Computing Entanglement In Quantum Matter

A new tool for the study of strongly-correlated systems

Roger Melko

University of Waterloo

NSERC CRSNG

SHARCNET™

Ontario
MINISTRY OF RESEARCH AND INNOVATION

IQC Quantum Computing

COLLABORATORS

Ann B Kallin

Ivan Gonzalez

Matt Hastings

Rajiv Singh

Sergei Isakov

Valence Bond and von Neumann Entanglement Entropy in Heisenberg Ladders
Phys. Rev. Lett., 103, 117203 (2009)

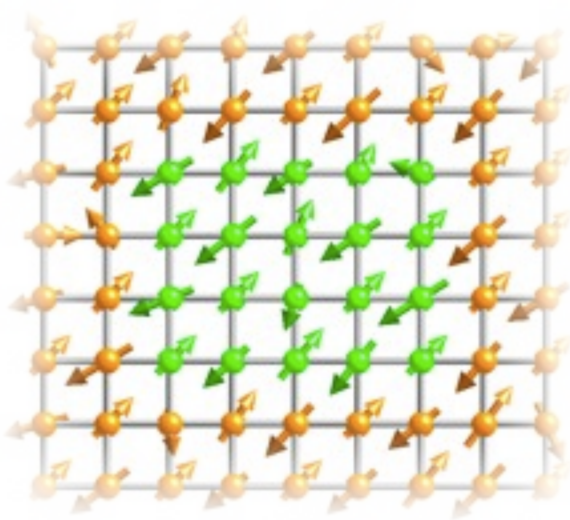
Measuring Renyi Entanglement Entropy with Quantum Monte Carlo
Phys. Rev. Lett. 104, 157201 (2010)

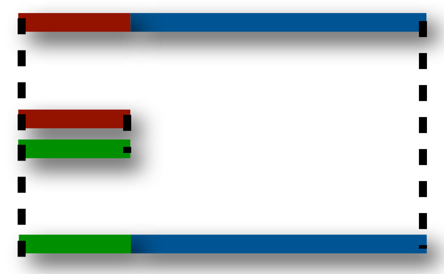
Finite-size scaling of mutual information in Monte Carlo simulations: Application to the spin-1/2 XXZ model
Phys. Rev. B, 82, 180504 (2010)

Finite temperature critical behavior of Mutual Information
Phys. Rev. Lett. 106, 135701 (2011)

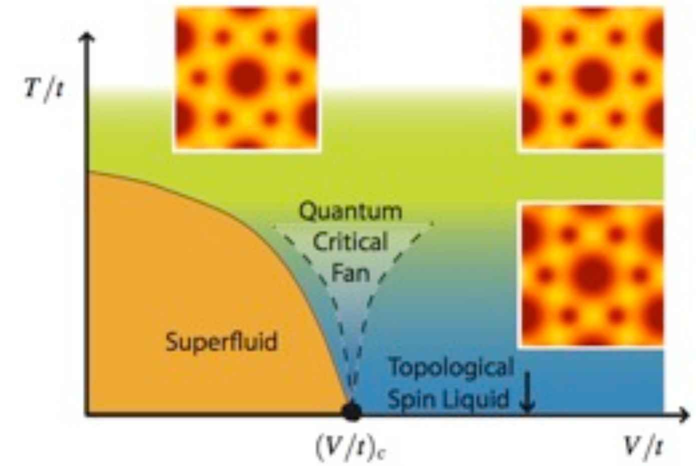
Topological Entanglement Entropy of a Bose-Hubbard Spin Liquid
arXiv:1102.1721 (Nature Physics in press)

- **Entanglement Entropy:**
  - a resource in condensed matter physics
  - accessible in scalable simulation methods (QMC)





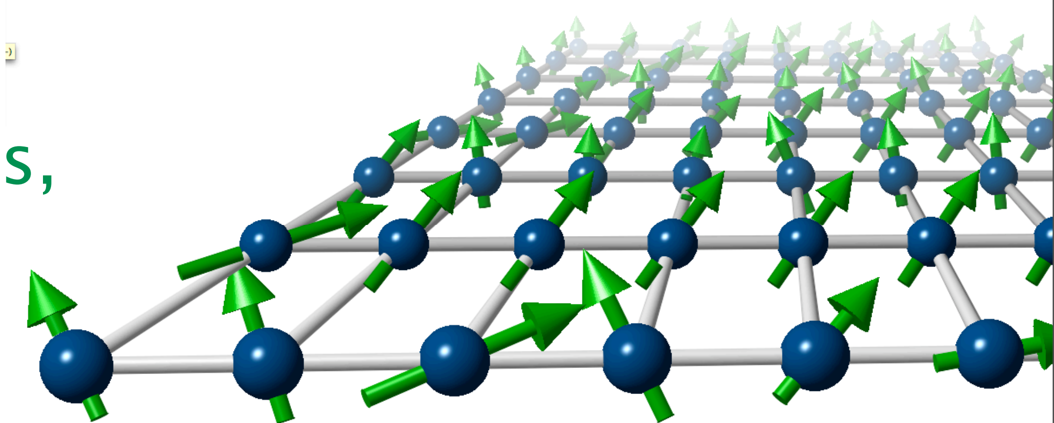
- **Topological entanglement entropy in a quantum Spin Liquid**



1) Identify models and materials with interesting, exotic or novel phenomena

Strongly-correlated quantum systems:

superconductivity, supersolids, spin liquids, fractionalization, spin-charge separation, exotic quantum criticality

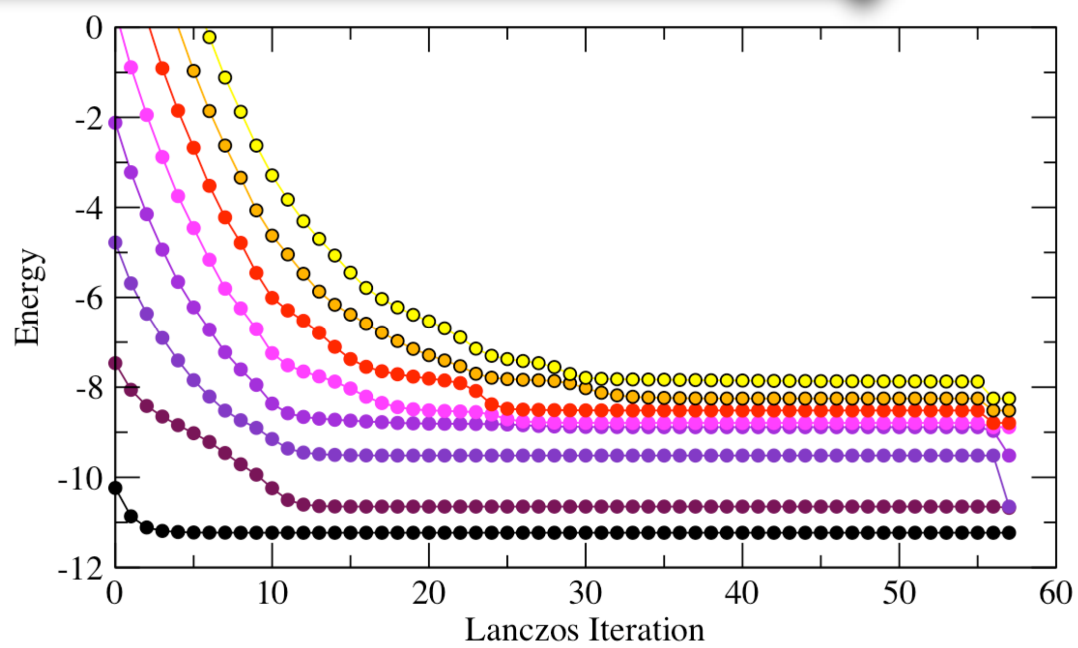


2) Develop tools to explore these systems

- Theoretical and numerical methods
- New measurements, observables, and estimators

- Lanczos exact diagonalization

2^N



- Density Matrix Renormalization Group

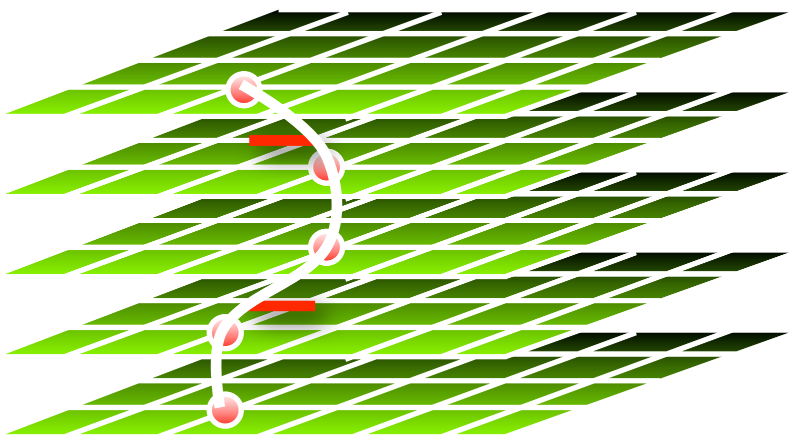
d=1 only

- Quantum Monte Carlo

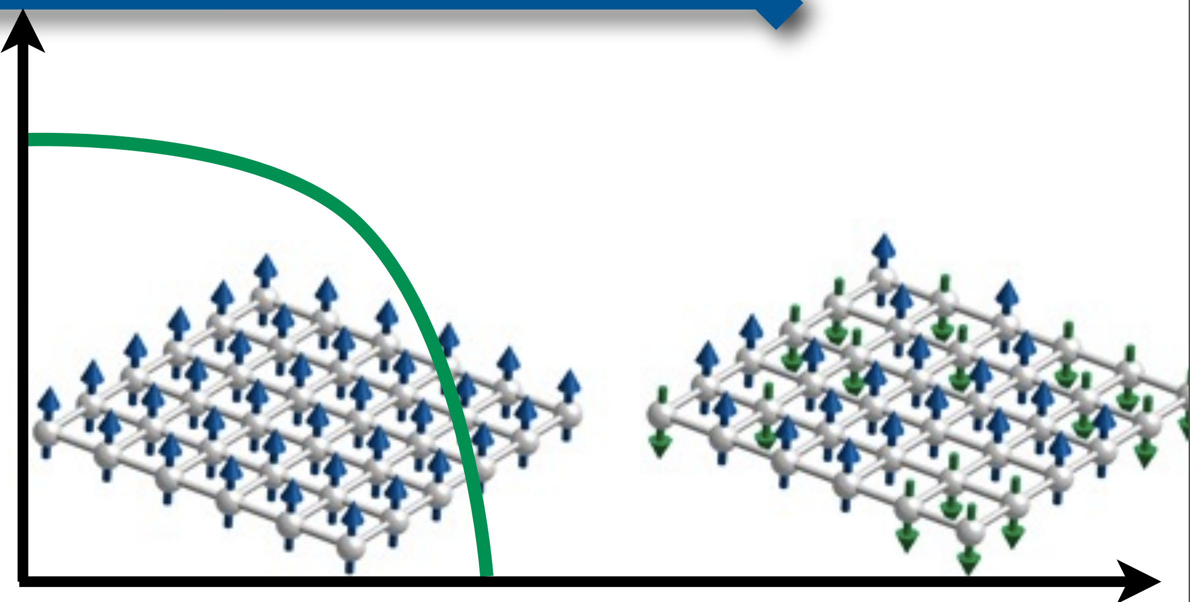
$\mathcal{O}(N)$

$N \approx 10^7 - 10^9$

spin 1/2 particles



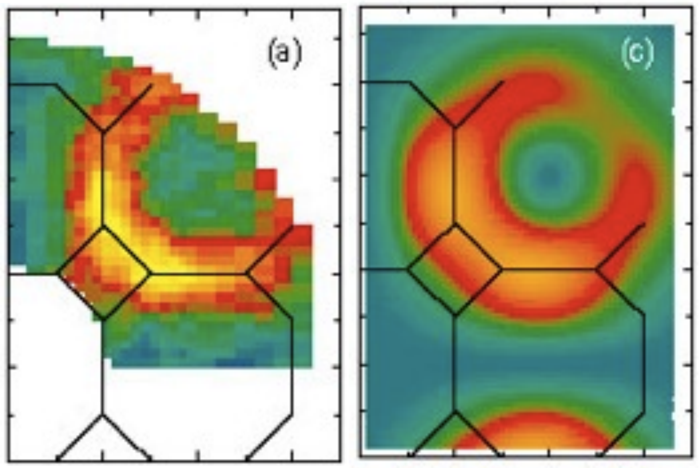
Traditional CMT tools



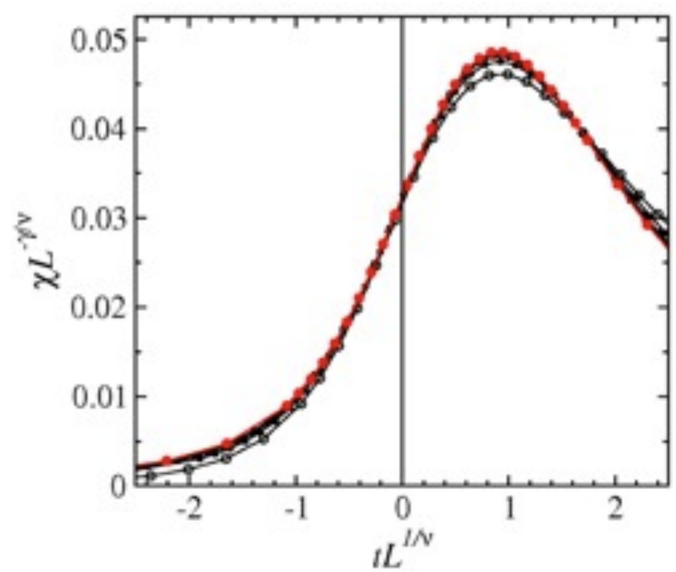
- Order Parameter
  (symmetry breaking)

- Correlation functions

$$\langle S_i^z S_j^z \rangle$$

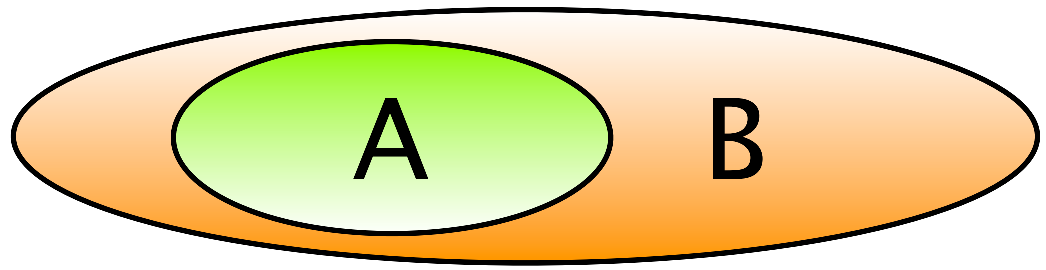


- Bulk properties C_v χ



- **Entanglement?** $|\Psi\rangle = \frac{1}{\sqrt{2}}$ (|↑↓⟩−|↓↑⟩)

von Neumann entanglement entropy



$$\rho_A = \mathrm{Tr}_B(\rho)$$

$$S_1(\rho_A) = -\mathrm{Tr}(\rho_A \ln \rho_A)$$

$$\rho = \sum_i \lambda_i |\Psi_i\rangle\langle\Psi_i|$$

- Quantifies the entanglement between subregions A and B
- Does not depend on any choice of observable
- $S_1(\rho_A) = S_1(\rho_B)$
- $S_1(\rho_A) = 0$ if region A and B are unentangled

$\uparrow = A$ (green)

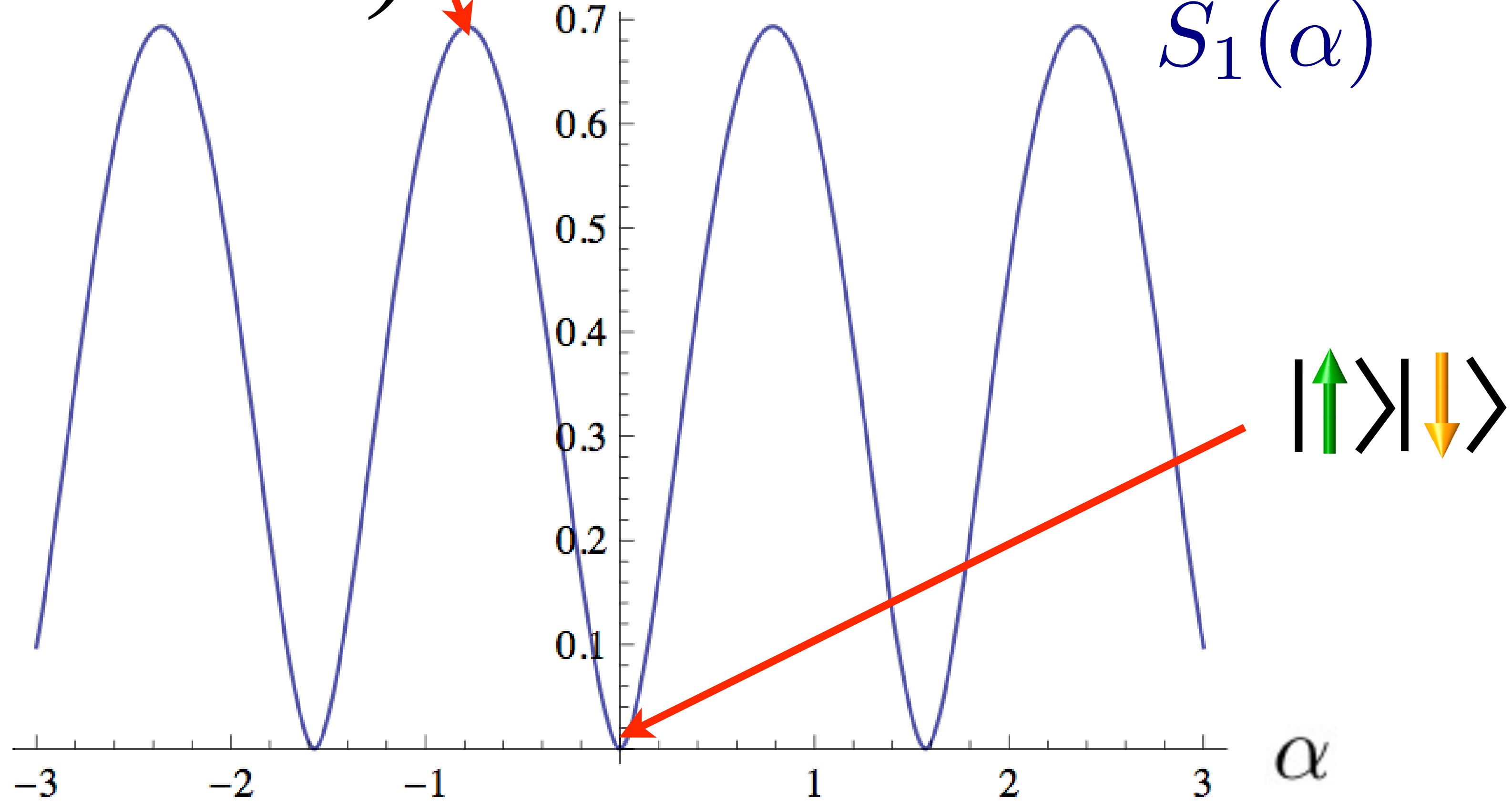
$\uparrow = B$ (orange)

$$|\Psi\rangle = \cos\alpha \, |\uparrow\rangle|\downarrow\rangle + \sin\alpha \, |\downarrow\rangle|\uparrow\rangle$$

$$\rho_A = \begin{pmatrix} \cos^2\alpha & 0 \\ 0 & \sin^2\alpha \end{pmatrix}$$

$$S_1 = -\cos^2\alpha \ln\cos^2\alpha - \sin^2\alpha \ln\sin^2\alpha$$

$$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$



Renyi Entropies

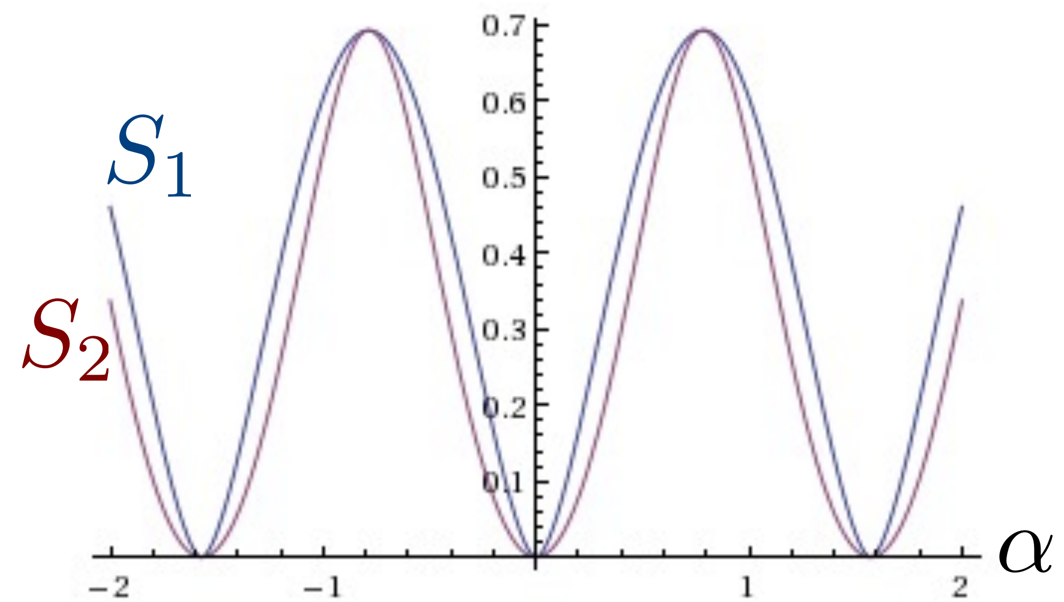
$$S_n(\rho_A) = \frac{1}{1-n} \ln \left[\mathrm{Tr}\left(\rho_A^n \right) \right]$$

$$S_1(\rho_A) = -\mathrm{Tr}(\rho_A \ln \rho_A)$$

$$S_2(\rho_A) = -\ln \left[\mathrm{Tr}(\rho_A^2) \right]$$

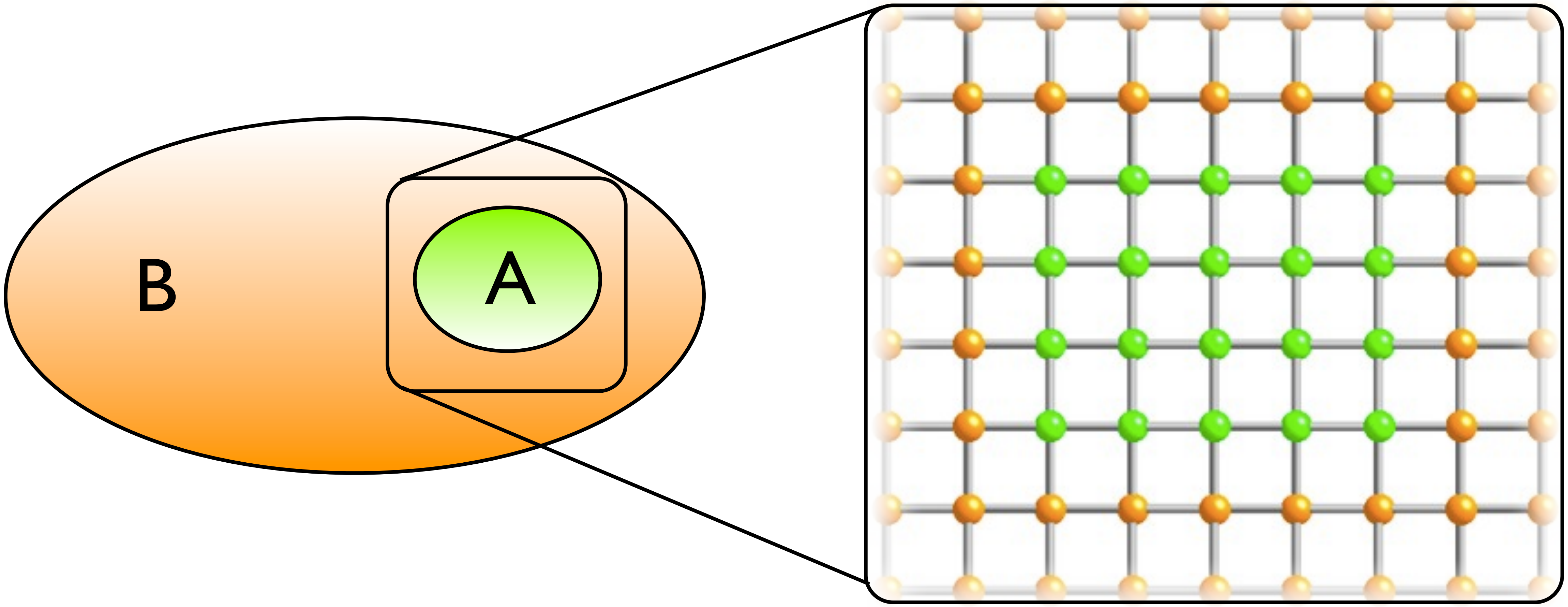
- **Gives a Lower bound**

$$S_n \geq S_m \quad \text{when} \quad n < m$$



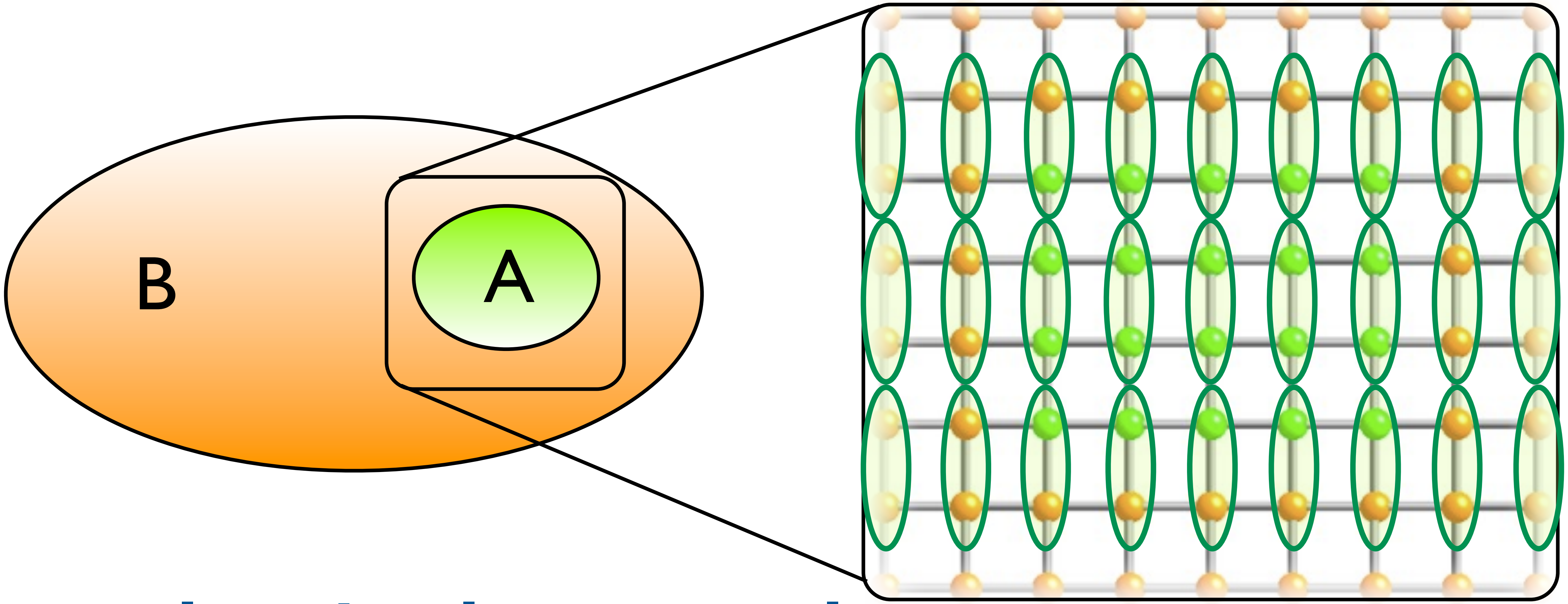
QUESTION:

- For many interacting quantum spins, how does the entanglement entropy depend on the size of the region A?

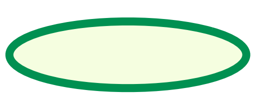


1) S depends on the “volume” of region A

2) S depends on the boundary size



Example: singlet crystal (valence bond solid)

 $= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

$S_1 \sim \ell$ **"area" or boundary law**

M. Srednicki, Phys. Rev. Lett. 71, 666 (1993)

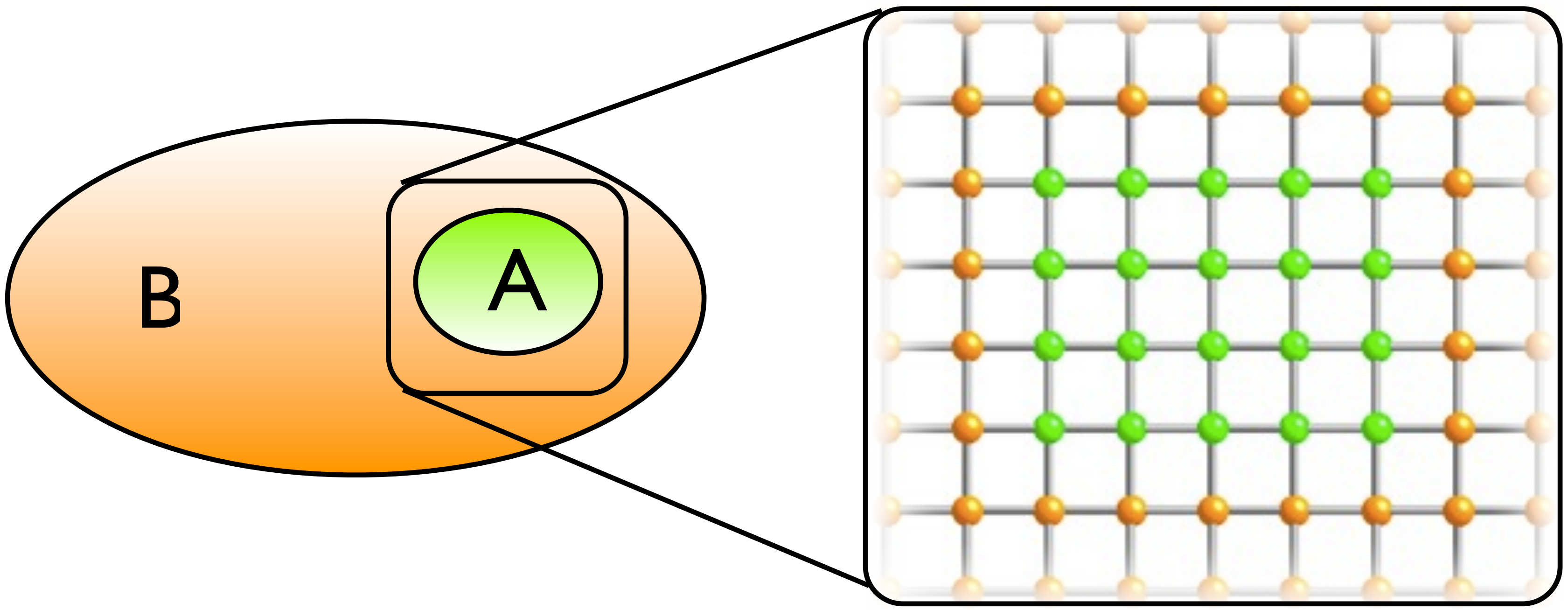
the Area Law in CM

Most "well behaved" quantum condensed matter groundstate wavefunctions are **expected** to obey an area law.

- Gapped wavefunctions
- Hamiltonians with local interactions

Implied heuristically by the existence of a characteristic length scale and/or localized correlations. Wolf et al. Phys. Rev. Lett. 100, 070502 (2008)

$$S_1 \sim \ell$$



Universal corrections

- **Subleading corrections** are believed to harbour new universal physics. These can be used as a resource to diagnose new phases and phase transitions in condensed matter systems.

gapped	$S_1 = a\ell + \cdots$
gapped spin liquid	$S_1 = a\ell - \gamma + \cdots$
gapless/critical	$S_1 = a\ell + c_1 \ln(\ell) + \cdots$
fermi surface	$S_1 = c\ell \ln(\ell) + \cdots$

- We have no proof and no exact calculations in d>1, apart from a few non-interacting systems.

1D example

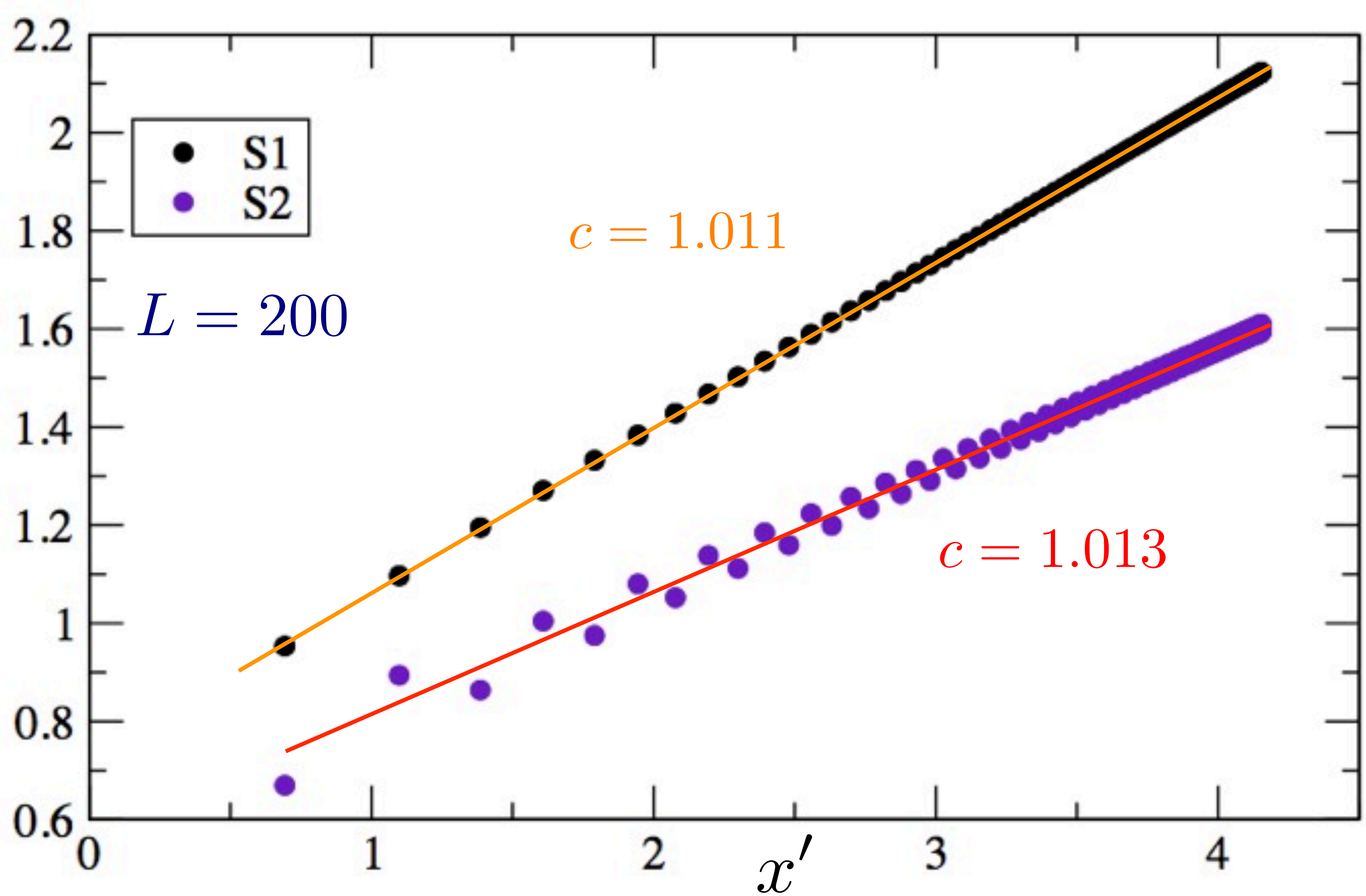
$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Conformal Field Theory:

$$S_n(x) = \frac{c}{6}\left(1 + \frac{1}{n}\right) \cdot \ln\left[x'\right] + \cdots$$

$$x' = \frac{L}{\pi} \sin\left(\frac{\pi x}{L}\right)$$

c=1: central charge of CFT

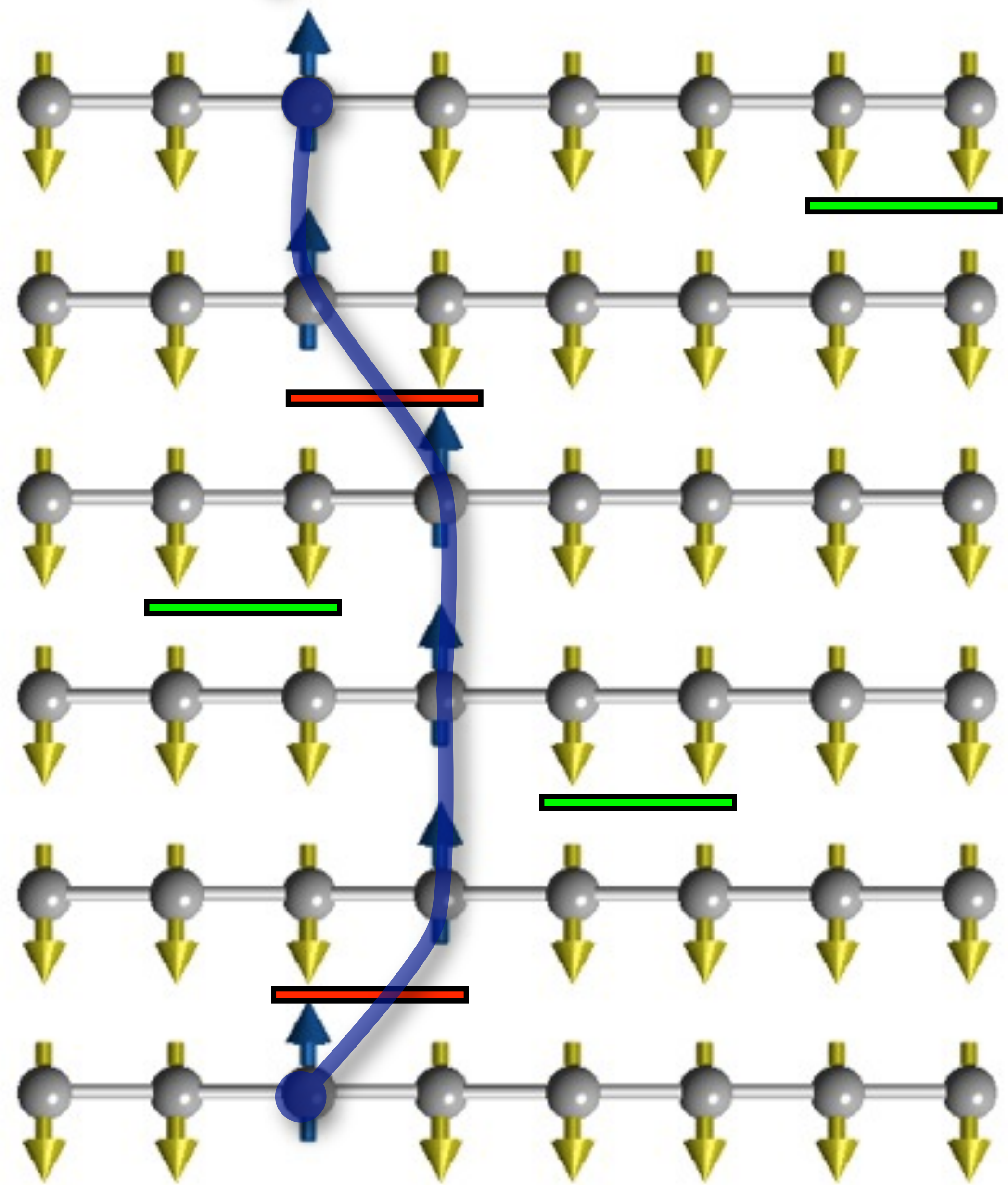


Holzhey, Larsen, Wilczek
Nucl. Phys. B 424 443 (1994)

Calabrese and Cardy,
J. Stat. Mech: Theory Exp. P06002 (2004)

Capponi, Alet, Mambrini,
arXiv:1011.6530

Quantum Monte Carlo



- A scalable simulation method applicable to any dimension

- Finite and zero-temperature methods available

$$Z = \sum_\alpha \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle \quad = \sum_\alpha \sum_n \frac{(-\beta)^n}{n!} \langle \alpha | H^n | \alpha \rangle$$

$$= \sum_\alpha \sum_n \sum_{S_n} \frac{(-\beta)^n}{n!} \langle \alpha | \prod_{i=1}^{n} H_{b_i} | \alpha \rangle$$

- Simulations don’t have access to the wavefunction

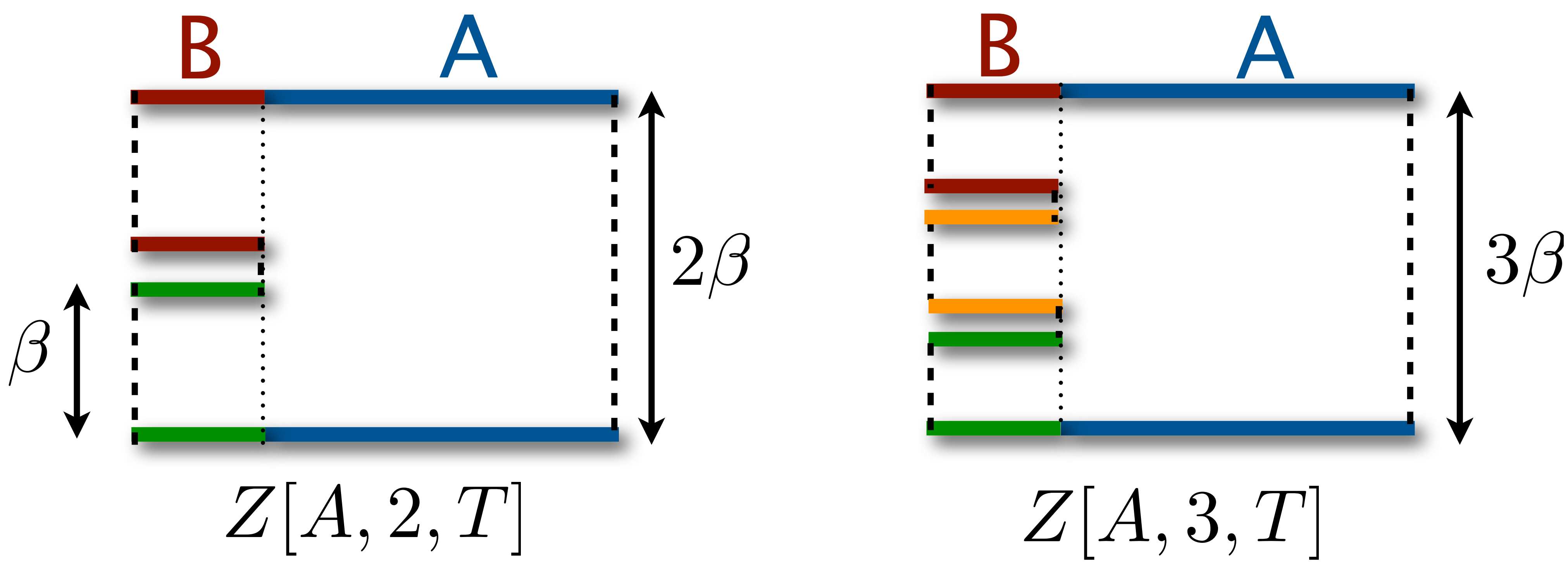
- The “sign problem” inhibits the simulation of frustrated spins or fermions

Replica Trick

Calabrese and Cardy, J. Stat. Mech. 0406, P002 (2004).
Fradkin and Moore, Phys. Rev. Lett. 97, 050404 (2006)
Nakagawa, Nakamura, Motoki, and Zaharov, arXiv:0911.2596
Buividovich and Polikarpov, Nucl. Phys. B, 802, 458 (2008)
M. A. Metlitski, et.al, Phys.Rev. B 80, 115122 (2009).

$$S_n(\rho_A) = \frac{1}{1-n} \ln \left[\mathrm{Tr}\left(\rho_A^n\right) \right] = \frac{1}{1-n} \ln \frac{Z[A,n,T]}{Z(T)^n}$$

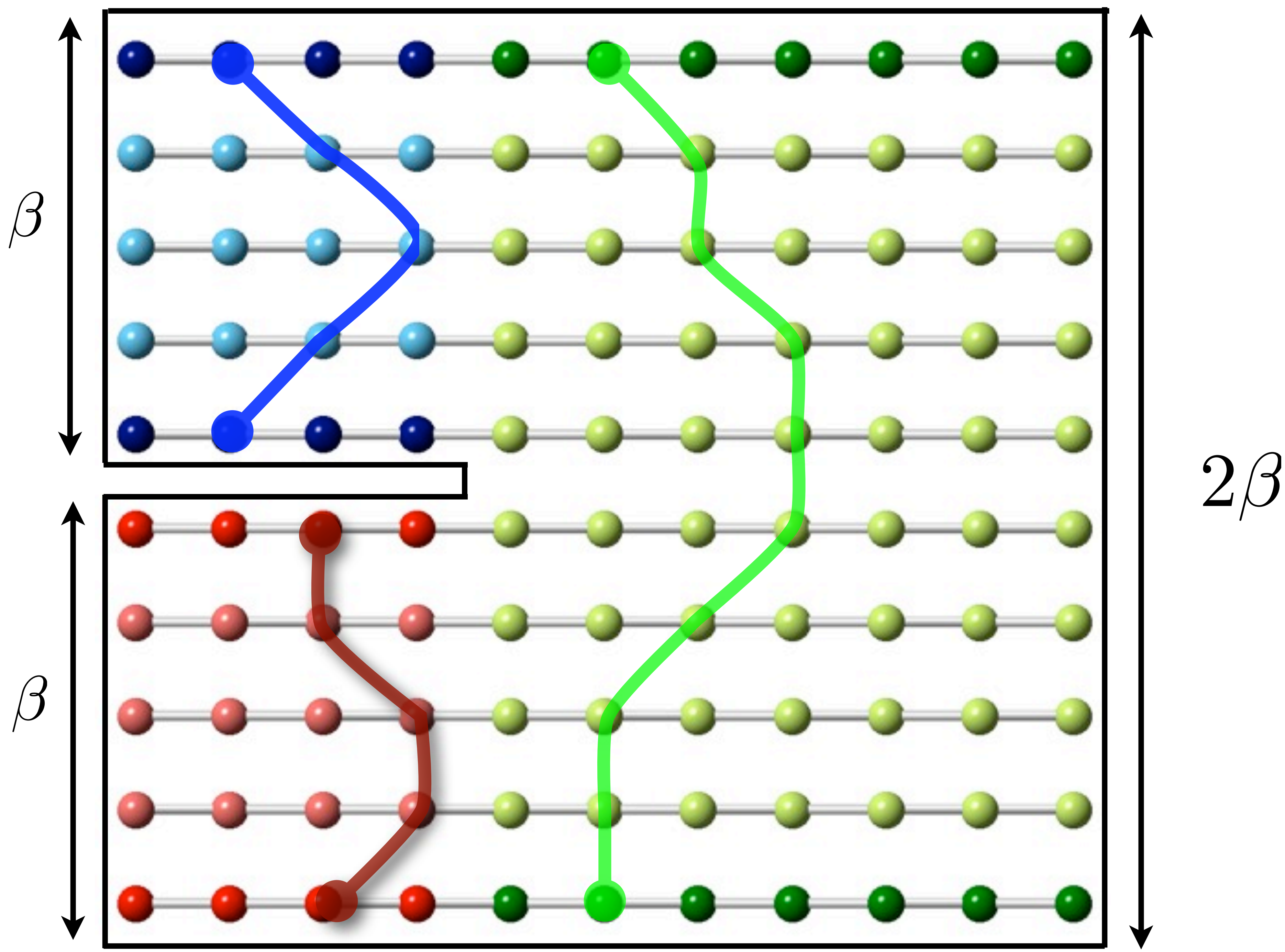
where $Z[A,n,T]$ is the partition function of the system with special topology - the n-sheeted Riemann surface.



QMC SIMULATION CELL

Phys. Rev. B, 82, 180504 (2010)

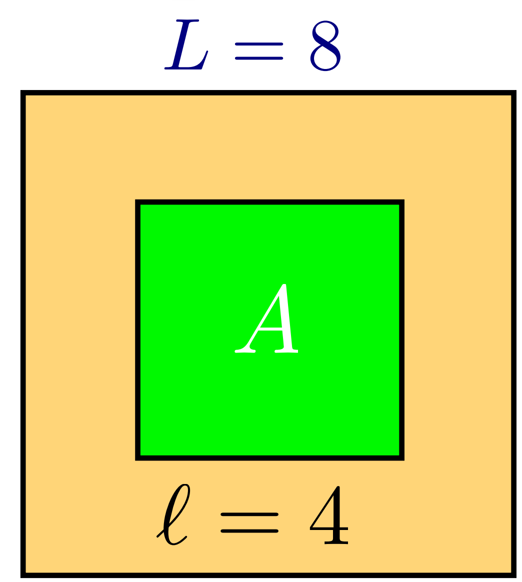
$$Z[A, 2, T]$$



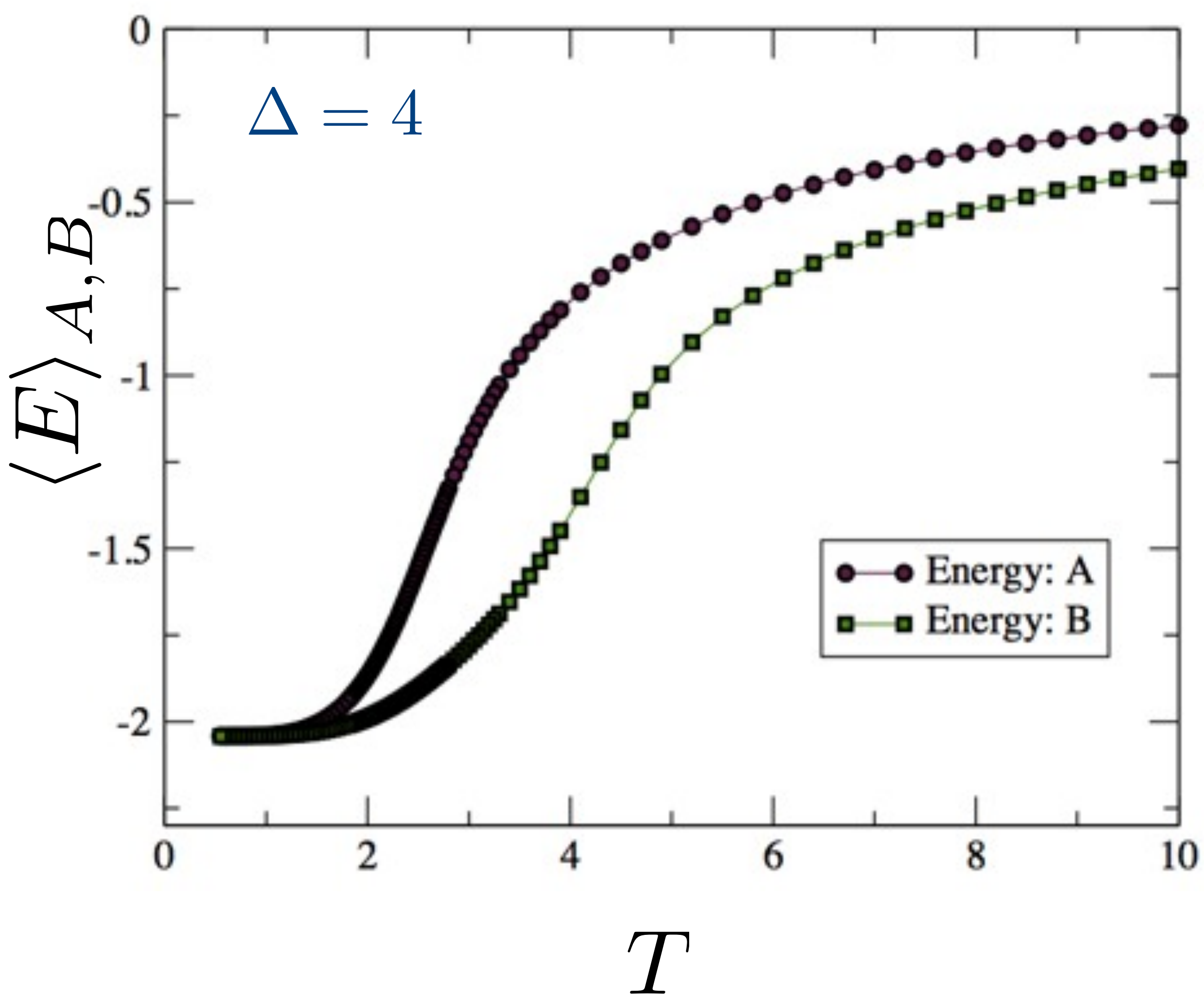
Thermodynamic Integration

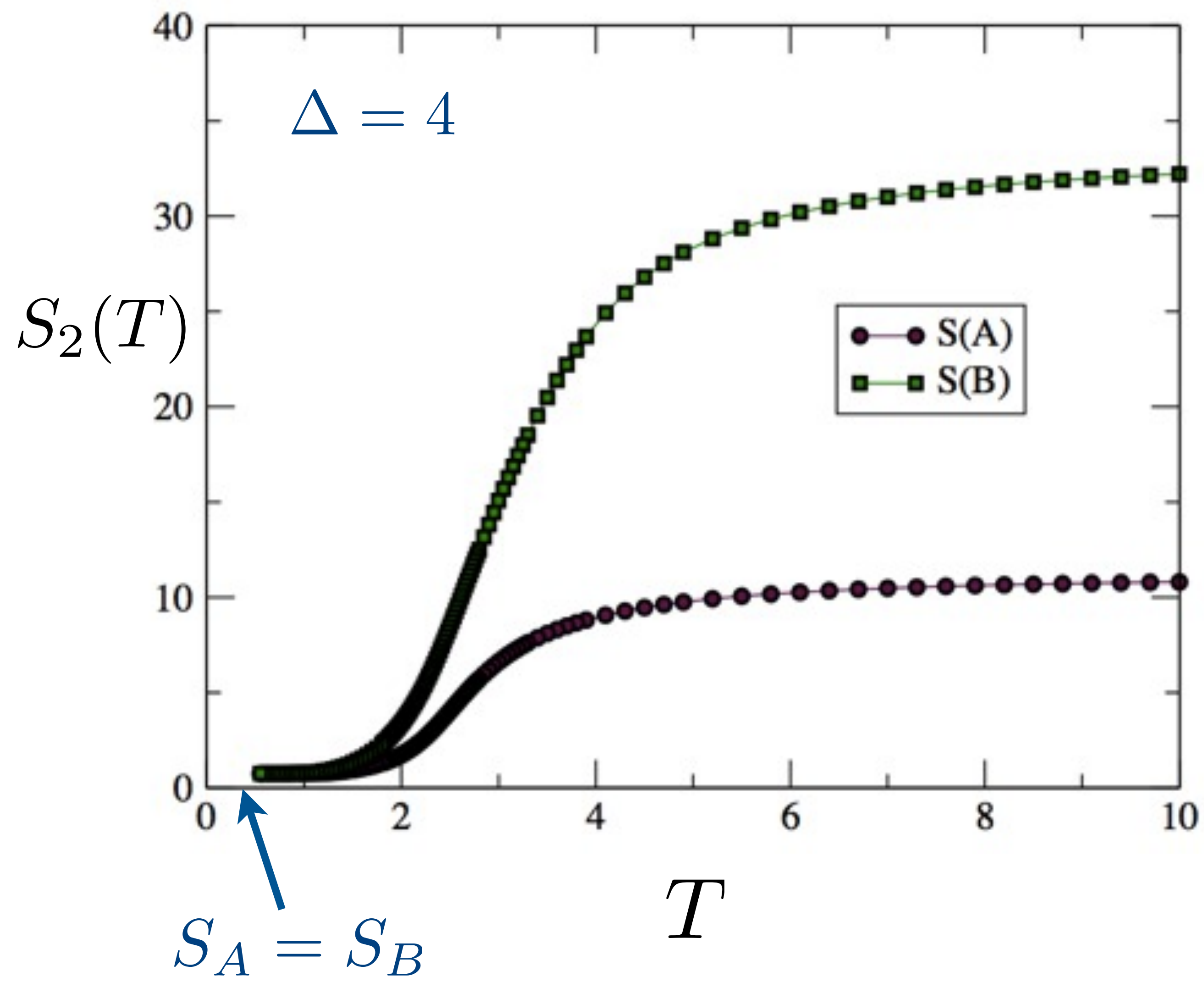
$$S_2 = -\ln \mathrm{Tr}(\rho_A^2) = -\ln \left\{ \frac{Z[A,2,\beta]}{Z(\beta)^2} \right\} = -\ln Z[A,2,\beta] + 2\ln Z(\beta)$$

$$= -S_A(\beta=0) + \int_0^\beta \langle E \rangle_A d\beta + 2S_0(\beta=0) - 2\int_0^\beta \langle E \rangle_0 d\beta$$



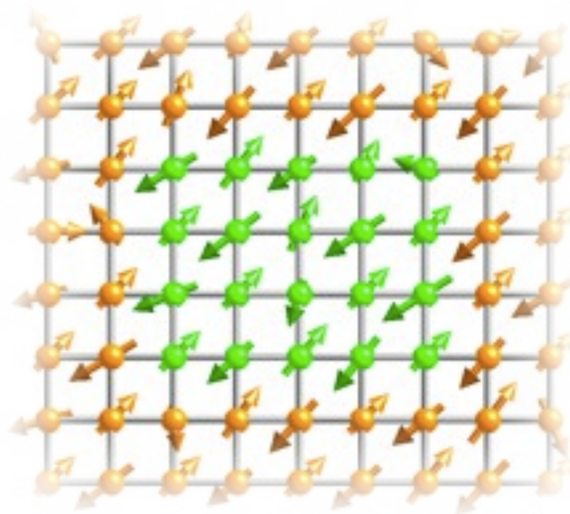
XXZ model $\quad H = \sum_{\langle ij \rangle} (\Delta S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y)$

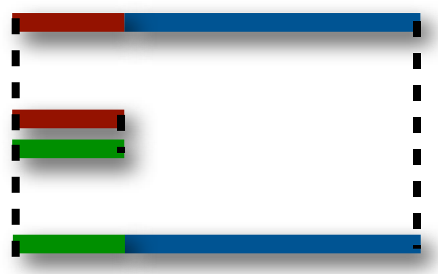




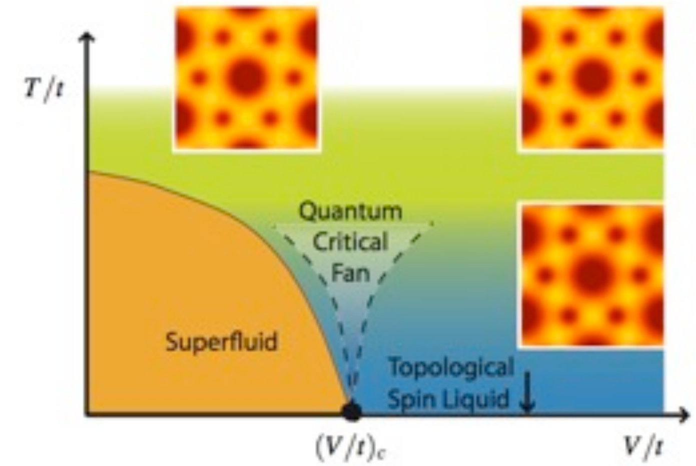
Outline

- **Entanglement Entropy:**
  - a resource in condensed matter physics
  - accessible in scalable simulation methods (QMC)





- **Topological entanglement entropy in a quantum Spin Liquid**



T=0 paramagnetic states ("spin liquids") have no local order parameters: it makes them notoriously difficult to find

Leon Balents Nature 464, 11 (2010)

Table 1 | Some experimental materials studied in the search for QSLs

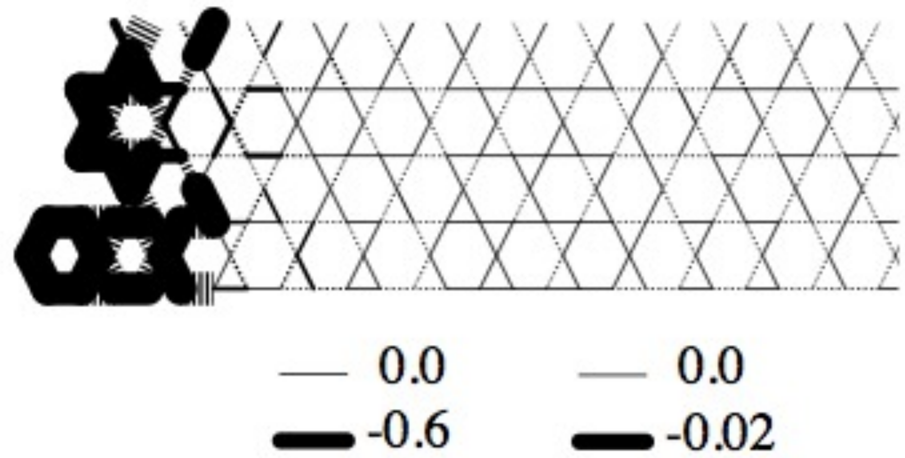
Material	Lattice	*S*	Status or explanation
κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$	Triangular†	½	Possible QSL
$EtMe_3Sb[Pd(dmit)_2]_2$	Triangular†	½	Possible QSL
$Cu_3V_2O_7(OH)_2 \cdot 2H_2O$ (volborthite)	Kagomé†	½	Magnetic
$ZnCu_3(OH)_6Cl_2$ (herbertsmithite)	Kagomé	½	Possible QSL
$BaCu_3V_2O_8(OH)_2$ (vesignieite)	Kagomé†	½	Possible QSL
$Na_4Ir_3O_8$	Hyperkagomé	½	Possible QSL
Cs_2CuCl_4	Triangular†	½	Dimensional reduction
$FeSc_2S_4$	Diamond	2	Quantum criticality

- The precise ingredients that are needed to make spin liquid states in microscopic models are unknown

- Frustration is a major player

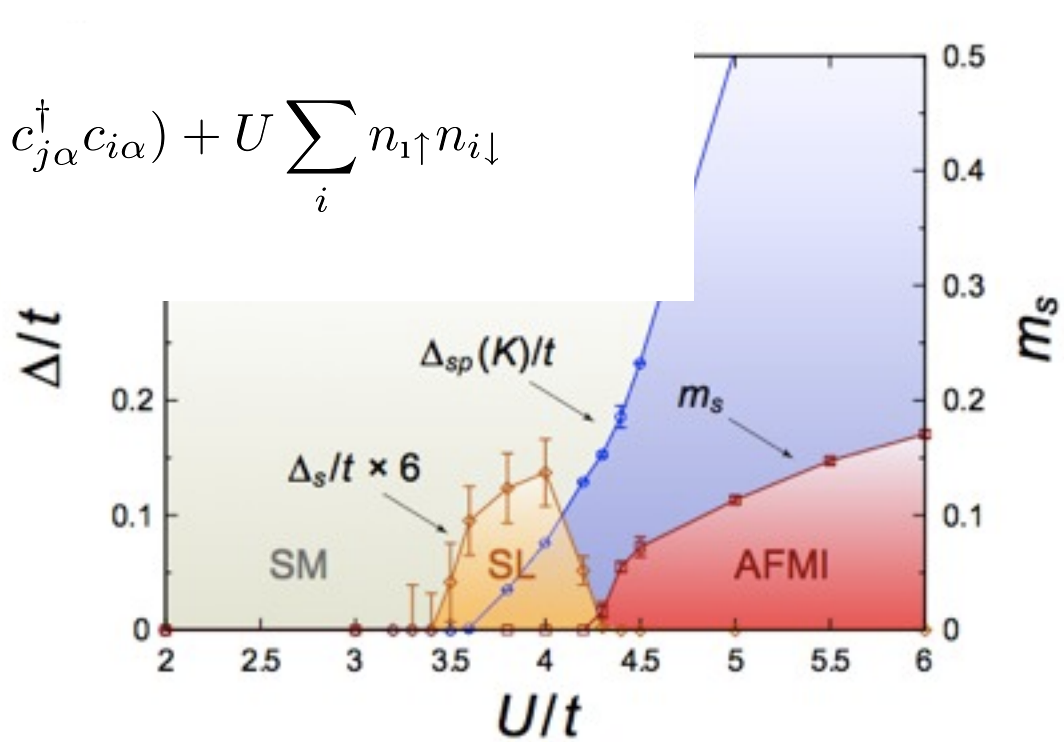
  Yan, Huse, White, **Science, 332 1173 (2011)**

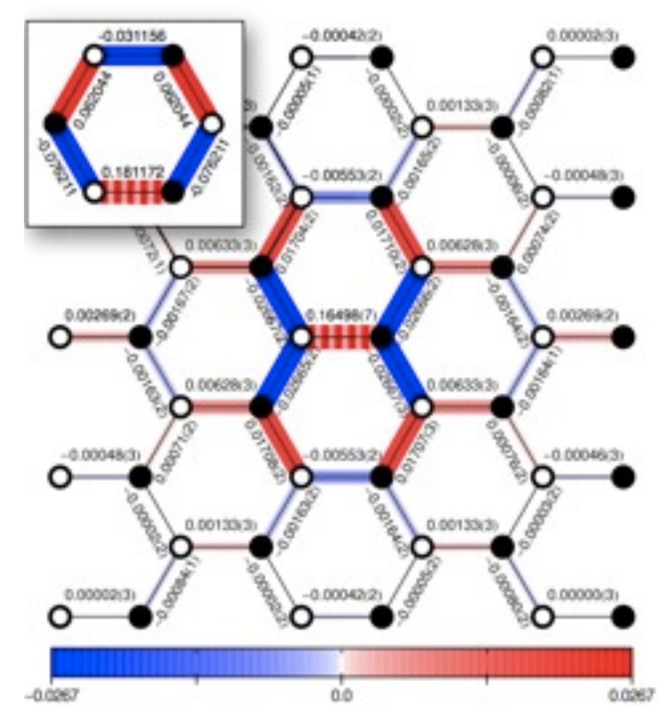
$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



- Or is it? Meng et. al. **Nature 464, 847 (2010)**

$$H = -t \sum_{\langle i,j \rangle,\alpha} (c^\dagger_{i\alpha} c_{j\alpha+} + c^\dagger_{j\alpha} c_{i\alpha}) + U \sum_i n_{1\uparrow} n_{i\downarrow}$$

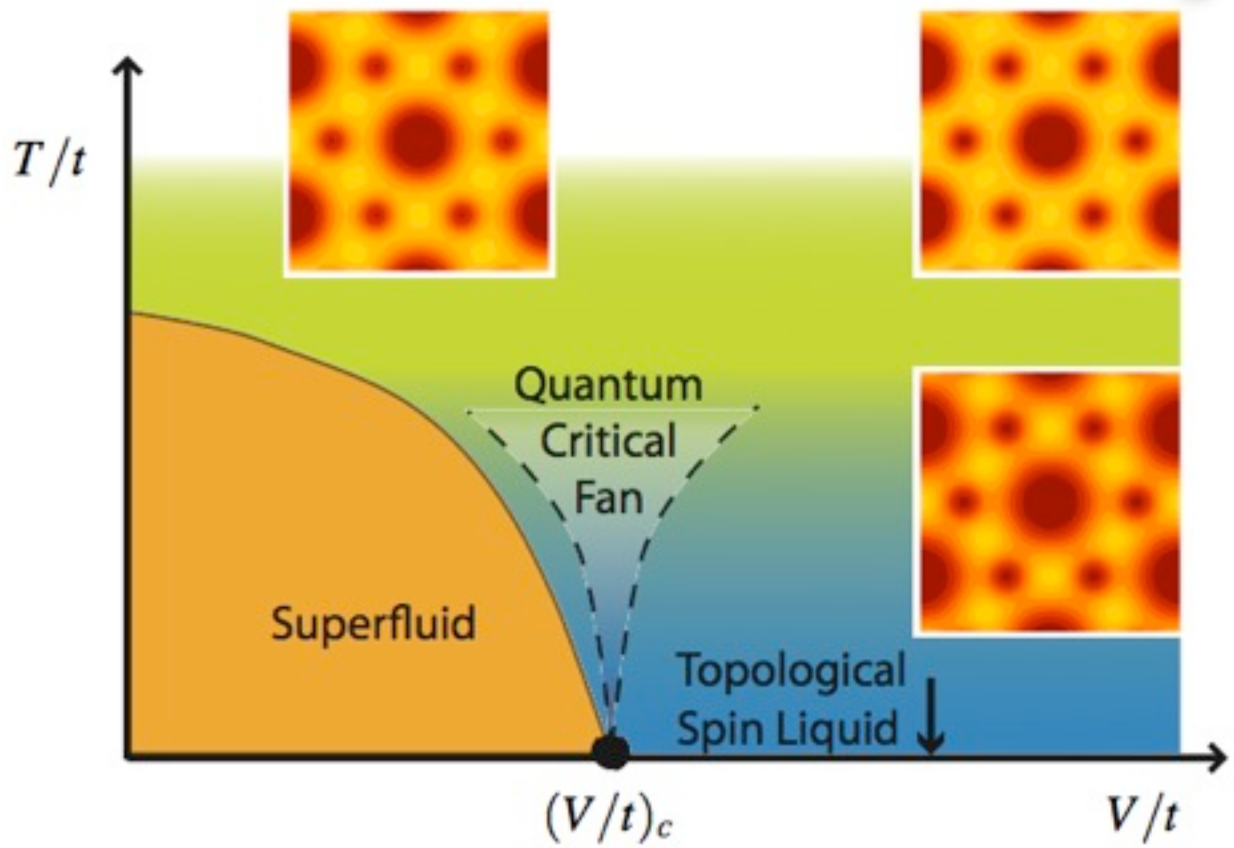




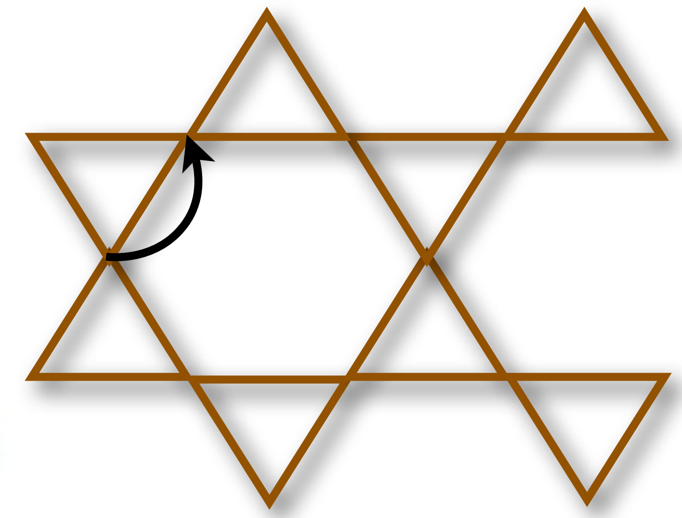
BFG Hamiltonians

Balents, Fisher, Girvin, Phys. Rev. B, 65 224412

Isakov, Hastings, RGM arXiv:1102.1721



$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

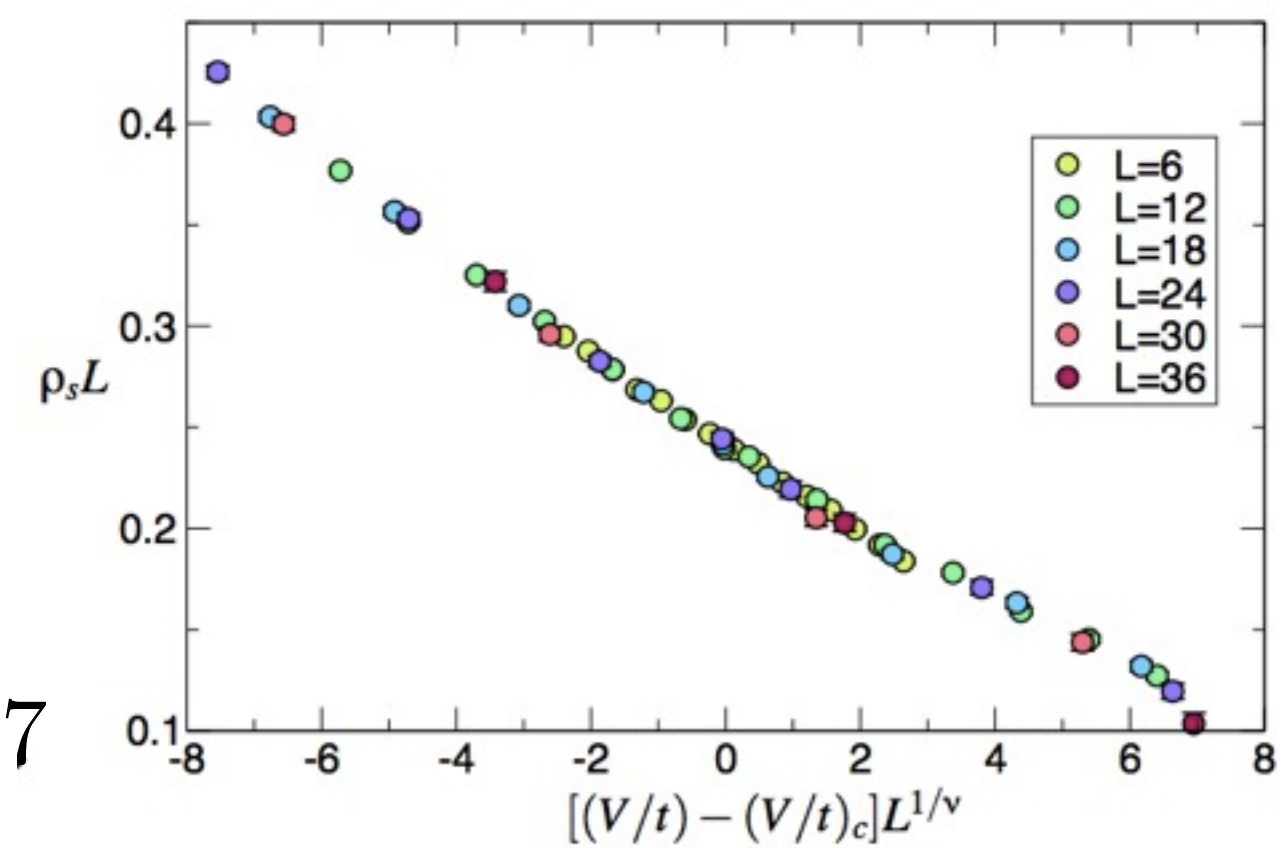


$$\mathcal{H}_0 = V \sum_{\hexagon} (S^z_{\hexagon})^2$$

$$\mathcal{H}_1 = -t \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_j^+ S_i^-)$$

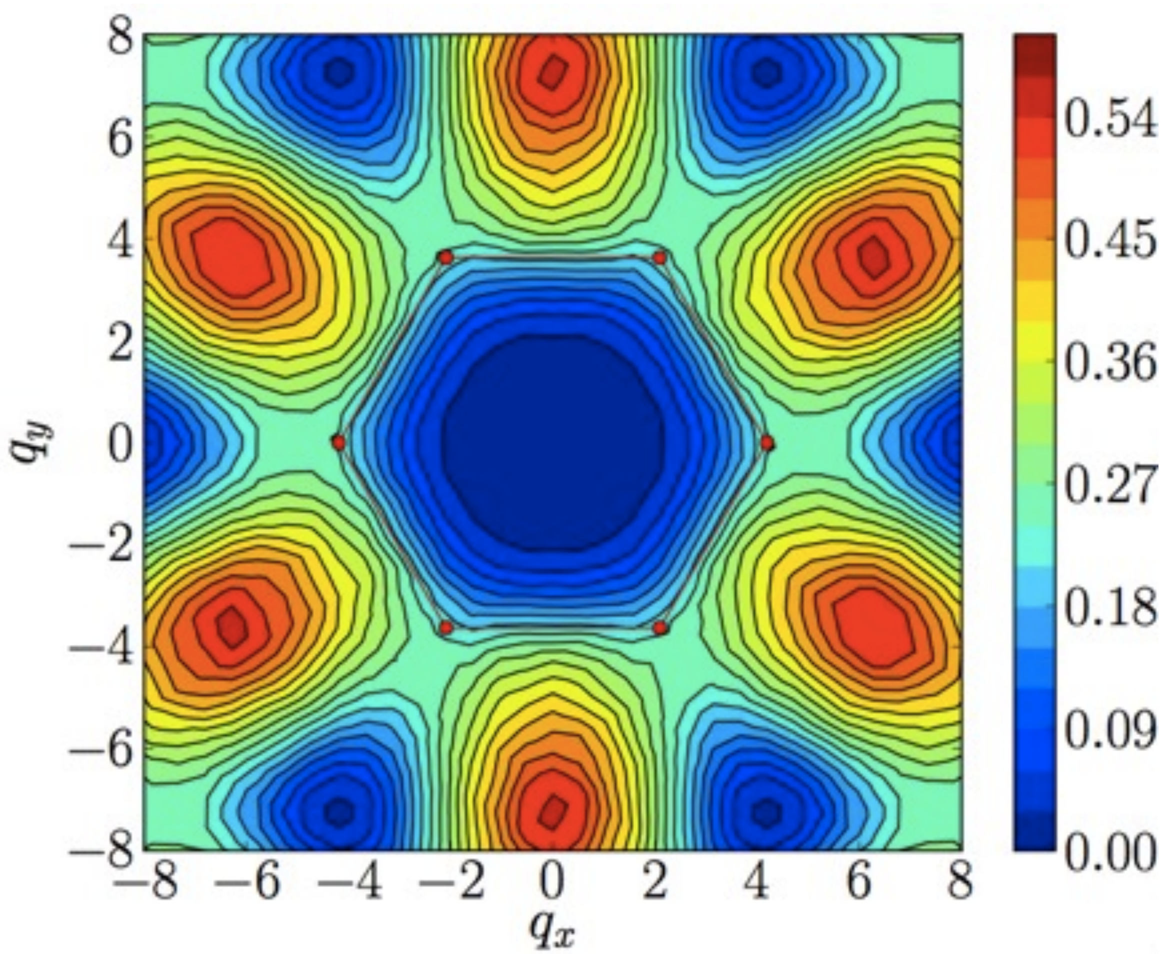
- QCP is in the 2D XY universality class

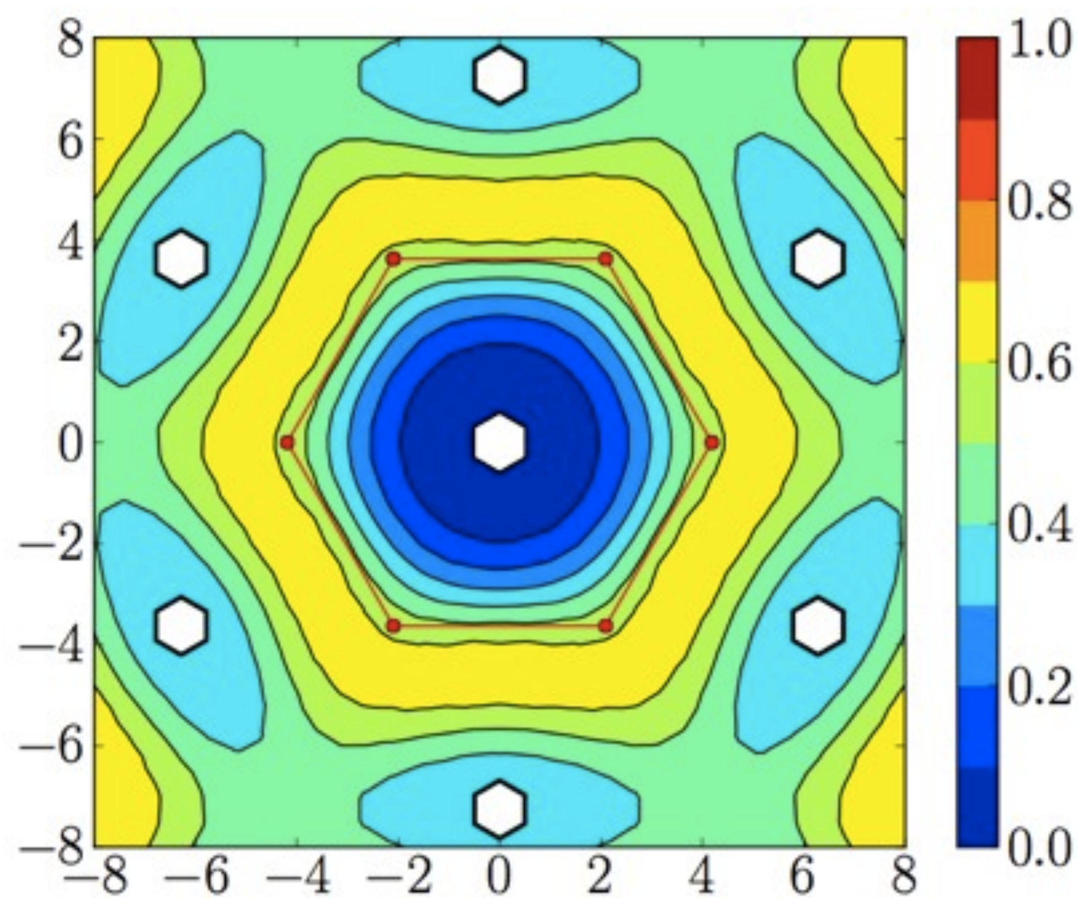
$$\nu = 0.6717$$



Spin Liquids: correlation functions

- The standard method of “detecting” spin liquids is negative signatures of ordering in two-point correlations functions

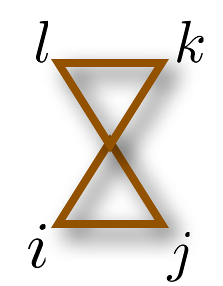




$$S_s(q_x, q_y) = \frac{1}{N} \sum_{k,l} e^{i(\mathbf{r}_k - \mathbf{r}_l).\mathbf{q}} \langle S_k^z S_l^z \rangle$$

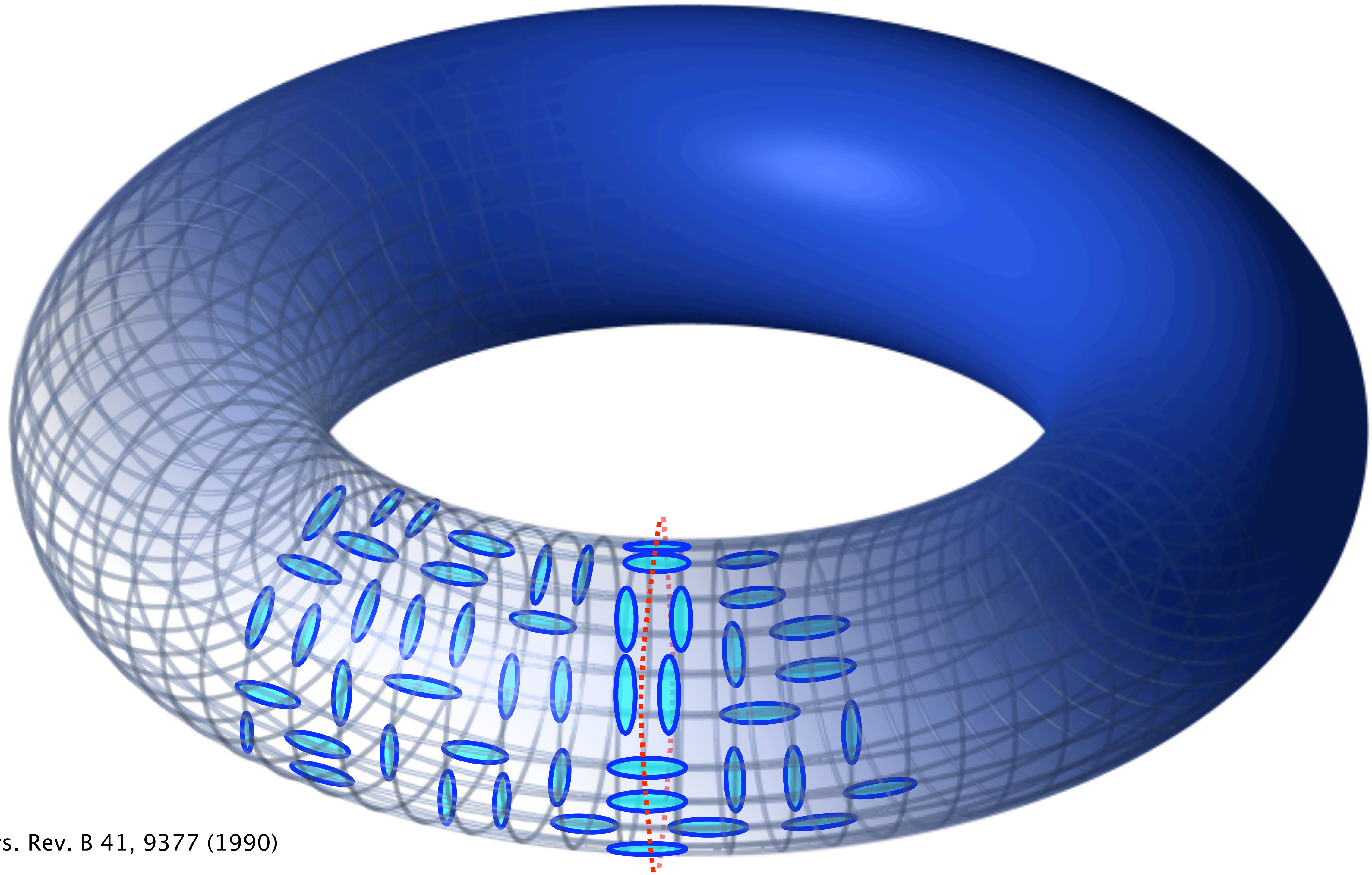
$$S_p(q_x, q_y) = \frac{1}{N} \sum_{a,b} e^{i(\mathbf{r}_a - \mathbf{r}_b).\mathbf{q}} \langle P_a P_b \rangle$$

$$P_a = (S_i^+ S_j^- S_k^+ S_l^- + \text{h.c.})$$



Z2 SPIN LIQUID

• Gapped spin liquids have a **topological order** (or degeneracy) in the ground state wavefunction

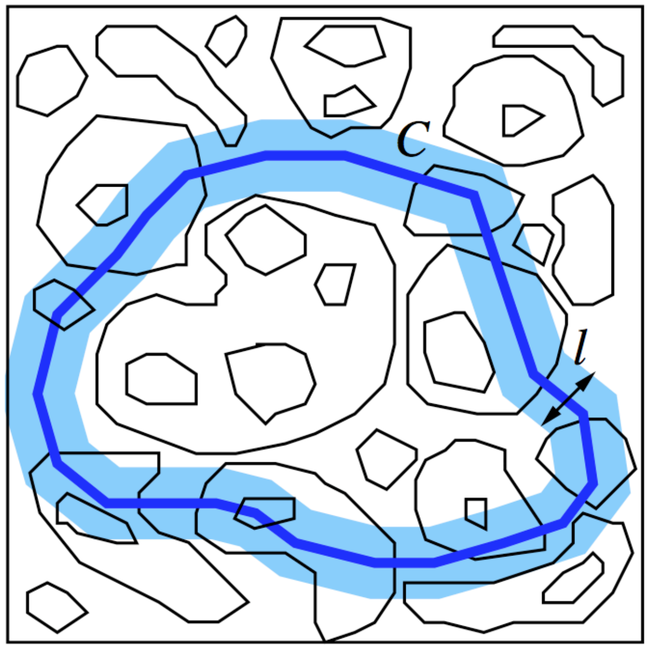


Wen, Niu, Phys. Rev. B 41, 9377 (1990)

Entanglement Entropy

Hamma, Ionicioiu, Zanardi - Phys. Lett. A 337, 22 (2005)
- Phys. Rev. A 71, 022315 (2005)
Kitaev and Preskill - Phys. Rev. Lett. 96, 110404 (2006)
Levin and Wen, - Phys. Rev. Lett. 96, 110405 (2006)

- Topological order is manifest as a universal correction in the entanglement entropy



$$S_1 = a\ell - \gamma + \cdots$$

Flammia, Hamma, Huges, Wen,
Phys. Rev. Lett. 103, 261601 (2009)

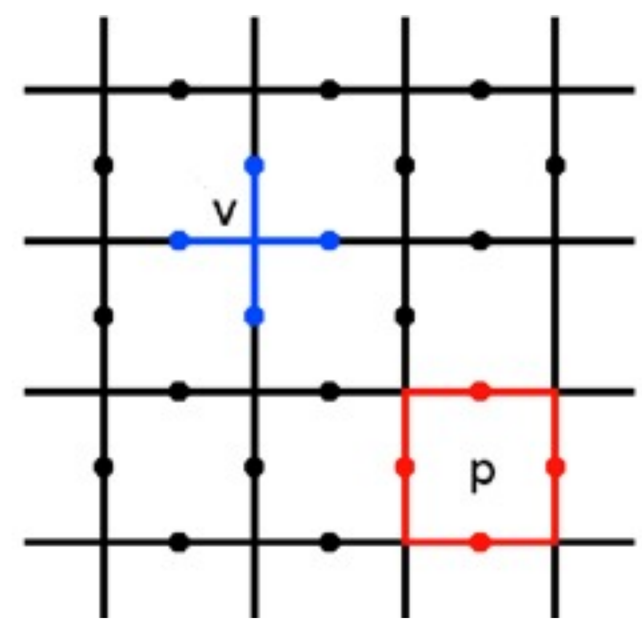
for a Z2 spin liquid $\gamma = \ln(2)$

from the description of the groundstate as a “loop gas”

exhaustively studied as the groundstate wavefunction of Kitaev’s Toric Code

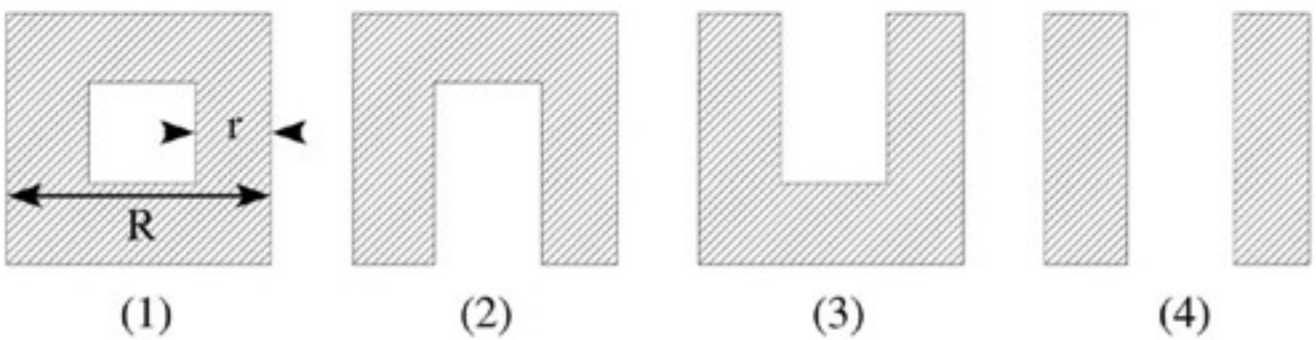
$$H = -\lambda_B \sum_p B_p - \lambda_A \sum_v A_v$$

$$B_p = \prod_{i \in p} \sigma_i^z \qquad A_v = \prod_{j \in v} \sigma_j^x$$



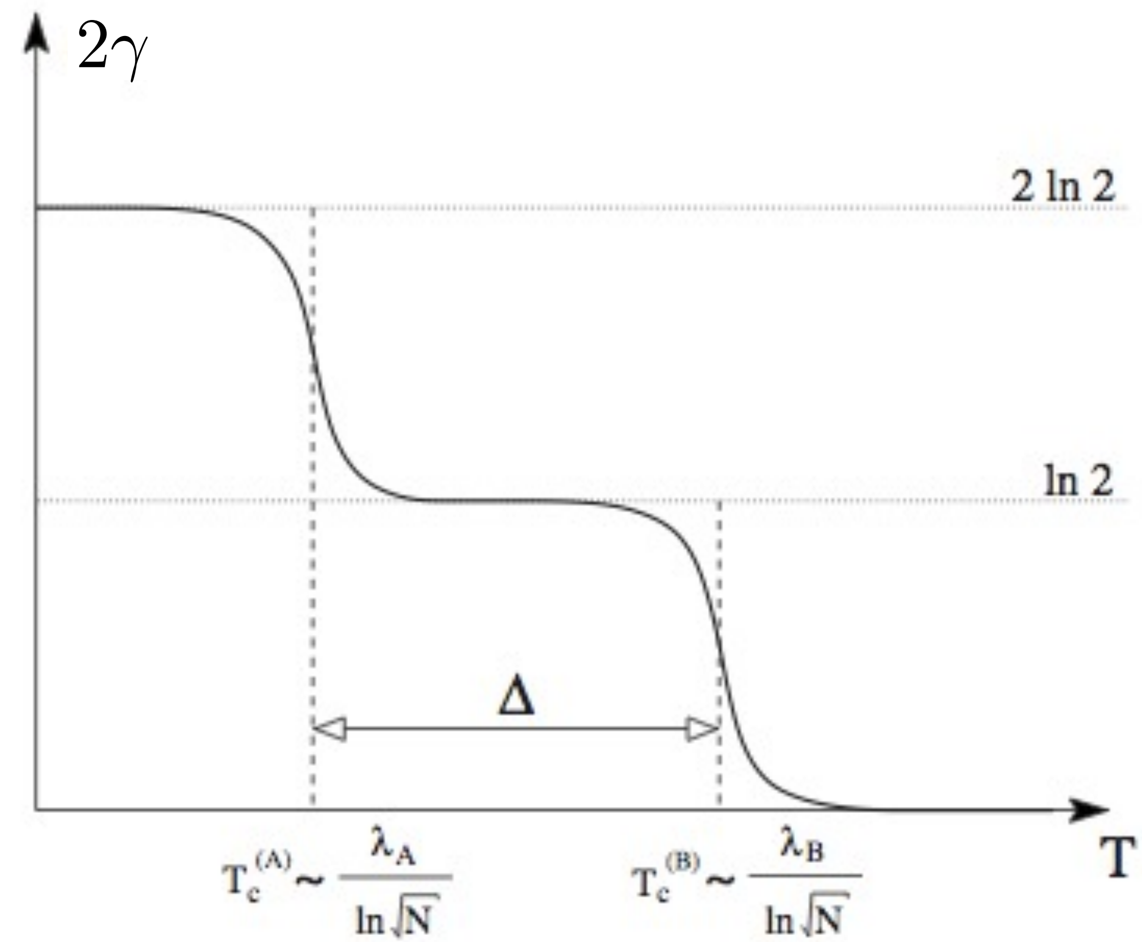
Levin and Wen, - Phys. Rev. Lett. 96, 110405 (2006)

- This γ can serve as an "order parameter" for a spin liquid (it identifies the underlying emergent gauge symmetry)



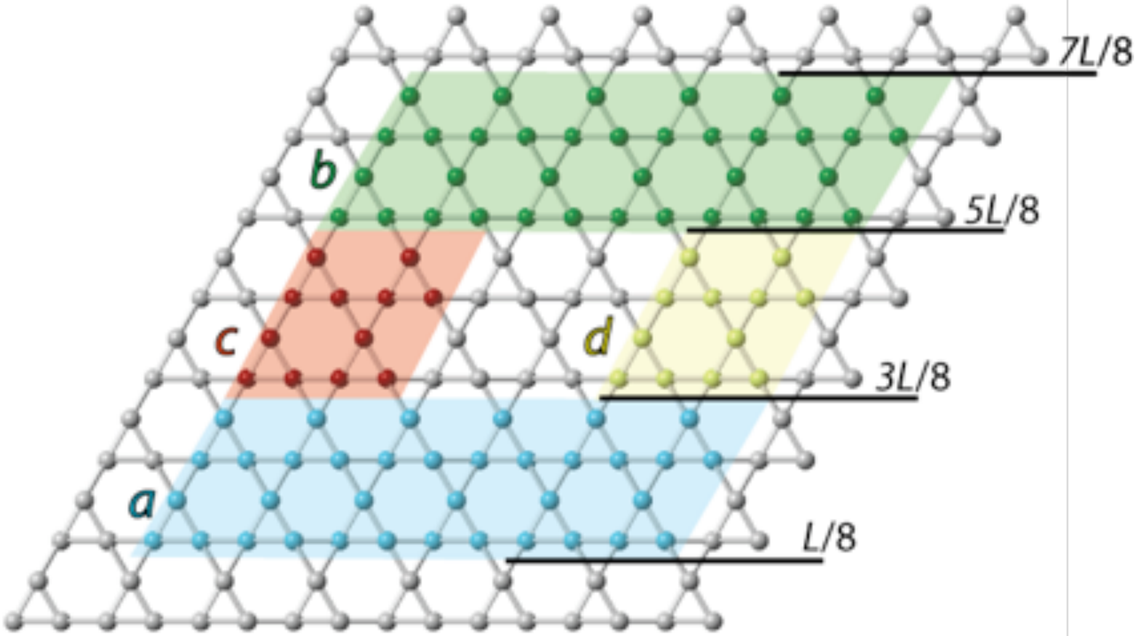
$$2\gamma = \lim_{r,R\to\infty} [-S_{VN}^{1A} + S_{VN}^{2A} + S_{VN}^{3A} - S_{VN}^{4A}]$$

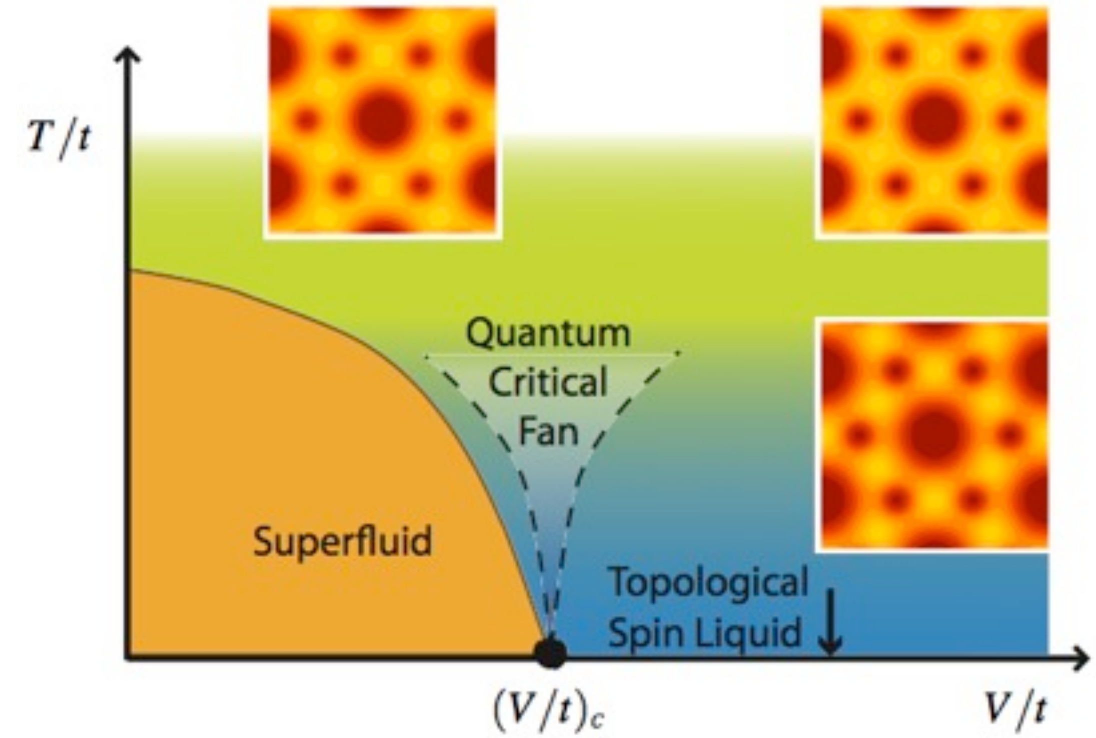
finite-size systems retain a statistical contribution to the topological EE

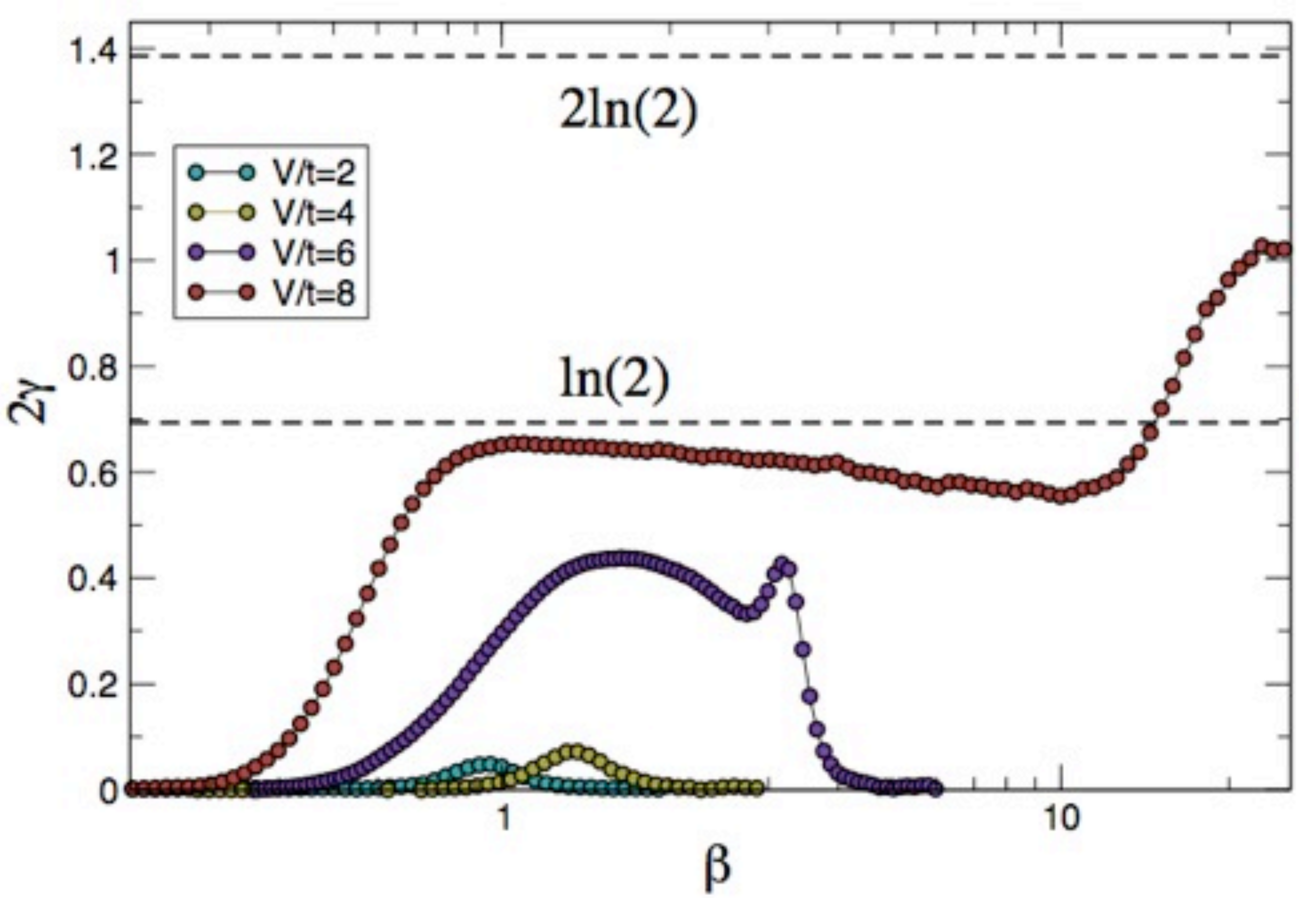


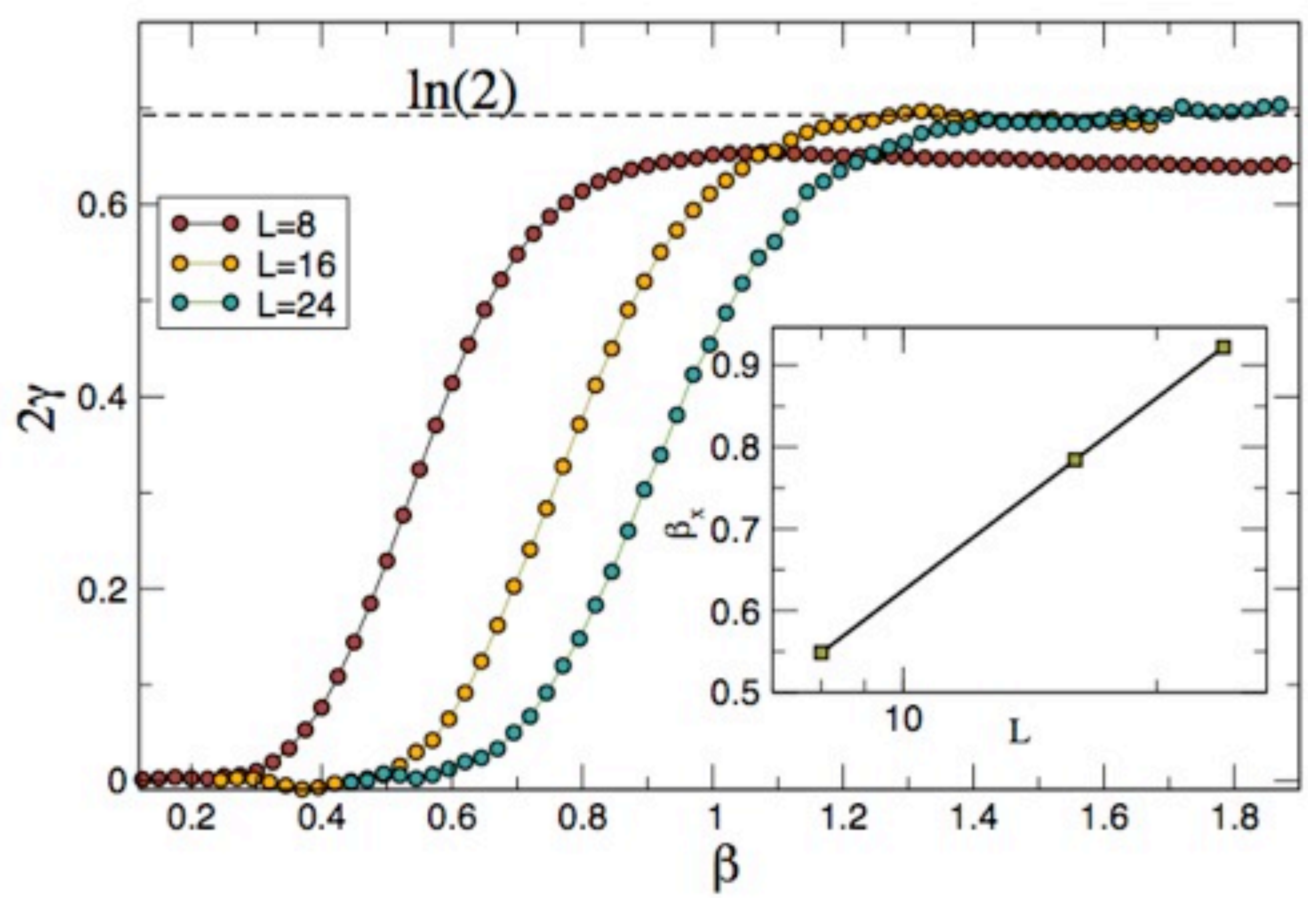
Entanglement and topological entropy of the toric code at finite temperature
Claudio Castelnovo and Claudio Chamon, PRB 76, 184442 2007

Topological Entanglement Entropy

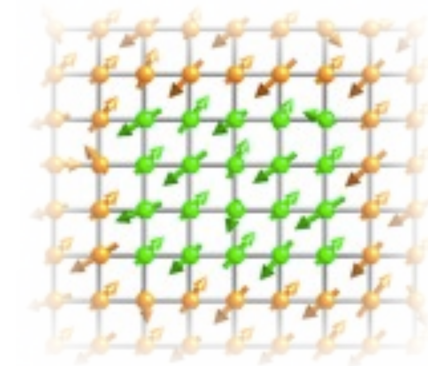




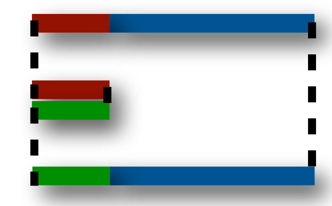




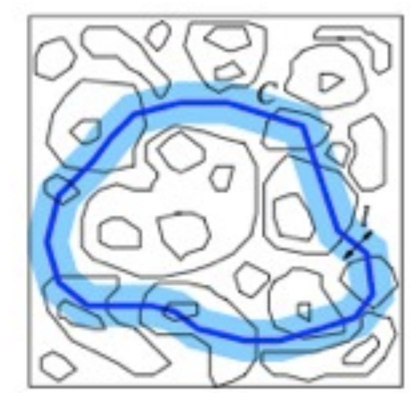
Conclusions



- **Entanglement entropy can be used as a resource to detect and classify phases and phase transitions**



- **Renyi entropies can be measured in large-scale numerical simulations with QMC methods**



- **Subleading corrections to the area law are a practical tool to detect topologically ordered spin liquid phases**

- **This effort is only about two years old - there are many more exciting applications to study**