Title: Chiral spin liquid phase of the triangular lattice Hubbard model: evidence from iDMRG in a mixed real- and momentum-space basis

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Abstract: <p>Experiments on organic crystals whose structure is well-described by the two-dimensional triangular lattice have found a lack of magnetic ordering down to the lowest accessible temperatures, indicative of a quantum spin liquid phase; however, the precise nature of this phase remains an open question. In this talk, I present strong evidence that the triangular lattice Hubbard model at half filling, a physically motivated model of these organic crystals, realizes a chiral spin liquid phase. In particular, I show that the model has a nonmagnetic insulating phase between a metallic phase for weak interactions and a magnetically ordered phase for strong interactions, and that the intermediate phase exhibits the expected properties of a chiral spin liquid: spontaneous breaking of time-reversal symmetry, topological ground state degeneracy, a quantized spin Hall effect, and characteristic level counting in the entanglement spectrum. These results were obtained using the infinite-system density matrix renormalization group (iDMRG) method in a mixed real- and momentum-space basis; in the talk, I will also discuss the benefits of this mixed-space approach to DMRG in general, including its applicability to systems such as twisted bilayer graphene for which a large unit cell makes real-space DMRG impractical. </p>

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

Outline

1. Introduction
2. Calculation methods
3. Phase diagram
4. Chiral spin liquid phase
5. Implications for experiments 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

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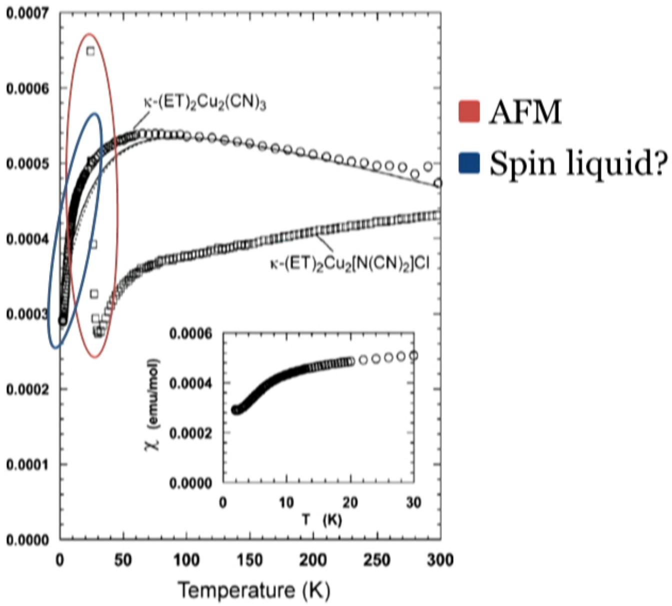
Nonmagnetic at low T:

Magnetic susceptibility



Shimizu et al., PRL 2003

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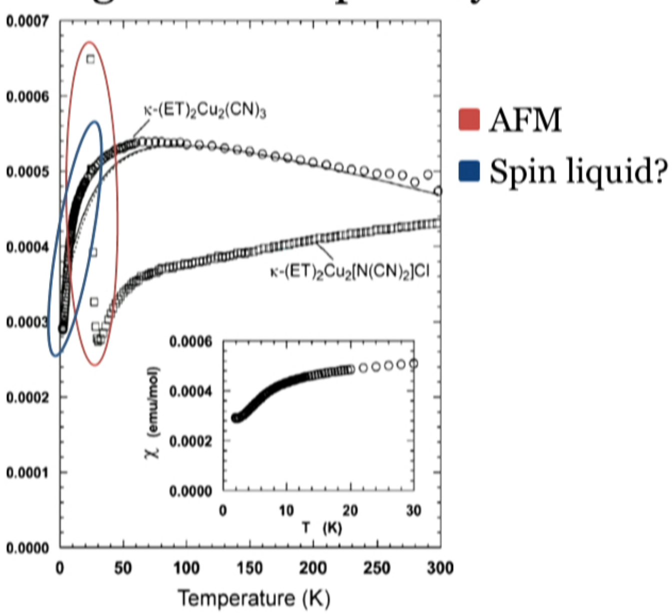
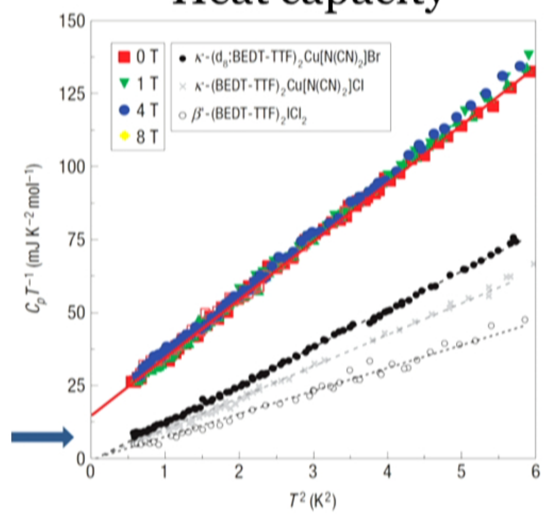


Shimizu et al., PRL 2003

Gapless?

Heat capacity



Yamashita et al., Nat. Phys. 2008

Spin liquids

Anderson 1973

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Pratt 2011

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Gapless states:

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Gapless states:

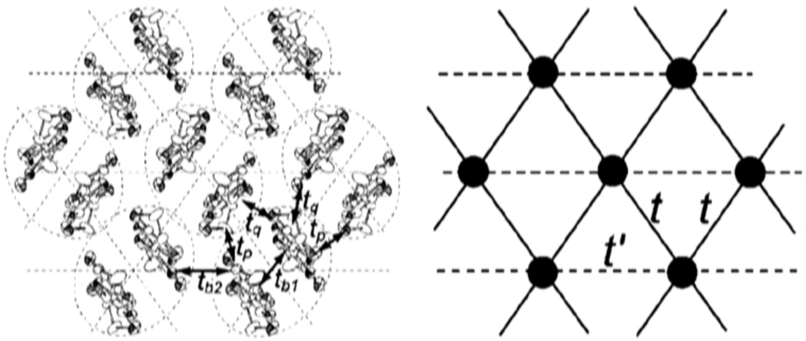
- U(1) spin liquid: spinon Fermi surface
- Dirac spin liquid: gapless Dirac cones at specific points in Brillouin zone
- Quadratic band-touching

Gapped states:

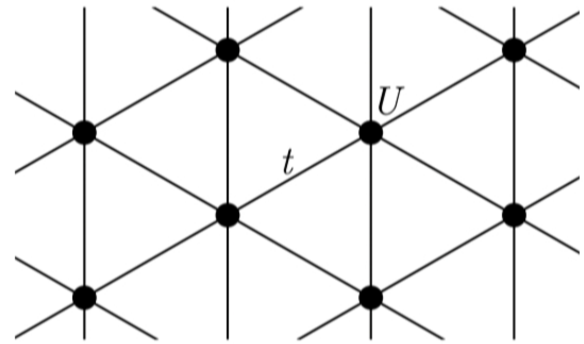
- Z_2 spin liquid: equivalent to Toric code
- Chiral spin liquid:
  - Time-reversal symmetry breaking
  - Gapless edge modes
  - More later!

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]
- $t'/t = 0.8,\ U/t \approx 12\text{-}15$ [Nakamura et al., J. Phys. Soc. Jpn. 2009]

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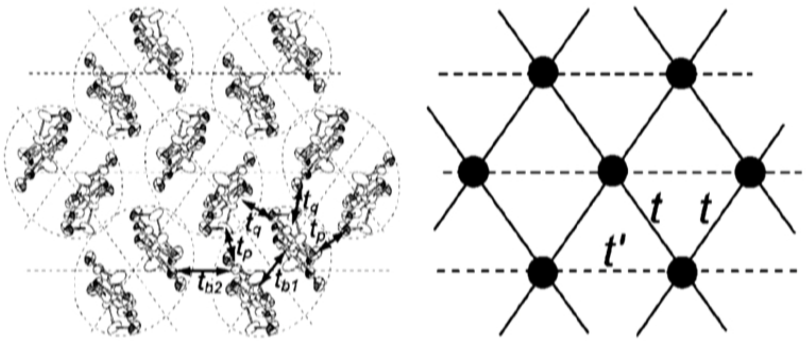

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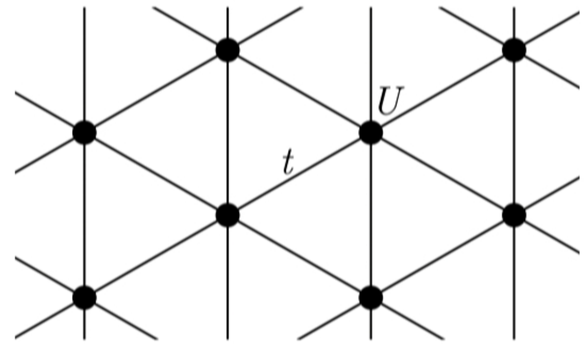

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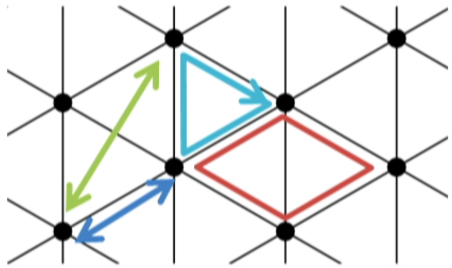
Try to simplify: t/U expansion

½ filling → extended Heisenberg model

Existing results – theory

Spin models:

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



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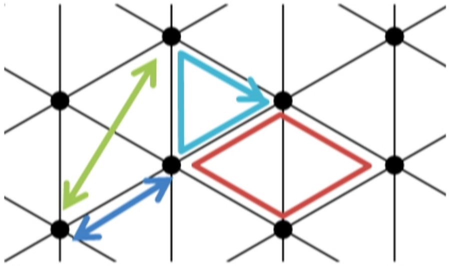
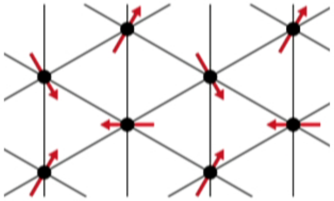


Heisenberg:



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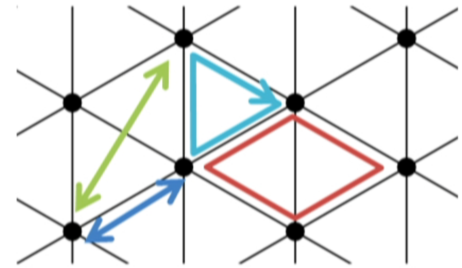

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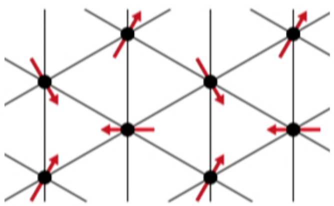
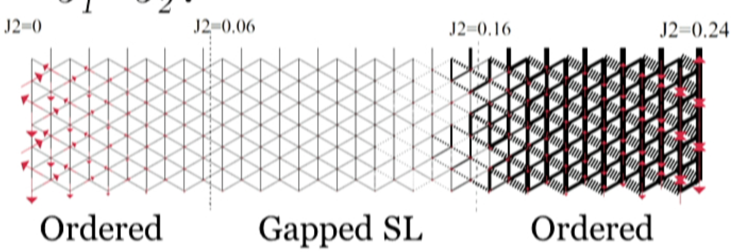


J_1—J_2:



Zhu & White, PRB 2015

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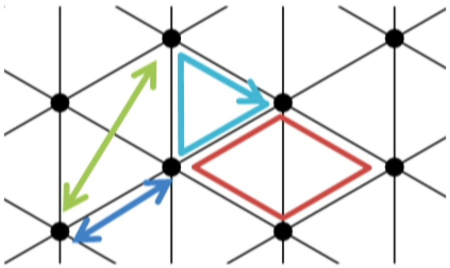

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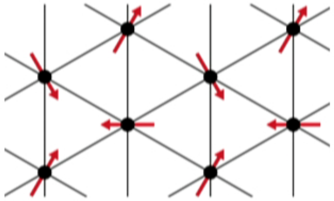

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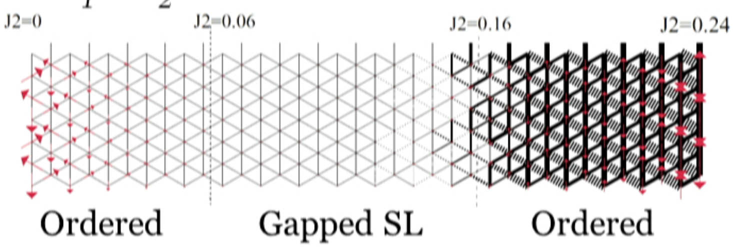

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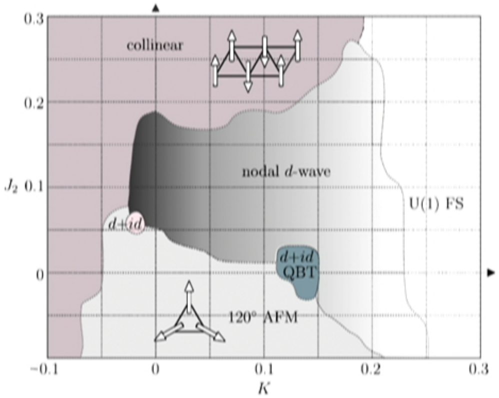
J_1, J_2, K:

Spinon Fermi surface

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



Mishmash et al, PRL 2013

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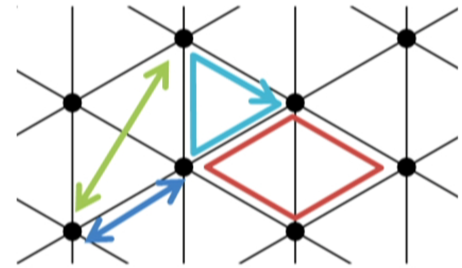

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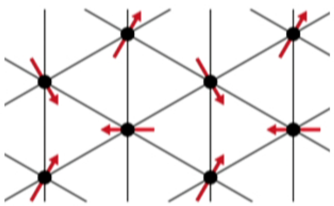

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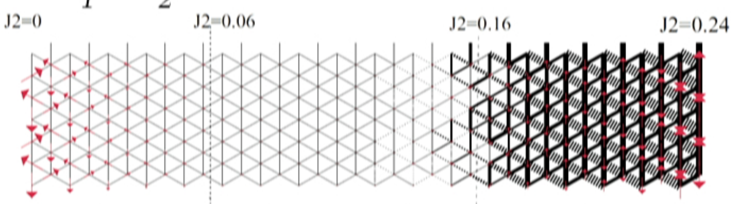

Ordered Gapped SL Ordered

Zhu & White, PRB 2015

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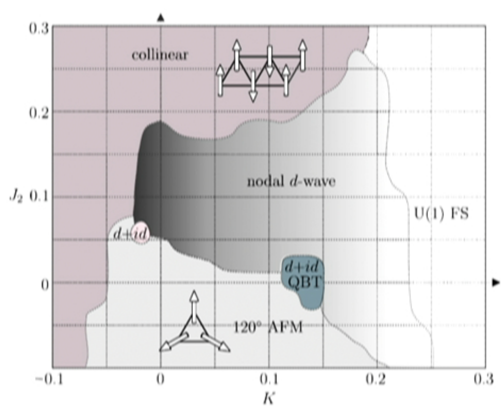
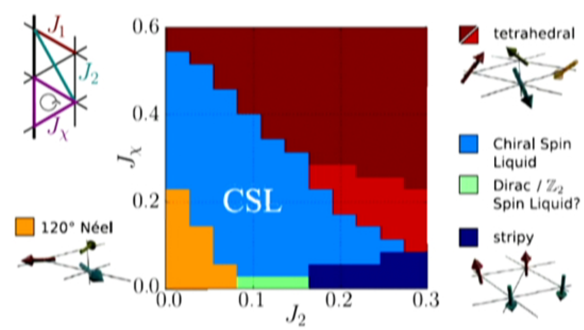


Mishmash et al, PRL 2013

J_1, J_2, χ:

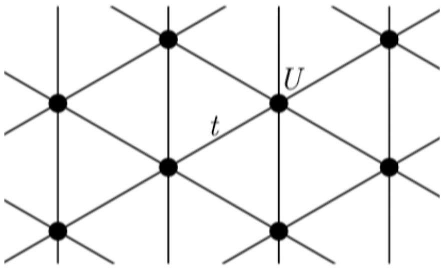


Wietek & Lauchli, PRB 2017

Existing results – theory

Hubbard model:

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



Via spin models:

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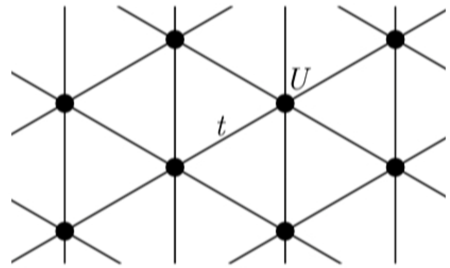

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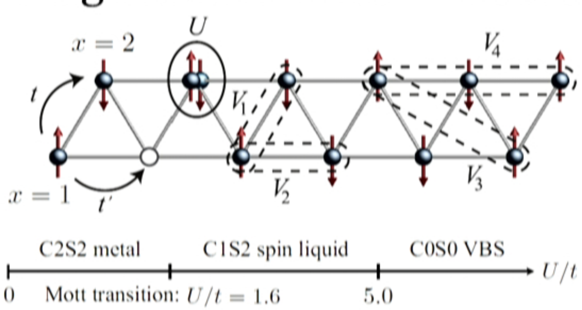

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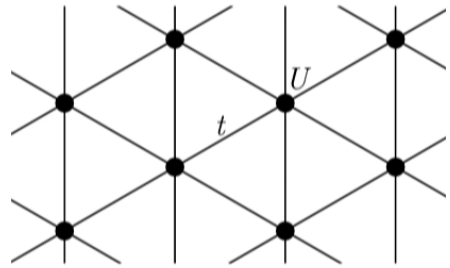

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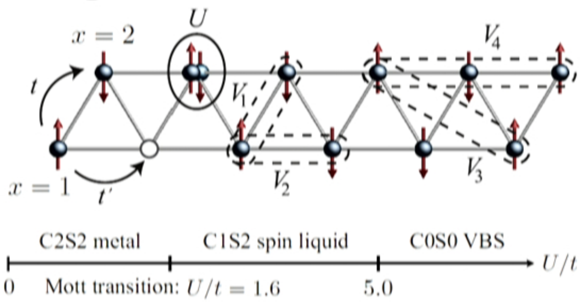

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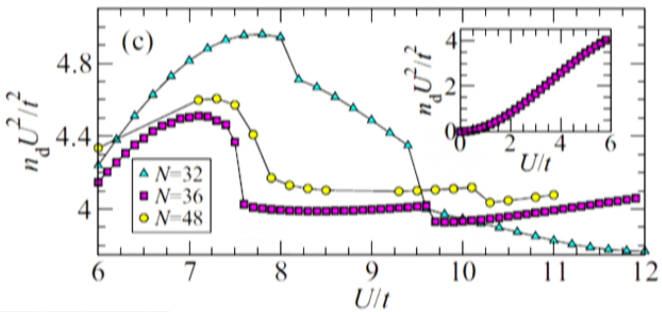
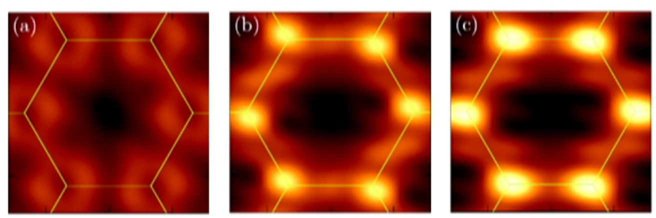
DMRG on finite cylinder:

Three phases:

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





SL spin correlations:

- No Fermi surface
- Gapped/gapless unclear

Shirakawa et al, PRB 2017

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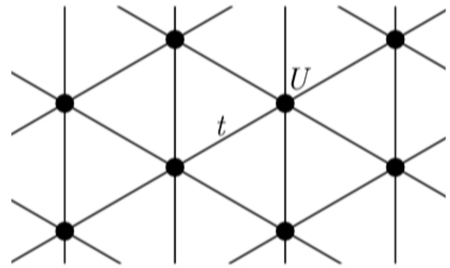

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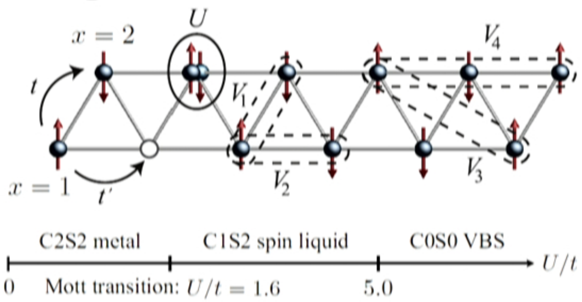

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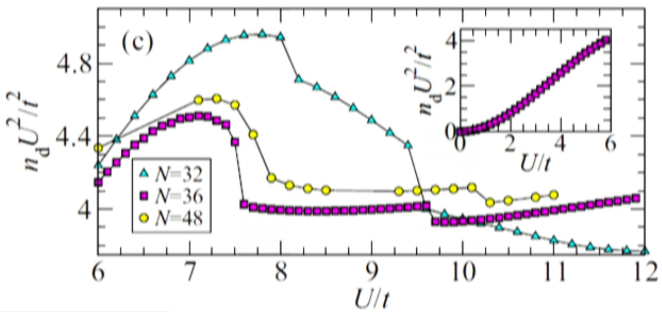

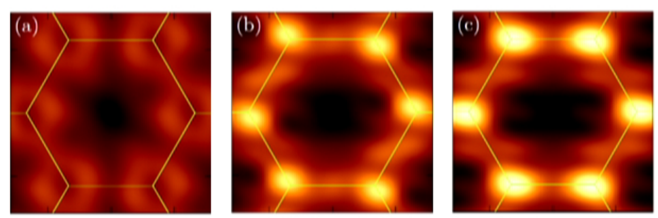

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Nature of spin liquid unclear!

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

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

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

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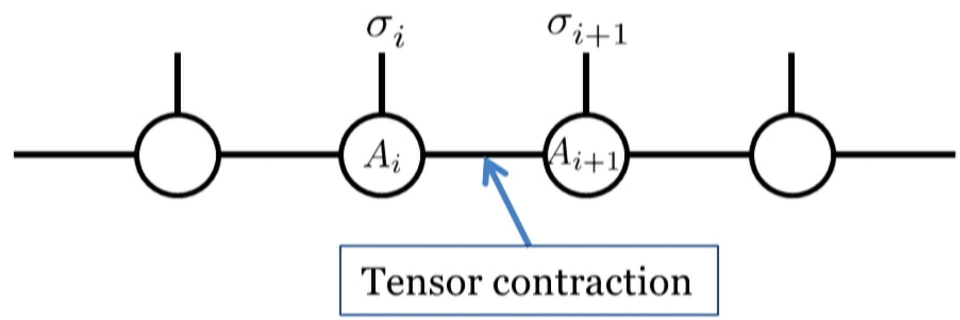

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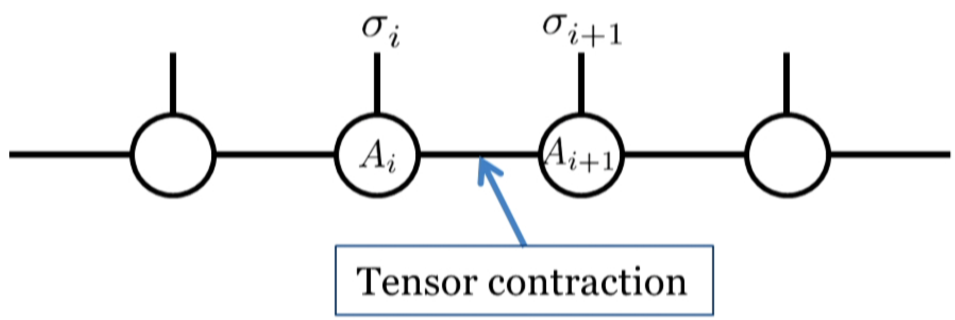

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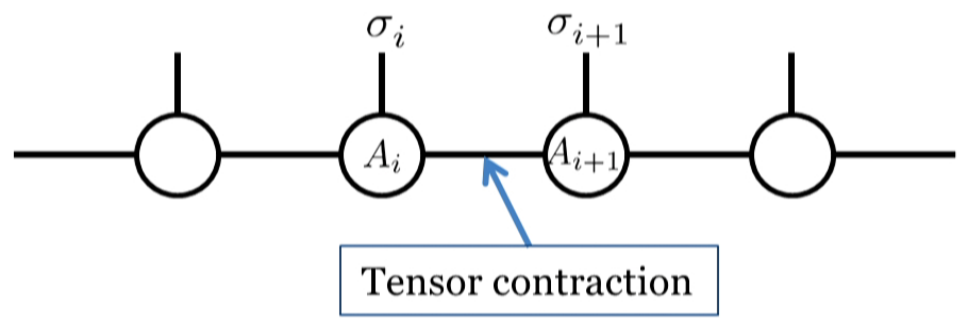
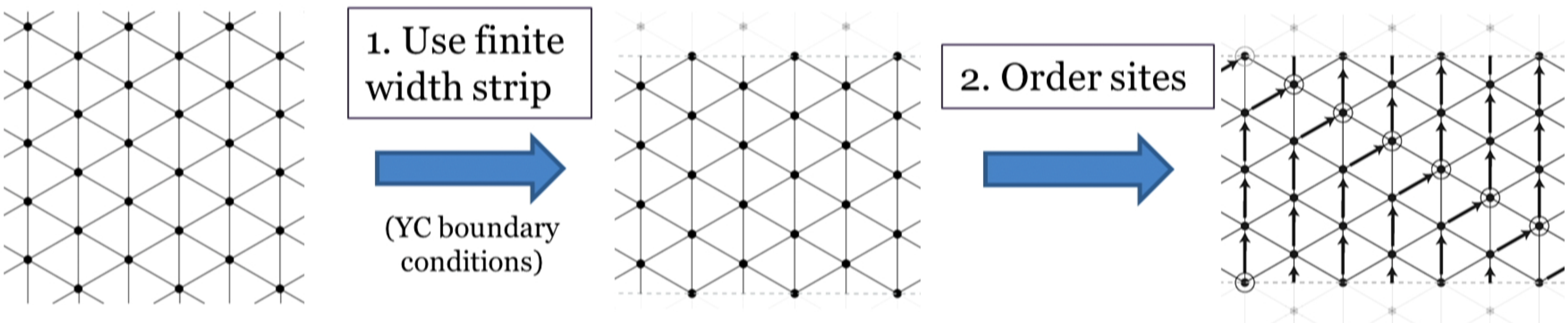


- Max entanglement $\rightarrow$ log(χ)
  - Necessary χ scales with exp(S)
  - MPS is efficient for 1D *area law* states (eg. gapped ground states!)

Calculation methods – cylinder DMRG

Apply DMRG to 2D system:



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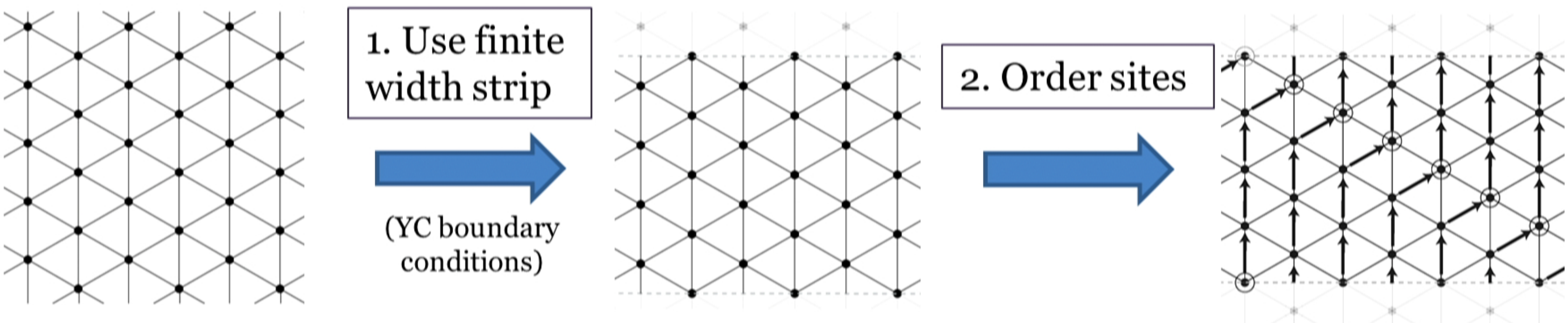

Consequences & Limitations:

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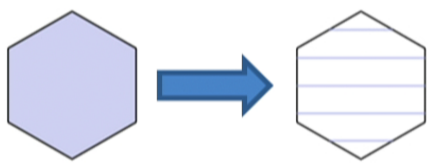

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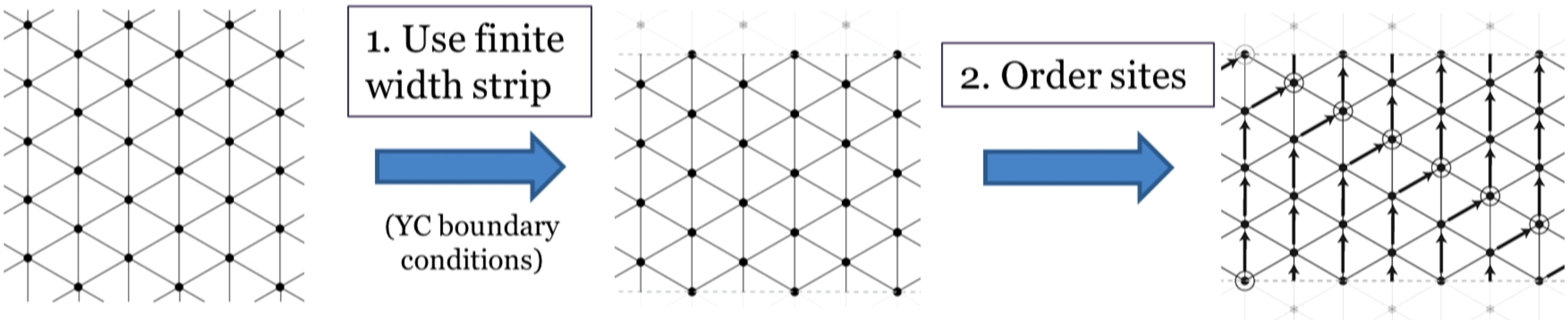

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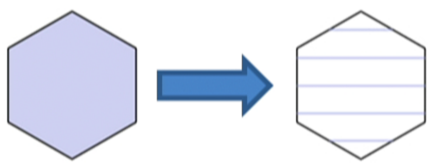
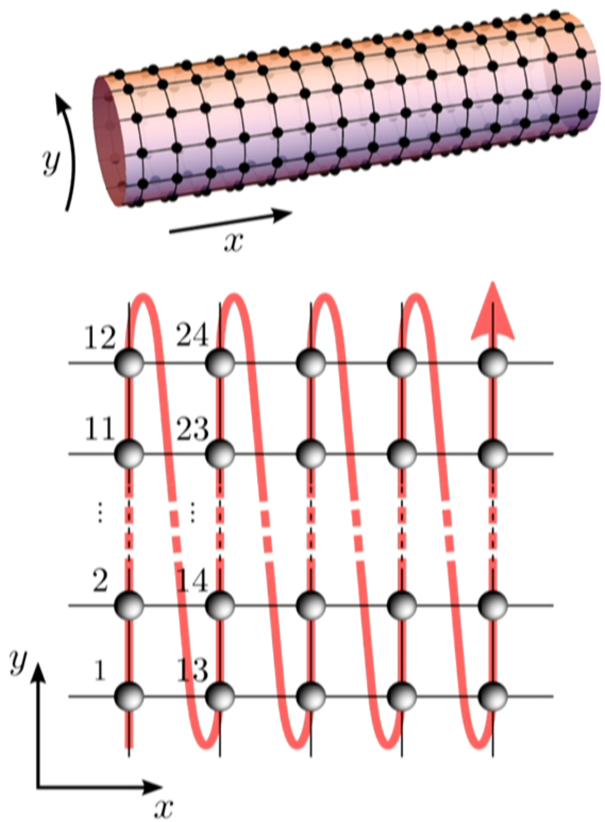


2. Entanglement growth

$$\xrightarrow{\text{(Area law)}} S \propto L \longrightarrow \chi \propto \exp(L) \longrightarrow L \lesssim 6$$

Calculation methods – mixed-space DMRG



Motruk et al, PRB 2016

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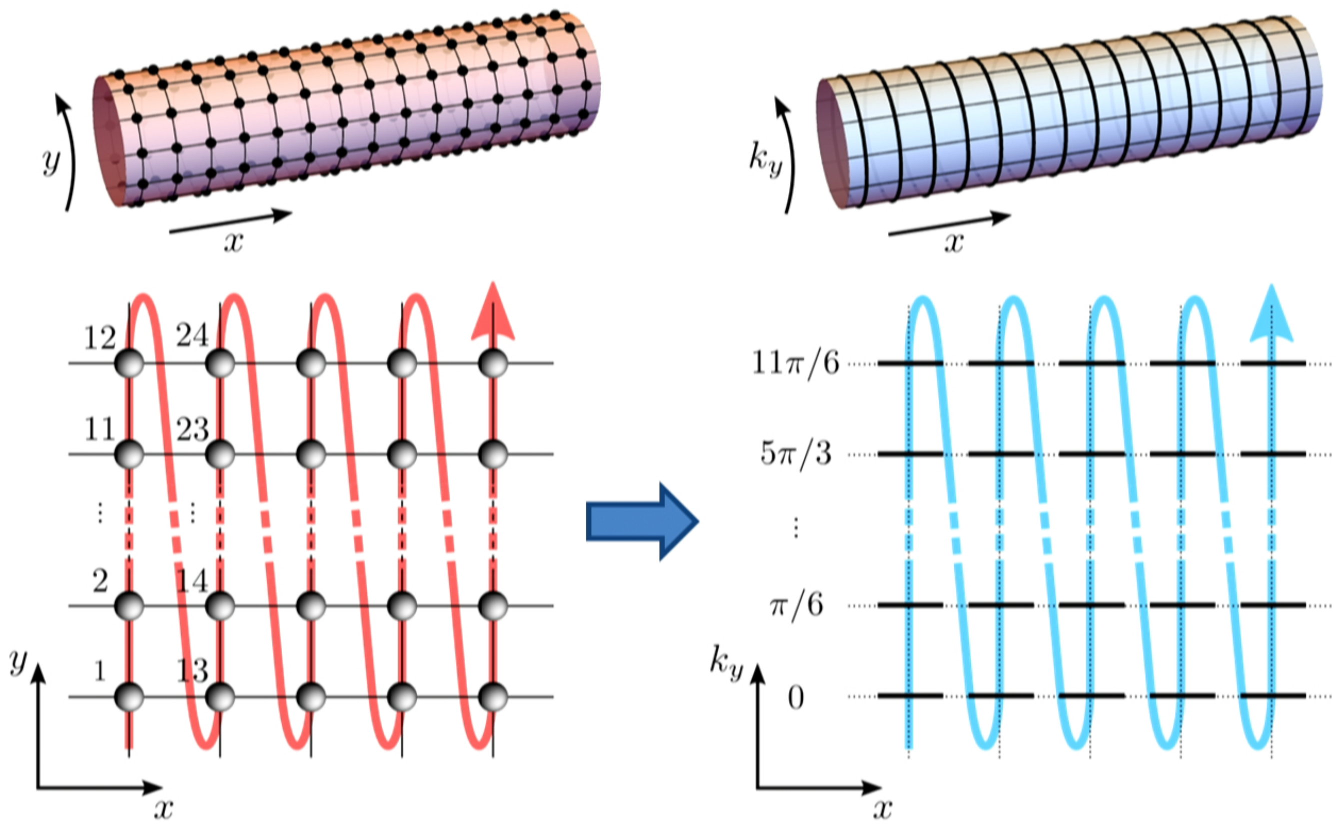

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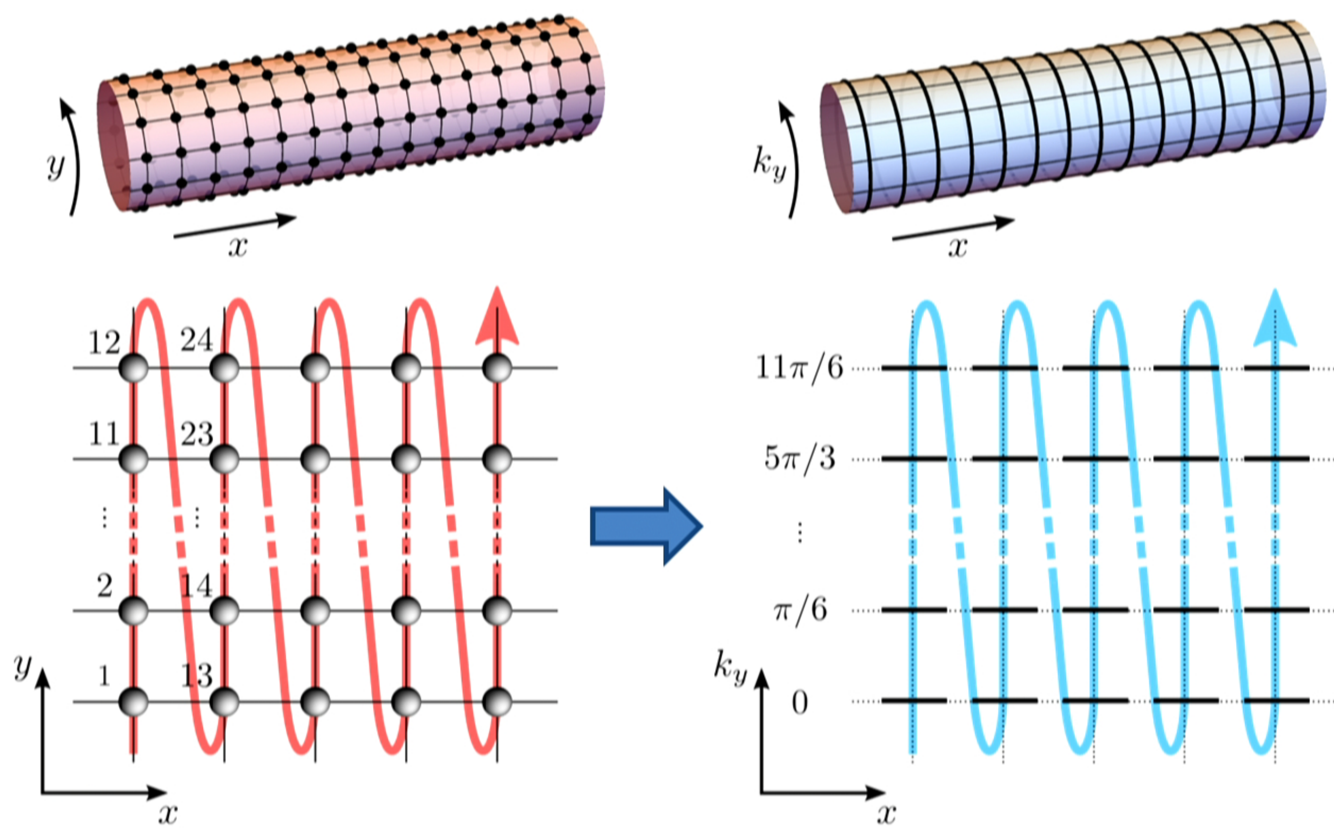
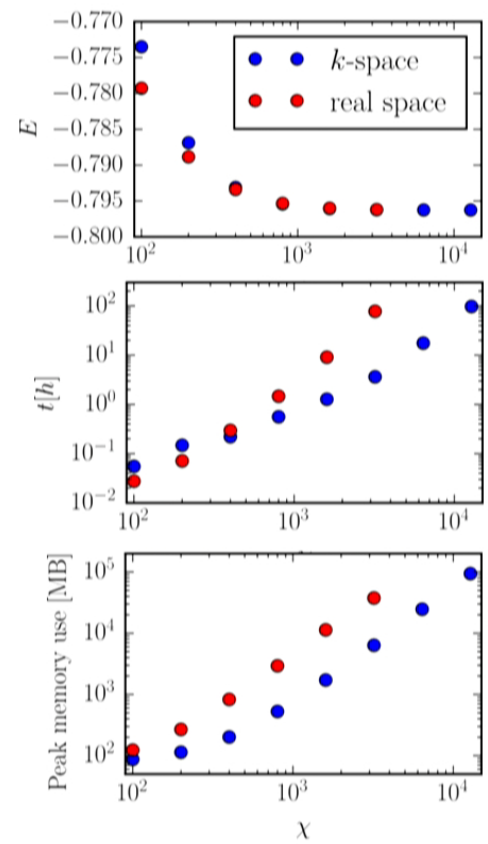
Calculation methods – mixed-space DMRG



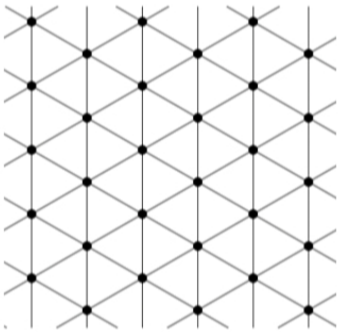
Motruk et al, PRB 2016

Benchmark:
Hofstadter model



Calculation methods – mixed-space DMRG

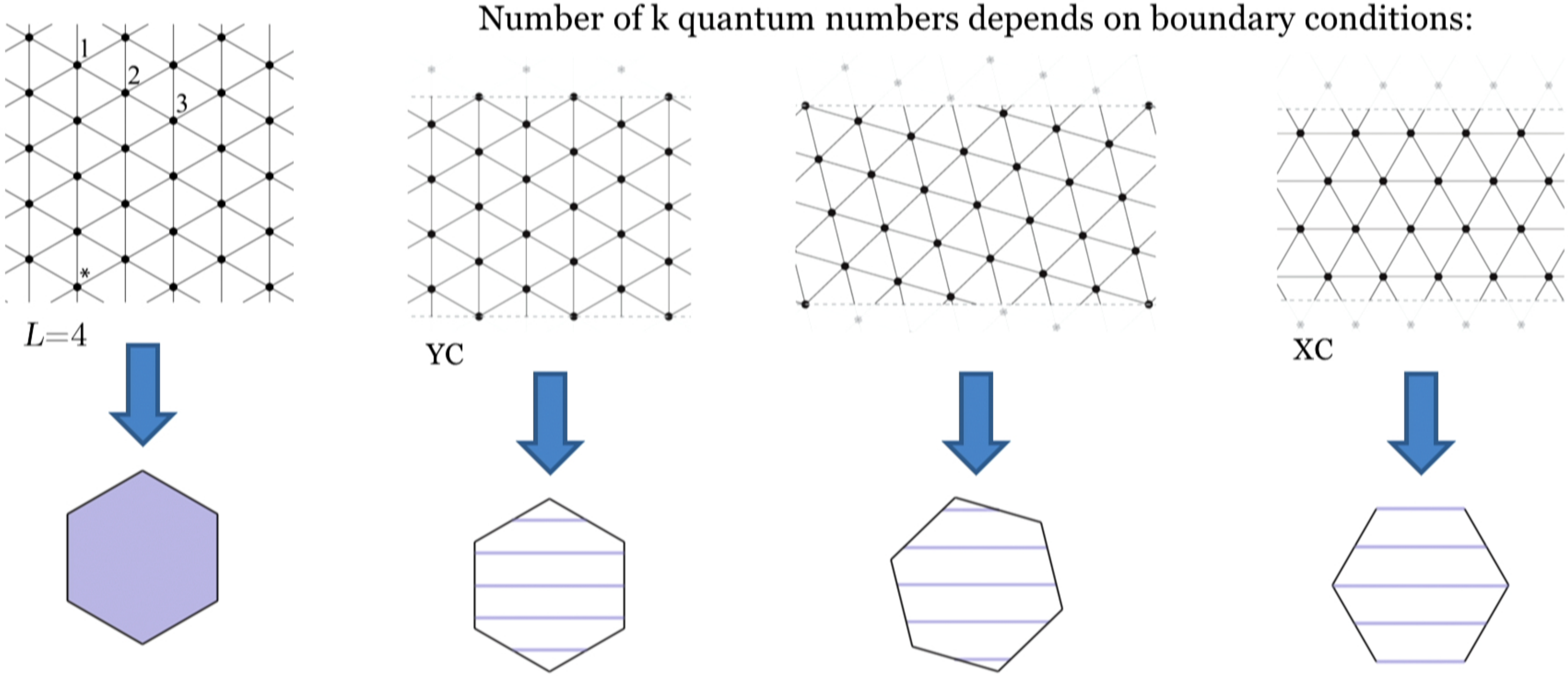
On triangular lattice



Calculation methods – mixed-space DMRG

On triangular lattice

Number of k quantum numbers depends on boundary conditions:



Calculation methods – mixed-space DMRG

On triangular lattice

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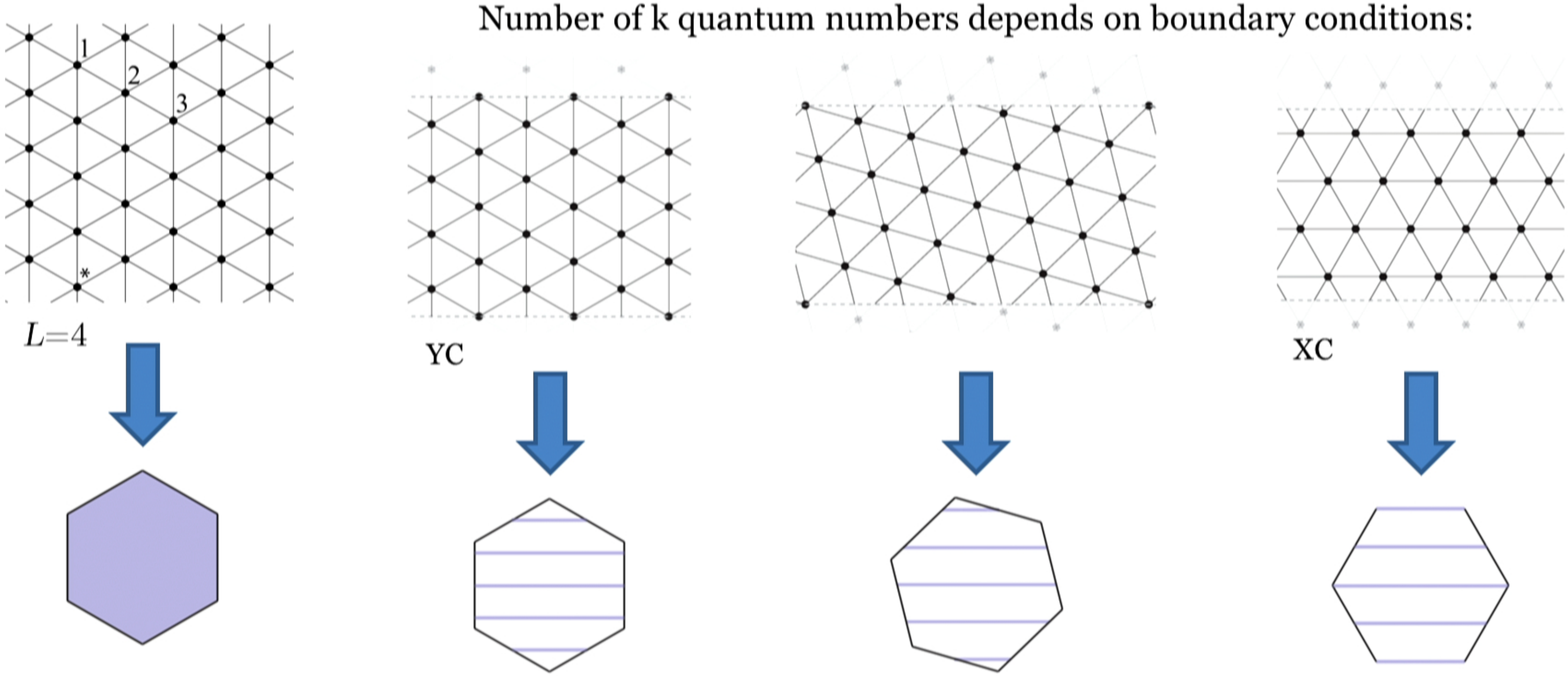
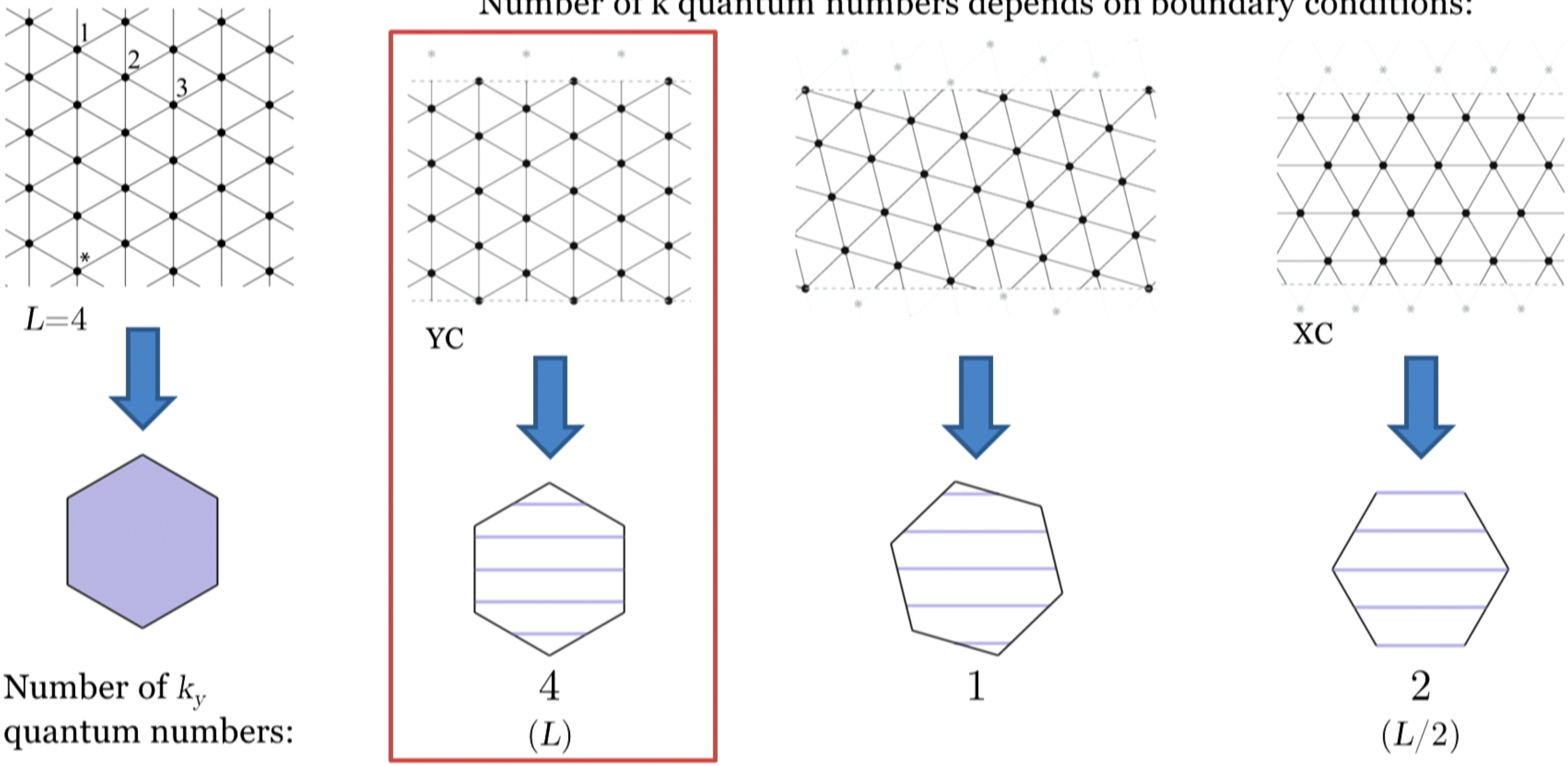


Number of k_y quantum numbers: 4 (L) | 1 | 2 ($L/2$)

Calculation methods – mixed-space DMRG

On triangular lattice

Number of k quantum numbers depends on boundary conditions:



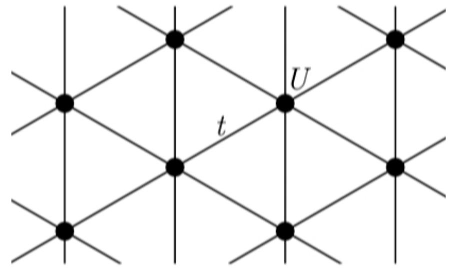
Outline

1. Introduction
2. Calculation methods
3. Phase diagram
4. Chiral spin liquid phase
5. Implications for experiments 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):

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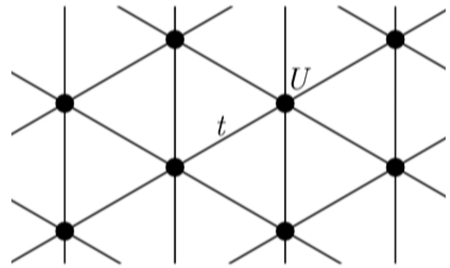

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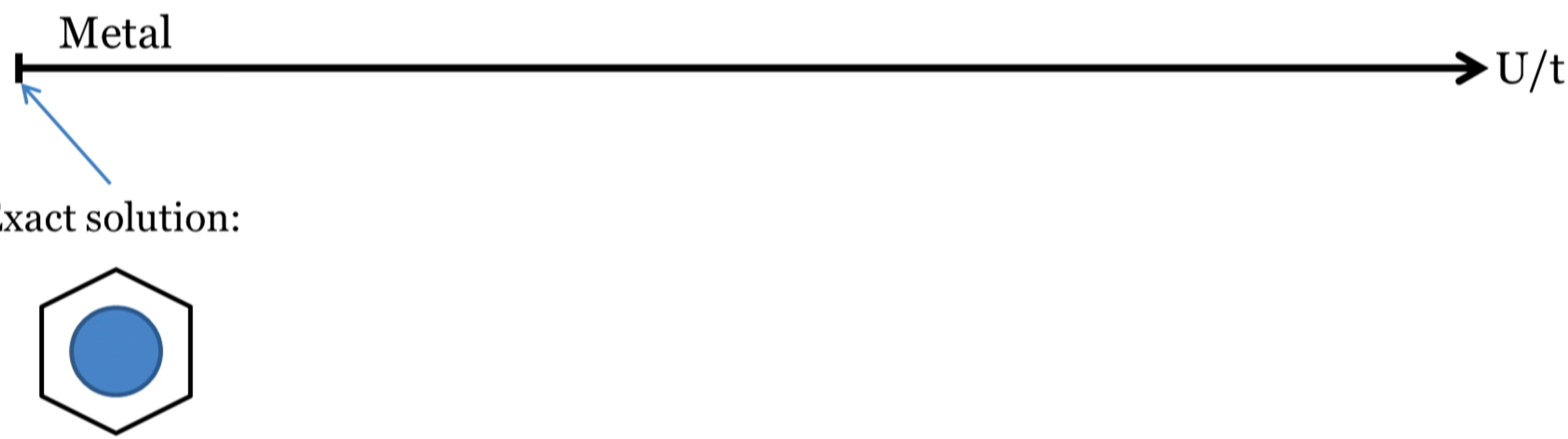

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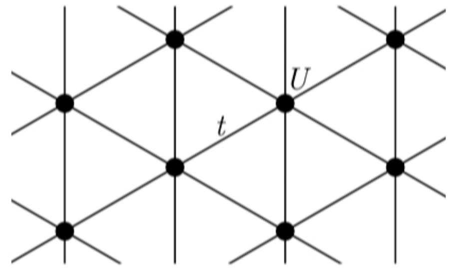


Phase diagram (expected):

Metal

Spin-ordered

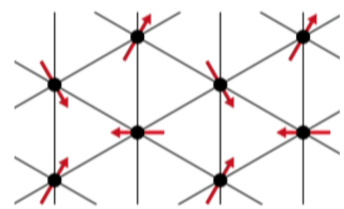
U/t

Reduces to Heisenberg:

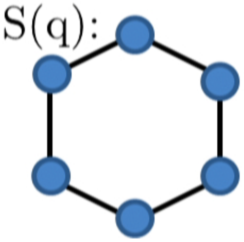
$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Exact solution:

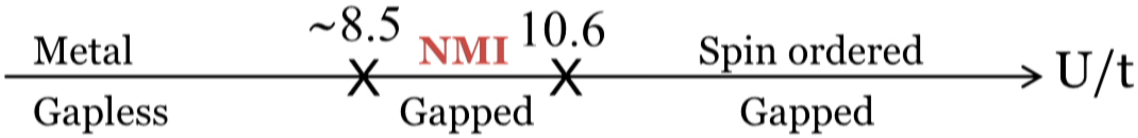
120° order:



S(q):

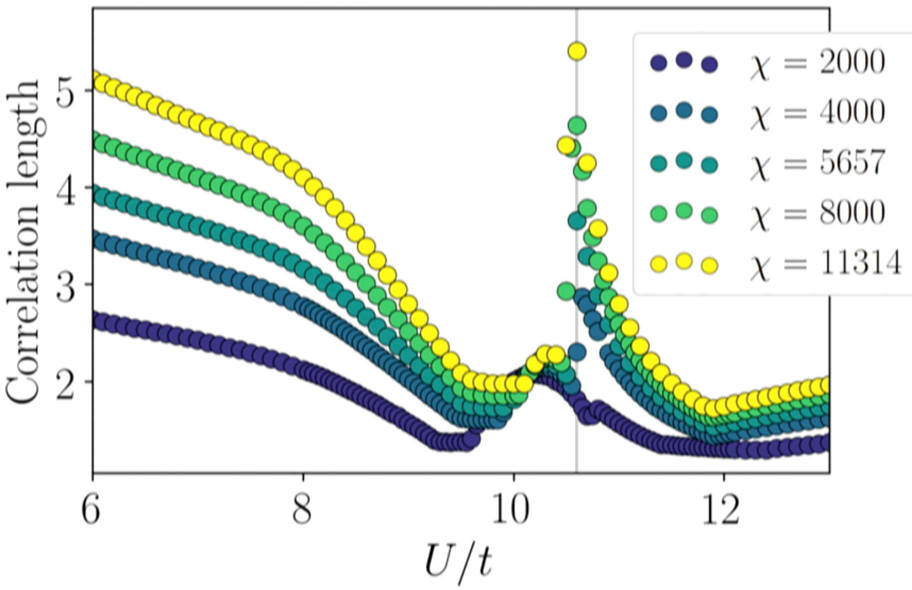


Phase diagram: L=4 cylinder



Phase diagram: L=4 cylinder

Correlation length

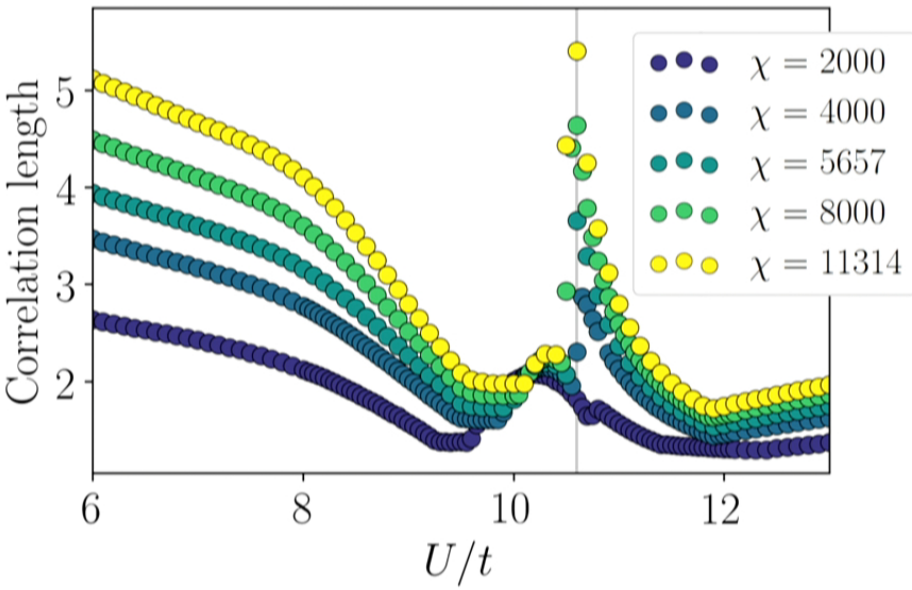


χ: MPS bond dimension

- Controls precision of DMRG

Phase diagram: L=4 cylinder

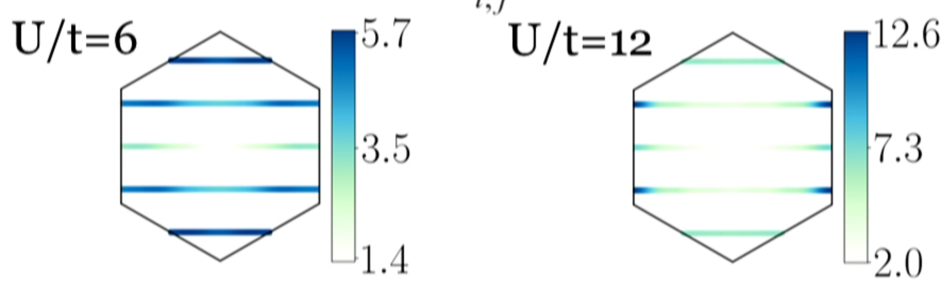
Correlation length



χ: MPS bond dimension

- Controls precision of DMRG

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



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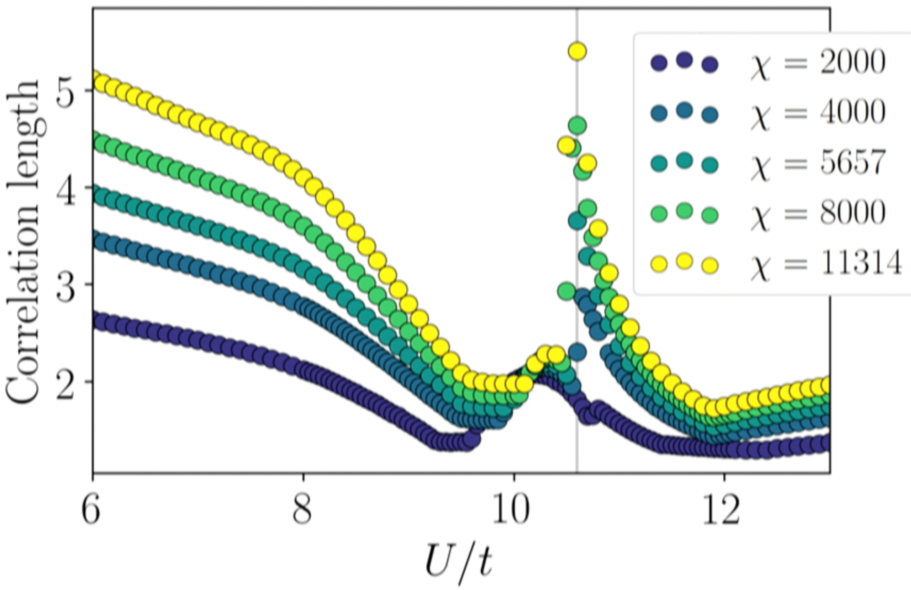

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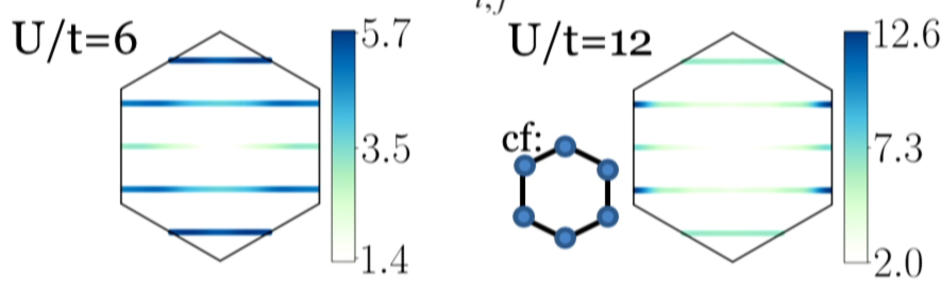
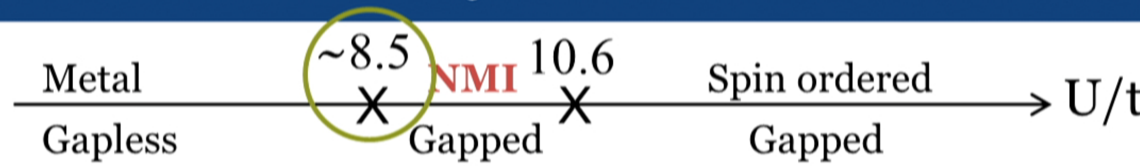
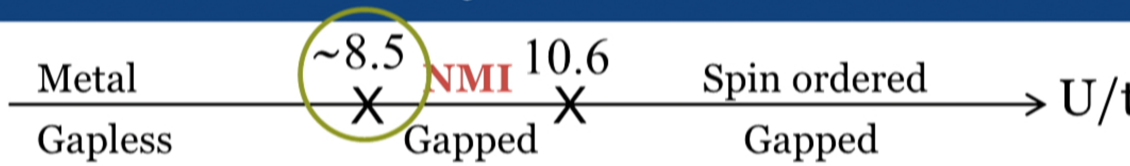


Phase diagram: L=4 cylinder



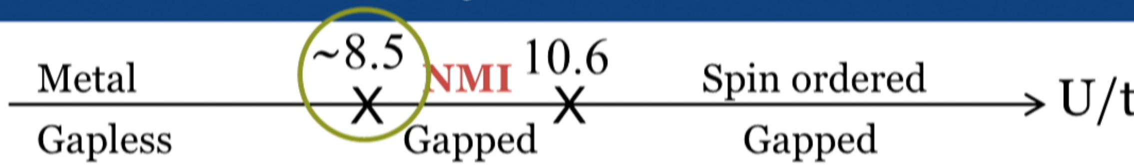
Phase diagram: L=4 cylinder



Entanglement:

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

Phase diagram: L=4 cylinder



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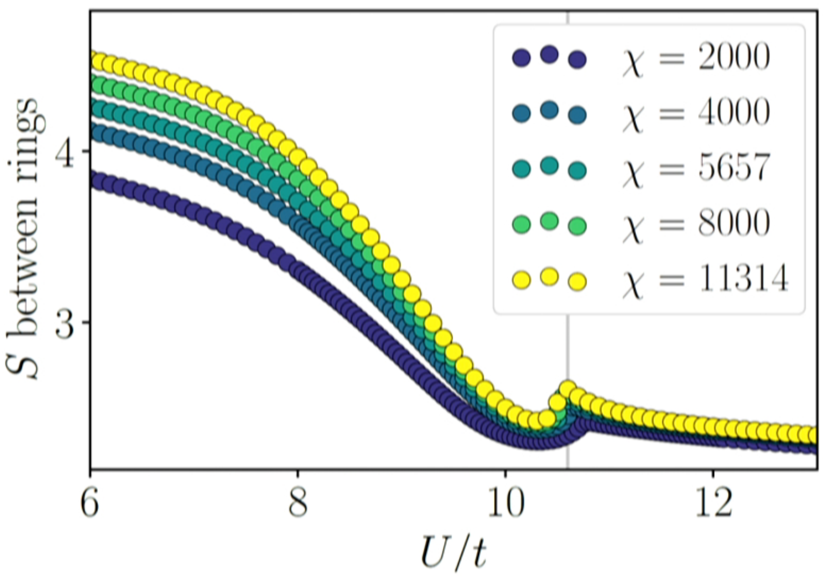

Phase diagram: L=4 cylinder

Metal ~8.5 NMI 10.6 Spin ordered U/t

Gapless Gapped Gapped

Entanglement:

A  B

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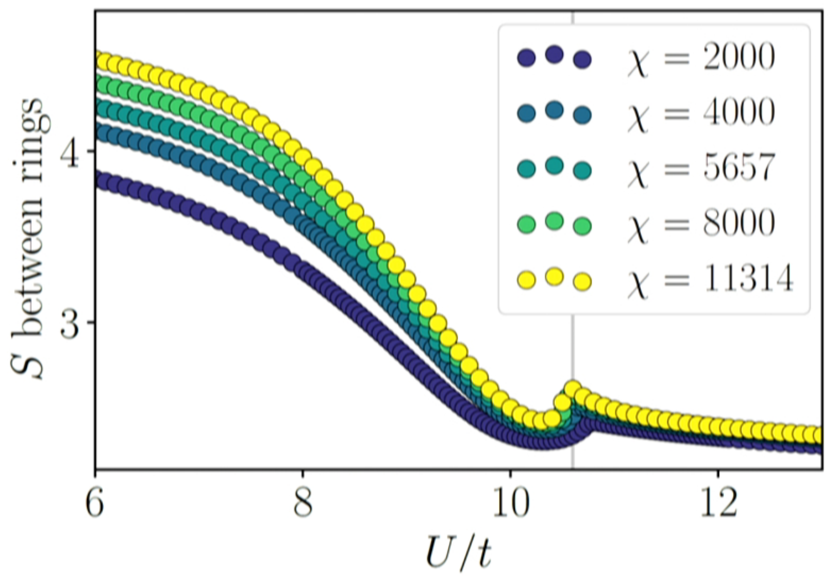
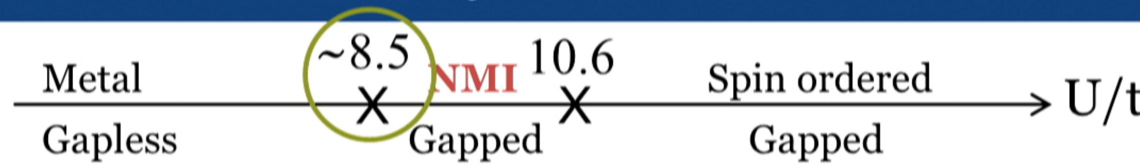


Finite entanglement scaling:

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

Calabrese & Cardy, J. Stat. Mech. 2004

Phase diagram: L=4 cylinder



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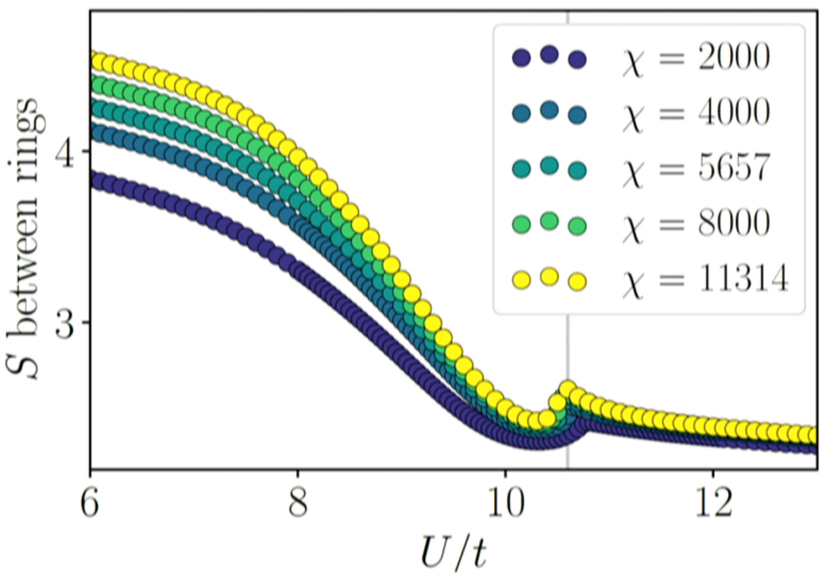

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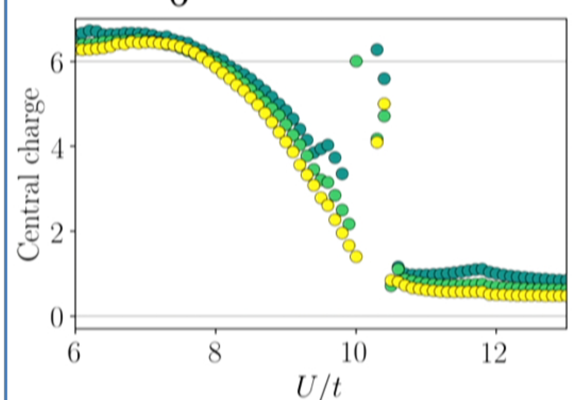

Calabrese & Cardy, J. Stat. Mech. 2004

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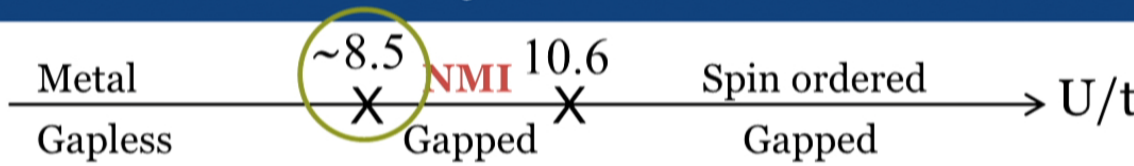

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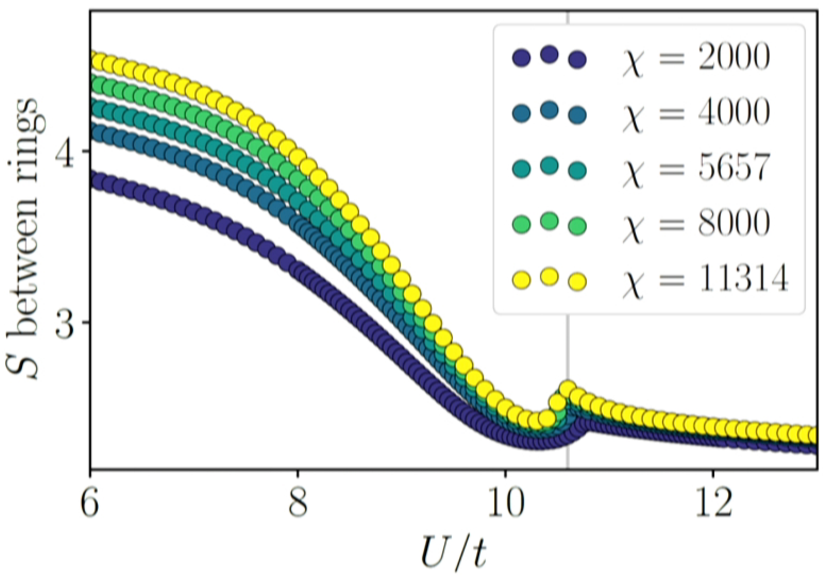

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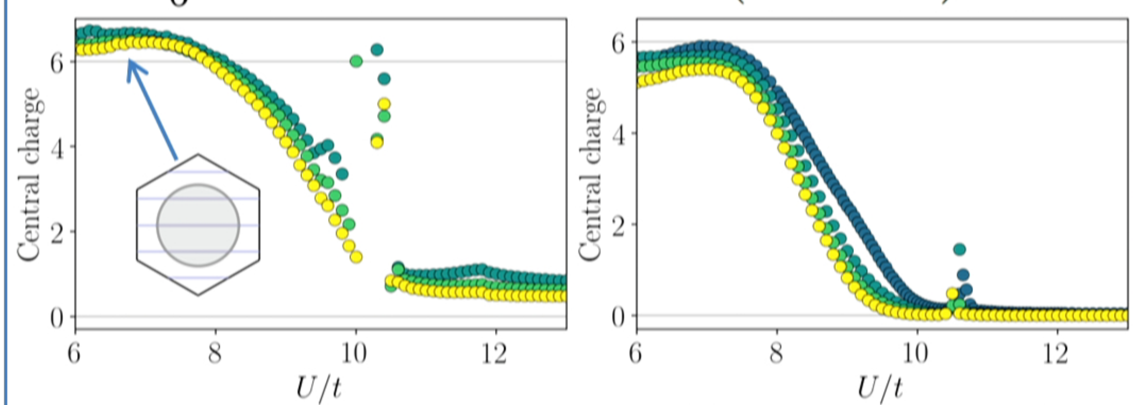

Calabrese & Cardy, J. Stat. Mech. 2004
Pollmann et al, PRL 2009

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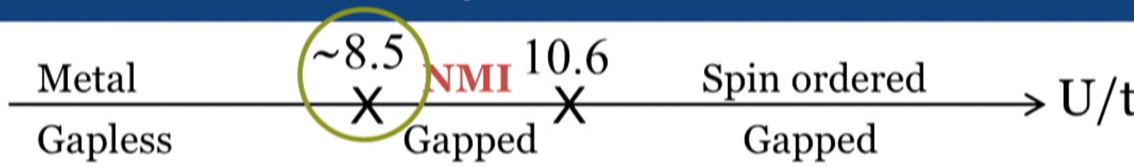

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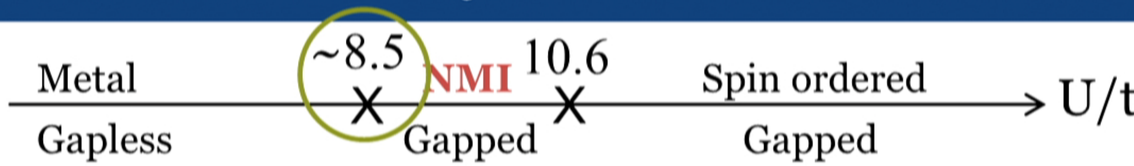
Entanglement spectrum: $\{-\log(\lambda_i)\}$

Phase diagram: L=4 cylinder



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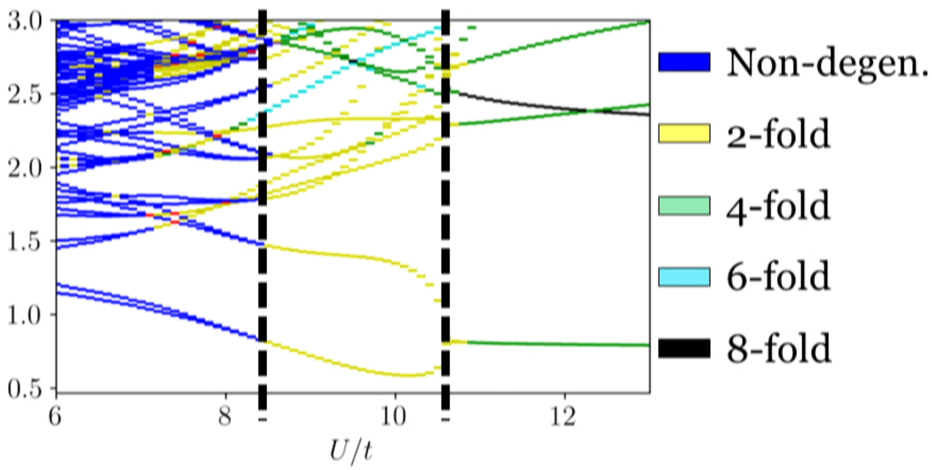
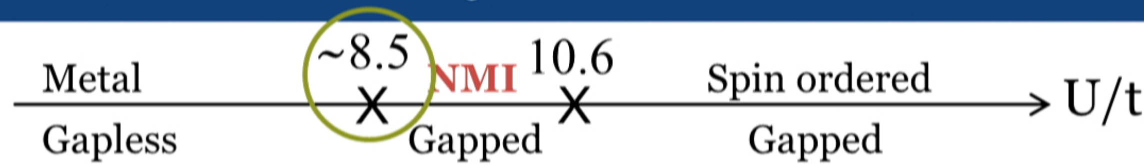


Phase diagram: L=4 cylinder



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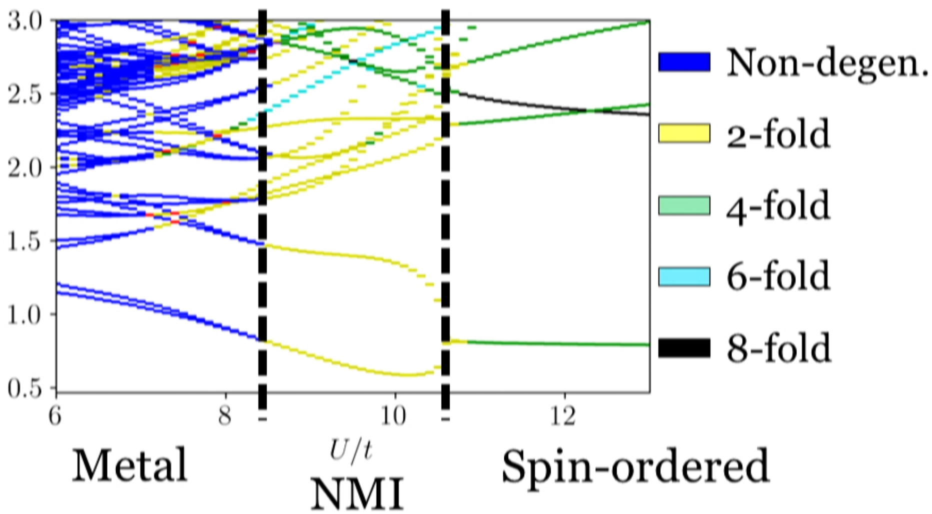

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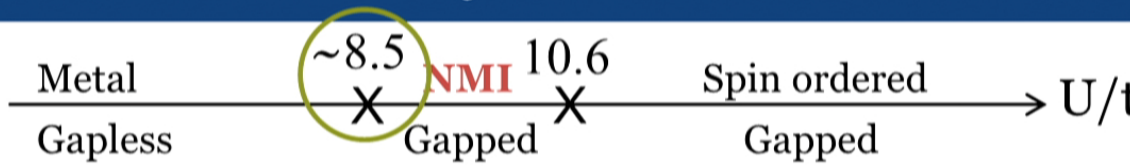

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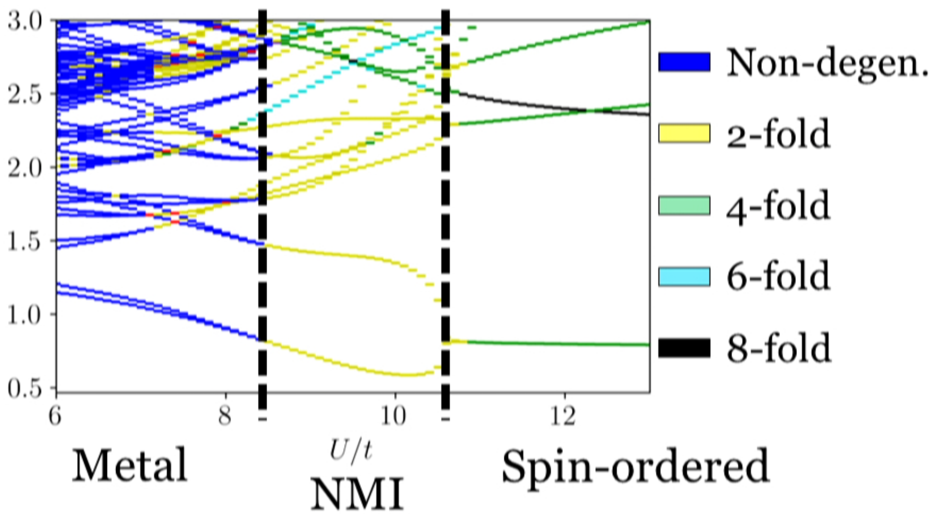
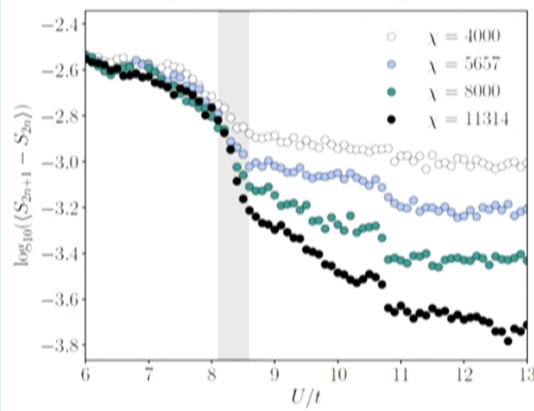


Separation of pairs



Phase diagram: L=4 cylinder

Occupation and Fermi surface:

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

Phase diagram: L=4 cylinder

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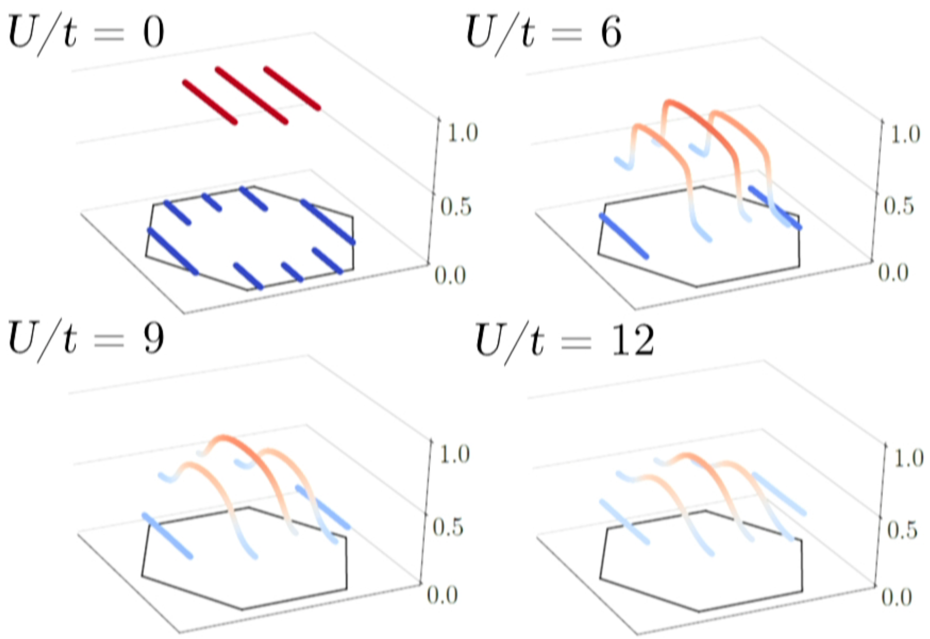

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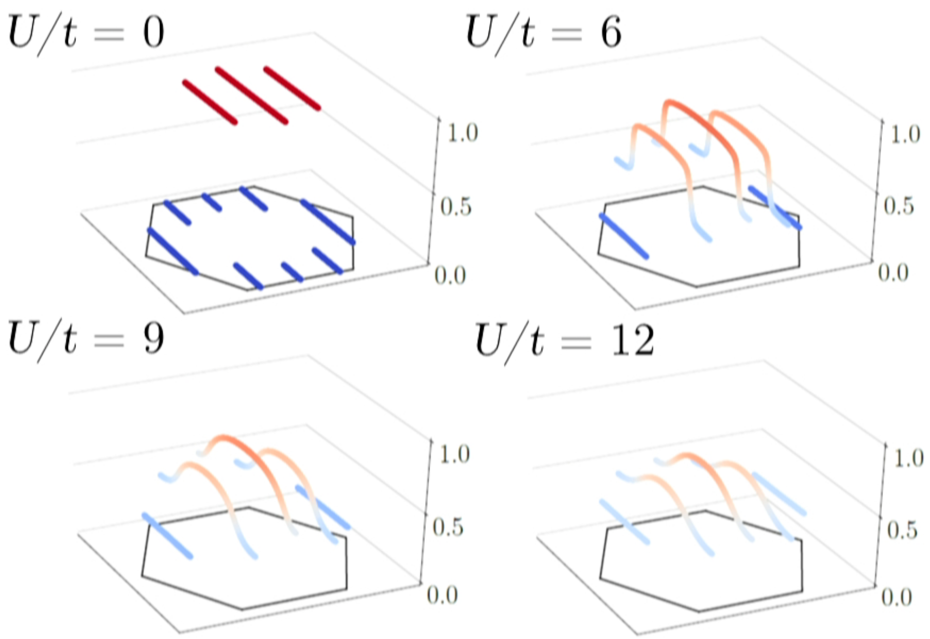
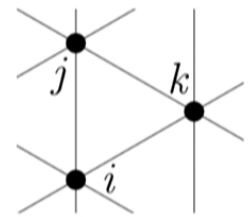
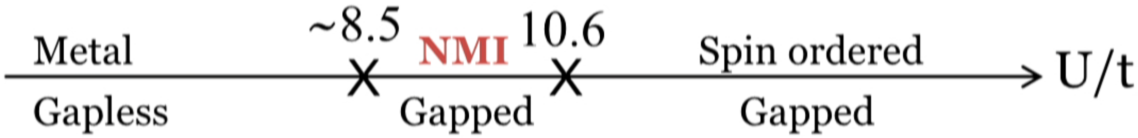


Scalar chiral order parameter:



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

Phase diagram: L=4 cylinder



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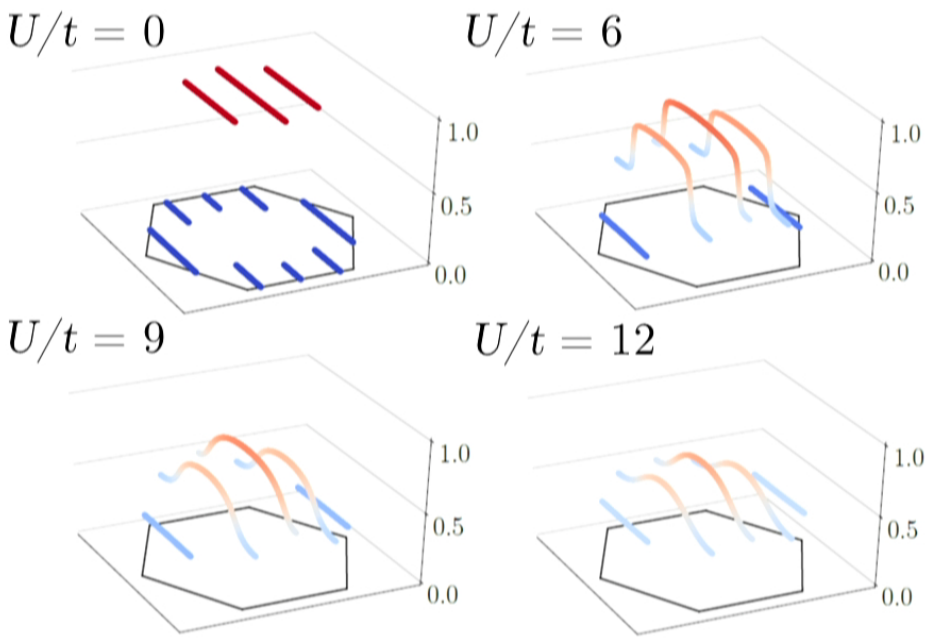

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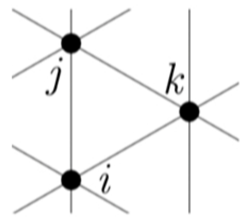

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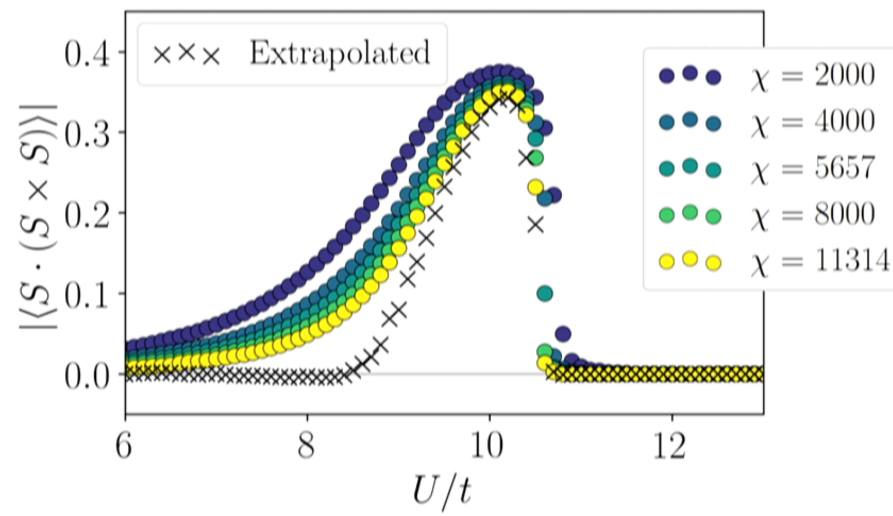
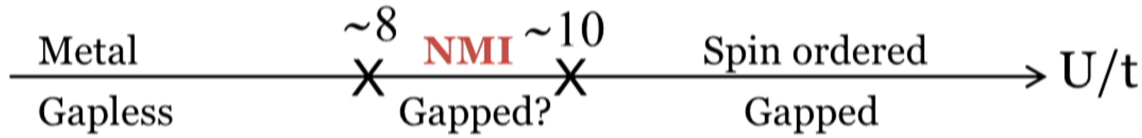


Phase diagram: L=6 cylinder



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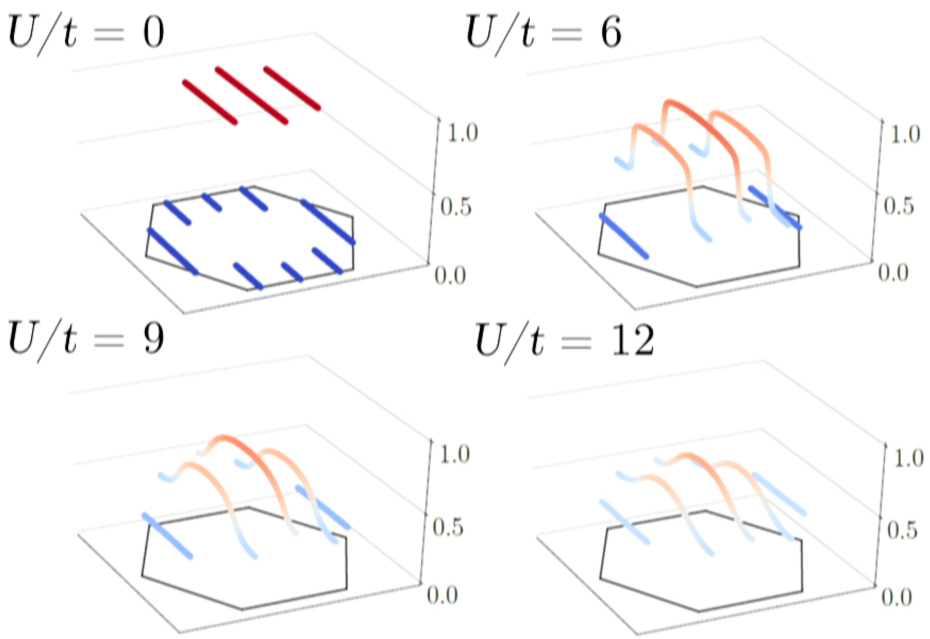
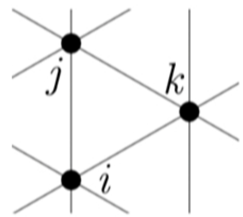


Scalar chiral order parameter:



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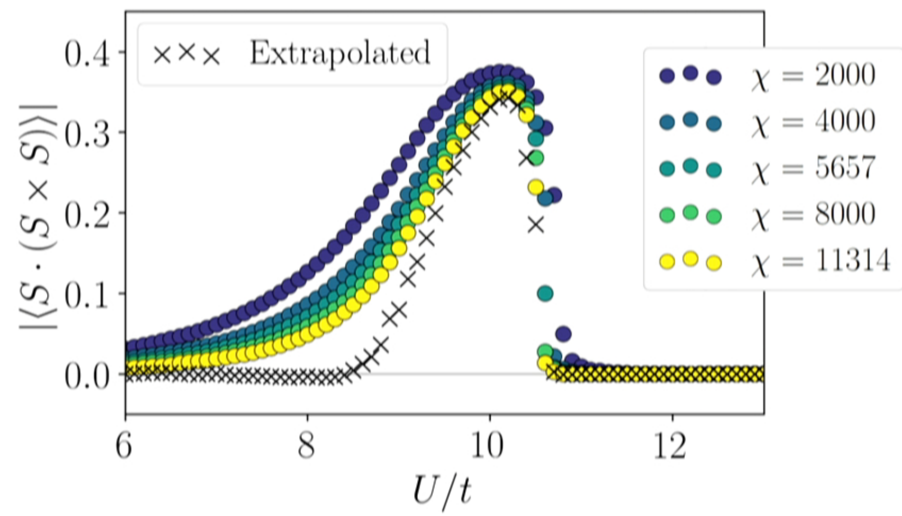
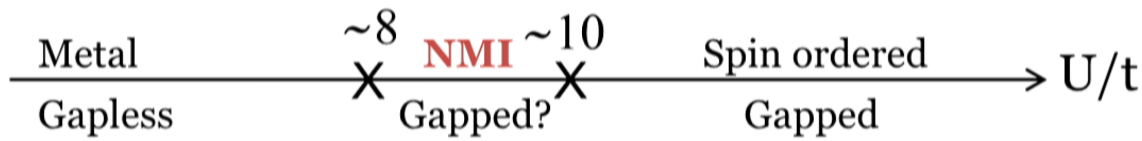
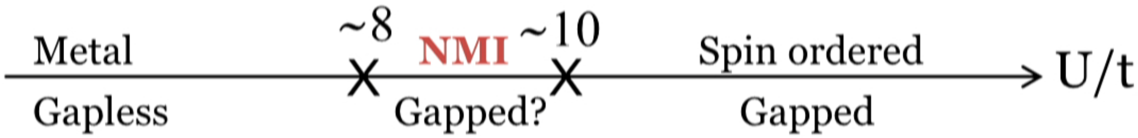


Phase diagram: L=6 cylinder



Phase diagram: L=6 cylinder



Two low-energy states:

$k=0$, $k=\pi$
per ring

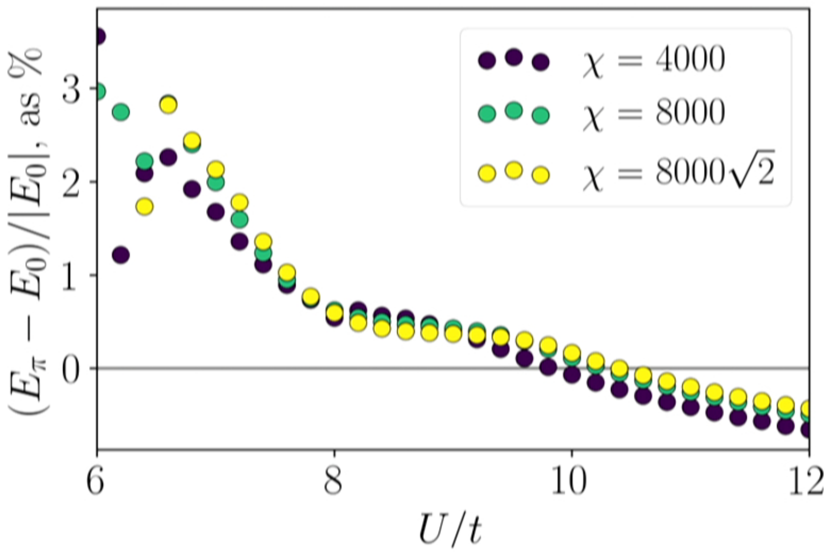
Phase diagram: L=6 cylinder

Metal — ~8 — **NMI** — ~10 — Spin ordered → U/t

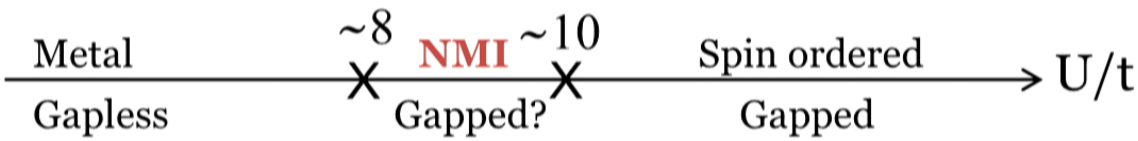
Gapless — Gapped? — Gapped

Two low-energy states:

k=0, k=π
per ring



Phase diagram: L=6 cylinder



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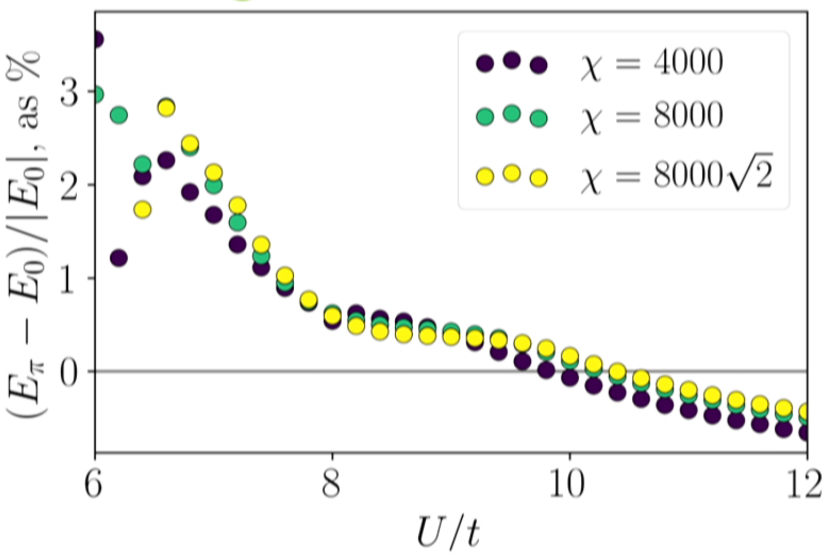
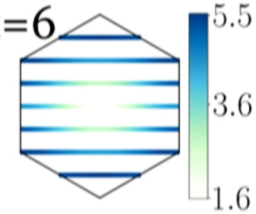
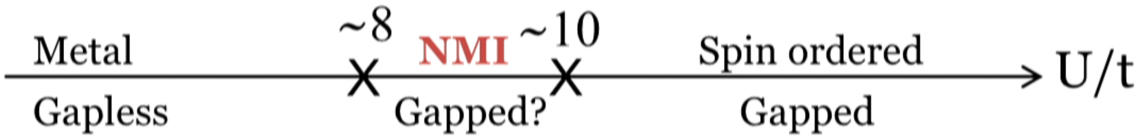


Spin order:

U/t=6



Phase diagram: L=6 cylinder



Two low-energy states:

k=0, k=π
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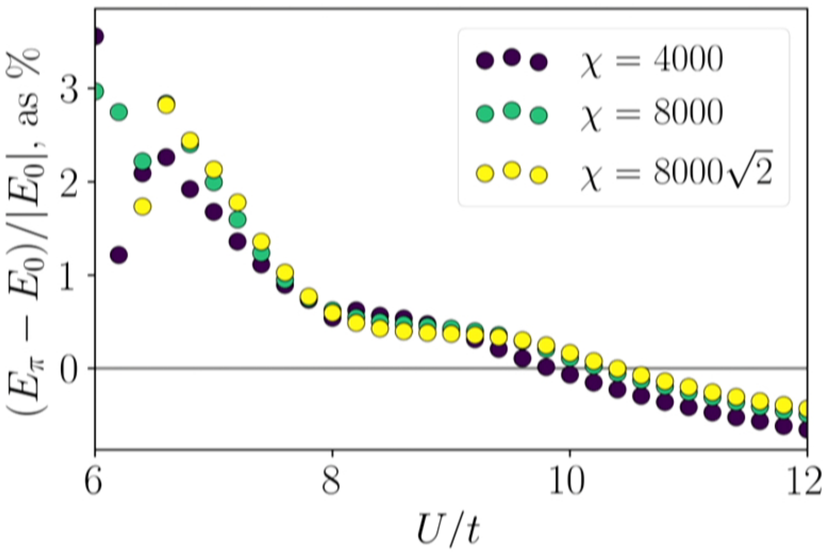
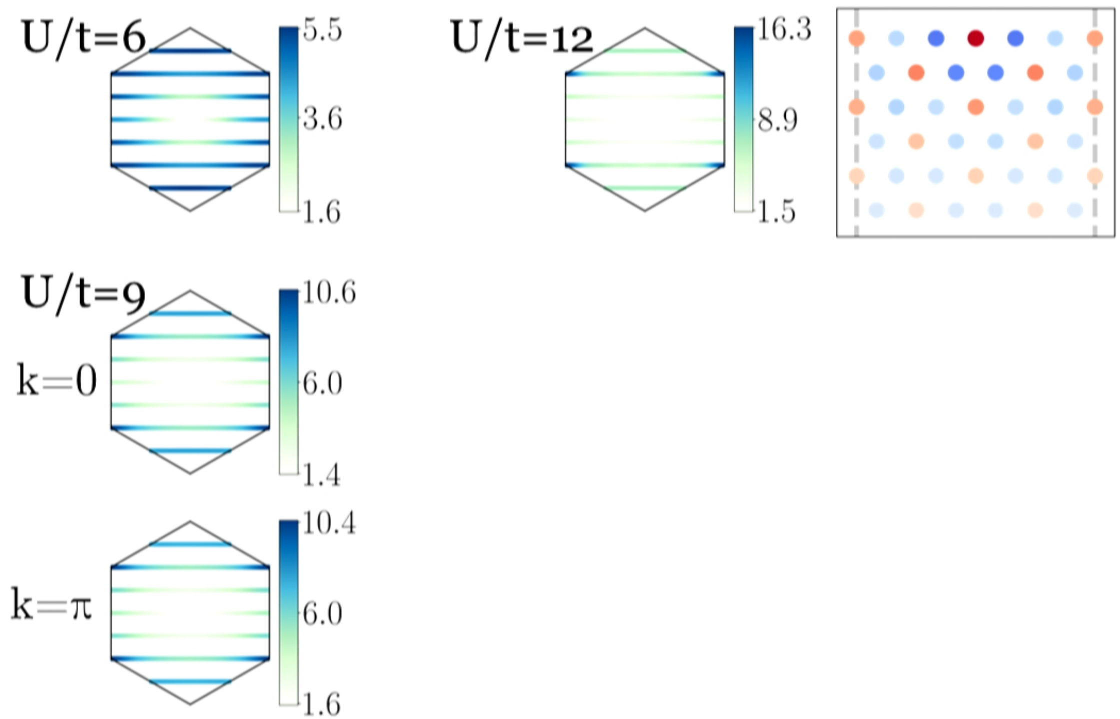


Spin order:



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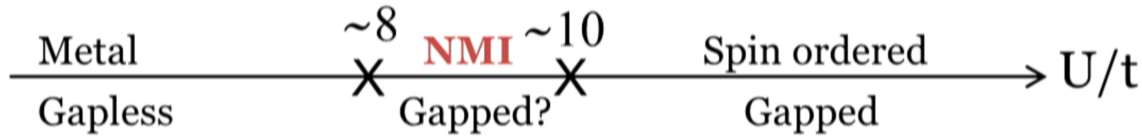

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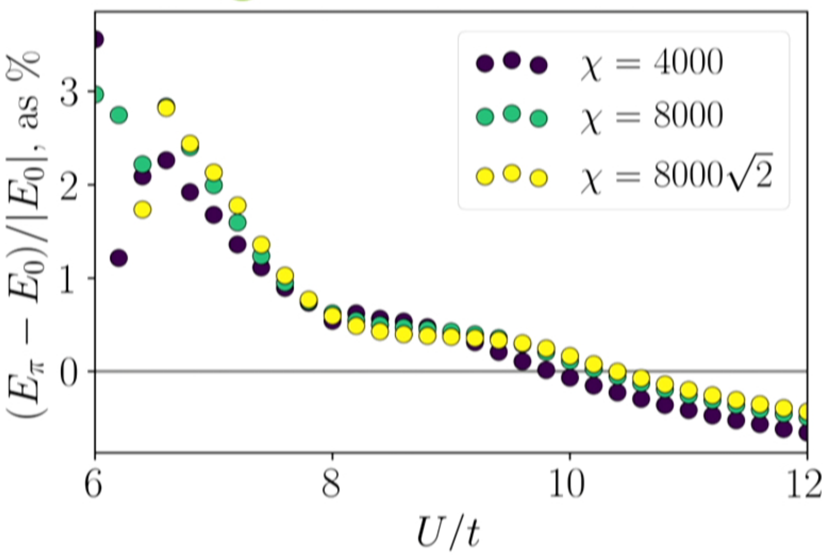

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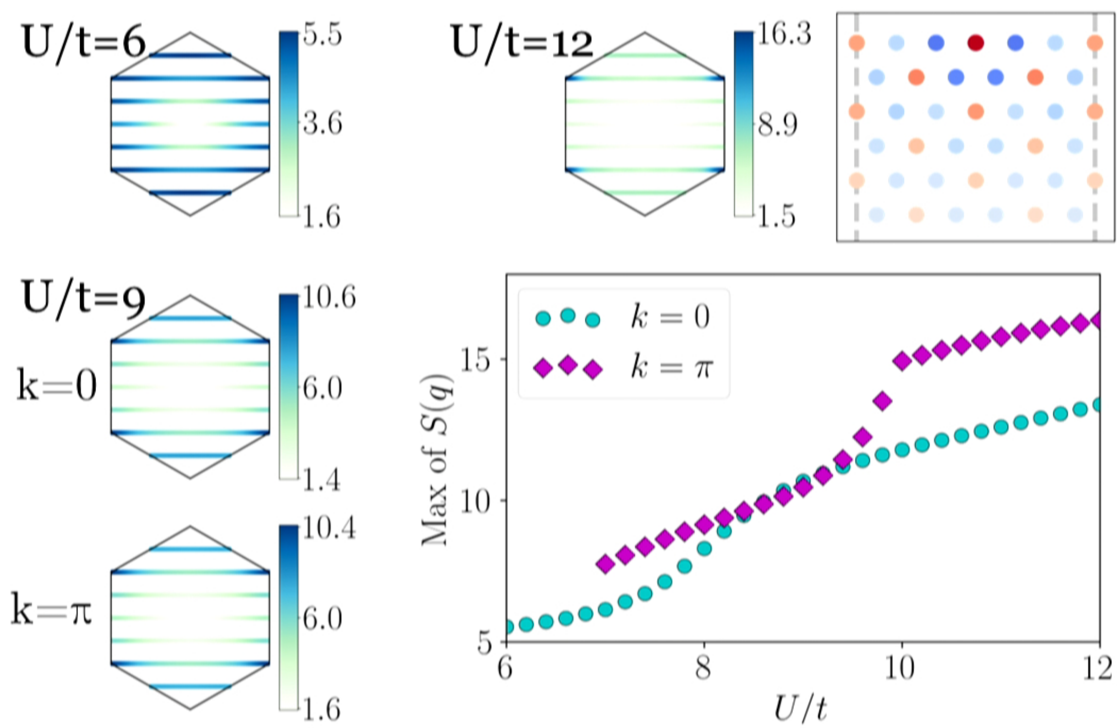

What is a chiral spin liquid?

- $\nu=1/2$ fractional quantum Hall effect state for spins

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

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  - Quantized spin Hall effect: 2π flux insertion $\rightarrow$ spin ½ pumping

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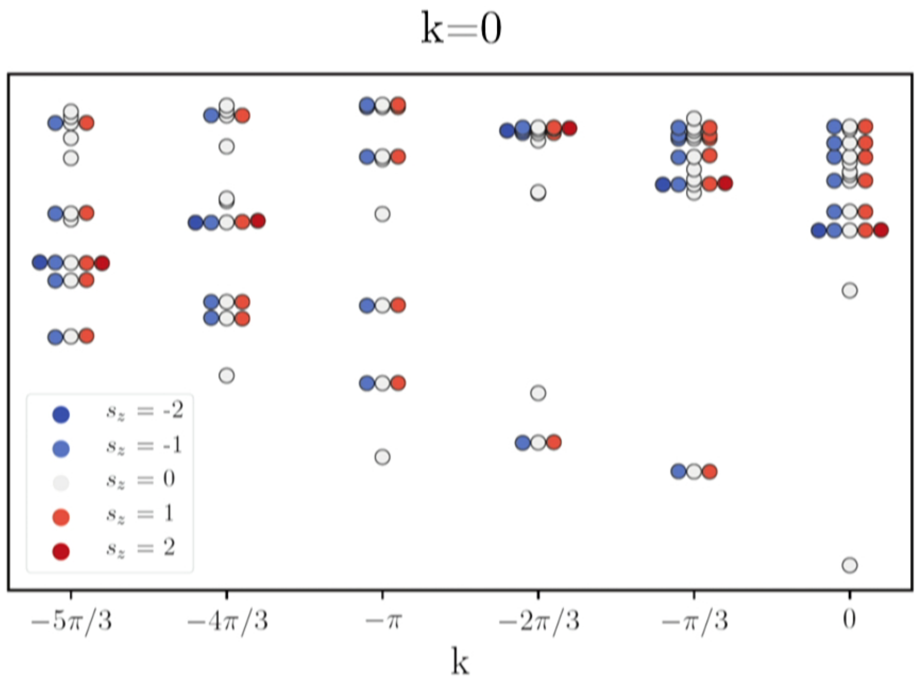
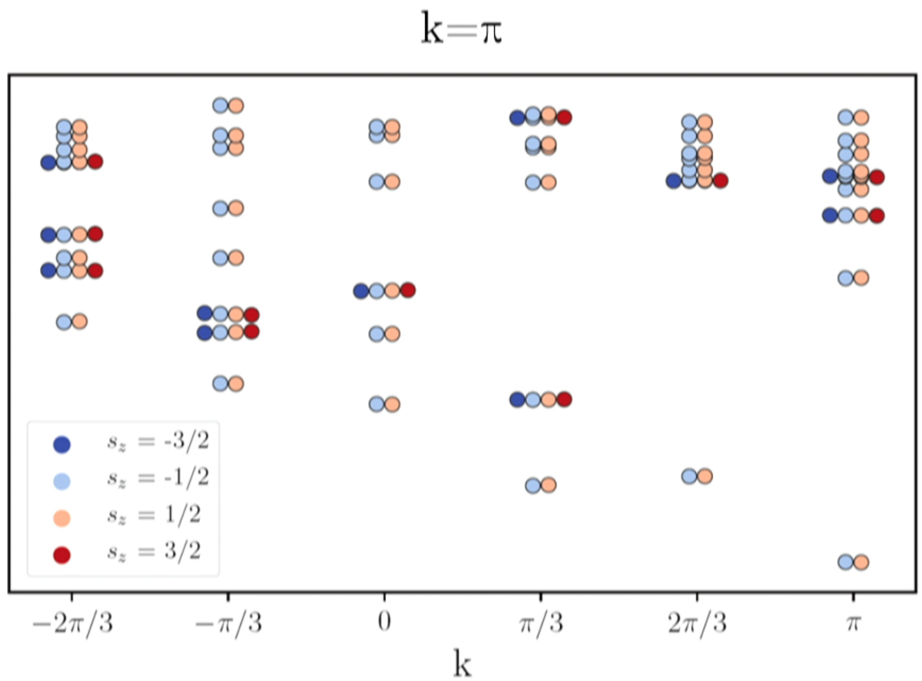
Identification as a CSL

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





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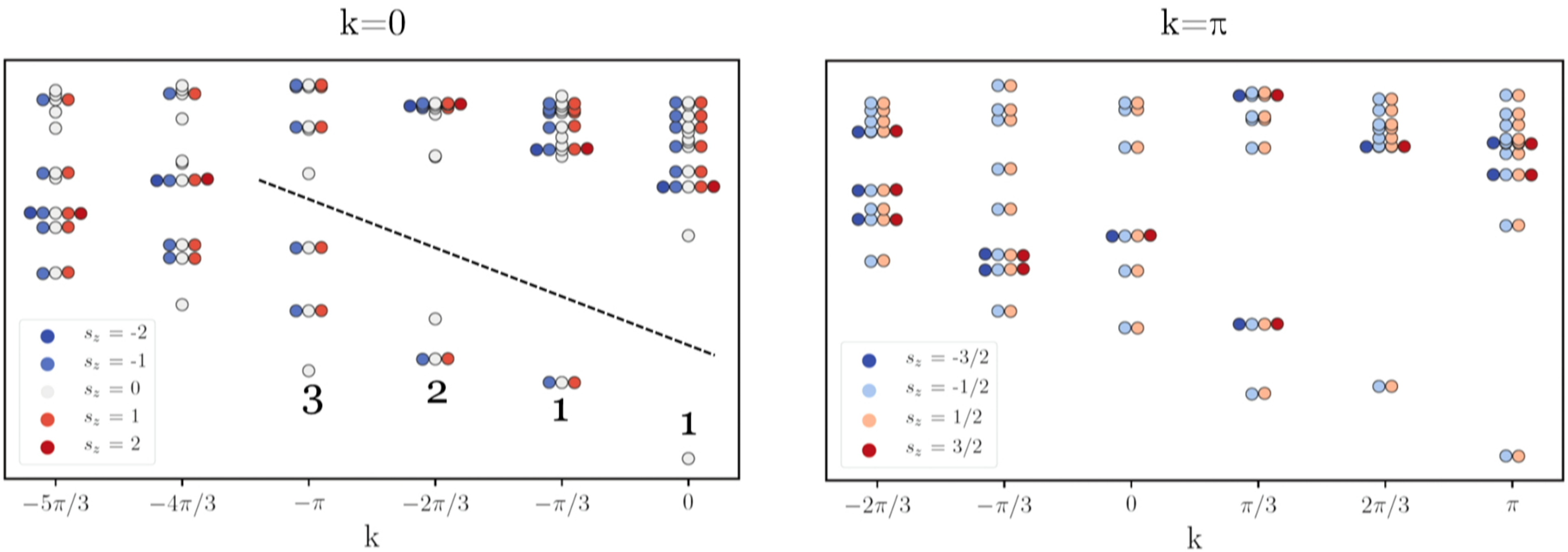
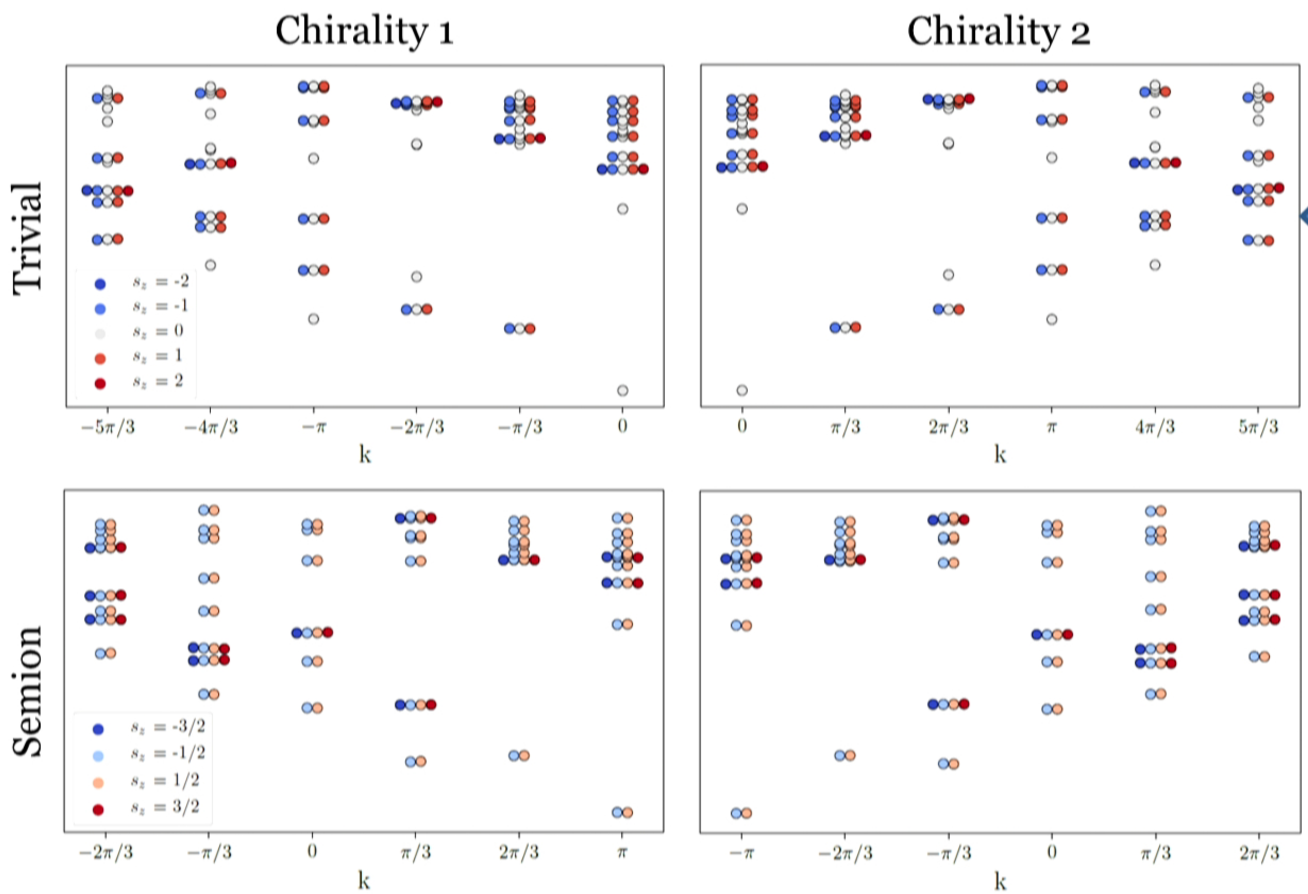


Trivial sector

Semion sector

Identification as a CSL

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

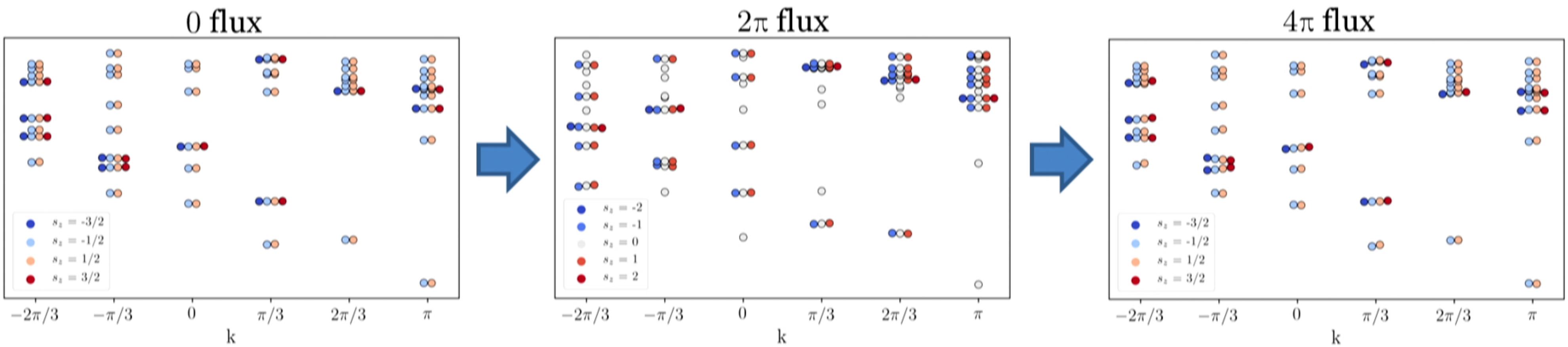


Initialize: 10 random product states

Identification as a CSL

Flux insertion and spin Hall effect:

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



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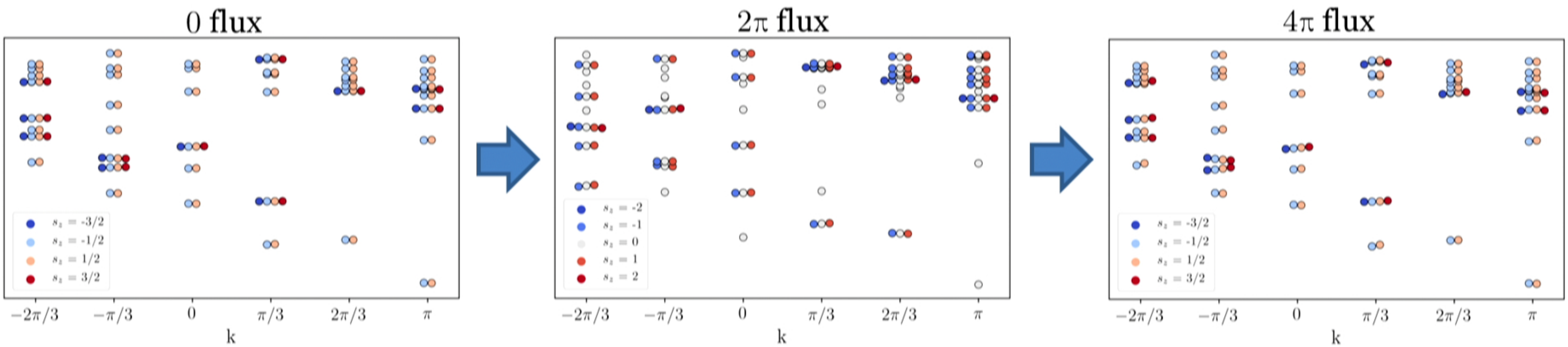
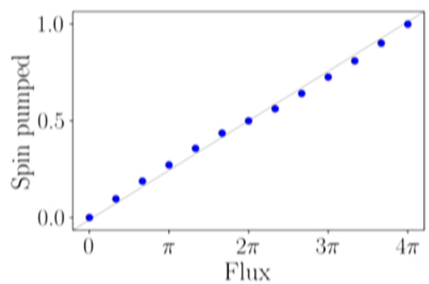


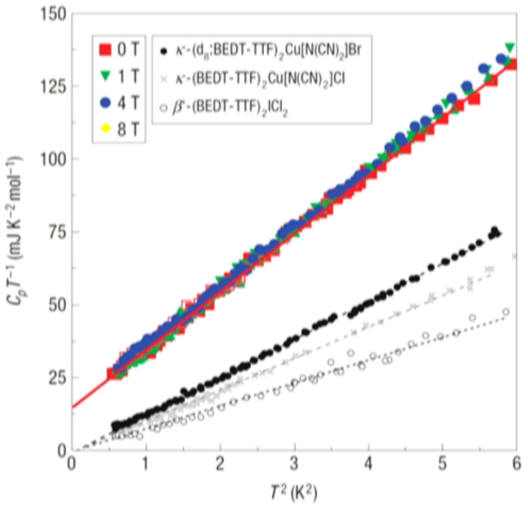
Spin Hall effect:



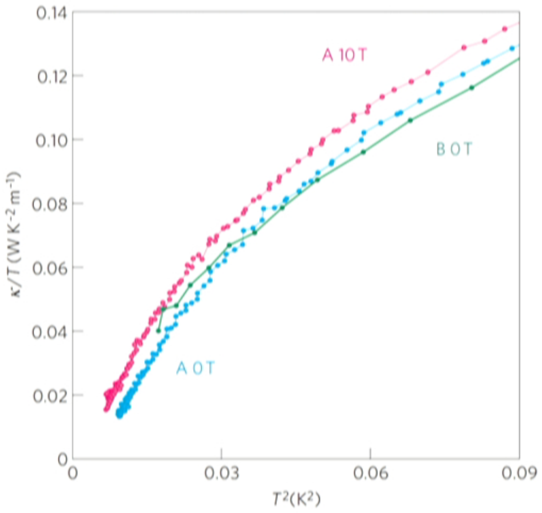
Outline

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

Comparison with experiments



Gapless heat capacity



Gapped conductivity

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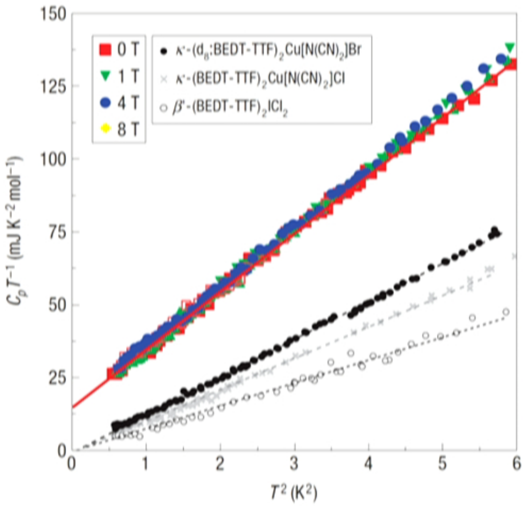

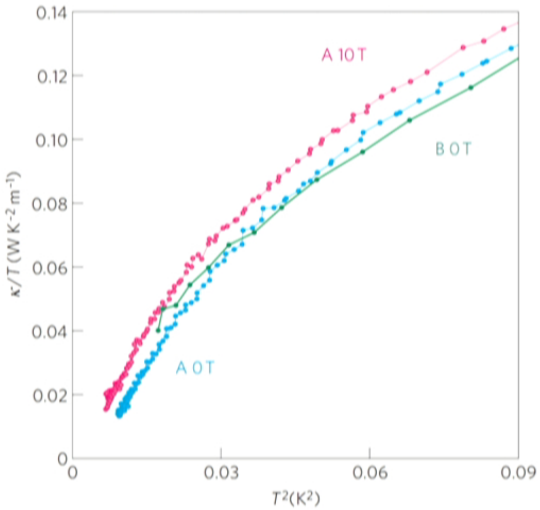

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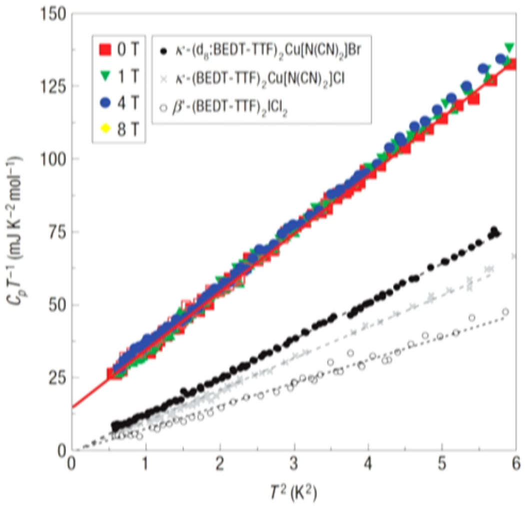

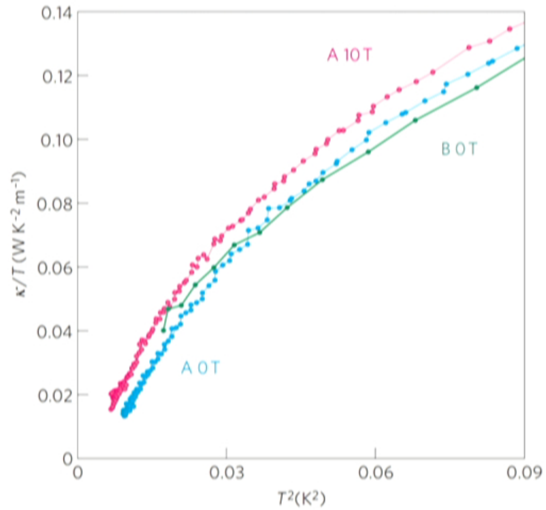

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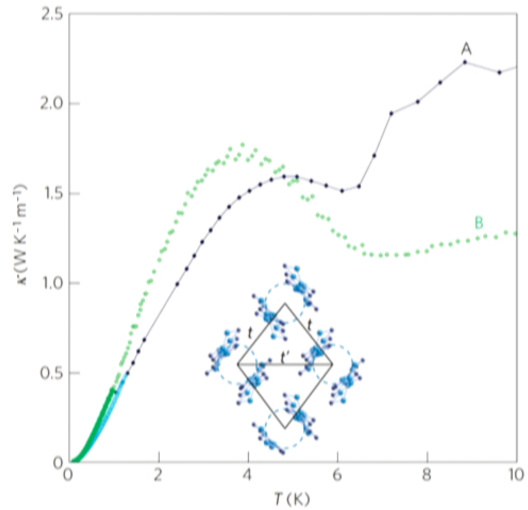

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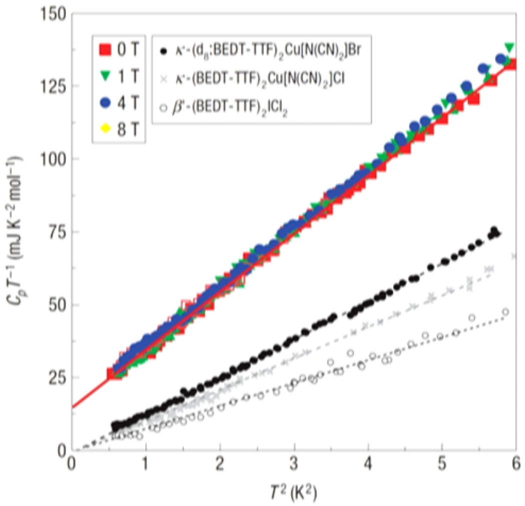

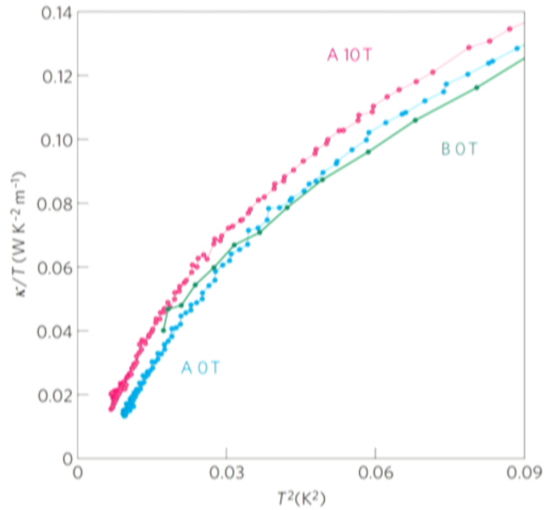

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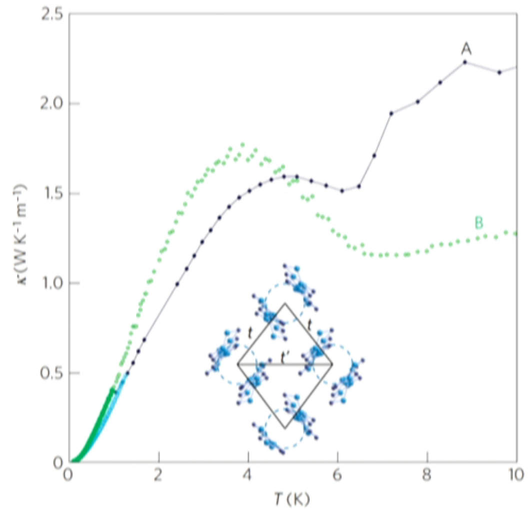

Maybe a finite T phase transition?

Ising-like ordering transition for two chiralities?

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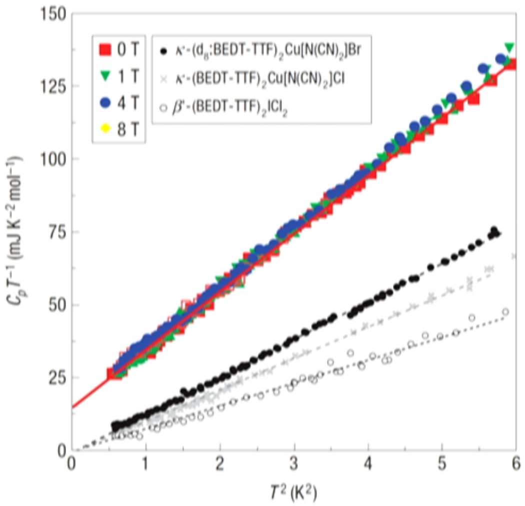

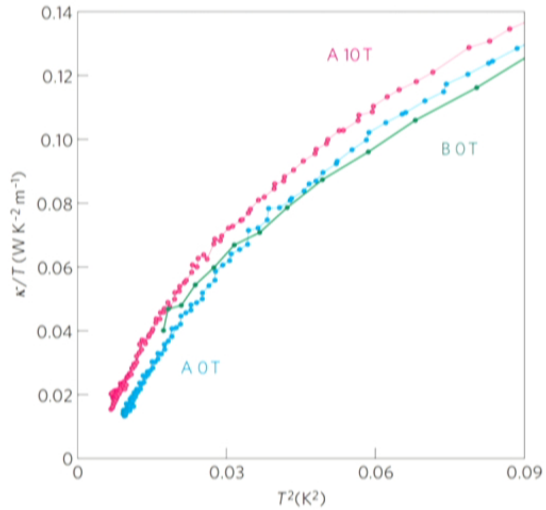

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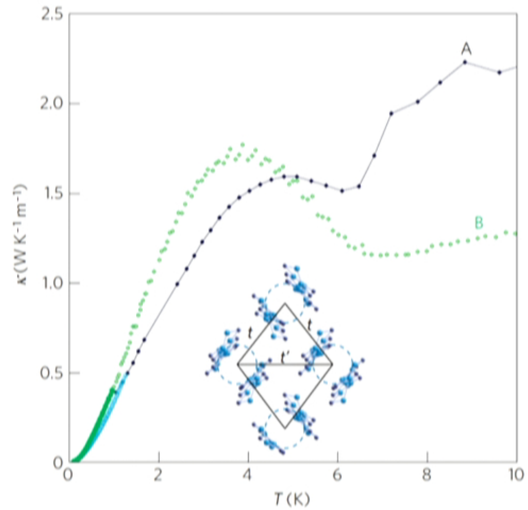

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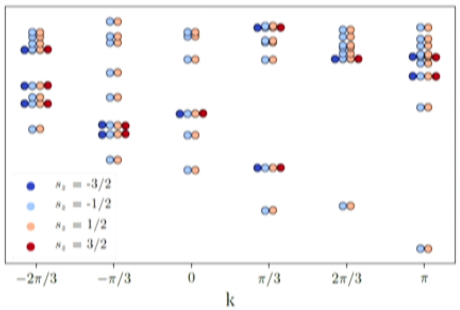
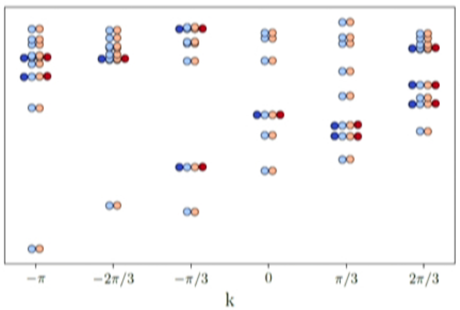
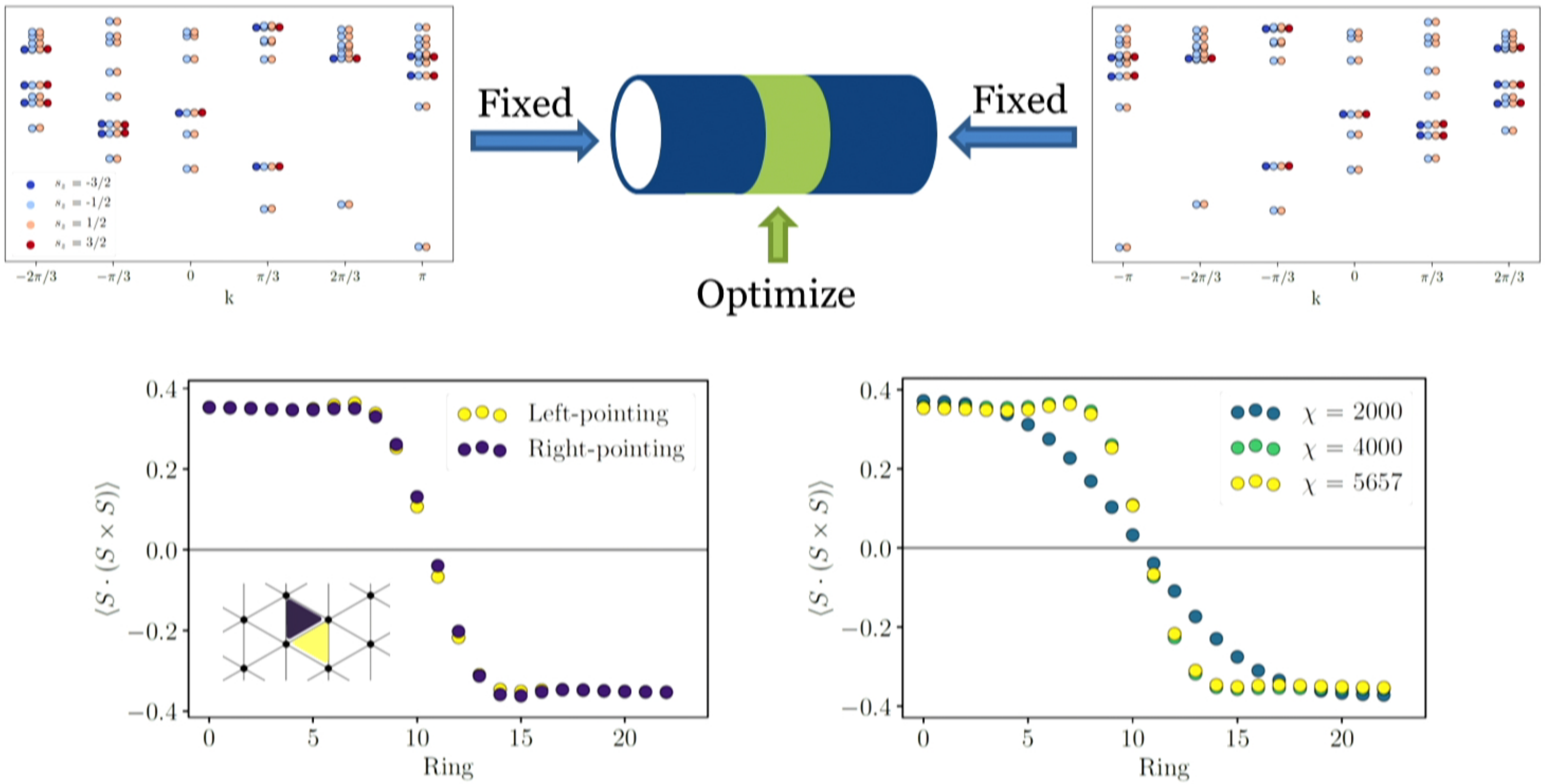
Look at chiral domain wall tension

Chiral domain wall

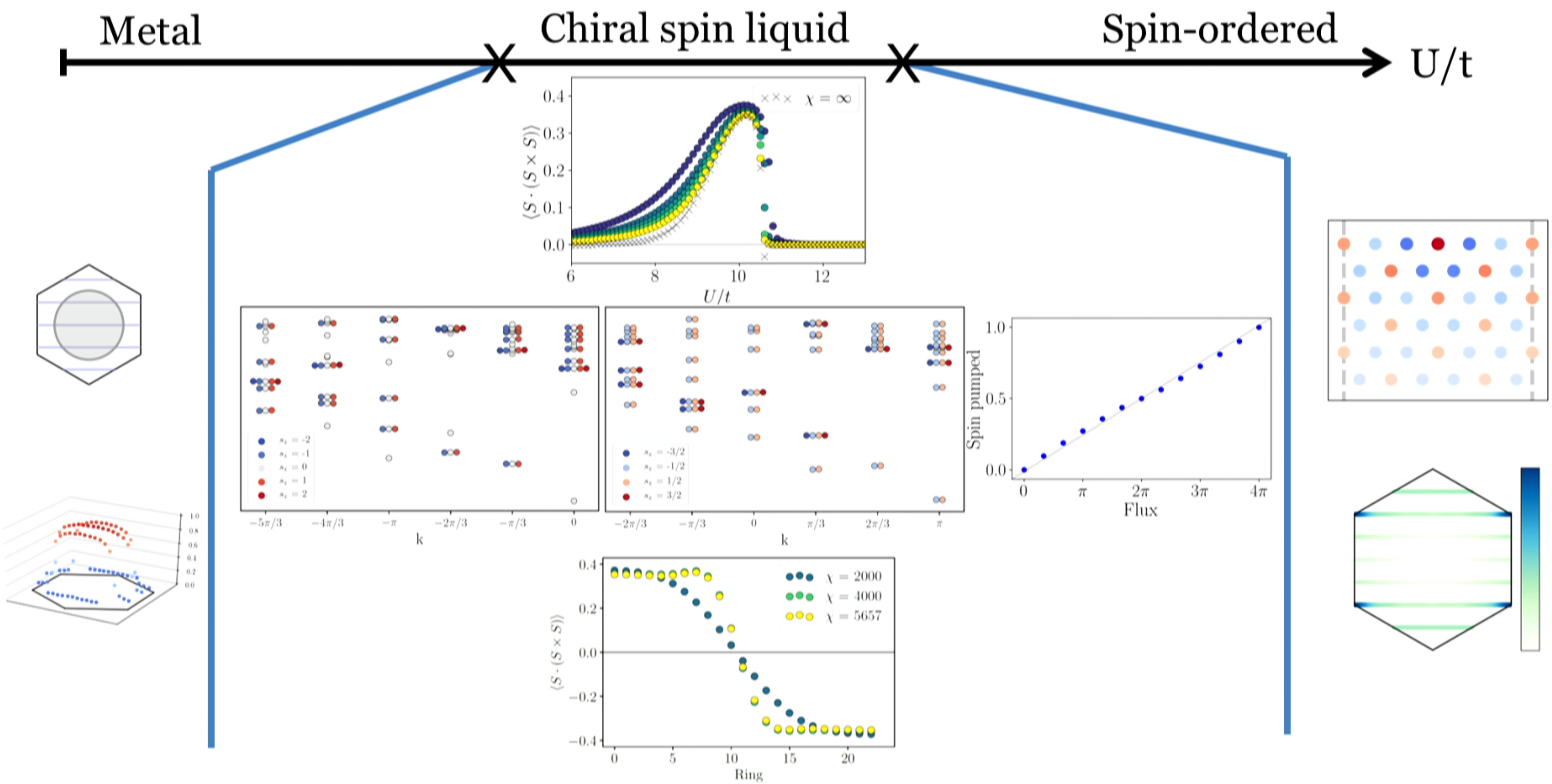




Chiral domain wall

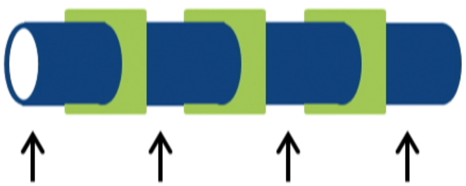


Summary


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

Spin gap

Version 1: Flip 1 spin per N rings:



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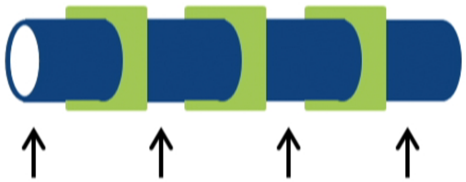

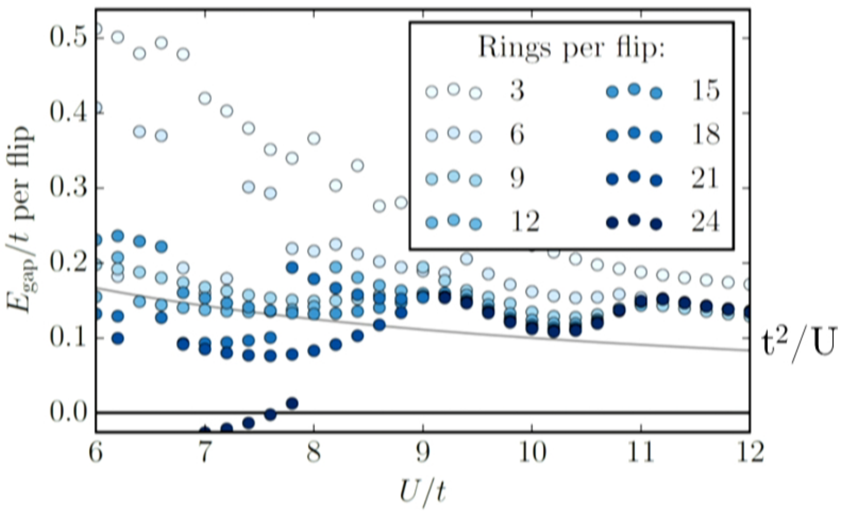

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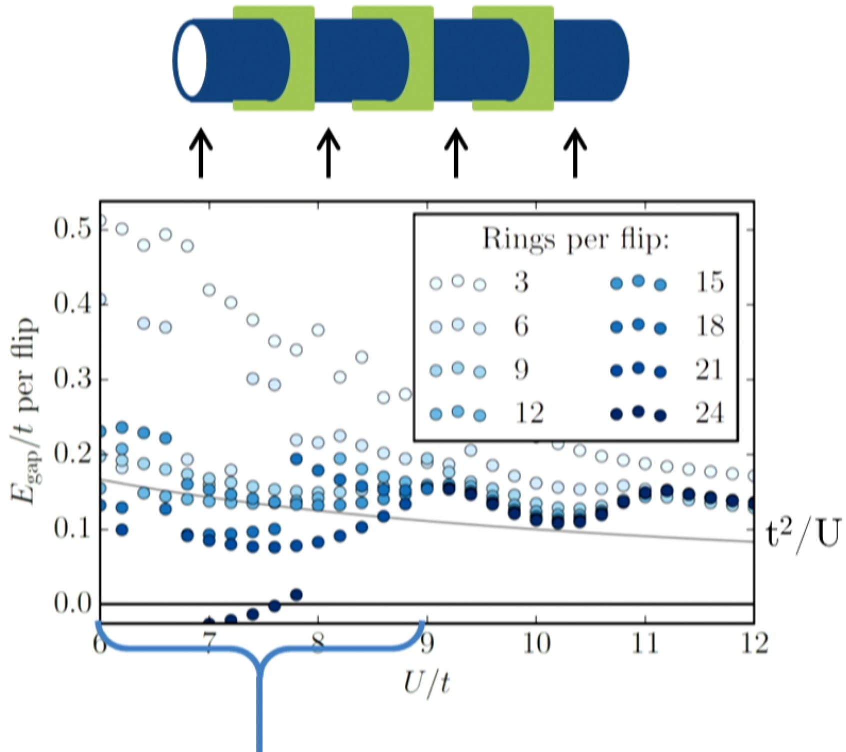
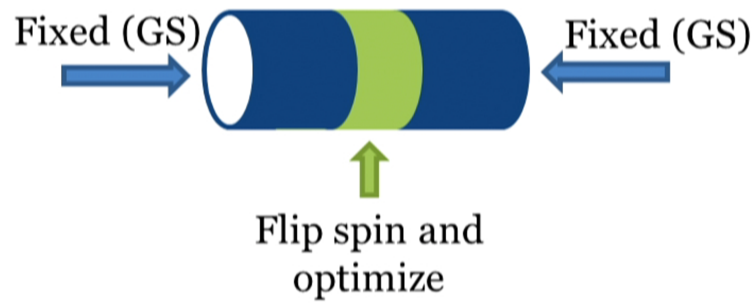


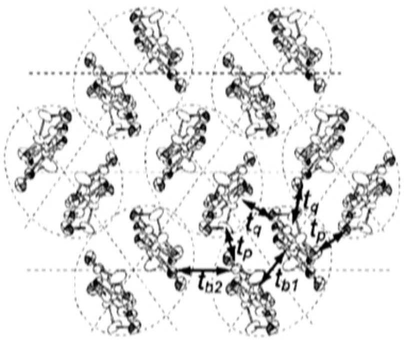
???: Take it with a grain of salt!

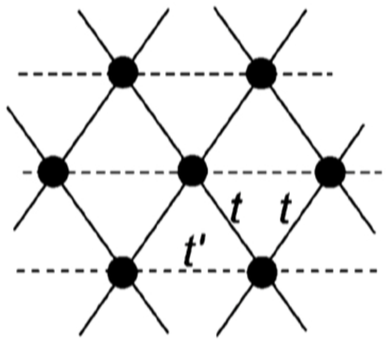
Version 2: Fixed edges



Anisotropy

Real material has some anisotropy:





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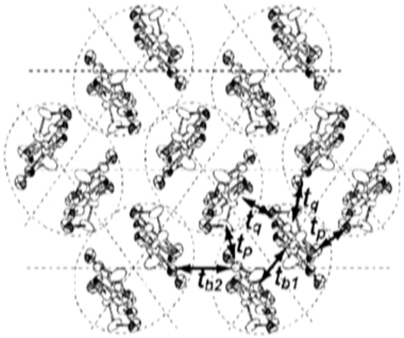

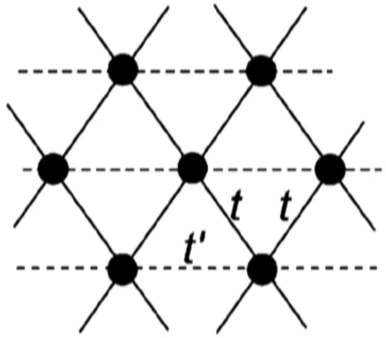

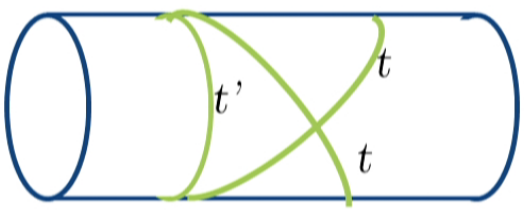

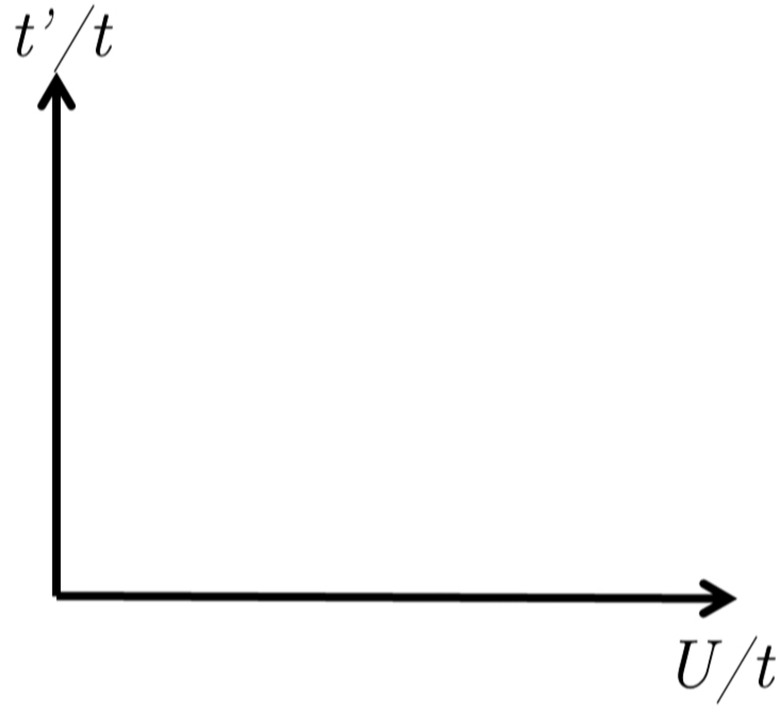

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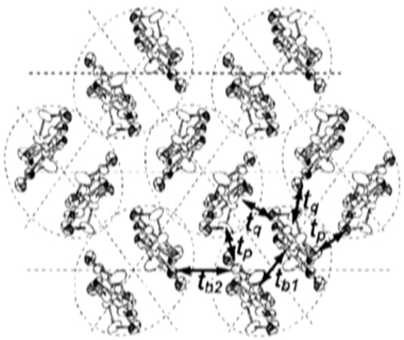

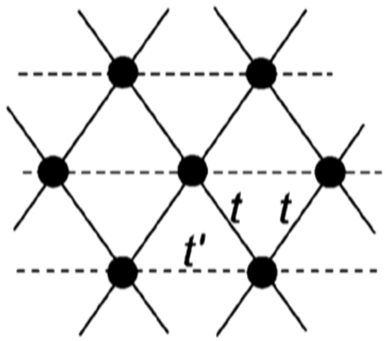

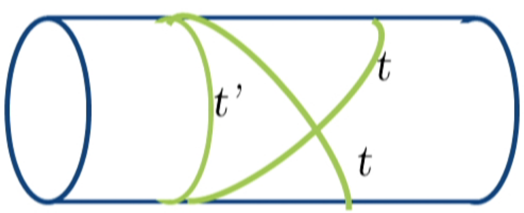

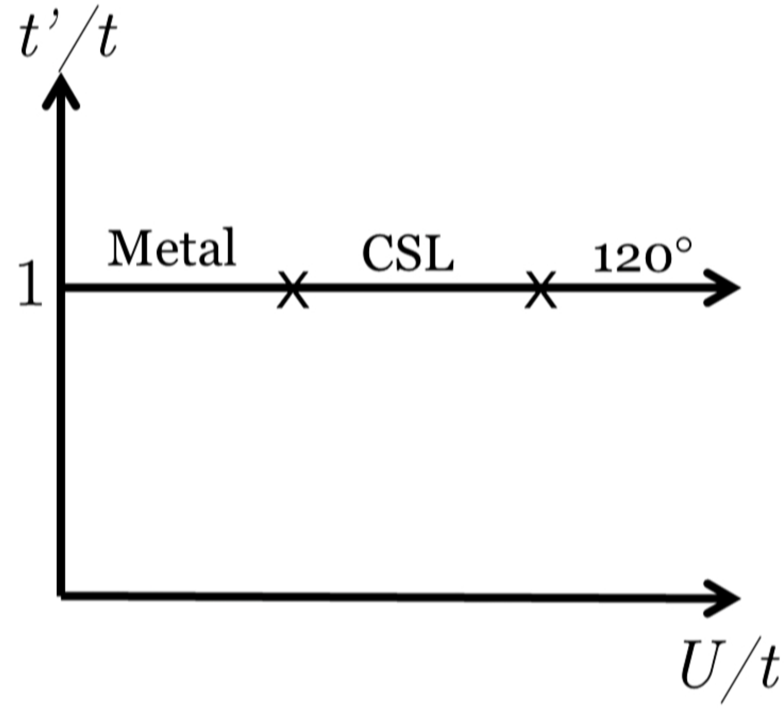

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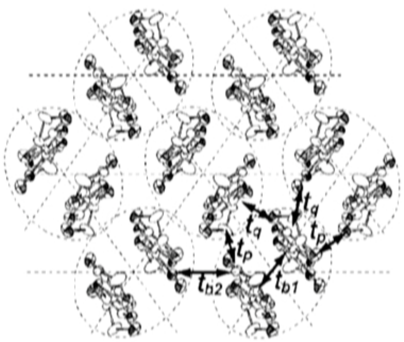

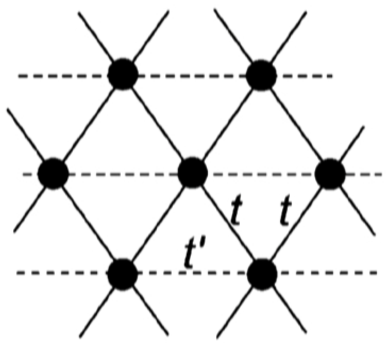

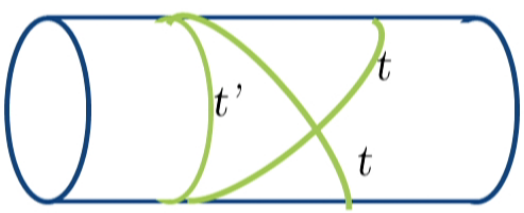

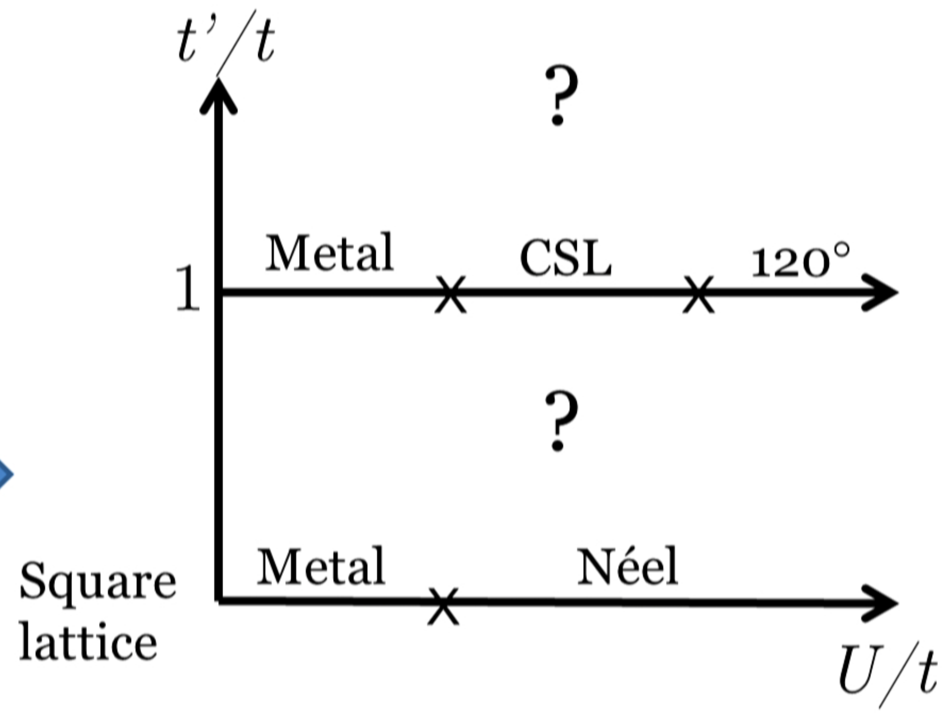

- Interesting phase transitions to observe!

Mixed-space DMRG

For triangular lattice:

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

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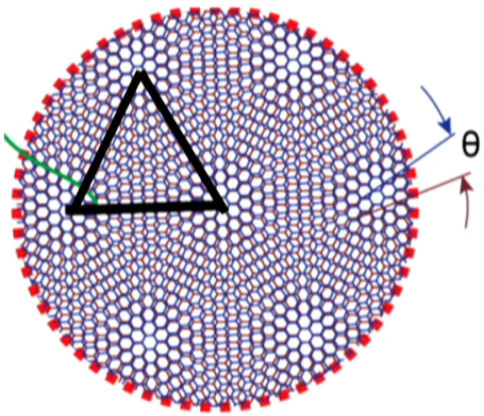
Can be even more useful!

Consider system with Moiré pattern
eg. twisted bilayer graphene



Cao et al., Nature 2018

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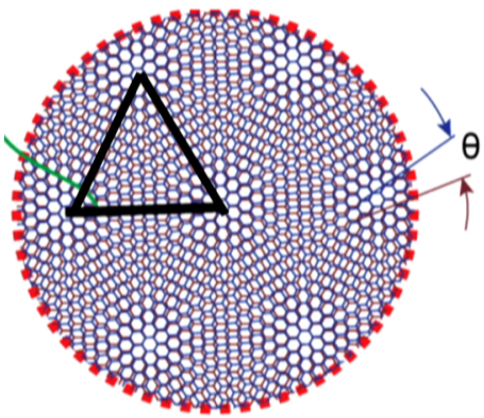
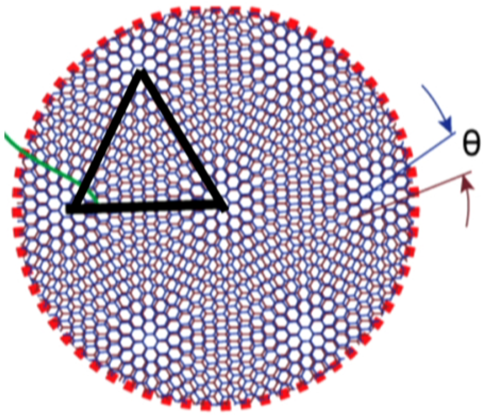


Cao et al., Nature 2018

Extremely large unit cell → ~~DMRG~~

Mixed-space DMRG



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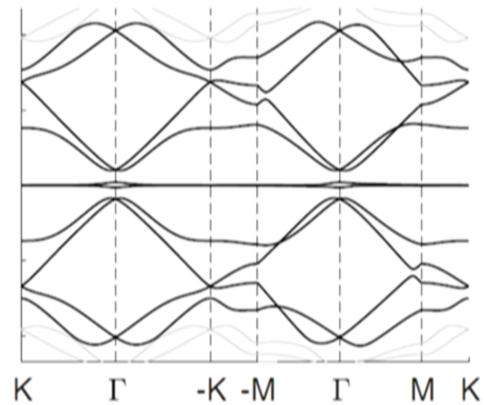
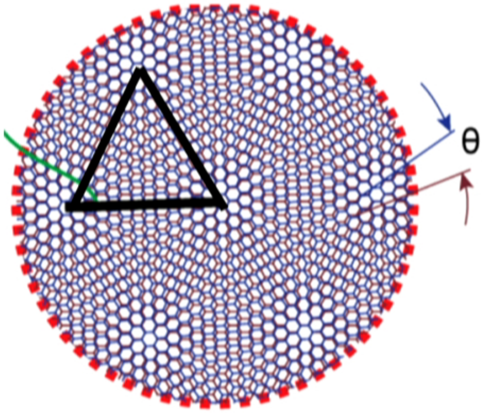


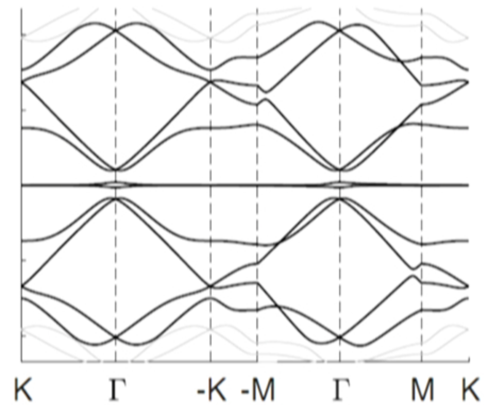
Po et al., 1808.02482

Only need flat bands

Mixed-space DMRG



Cao et al., Nature 2018



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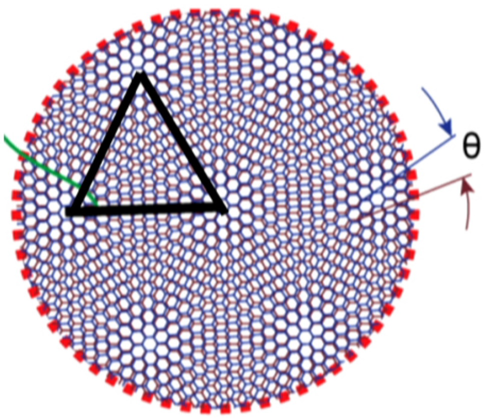
Mixed-space DMRG



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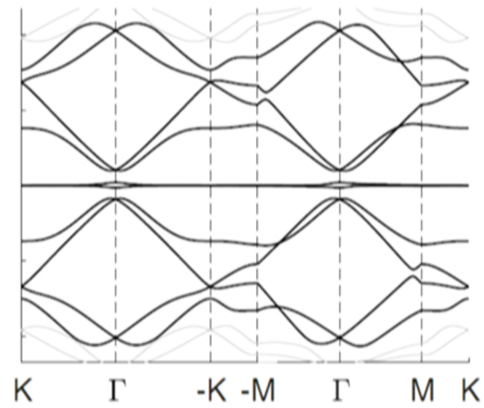

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Automatically generate and compress MPO

$\boxed{\text{DMRG}}$

Acknowledgements

Collaborators:

Johannes Motruk
(UC Berkeley)

Michael P. Zaletel
(Princeton,
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!