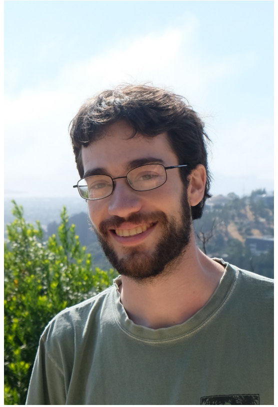
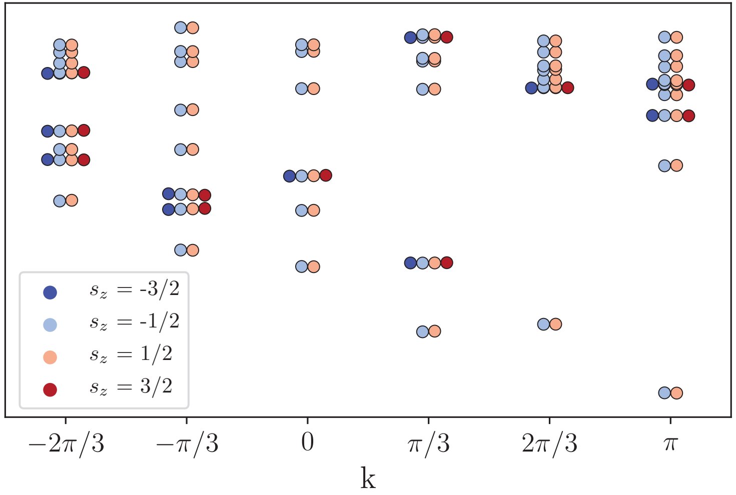
Chiral spin liquid phase of the triangular lattice Hubbard model

An iDMRG study



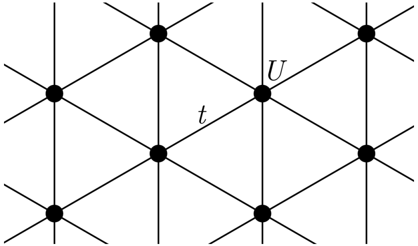


Aaron Szasz
Berkeley, now Perimeter

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

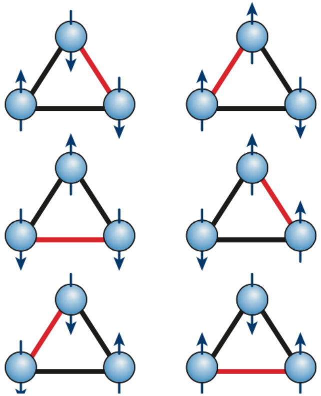
The model

Half-filled Triangular Lattice Hubbard model:



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

Triangles = frustration



ABSTRACT

The possibility of a new kind of electronic state is pointed out, corresponding roughly to Pauling's idea of "resonating valence bonds" in metals. As observed by Pauling, a <u>pure</u> state of this type would be insulating; it would represent an alternative state to the Néel antiferromagnetic state for S = 1/2. An estimate of its energy is made in one case.

[Anderson 73]

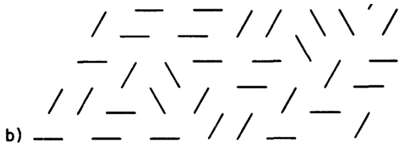
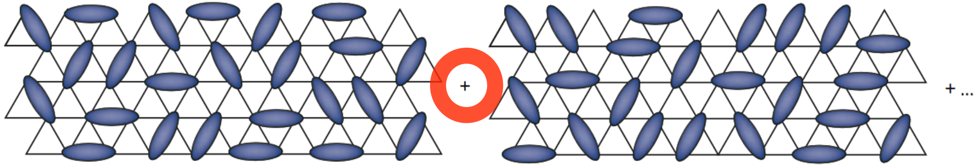


FIG. 3

“Resonating valence bonds:”
spin liquid

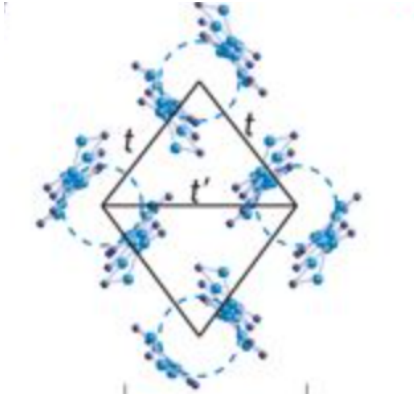


Motivation from experiments

Possible spin liquids in organic triangular compounds

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

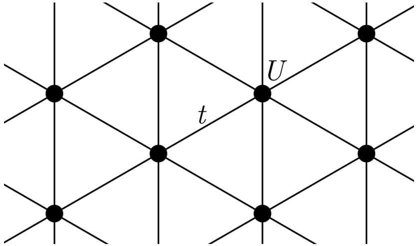
$EtMe_3Sb[Pd(dmit)_2]_2$ "dmit-131"



$\approx$

2D triangular layers

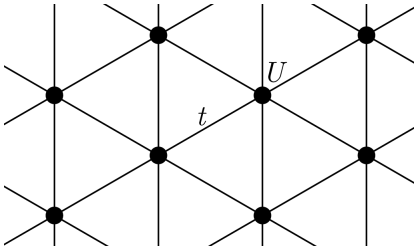
Approximated by Hubbard model



[from Yamashita et al., Nat. Phys. **5**, 44 (2008)]

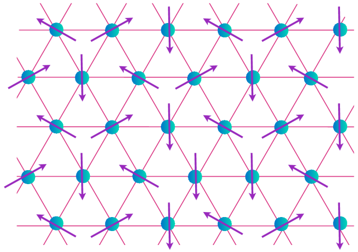
Motivation from experiments

Approximated by Hubbard model



Key parameter: U/t

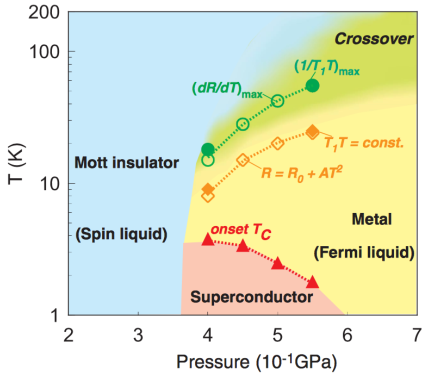
At ambient pressure, material is a Mott insulator: spin degree of freedom



Biggish U/t

Under 0.5 Gpa pressure transitions to metal or superconductor

$\kappa - (ET)_2(Cu)_2(CN)_3$



Smaller U/t

[from Kurosaki et al., PRL (2005)]

"Weak" Mott insulator:

$$H \approx 4\frac{t^2}{U}\sum_{\langle i,j\rangle} S_i \cdot S_j + g\frac{t^4}{U^3}\sum_{\Diamond} P_{ijkl} + \cdots$$

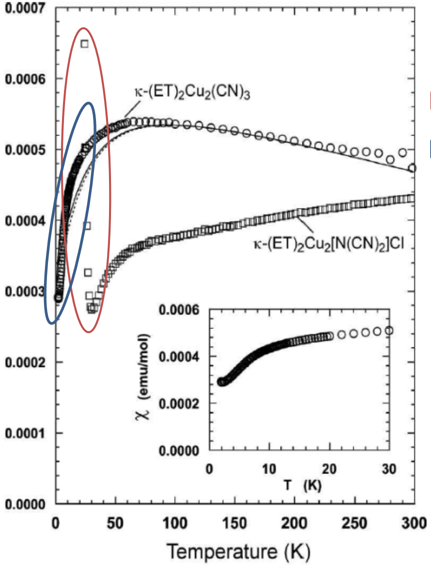
"ring exchange"

Experiment: absence of magnetic order

Eg: $\kappa-(ET)_2(Cu)_2(CN)_3$ "BEDT"

Nonmagnetic at low T:

Magnetic susceptibility



AFM

Spin liquid?

Figure from [1]

Gapless?

Linear-T Heat capacity

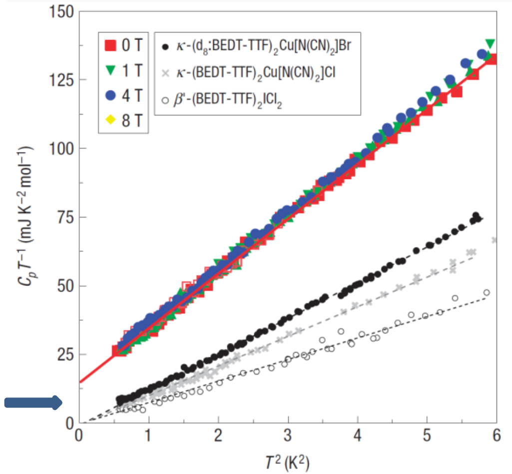


Figure from [2]

Gapped?

Thermal conductivity

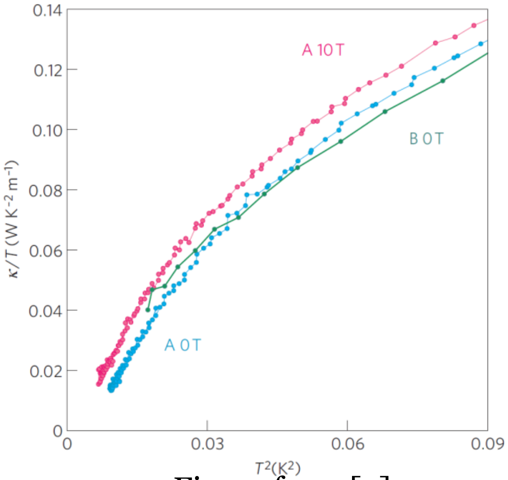


Figure from [3]

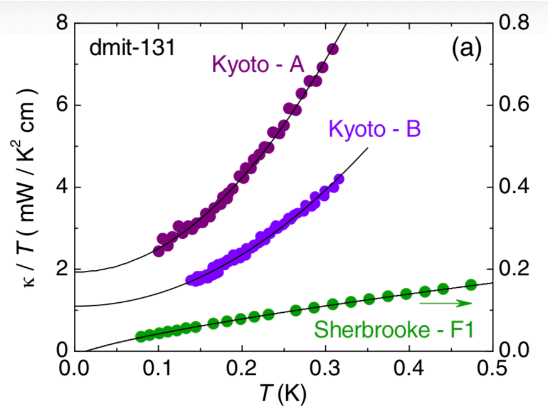
[1] Shimizu et al., PRL **91**, 107001 (2003)
[2] Yamashita et al., Nat. Phys. **4**, 459 (2008)
[3] Yamashita et al., Nat. Phys. **5**, 44 (2008)

Experiment: thermal conductivity in dmit-131

$EtMe_3Sb[Pd(dmit)_2]_2$ “dmit-131”

First thermal conductivity experiments: linear-T. “spinon-Fermi surface?”

[Yamashita, et al. Science 2010 (Kyoto)]



More recently: no linear-T (but not activated either)

$$\kappa/T = bT^c + \cdots\,, \qquad c \sim 0.7$$

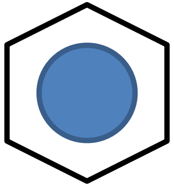
[Bourgeois-Hope et al, PRX 2019 (Sherbrooke); Ni et al. PRL 2019 (Fudan)]

Phase diagram (expected)

Single parameter: U / t

Metal (SC?) **Nonmagnetic insulator** Spin-ordered U/t

Exact solution:



$$H \approx 4\frac{t^2}{U}\sum_{\langle i,j\rangle} S_i \cdot S_j + g\frac{t^4}{U^3}\sum_{\Diamond} P_{ijkl} + \cdots$$

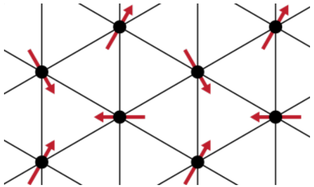
Ring exchange, other terms destroy Neel order?

[Misguich et al. PRB 1999; LiMing et al. PRB 2000; Imada 2003; Motrunich 2004]

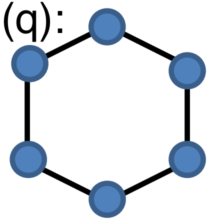
Reduces to Heisenberg:

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

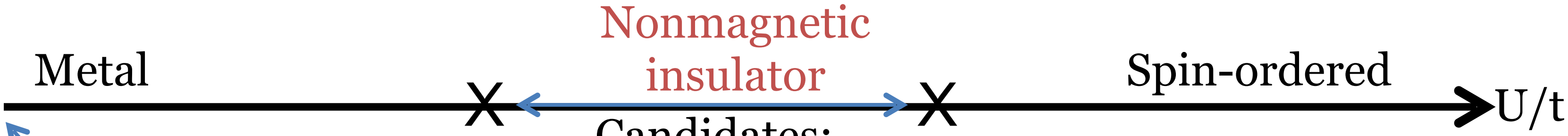
120° order:



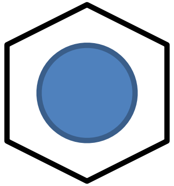
S(q):



Phase diagram (expected)



Exact solution:



Candidates:

- U(1) spin liquid with spinon Fermi surface[3]
- Gapped Z_2 spin liquid[4]
- Nodal gapless spin liquid[5]
- Chiral spin liquid[6]
- Others …

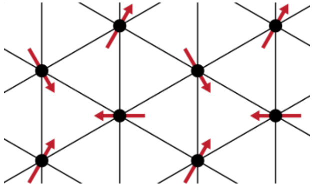
With DMRG:

- Two-leg ladder: U(1) gapless[7]
- Finite DMRG: likely gapped[8]

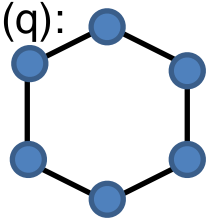
Reduces to Heisenberg:

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

120° order:



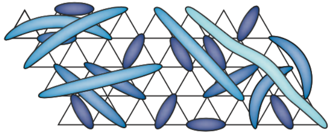
S(q):



[3] Motrunich, PRB 72, 045105 (2005)
[4] Zhu & White, PRB 92, 041105 (2015)
[5] Mishmash et al., PRL 111, 157203 (2013)
[6] Kalmeyer & Laughlin, PRL 59, 2095 (1987)
[7] Mishmash et al., PRB 91, 235140 (2015)
[8] Shirakawa et al., PRB 96, 205130 (2017)

Spin liquid candidates

Gapless: “Spinon Fermi surface”



Gutzwiller projected Fermi surface

$$|\Psi\rangle = \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) \, |\mathrm{FS}\rangle$$

$$c_\sigma = b f_\sigma$$

$$b = \text{Mott Ins.}$$

$$f_\sigma = \text{Fermi Sur. (“spinon”)}$$

$$C \sim T^{2/3}$$

Motrunich, PRB 72, 045105 (2005)

Experiment: C “=” T

Gapped spin liquid

Many possible types!

Z2 spin liquid: preserves time reversal

Topology of the resonating valence-bond state: Solitons and high-T_c superconductivity

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Institute for Theoretical Physics, University of California, Santa Barbara, California 93106
(Received 9 March 1987; revised manuscript received 12 May 1987)

We study the topological order in the resonating valence-bond state. The elementary excitations have reversed charge-statistics relations: There are neutral spin-$\frac{1}{2}$ fermions and charge $\pm e$ spinless bosons, analogous to the solitons in polyacetylene. The charged excitations are very light, and form a degenerate Bose gas even at high temperatures. We discuss this model in the context of the recently discovered oxide superconductors.

“Chiral spin liquid:” breaks it

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Equivalence of the Resonating-Valence-Bond and Fractional Quantum Hall States

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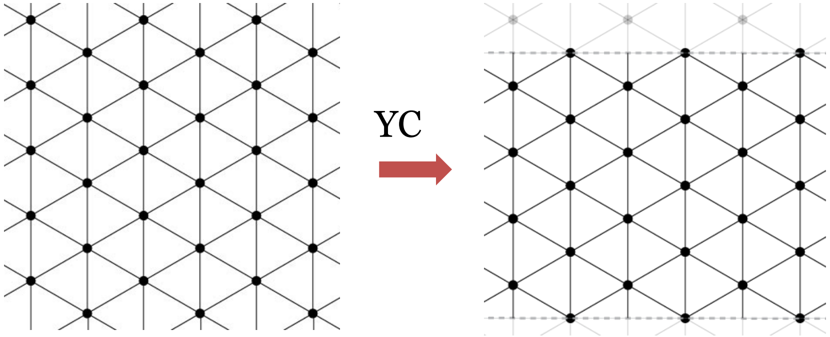
University of California, Lawrence Livermore National Laboratory, Livermore, California 94550
(Received 24 July 1987)

Calculation methods

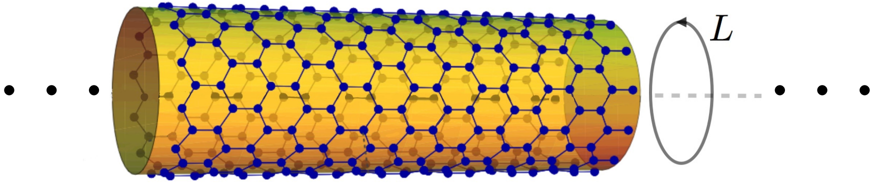
Find ground state with **infinite density matrix renormalization group (iDMRG)**.

- An unbiased variational method for solving infinite **1D** spin and fermion chains
- Efficient for 1D systems: how to do 2D?

1. Convert to cylinder



- *Infinite* along the length of the cylinder



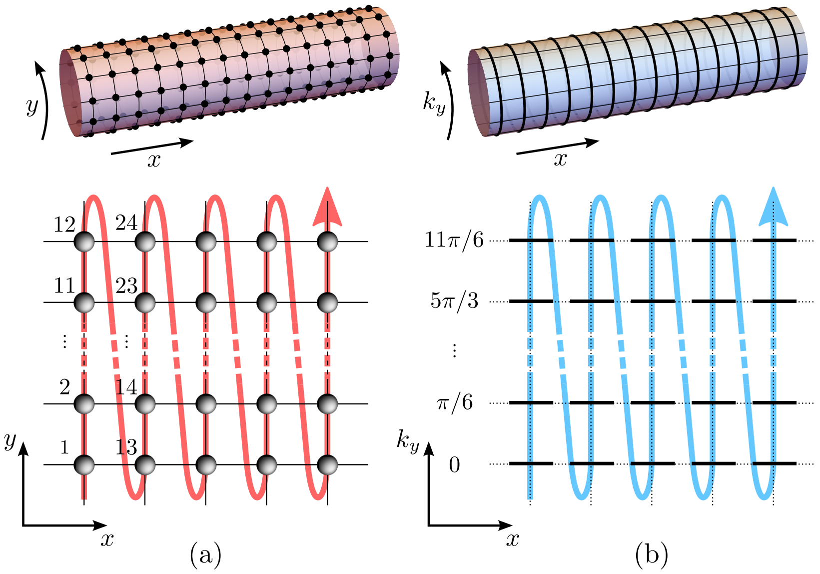
- Allowed momenta:

- YCL has conserved momentum with L eigenvalues

Different about our DMRG: “mixed” k-space

$$\psi_{x,y,\sigma} \rightarrow \psi_{x,k_y,\sigma}$$

[Motruk et al, PRB 2016; Hubig et al. PRB 2017]



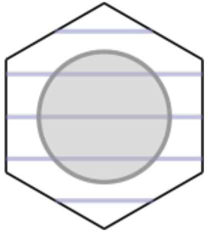
1. To momentum space **around** the cylinder
   - “Mixed real- and momentum-space basis”

$$c_{xk_y\sigma} = \frac{1}{\sqrt{L}} \sum_y e^{-ikay} c_{xy\sigma}$$

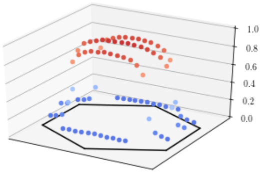
   - Fixed momentum sector: (a) smaller Hilbert space ⇒ reduced computation time, memory; (b) find multiple low-lying states
2. Use L=4, L=6 cylinders
   - 4-dimensional local Hilbert space, vs 2D for spin models ⇒ need smaller circumference

Summary of Phase diagram

Metal — Chiral spin liquid — Spin-ordered → U/t



n_k



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Equivalence of the Resonating-Valence-Bond and Fractional Quantum Hall States

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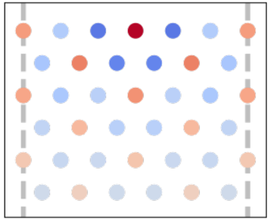
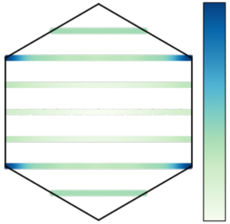
(Received 24 July 1987)

Gapped

Spin analog of FQHE

Spontaneously broken time-reversal

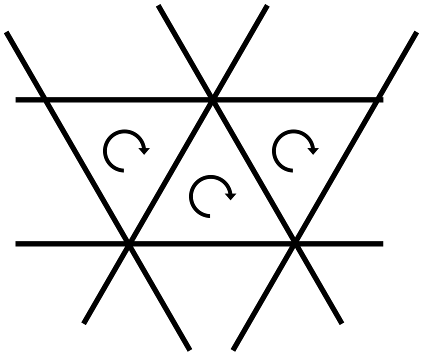




Chiral spin liquid

Preserves spin rotation, but breaks P, T:

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \times \mathbf{S}_k \rangle_\triangle \neq 0$$

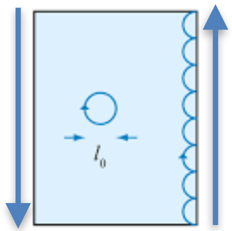


Gapped, fractionalized spin liquid:

Spin $\longleftrightarrow$ hard-core boson: $\uparrow$ = empty, $\downarrow$ = full

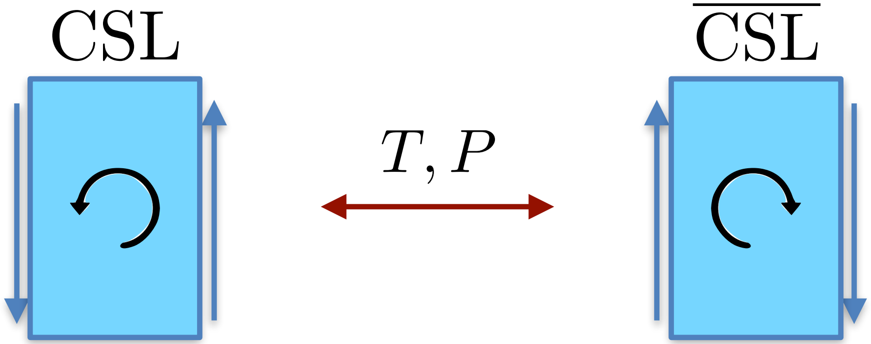
CSL: $\nu = \dfrac{1}{2}$ bosonic fractional QHE (Laughlin state).

Incompressible FQHE $\longleftrightarrow$ spin-gap in bulk



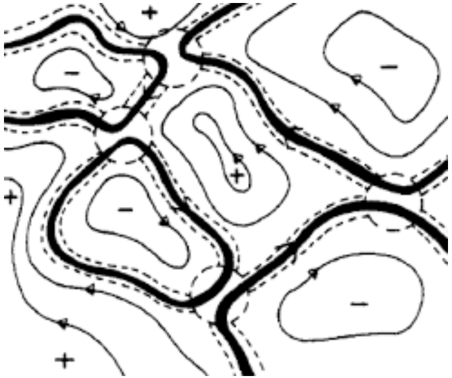
Gapless chiral edge states:
Thermal Hall Effect (c=1), spin-Hall effect

Spontaneous symmetry breaking

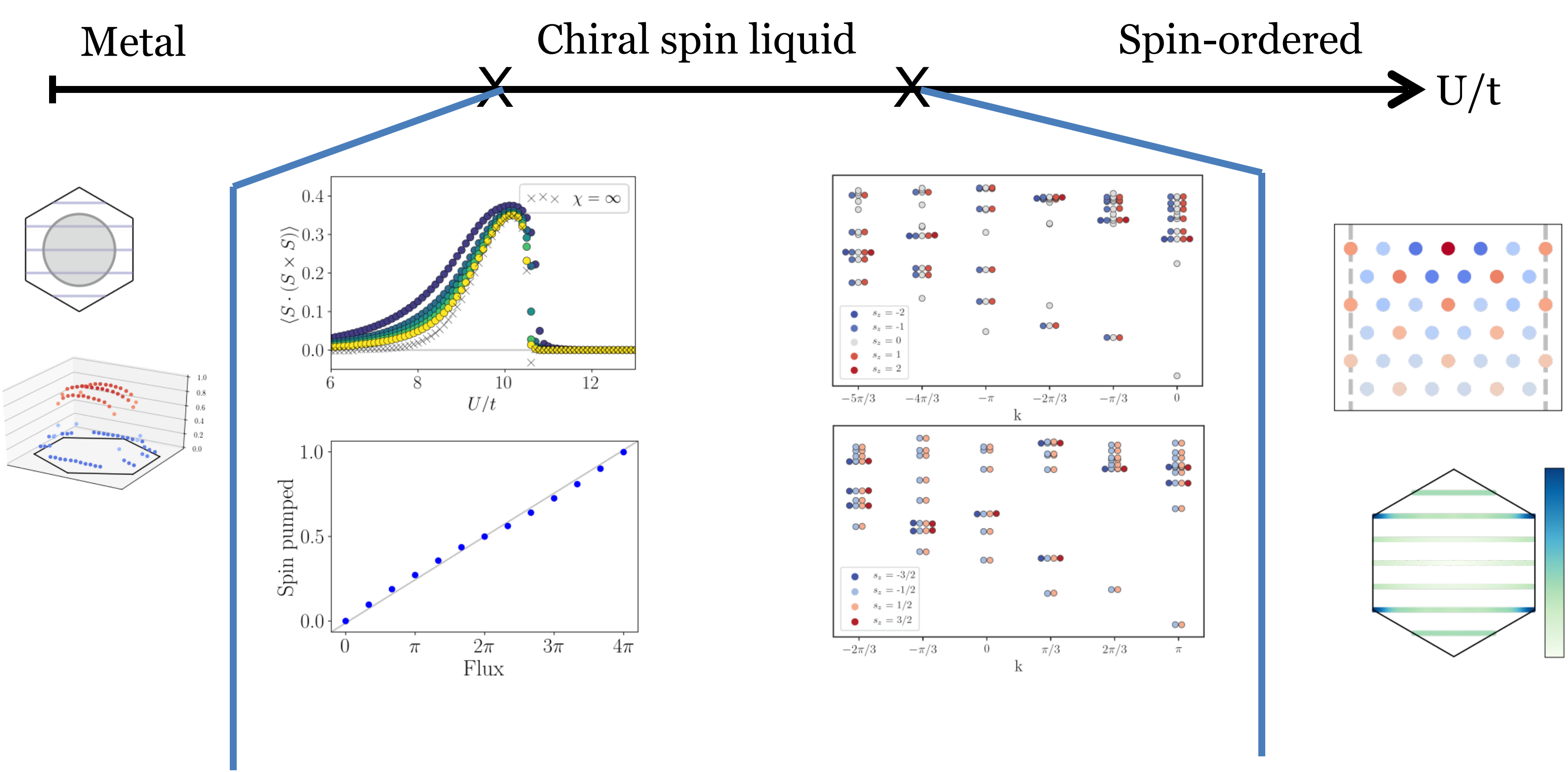


Above Ising T_c (or T-disorder):
puddles?

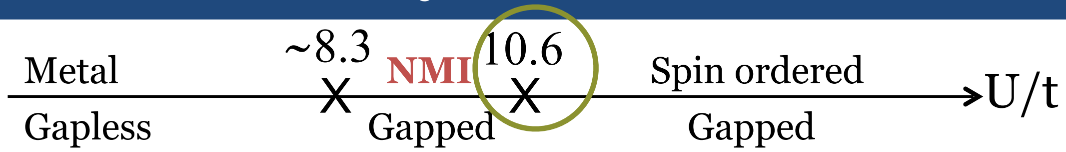
Domain walls have chiral edge states: linear-T specific heat



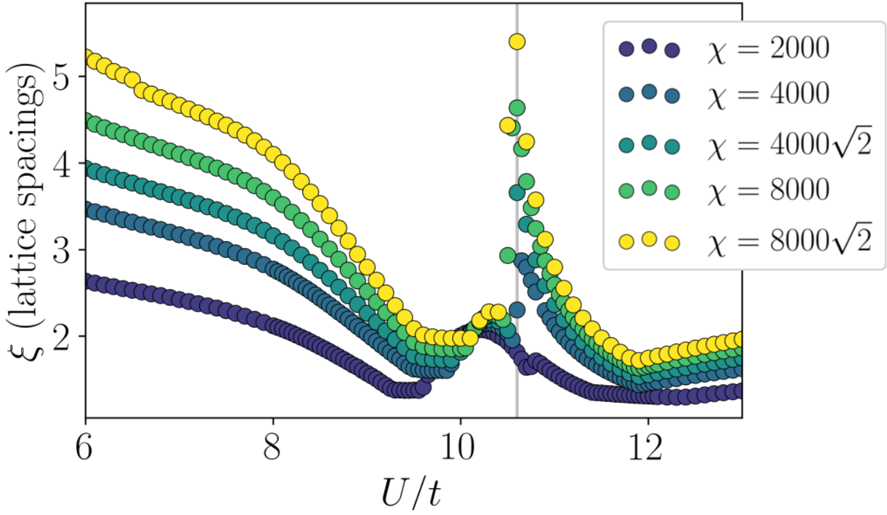
Phase diagram: numerical evidence



Phase diagram: L=4 cylinder



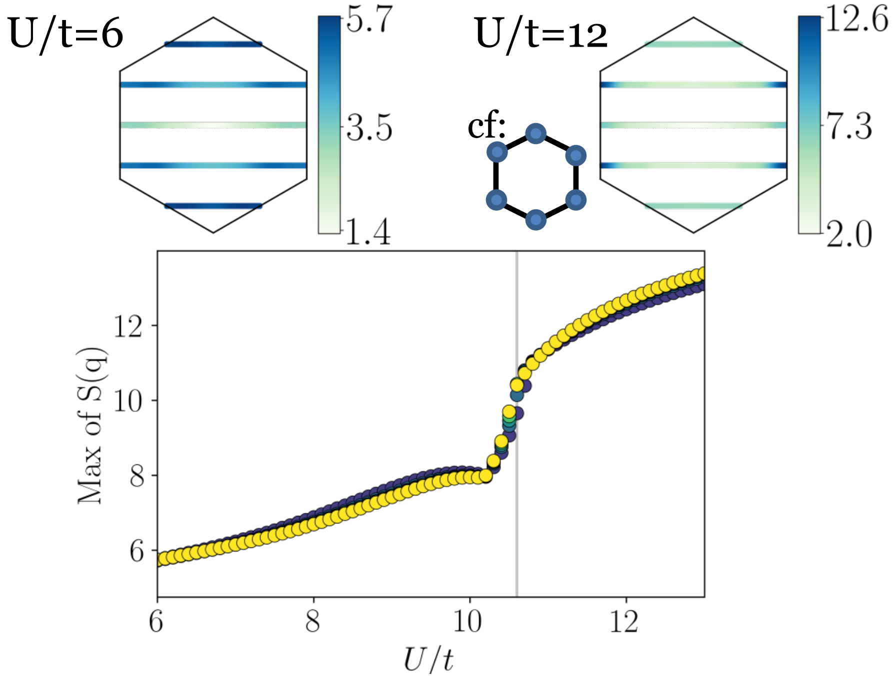
Correlation length



χ: MPS "bond dimension"

- Controls precision of DMRG

Spin order: structure factor $S(q)$



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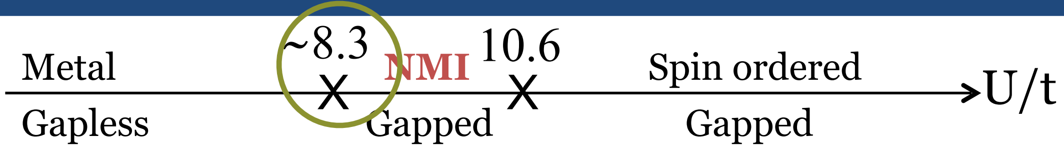
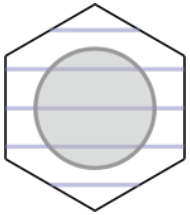




$c = 6 = 3 \cdot 2$

On cylinder, metal characterized by # of gapless modes "c" (2 per "wire")

Can be measured from entanglement:

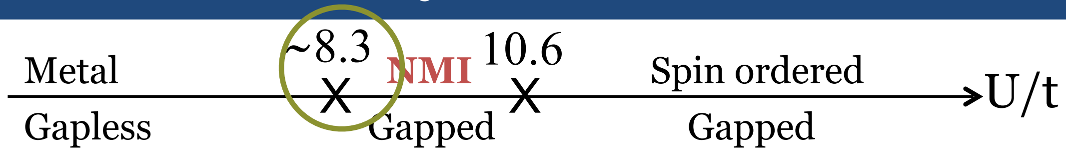
A  B

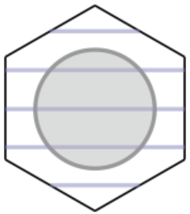
$$|\psi\rangle = \sum_{i=1}^{\cancel{\infty}\ \chi} \lambda_i |\psi_i^A\rangle |\psi_i^B\rangle \longrightarrow S = \sum_{i=1}^{\cancel{\infty}\ \chi} -\lambda_i^2 \log(\lambda_i^2)$$

Finite entanglement scaling:[8,9]

[8] Calabrese & Cardy, J. Stat. Mech. 06, P06002 (2004)
[9] Pollmann et al, PRL 102, 255701 (2009)

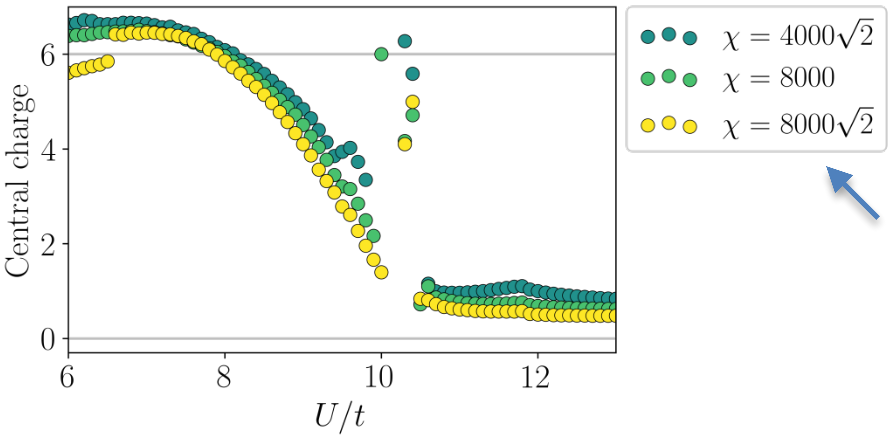
Phase diagram: L=4 cylinder



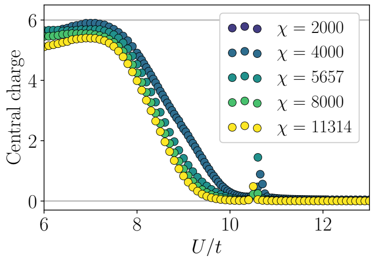


$c = 6 = 3 \cdot 2$

Gapped: c = 0



Accuracy of DMRG



Consistent with metal-insulator transition, though rounded out by finite DMRG accuracy

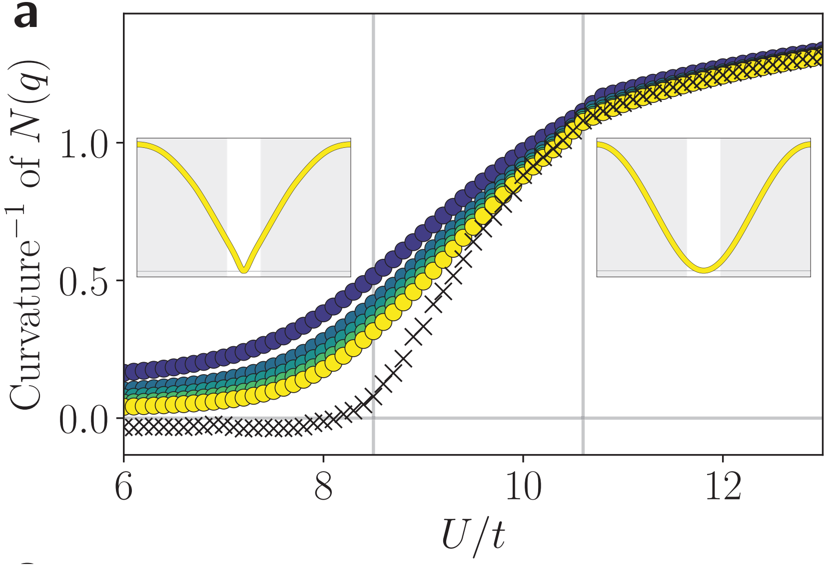
(give us bigger computers)

Metal-insulator transition

Density-density structure factor (along cylinder):

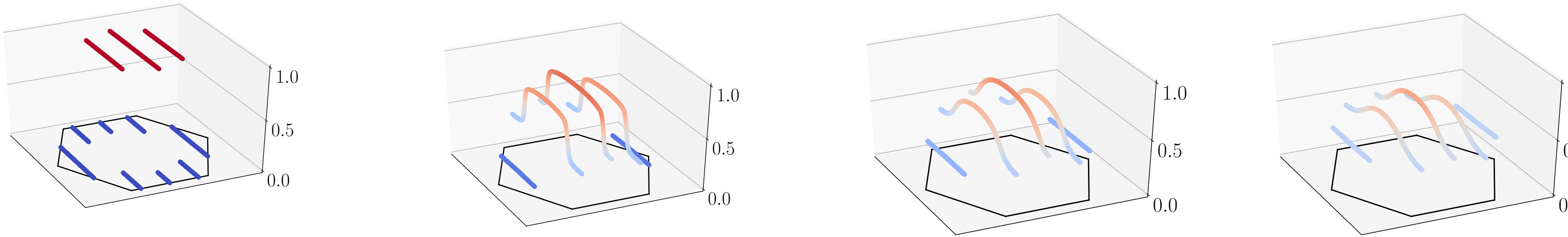
$$N(q) = \langle n(q) n(-q) \rangle$$

a



Destruction of Fermi surface

Electron occupation n_k



U=0 U=6 U=9 U=12

(metal) (spin liquid)

But on 1D cylinder, coupled Luttinger liquids (Z=0) for any U > 0
Metal-insulator —-> BKT transition

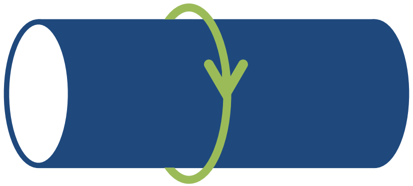
Suggestive of continuous destruction of Fermi surface (!!)
But how to infer 2D physics from 1D cylinders?

Phase diagram: L=6 cylinder consistent with 4

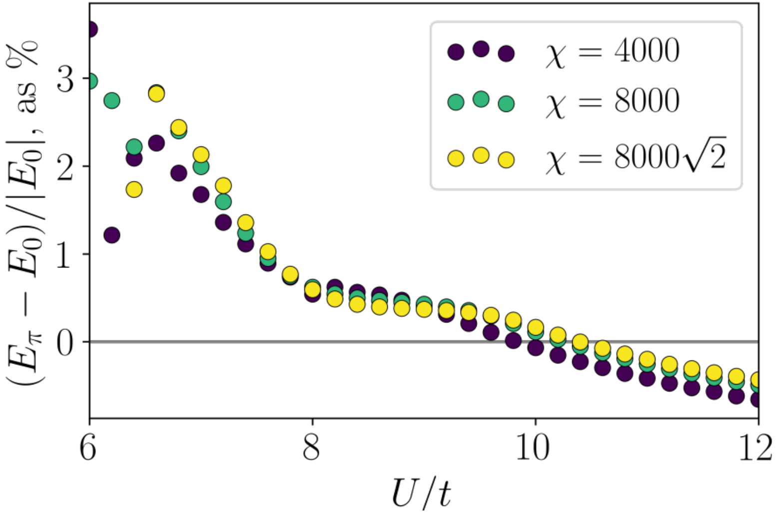
Metal | ~8 | **NMI** | ~10 | Spin ordered | → U/t

Gapless | | Gapped? | | Gapped

Two low-energy states per chirality:

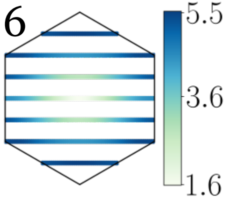


k=0, k=π per ring

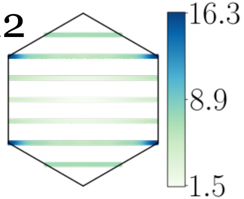


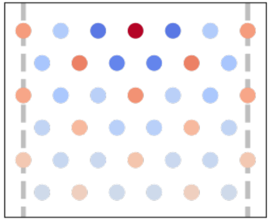
Spin order:

U/t=6



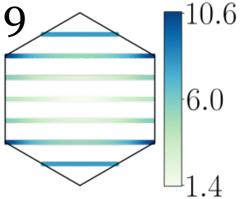
U/t=12



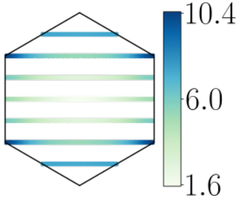


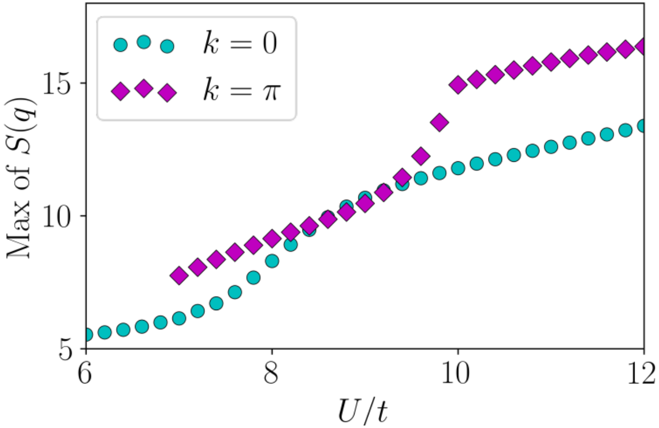
U/t=9

k=0

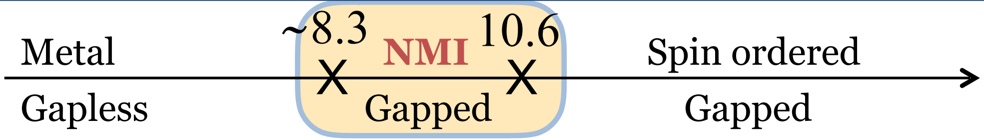


k=π



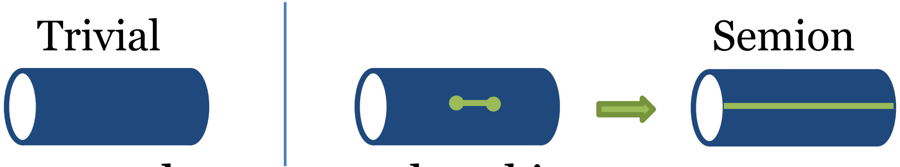


Identification as a CSL



What is a chiral spin liquid?

- ν=1/2 fractional quantum Hall effect state for spins[6,10]
- Signatures:
  - Topological ground state degeneracy and fractionalized quasiparticles (semions)
    - 2x on infinite cylinder (in addition to the symmetry-breaking)

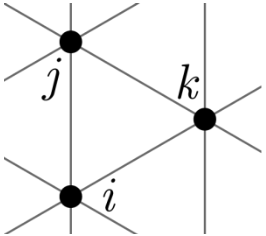


  - Time-reversal symmetry breaking
    - eg: scalar chiral order parameter
  - Chiral edge modes in 2D → entanglement spectrum on cylinder
    - Characteristic level counting vs momentum: 1, 1, 2, 3, 5, …
    - 2x degeneracy for semion sector
  - Quantized spin Hall effect: 2π flux insertion → spin ½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

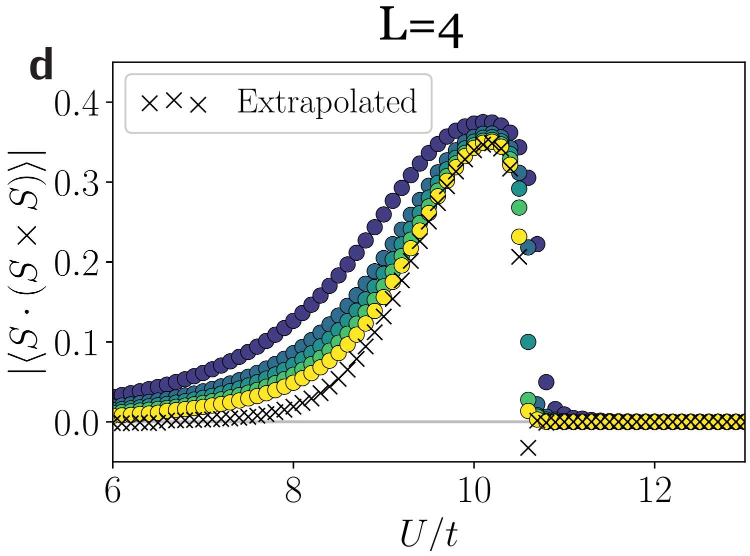
[6] Kalmeyer & Laughlin, PRL 59, 2095 (1987)
[10] Wen et al., PRB 39, 11413 (1989)

Identification as a CSL

Chiral order parameter:



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



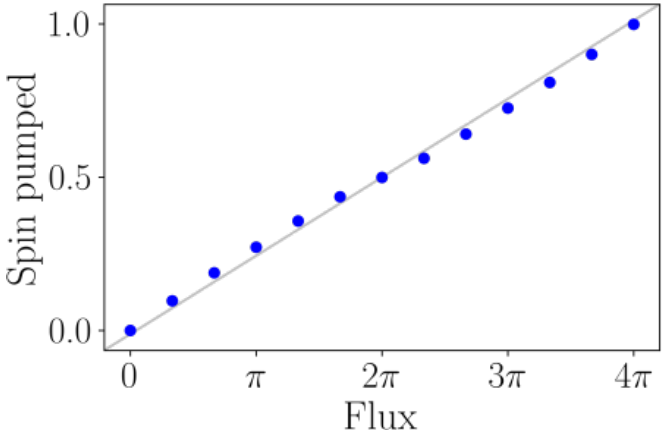
Seems like continuous onset of SSB at metal-insulator transition?
(uncertainty from finite DMRG accuracy)

Identification as a CSL

Flux insertion and spin Hall effect:

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

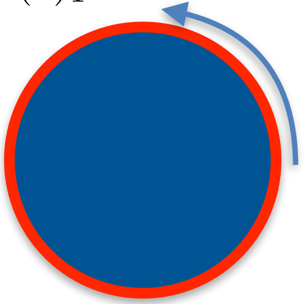
Spin Hall effect:



Identification as a CSL: chiral edge states

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

$\mathrm{SU}(2)_1$ WZW CFT

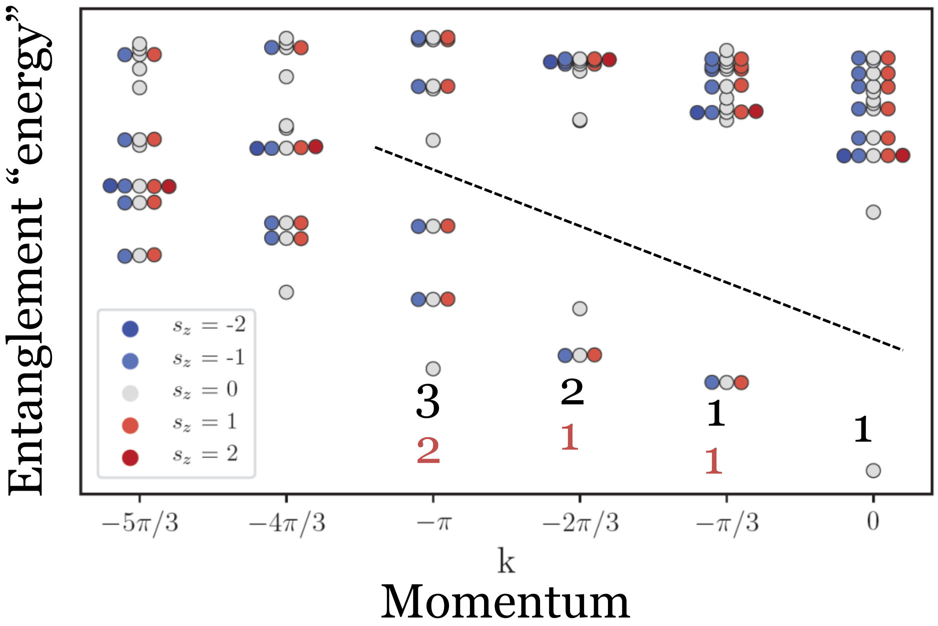


Simulate edge with entanglement cut

$$\rho_A \sim e^{-\beta H_E}$$

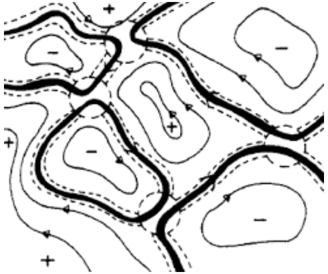
Li & Haldane 2008
Kitaev & Preskill 2006

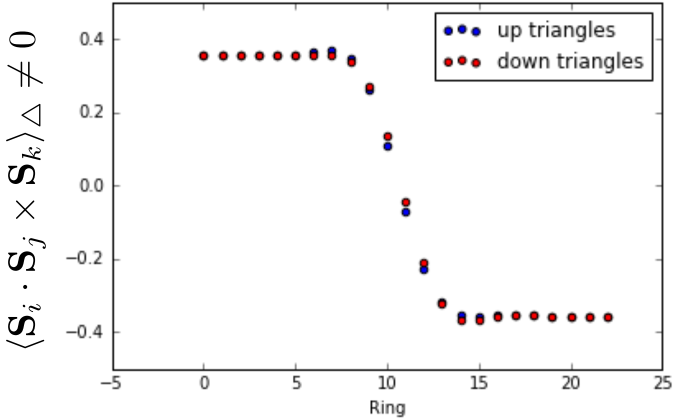
Chiral dispersion relation



CSL, CSL* domain-wall tension

What's the energy cost per unit length of a domain wall?
Will determine *T* of finite-temperature Ising transition



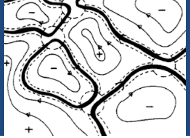


$$5 \cdot 10^{-3} t/a \sim 3\mathrm{K/unit\ length}$$

$$T_c \sim 3\mathrm{K}\ \log(2+\sqrt{3}) \sim 4\mathrm{K}$$

Expect Kerr effect,
small thermal-Hall below this

CSL, CSL* domains



“Hump” in heat capacity @ 5 - 6K

Linear-T Heat capacity

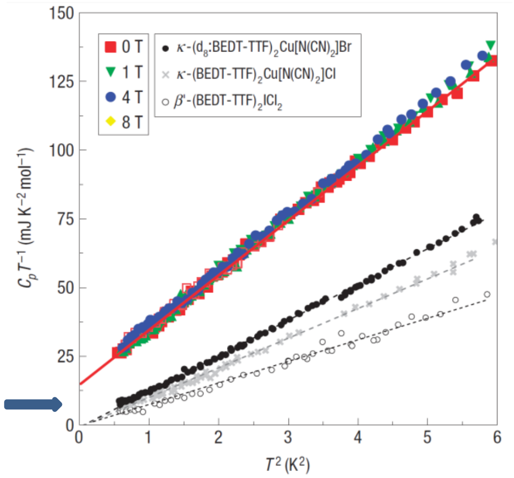
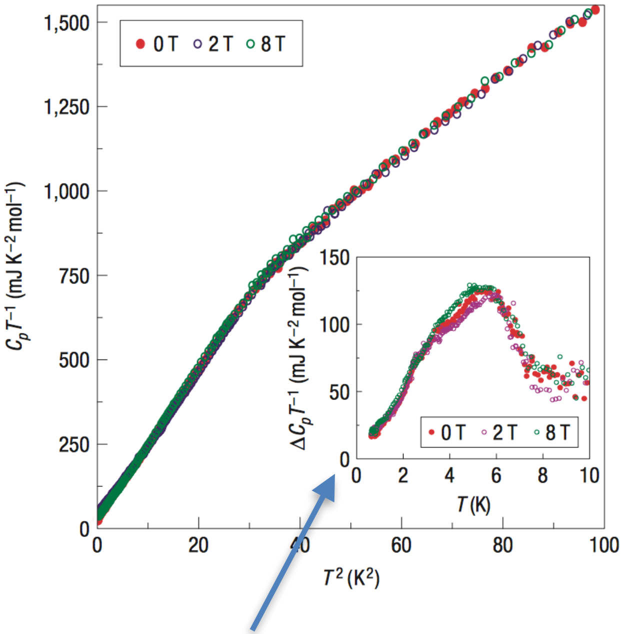


Figure from [2]



Excess heat capacity relative to AFM version

Magnetic field will split CSL, CSL* by

$$h = 10^{-4}\ \mathrm{meV/T}$$

per spin

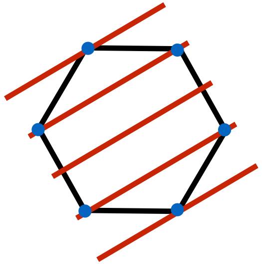
(small compared to J, T)

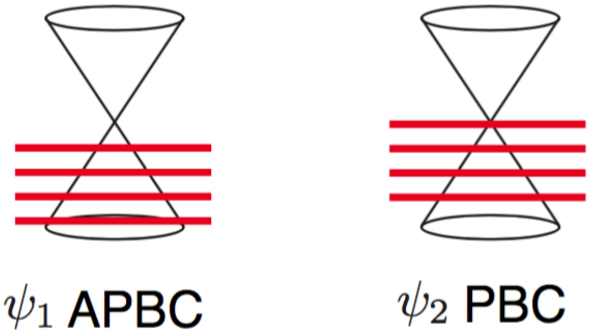
[1] Shimizu et al., PRL **91**, 107001 (2003)
[2] Yamashita et al., Nat. Phys. **4**, 459 (2008)
[3] Yamashita et al., Nat. Phys. **5**, 44 (2008)

Cautions: inferring 2D physics from 1D cylinders is tricky

The DMRG does NOT seem consistent with a spinon-Fermi surface.
However, ruling out a *nodal* gapless state (U(1) Dirac Spin Liquid) is trickier:

1D cylinder reduction can lead to instabilities, gap on cylinder





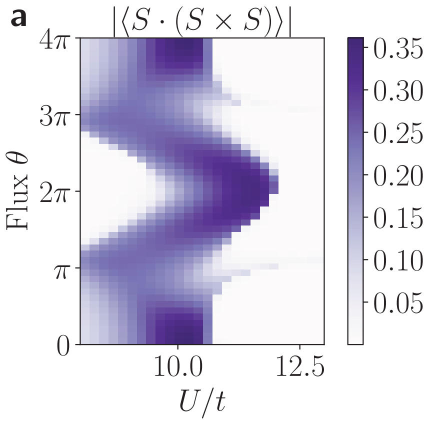
[He, et al., PRX 7, 031020]

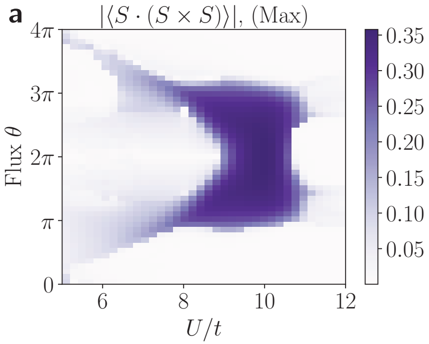
This (I believe) tricked us with Kagome-Heisenberg (“Herbertsmithite”) model: early DMRG suggested gapped, but our work suggests Dirac S.L.

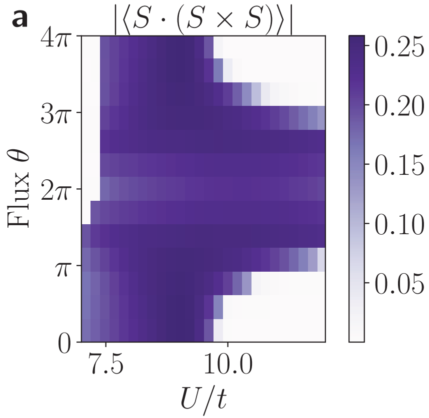
Can be probed by threading spin-flux through the cylinder to change BC

Cautions: inferring 2D physics from 1D cylinders is tricky

Effect of spin-flux on chiral order:







L=4

L=5

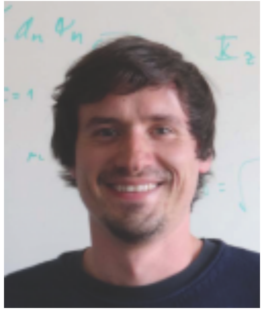
L=6

Clearly still large finite-circumference effects, but more consistent with 120 - CSL competition, not Dirac spin liquid

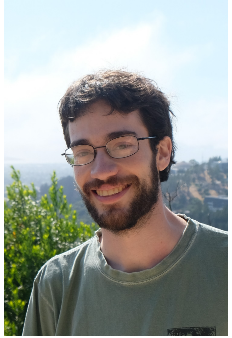
iPEPS study of Hubbard would be very interesting!

Acknowledgements

Collaborators:



Johannes Motruk
(UC Berkeley)



Aaron Szasz
(UC Berkeley)

Joel E. Moore
(UC Berkeley)

DMRG code base “TenPy”:

- Michael Zaletel
- Frank Pollmann (Munich)
- Roger Mong (Pittsburgh)

Computing resources:

- Lawrence Berkeley National Laboratory

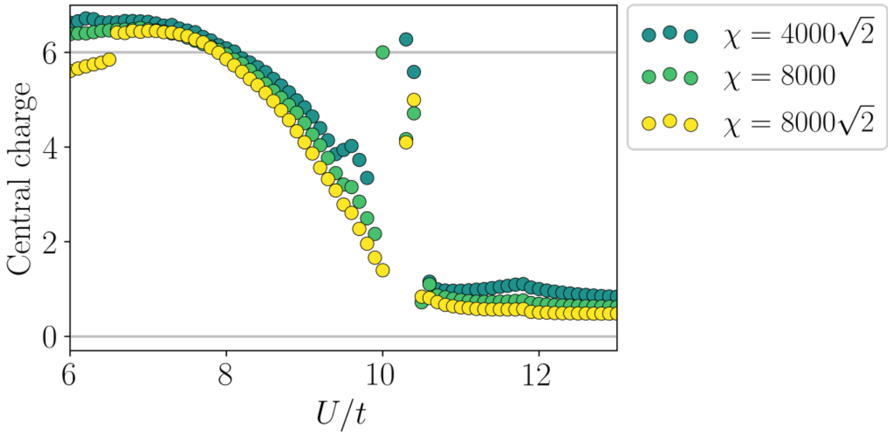
Summary

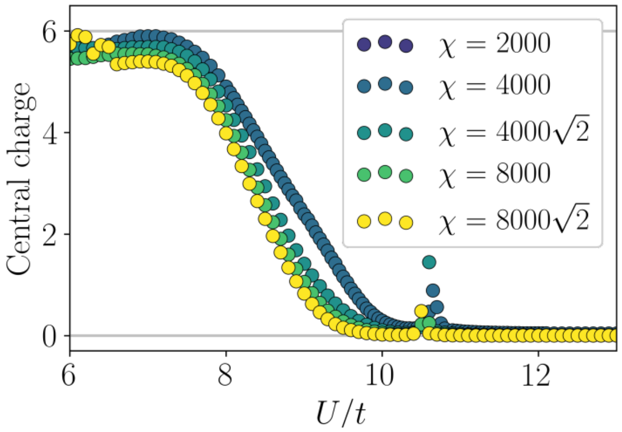
- Three phases of Hubbard model on triangular lattice
  - Metal, nonmagnetic insulator (NMI), magnetically ordered
- NMI phase is a chiral spin liquid!
  - Chiral order parameter → spontaneous breaking of time-reversal symmetry
  - Two topologically degenerate ground states: trivial, semion sectors
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

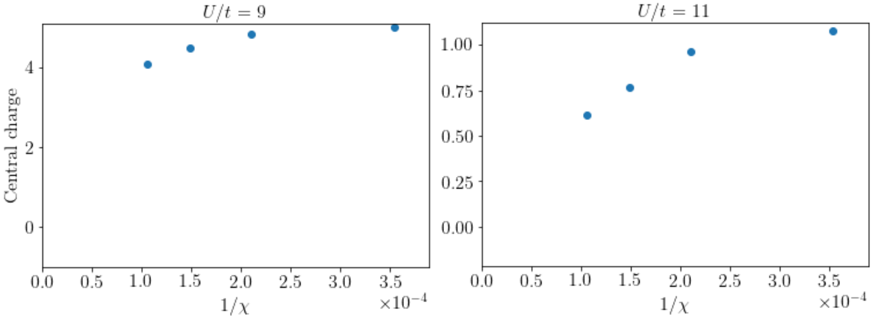
Thanks for your attention!

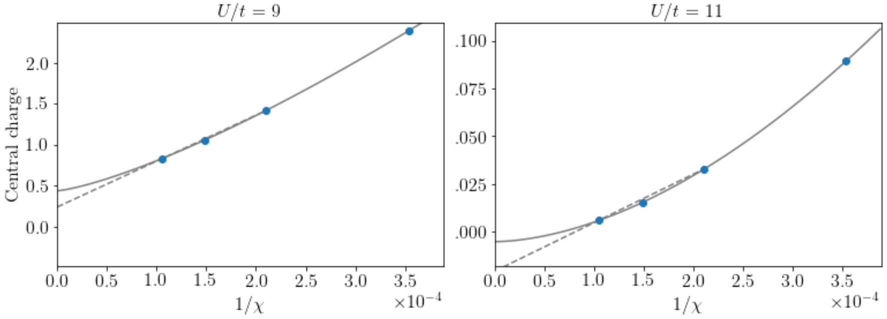
Extra slides: central charge scaling

$$S = \frac{1}{\sqrt{\frac{12}{c}} + 1} \log(\chi)$$





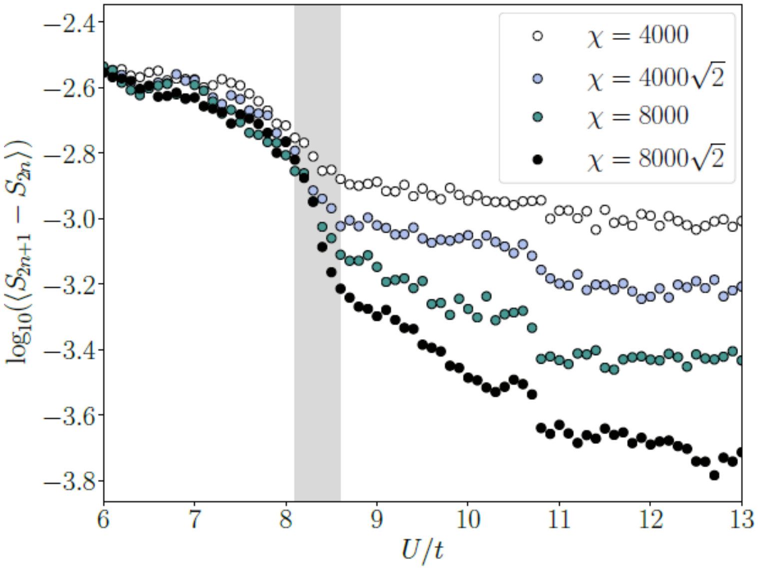


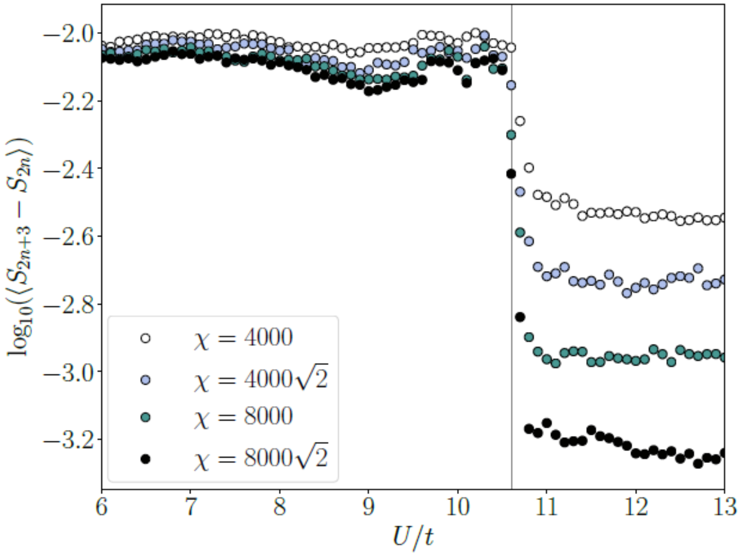


Extra slides: degeneracy onset

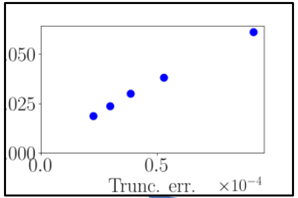
Proof of entanglement spectrum degeneracy:

Group entanglement levels into pairs/quadruplets, look at average splitting in each group.

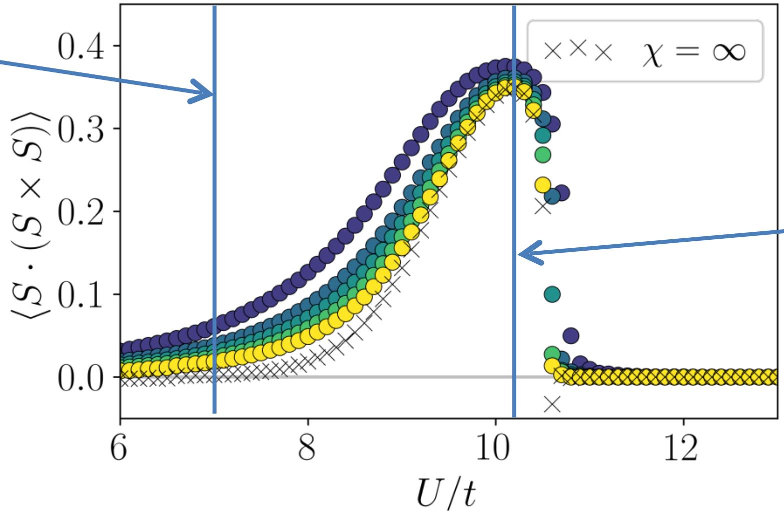


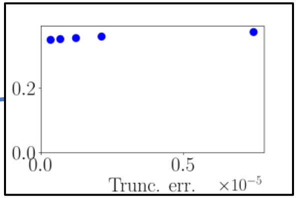


Extra slides: chiral order parameter extrap.

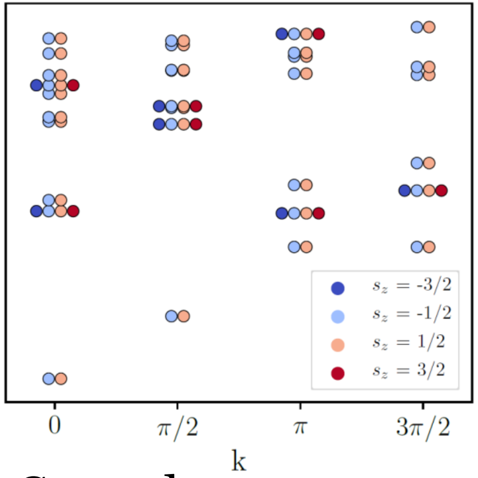


L=4

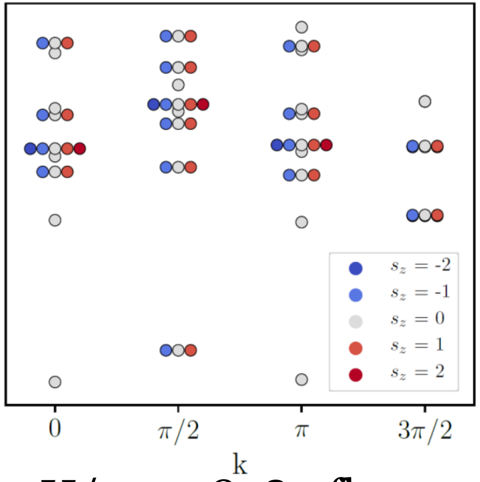




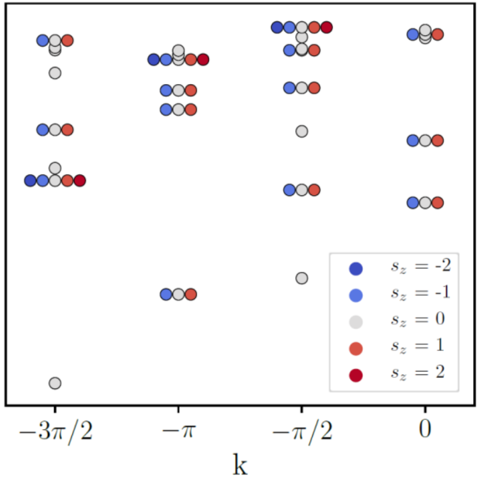
Extra slides: L=4 entanglement spectrum



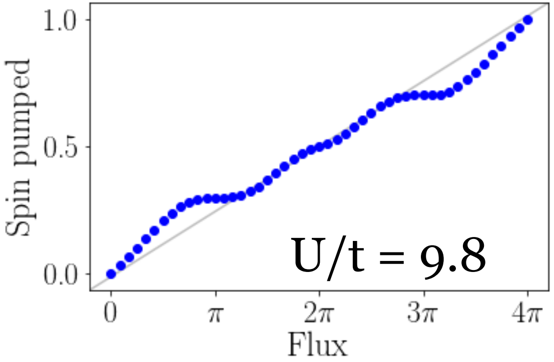
Ground state,
U/t = 9.8



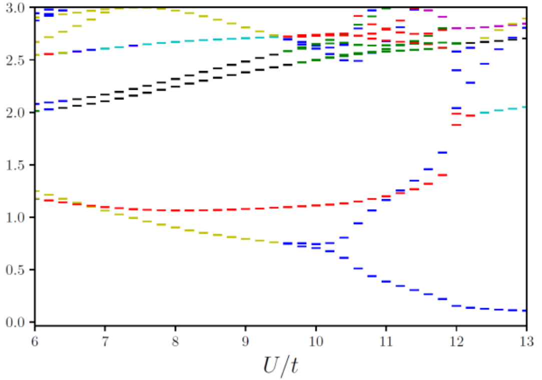
U/t = 9.8, 2π flux



U/t = 11.8,
2π flux

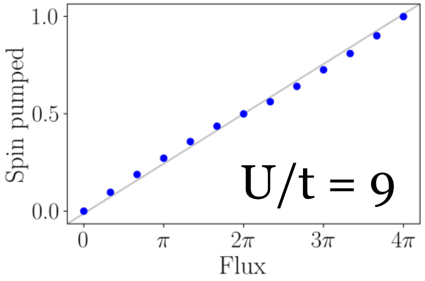


Phase boundaries moved

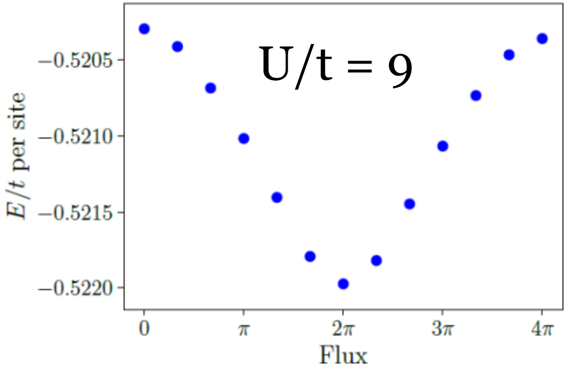


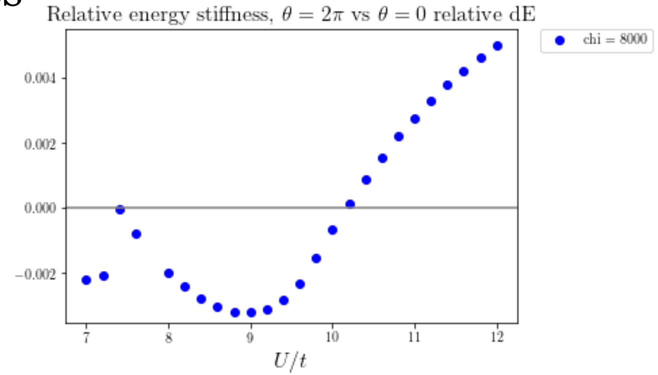
Extra slides: flux insertion

L=6



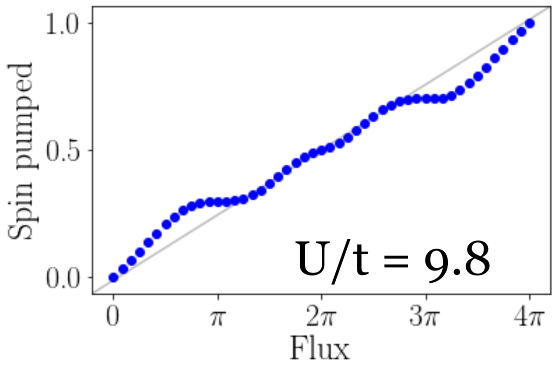
Energy stiffness

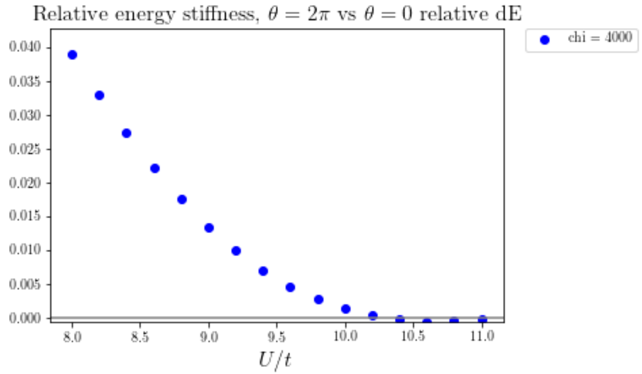




(Starts from k=π)

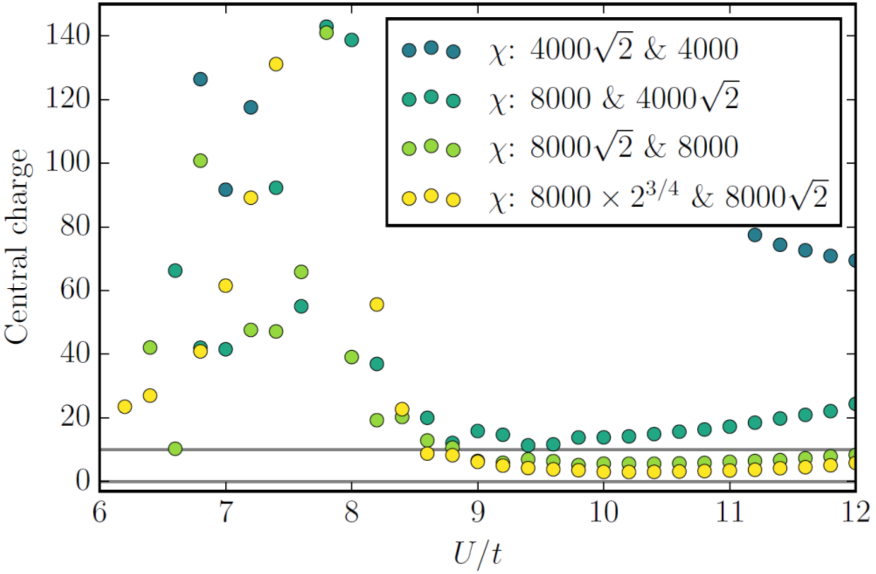
L=4



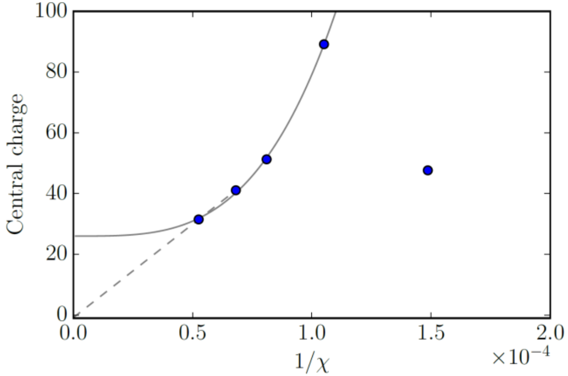


Extra slides: L=6 gapped?

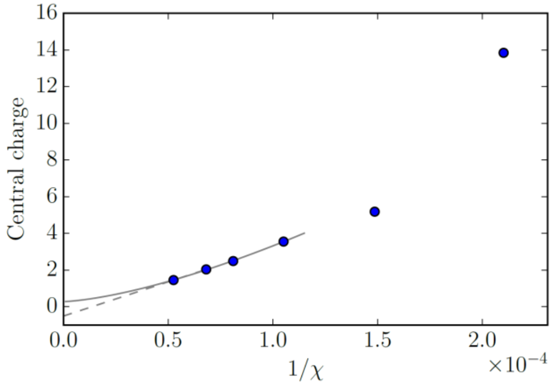
Central charge scaling with χ



U/t = 7.2

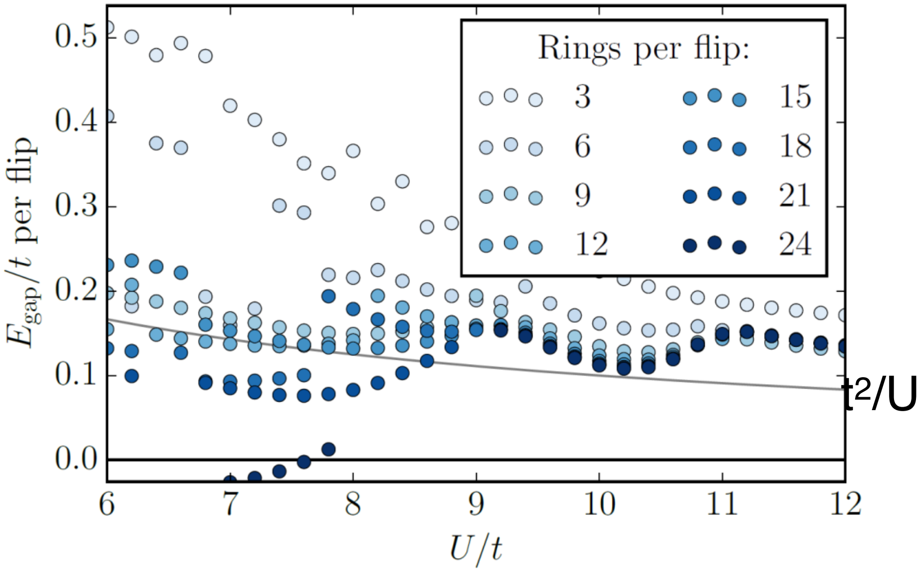


U/t = 9.8

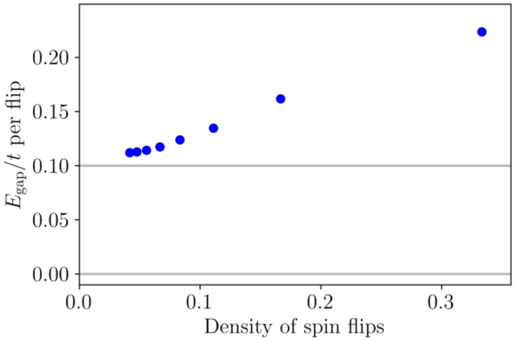


Extra slides: spin gap

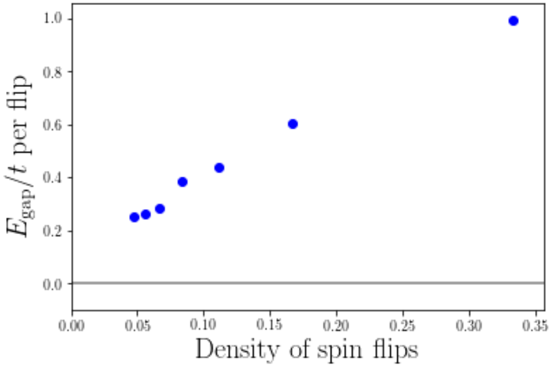
Excitation energy to state with <Sz> = 1 per N rings, L = 4



U/t = 10



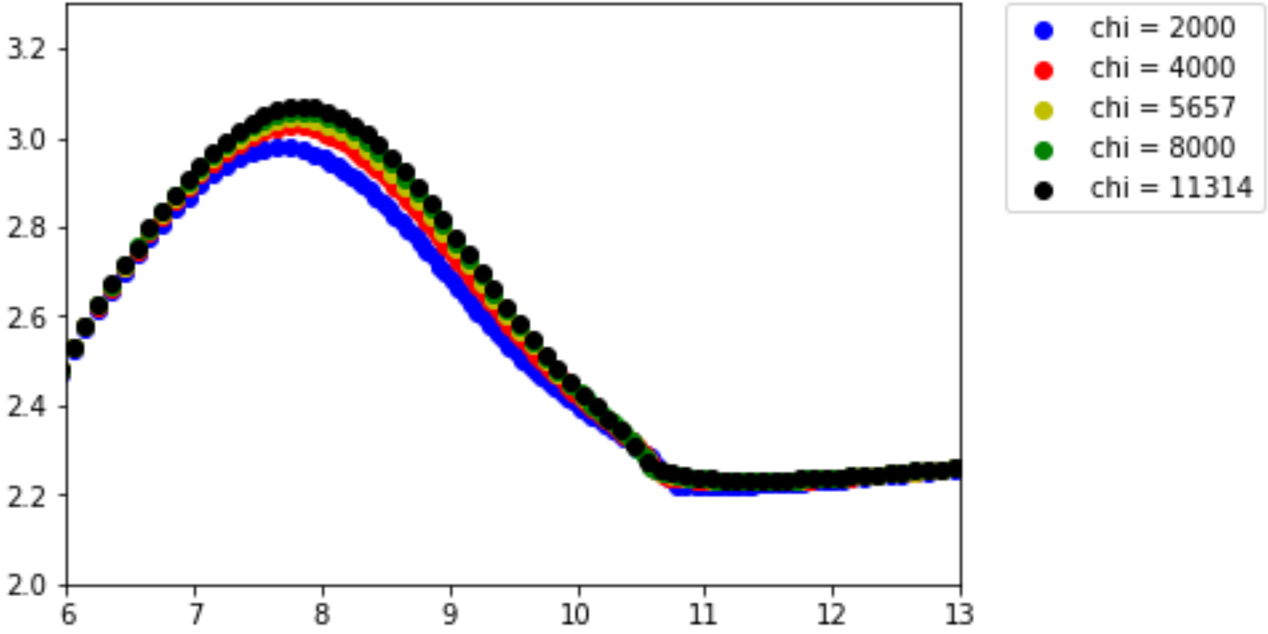
U/t = 0.01



Take it with a grain of salt for now!

Extra slides: nature of phase transitions

$(U/t)^2 \times dE/d(U/t)$



Some notes on experiments:

- T'/t = 1.06, U=8.2 for the first experiment
- EtMe3SbTPd(dmit)2U2 has J=220-250K => 10% anisotropy
- Nakamura paper, ab initio, says that three triangle hoppings are -55, -55, 44, in meV, and a second neighbor hopping of 7 meV, and U~0.85 eV, so U/t ~ 12-15

- This ``topological degeneracy'' arises because the CSL contains a fractionalized excitation, the semionic spinon, which carries spin-1/2 but no charge; if a pair of these semions are separated out to the ends of the cylinder at $\pm \infty$, the process toggles between the two ground states
- Wen **Phys. Rev. B 40, 7387**