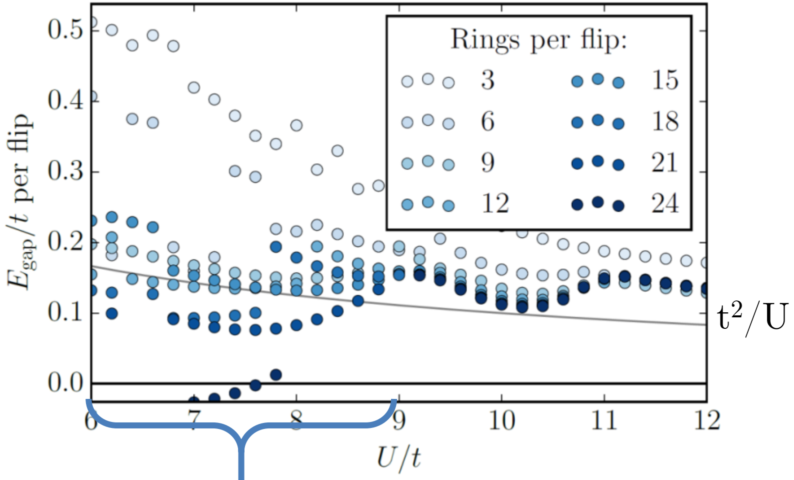
Outline

1. Introduction
2. Calculation methods
3. Phase diagram
4. Chiral spin liquid phase
5. Implications/comparisons and summary
6. Future directions

Spin gap

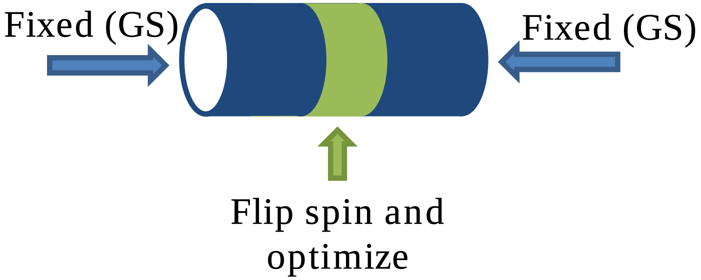
Version 1: Flip 1 spin per N rings:

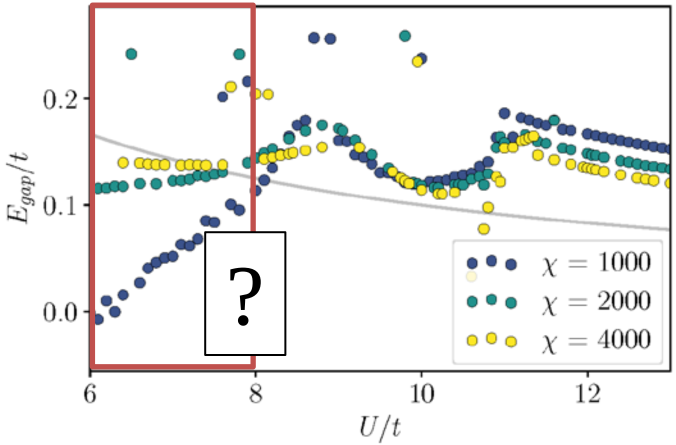




???: Take it with a grain of salt!

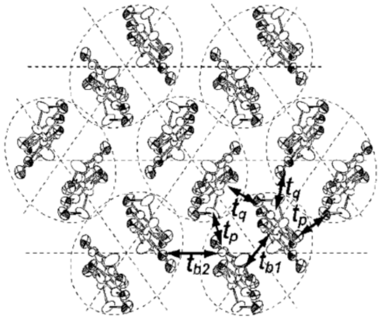
Version 2: Fixed edges

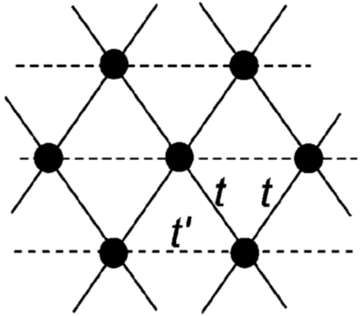


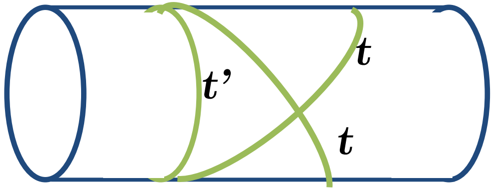


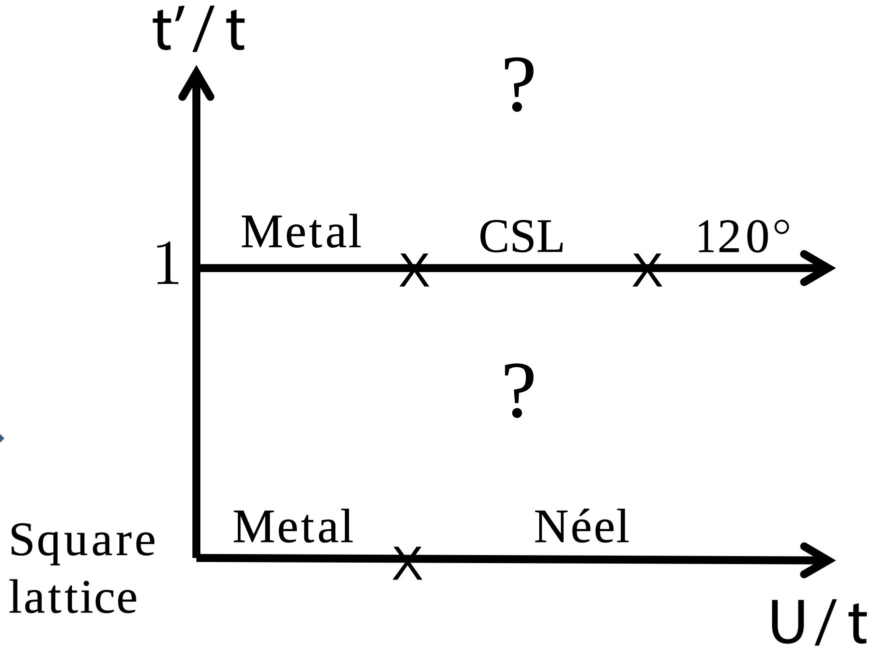
Anisotropy

Real material has some anisotropy:









- Interesting phase transitions to observe!
- Insight for isotropic case phase transitions?

Mixed-space DMRG

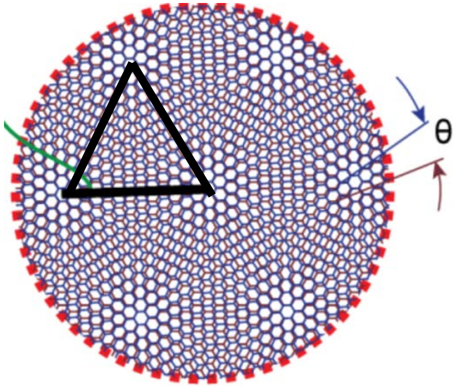
For triangular lattice:

- Extra quantum number $\rightarrow$ computational efficiency
- Find ground state in specific momentum sector

Can be even more useful!

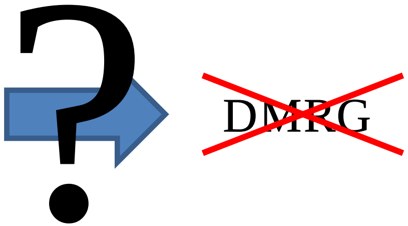
Consider system with Moiré pattern

eg. twisted bilayer graphene

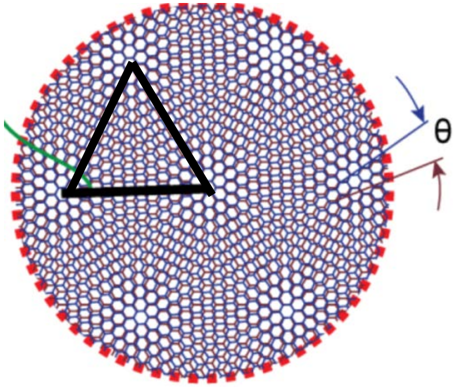


Cao et al., Nature 2018

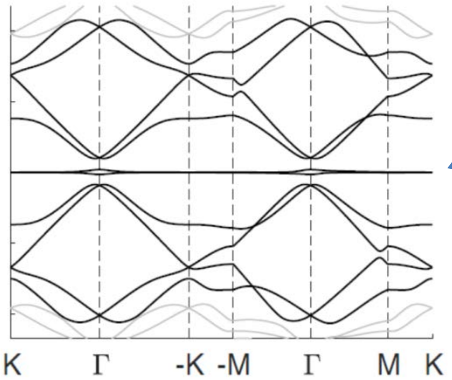
Extremely large unit cell



Mixed-space DMRG



Cao et al., Nature 2018



Po et al., 1808.02482

Only need flat bands

Use Wannier states (k_y, x)

$$\{t_{k_1 k_2, x_1 x_2}\}$$

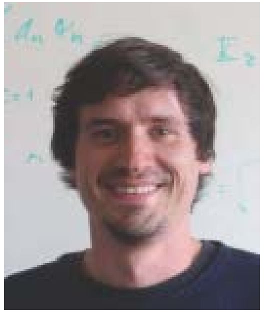
$$\{V_{k_1 k_2 k_3 k_4, x_1 x_2 x_3 x_4}\}$$

Automatically generate and compress MPO

DMRG

Acknowledgements

Collaborators:



Johannes Motruk
(UC Berkeley)

Michael P. Zaletel
(UC Berkeley)

Joel E. Moore
(UC Berkeley)

TenPy DMRG code:
- Michael Zaletel
- Frank Pollmann (Munich)
- Roger Mong (Pittsburgh)

Computing resources:
- Lawrence Berkeley National Laboratory

Summary

- Three phases of Hubbard model on triangular lattice
  - Metal, nonmagnetic insulator (NMI), magnetically ordered
- NMI phase is a chiral spin liquid!
  - Chiral order parameter $\rightarrow$ spontaneous breaking of time-reversal symmetry
  - Two topologically degenerate ground states: trivial, semion sectors
  - Spin Hall effect: 2π flux insertion pumps spin ½
  - May explain features observed in experiments

For more see arXiv: 1808.00463

Thanks for your attention!