

Entanglement, quantum spin liquids, and DMRG

Leon Balents, KITP



\$\$\$: NSF, DOE

Plan

- Introduction
- Topological entanglement entropy
- Calculations of TEE with DMRG, and minimally entangled states
- Comparison of scaling of Renyi and von Neumann entropies
- Application of MES to less exotic problems

People



Hong-Chen Jiang
KITP



Rajiv Singh
UC Davis

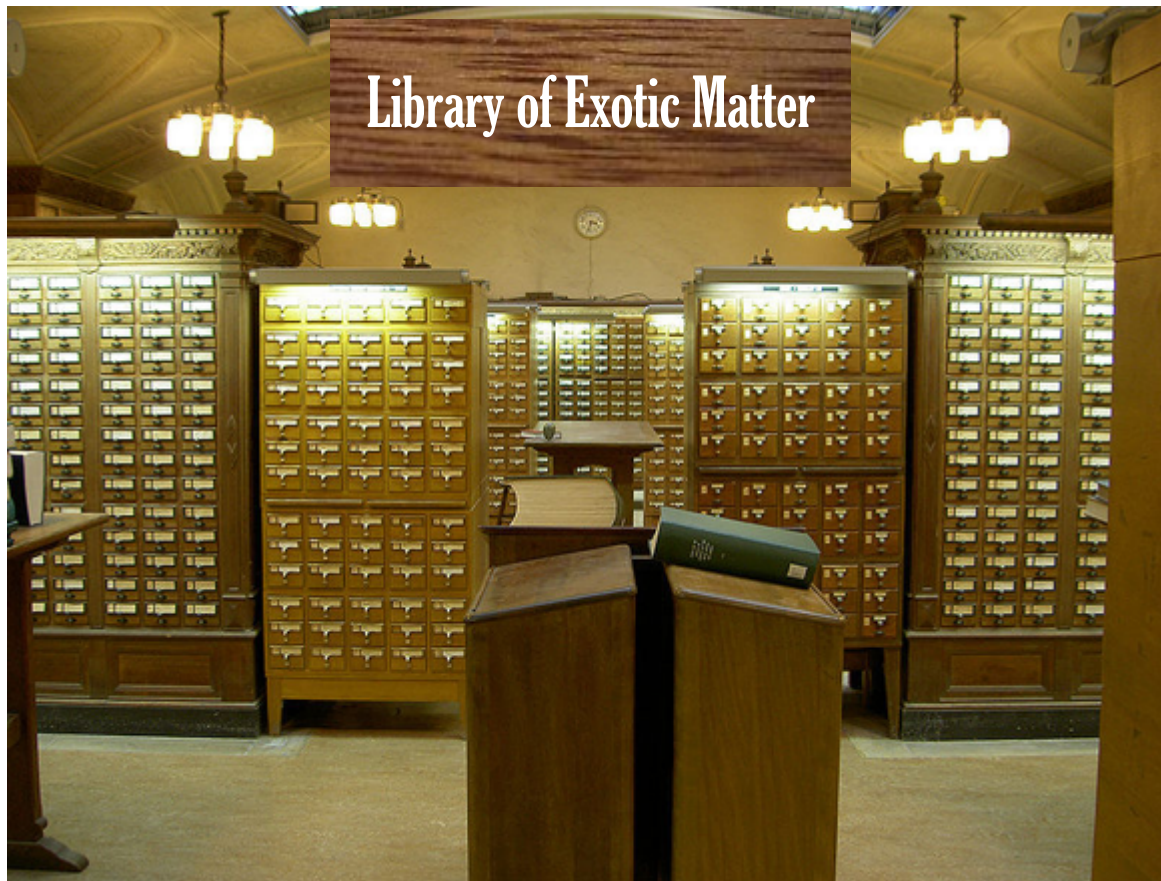


Zhenghan Wang
Microsoft Q



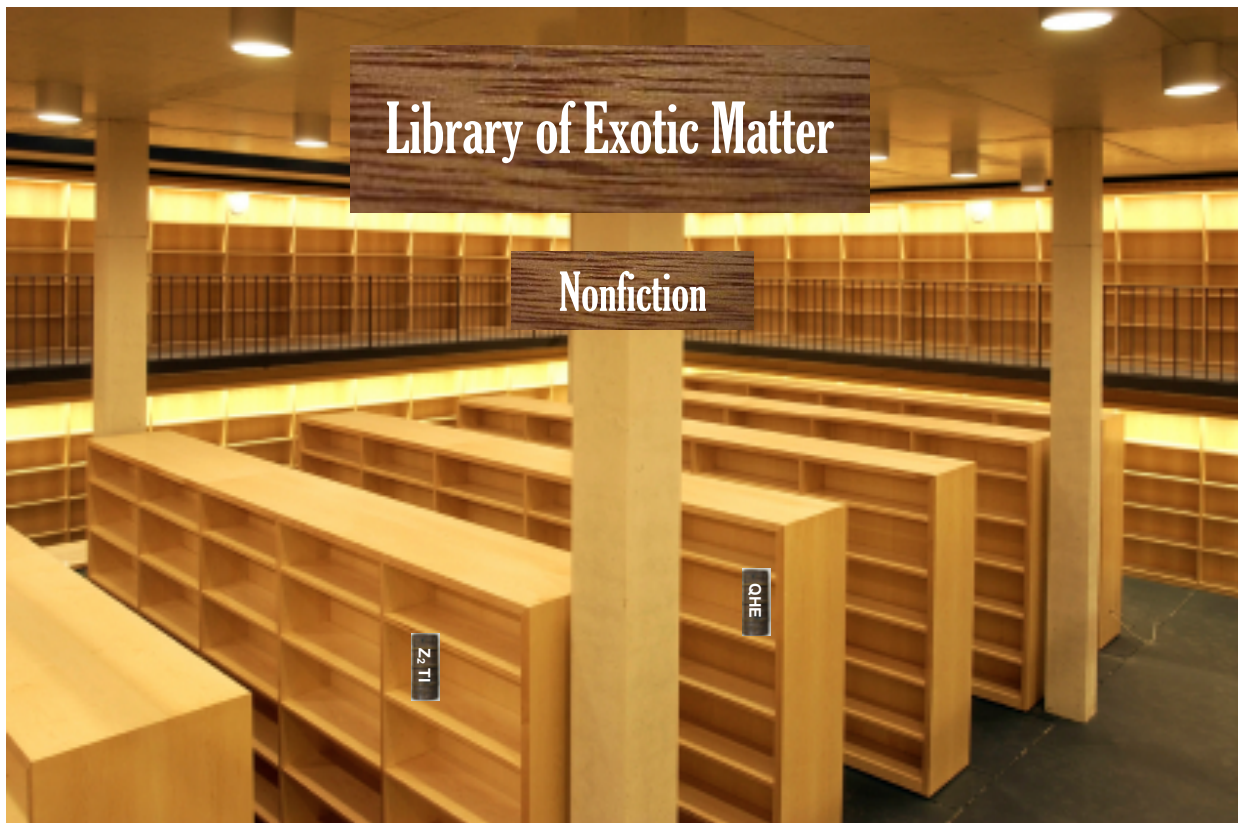
Hong Yao
Tsingua

Classification



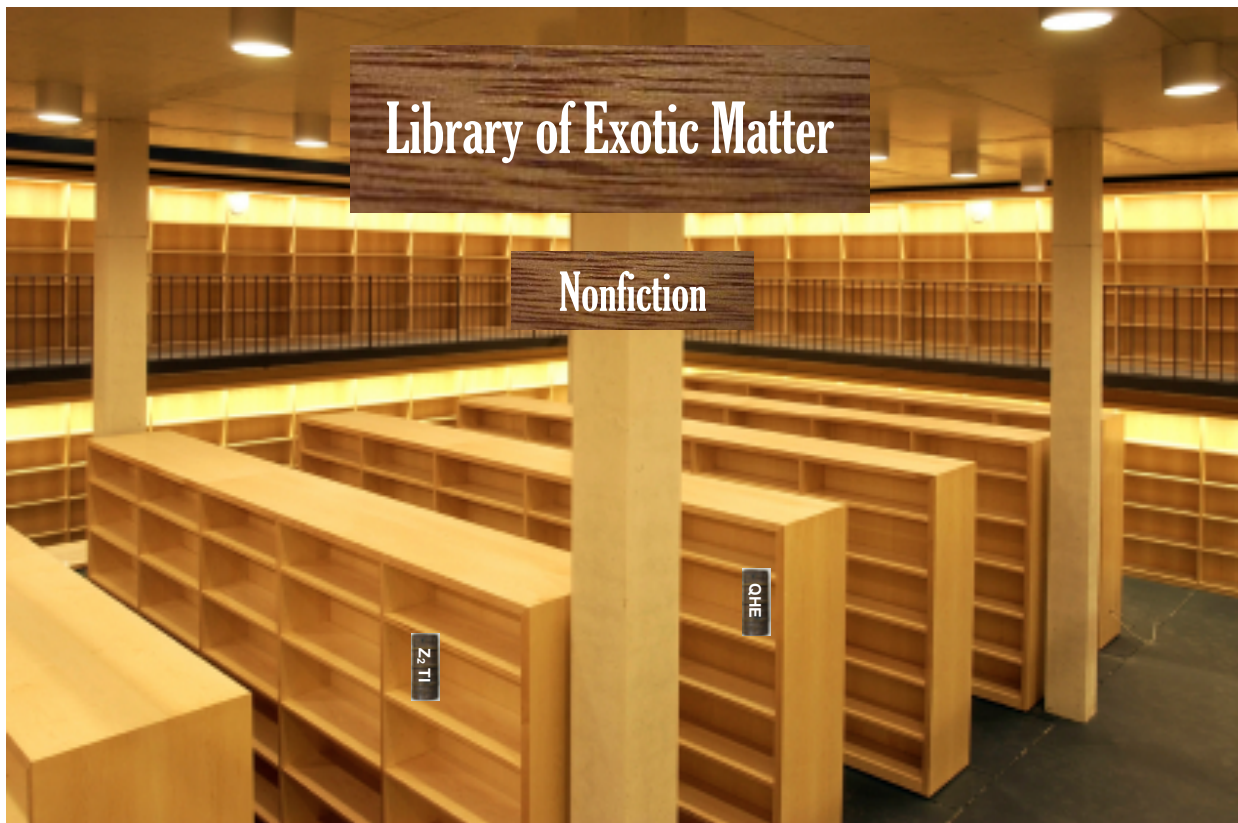
cohomology	K-matrix	General Subject
000, 040, 080	AC	Z_2 TI
010, 020, 090	Z	fibonacci
030	AE	IQHE
050	AP	ASL
060	AS	E8
070	PN	$SO(6)_3$
100	B-BJ	Philosophy (Gen.)
110-120	BD	Speculative Philosophy
130, 150	BF	Psychology
140, 180, 190	B	Philosophy (Gen.)
160	BC	Logic
170	BJ	Ethics
200, 210, 290	BL	Religions. Mythology
220	BS	The Bible
230	BT	Doctrinal Theology
240, 250	BV	Practical Theology
260, 270	BR	Christianity
280	BX	Christian Denominations
300	H	Soc. Sci. (General)
310	HA	Statistics
320	J	Gen. Legislative papers
330	HB	Economic Theory
340	K	Law
350	JF-JS	Political Institutions
360	HN, HV	Social History, Soc. Pathology
370	L	Education (General)
380	HD	Industries. Land Use. Labor
390	GT	Manners and customs

Classification



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Classification

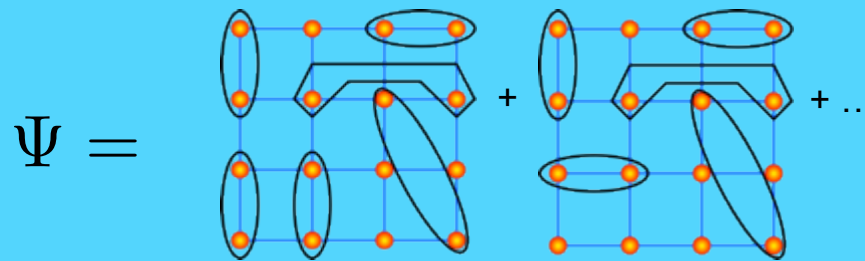
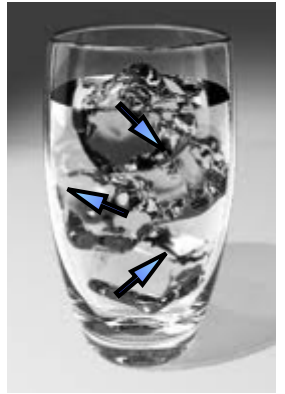


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I'd like to find some books

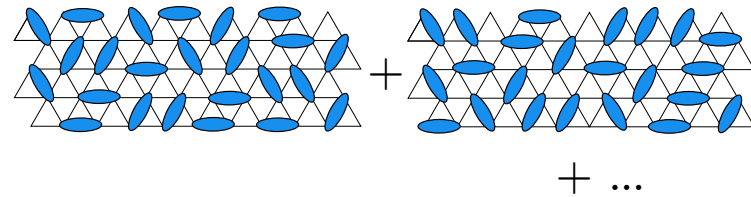
Quantum spin liquids

- Long sought non-magnetic ground states of quantum spin systems
- Interesting because of high degree of entanglement
- Anderson's RVB



Classes of QSLs

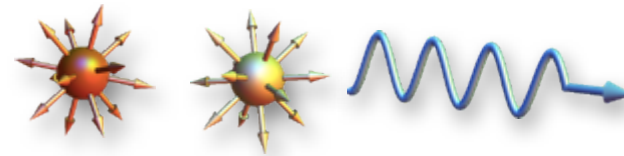
- Topological QSLs



TQFT

- full gap

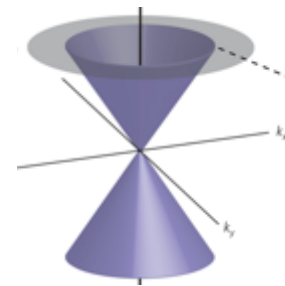
- U(1) QSL



compact
U(1) gauge
theory

- gapless emergent “photon”

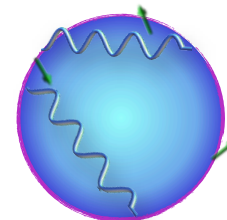
- Algebraic QSLs



QED₃

- Relativistic CFT (power-laws)

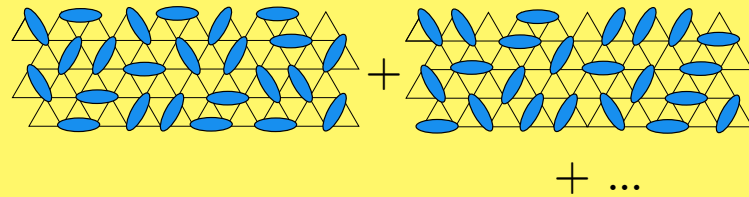
- Spinon Fermi surface QSL



QED₃
w/ $\mu > 0$

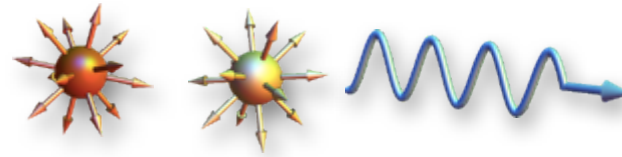
Classes of QSLs

- Topological QSLs
 - full gap



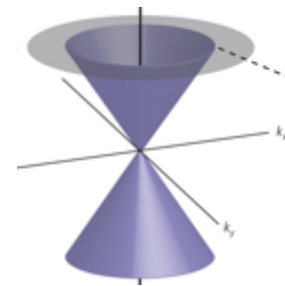
TQFT

- U(1) QSL
 - gapless emergent “photon”

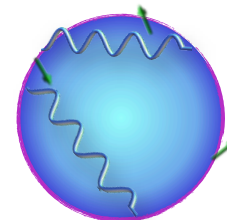


compact
U(1) gauge
theory

- Algebraic QSLs
 - Relativistic CFT (power-laws)
- Spinon Fermi surface QSL



QED₃




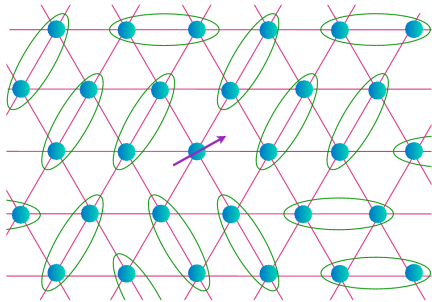
QED₃
w/ $\mu > 0$

Z_2 spin liquid

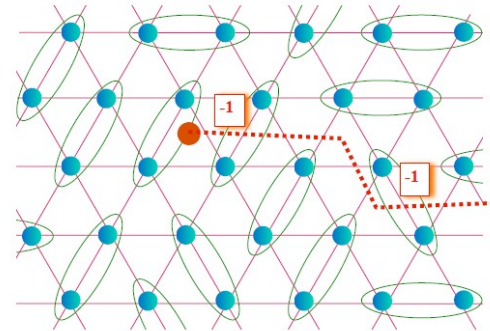
- Cartoon

$$\Psi = \text{[Diagram 1]} + \text{[Diagram 2]} + \dots$$


 spinon
 (e)



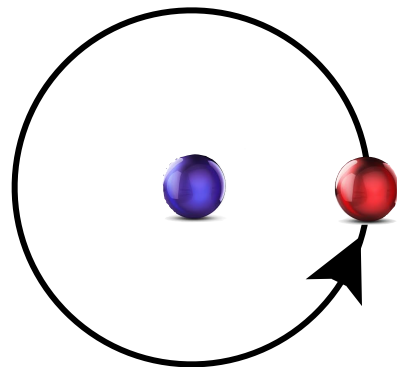

 vison
 (m)



$$\text{[Diagram of a blue and red sphere together]} = \text{[Diagram of a blue and red sphere together in an oval]}$$

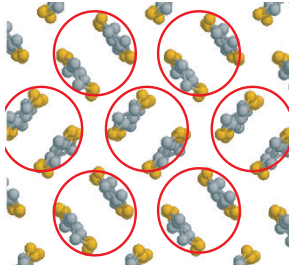
(ϵ)

$$\Psi \rightarrow -\Psi$$

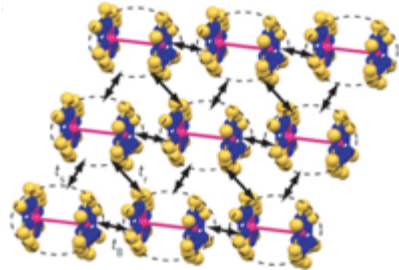


anyons characterized by
fusion rules and mutual
statistics

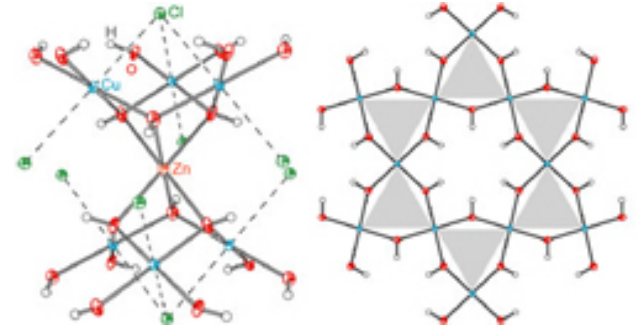
Materials



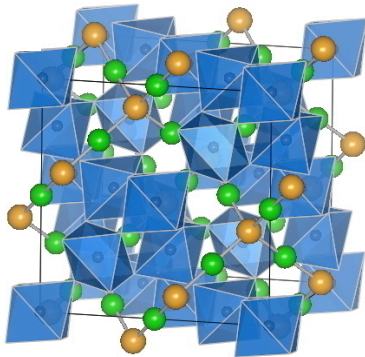
κ -(ET)₂X



β' -Pd(dmit)₂



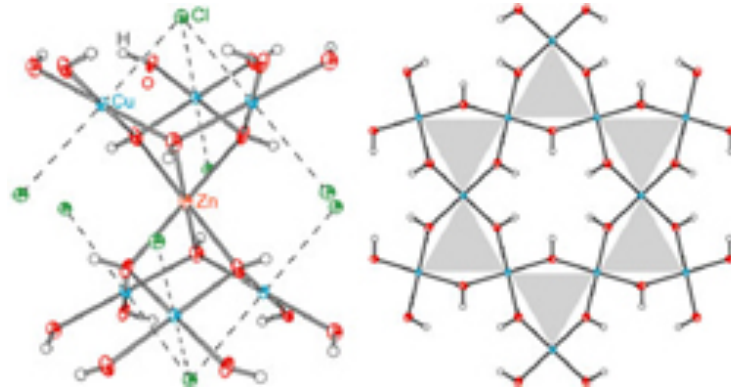
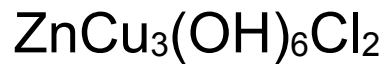
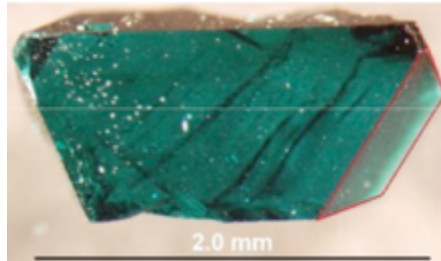
ZnCu₃(OH)₆Cl₂



Yb₂Ti₂O₇

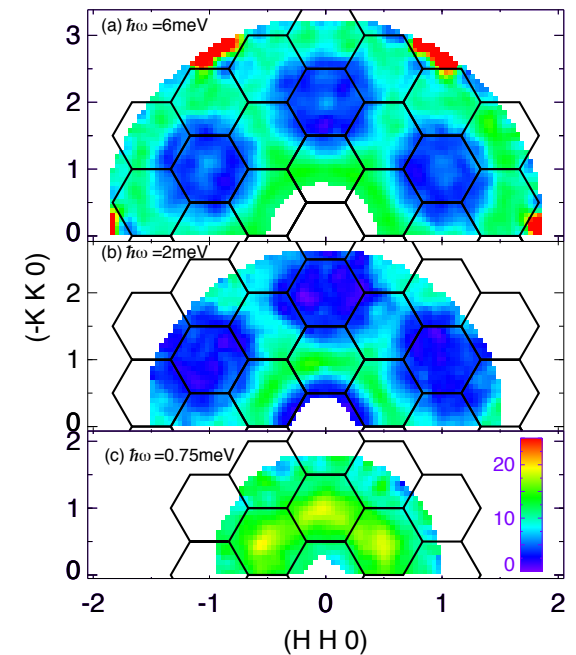
Pr₂Zr₂O₇

Herbertsmithite



Fractionalized excitations in the spin-liquid state of a kagome-lattice antiferromagnet

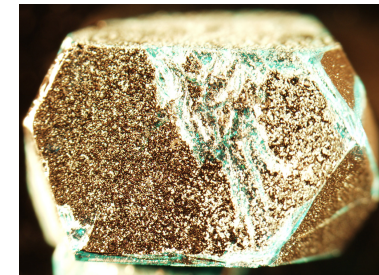
Tian-Heng Han, Joel S. Helton, Shaoyan Chu, Daniel G. Nocera, Jose A. Rodriguez-Rivera, Collin Broholm & Young S. Lee



The search is over?

MIT researchers discover a new kind of magnetism

Experiments demonstrate 'quantum spin liquid,' which could have applications in new computer memory storage.



Quantum spin liquid

From Wikipedia, the free encyclopedia



This article **may be too technical for most readers to understand**. Please help [improve](#) this article to [make it understandable to non-experts](#), without removing the technical details. The [talk page](#) may contain suggestions. *(December 2012)*

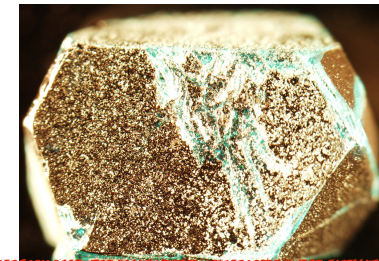
In [condensed matter physics](#), **quantum spin liquid** is a [state](#) that can be achieved in a system of interacting [quantum spins](#). The state is referred to as a "liquid" as it is a [disordered](#) state in comparison to a [ferromagnetic](#) spin state,^[1] much in the way liquid water is in a disordered state compared to crystalline ice. However, unlike other disordered states, a quantum spin liquid state preserves its disorder to very low temperatures.^[2]

The quantum spin liquid state was first proposed by physicist [Phil Anderson](#) in 1973 as the ground state for a system of spins on a [triangular lattice](#) that interact with their nearest neighbors via the so-called [antiferromagnetic](#) interaction. Quantum spin liquids generated further interest when in 1987 Anderson proposed a theory that described [high temperature superconductivity](#) in terms of a disordered spin-liquid state.^[3] A quantum spin liquid state was first realized experimentally in crystalline herbertsmithite by Young Lee and his group at the [Massachusetts Institute of Technology](#) in December 2012.^[4]

The search is over?

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Experiments demonstrate 'quantum spin liquid,' which could have applications in new computer memory storage.



Before we use nearly featureless data to declare victory, we should have some better understanding

Quantum
From Wikipedia

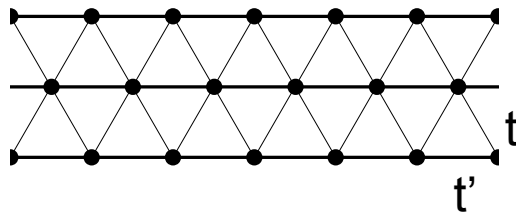


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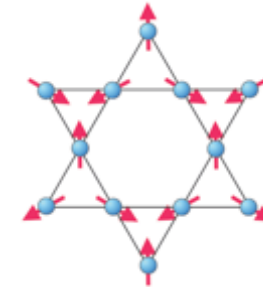
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Models



$$H = - \sum_{ij} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



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

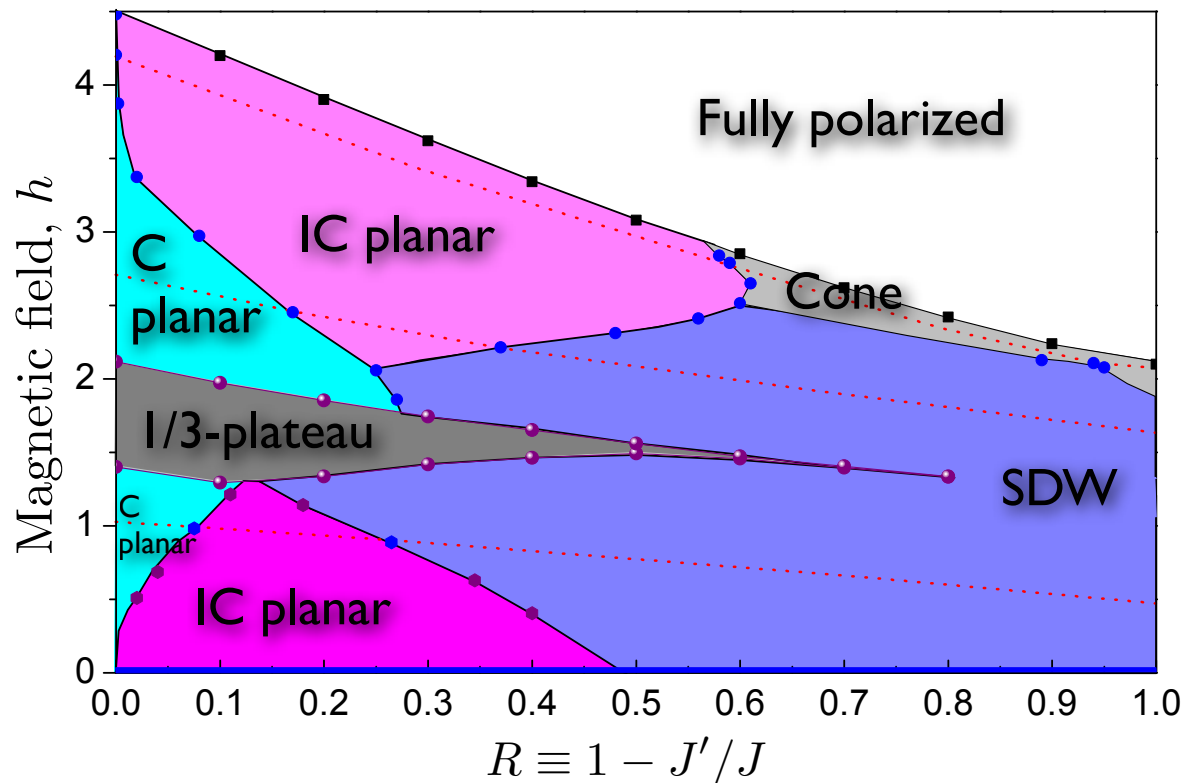


Yb₂Ti₂O₇
Pr₂Zr₂O₇

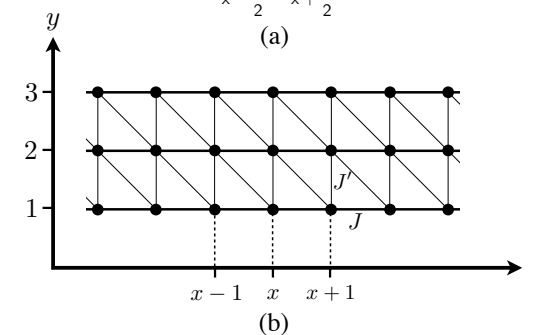
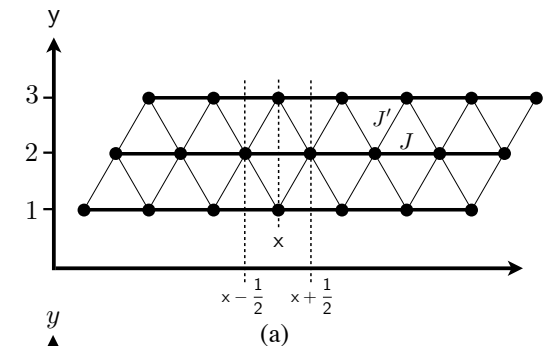
$$\begin{aligned}
 H = & J_{zz} \sum_{\langle i,j \rangle} S_i^z S_j^z \\
 & - J_{\pm} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+) \\
 & + J_{z\pm} \sum_{\langle i,j \rangle} [S_i^z (\zeta_{ij} S_j^+ + \zeta_{ij}^* S_j^-) + i \leftrightarrow j] \\
 & + J_{\pm\pm} \sum_{\langle i,j \rangle} (\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-)
 \end{aligned}$$

Phase diagrams

- DMRG gives powerful access to ground states of 1d strips of reasonable width

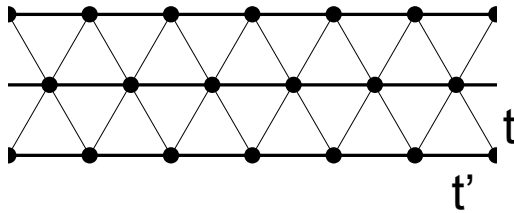


Heisenberg

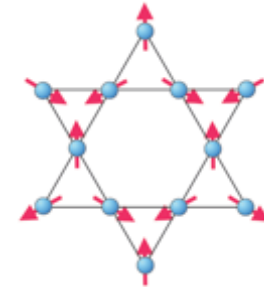


Ru Chen *et al*, 2013

Models



$$H = - \sum_{ij} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



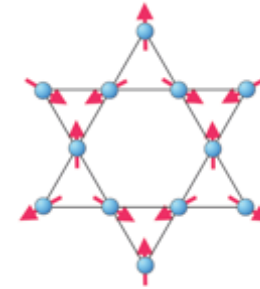
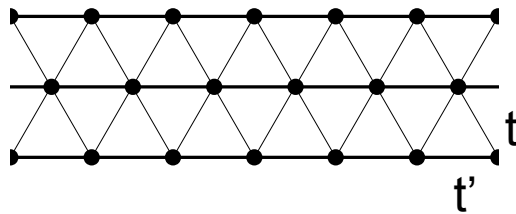
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Models



No “obvious” gauge structure/soluble limit.
 Diagnostics for QSL states in general models?

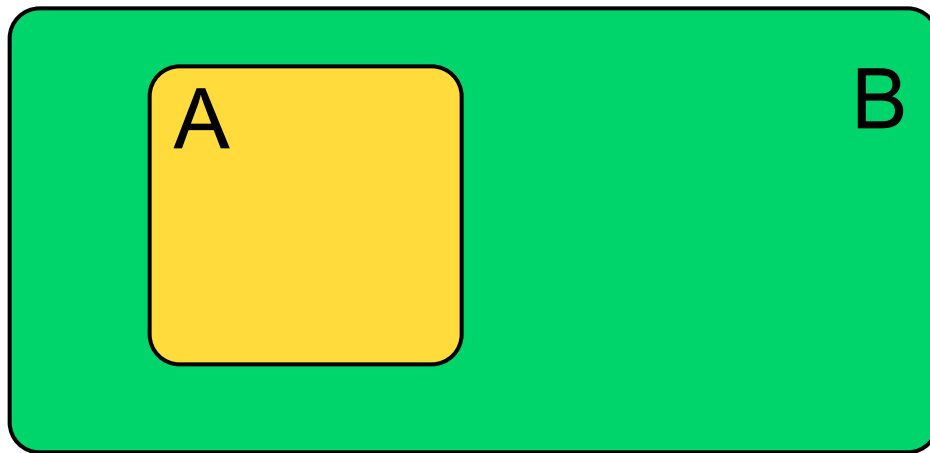
- ground state degeneracy
- topological entanglement entropy



Yb₂Ti₂O₇

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Entanglement entropy

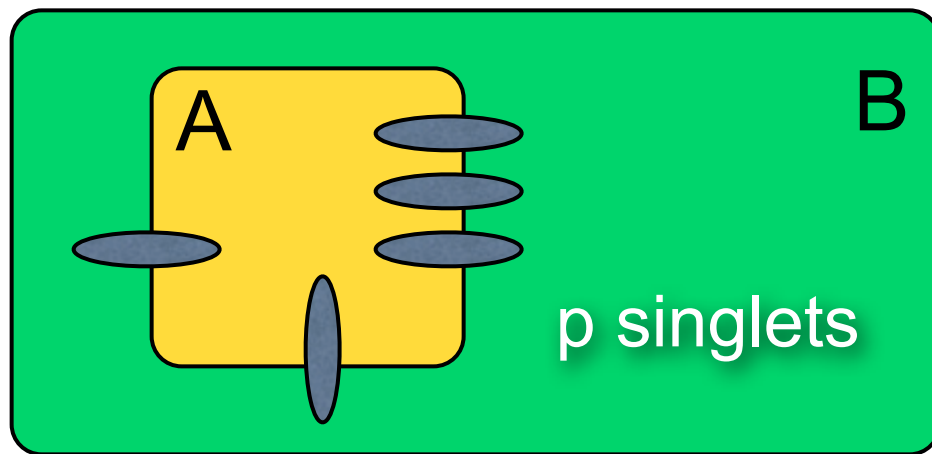


$$\rho_A = \text{Tr}_B |\psi\rangle\langle\psi|$$

von Neumann $S_{vN}(A) = -\text{Tr} [\rho_A \ln \rho_A]$

Renyi $S_\alpha(A) = -\frac{1}{1-\alpha} \ln \text{Tr} \rho_A^\alpha$

Entanglement entropy



$$\rho_A = \text{Tr}_B |\psi\rangle\langle\psi|$$

von Neumann

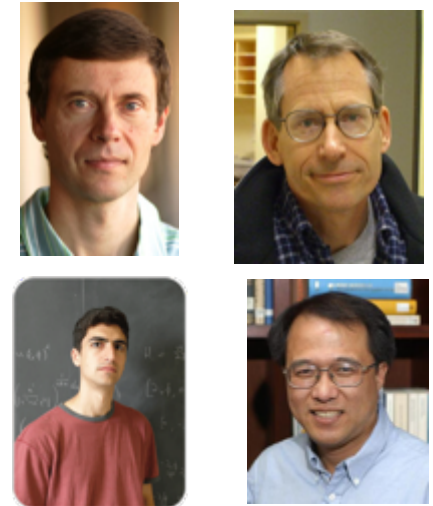
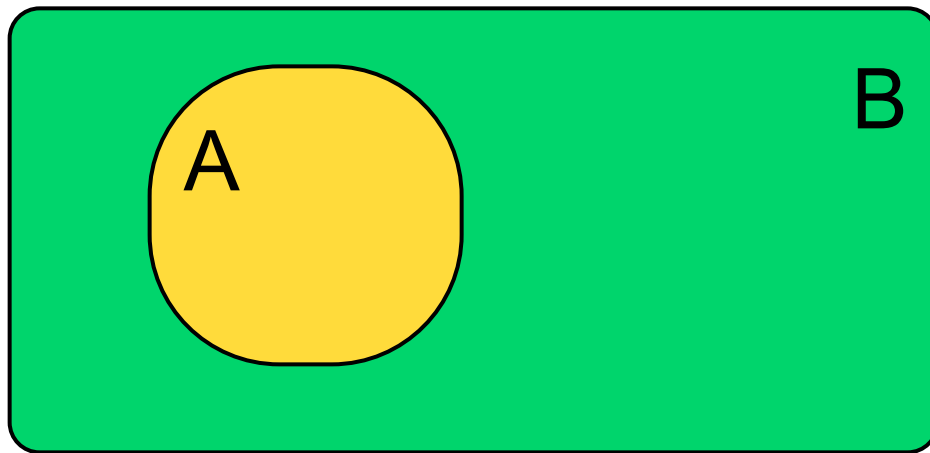
$$S_{vN}(A) = -\text{Tr} [\rho_A \ln \rho_A]$$

Renyi

$$S_\alpha(A) = -\frac{1}{1-\alpha} \ln \text{Tr} \rho_A^\alpha$$

$$= p \ln 2$$

Topological EE



2006

- TQFT result for a smooth boundary

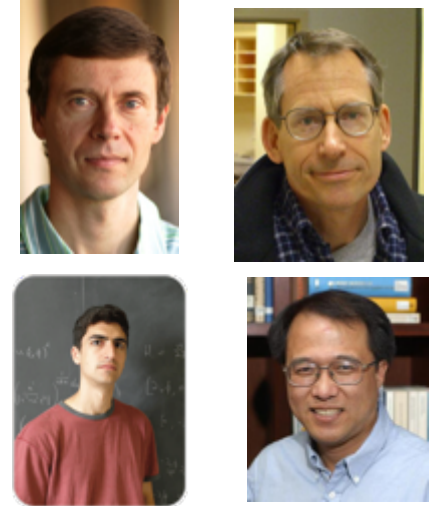
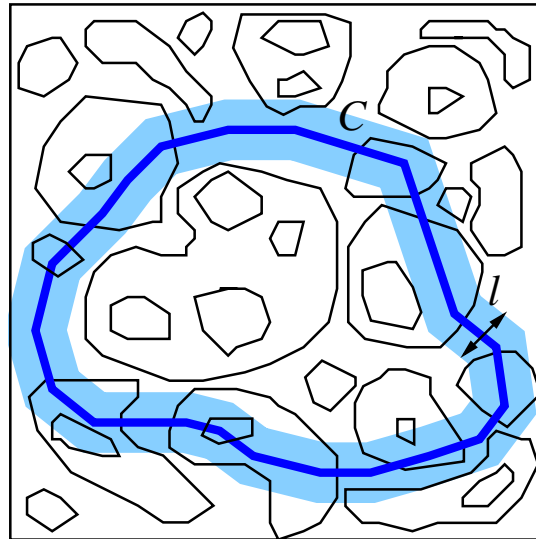
$$S_\alpha(A) \sim c_\alpha L - \gamma$$

$$\gamma = \ln \mathcal{D}$$

total quantum dimension

Topological EE

loops cross
boundary
even number
of times



2006

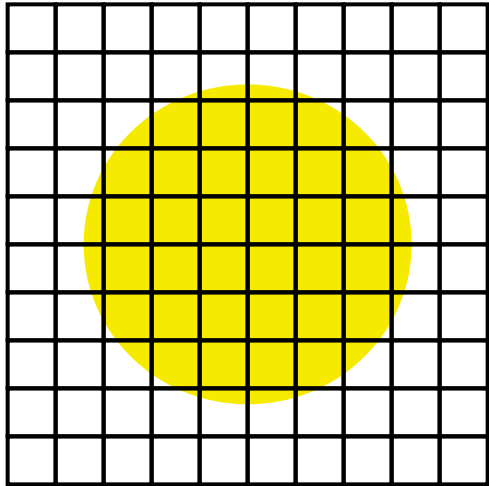
- TQFT result for a smooth boundary

$$S_\alpha(A) \sim c_\alpha L - \gamma$$

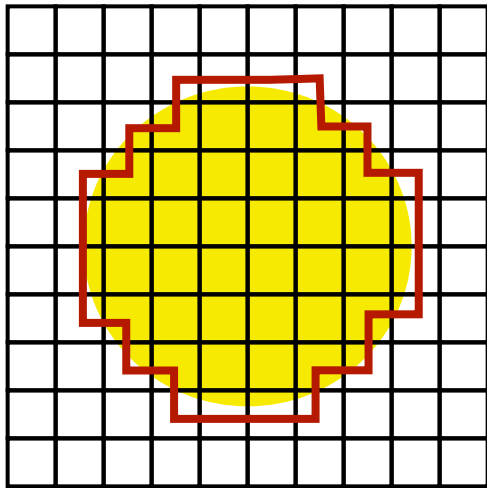
$$\gamma = \ln 2$$

Z_2 spin liquid

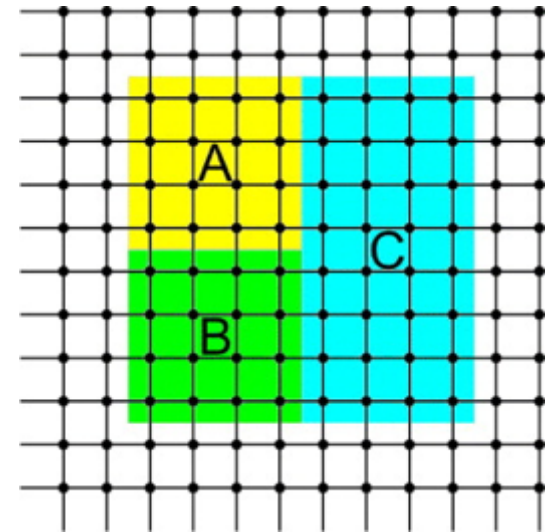
Smooth boundary?



Smooth boundary?

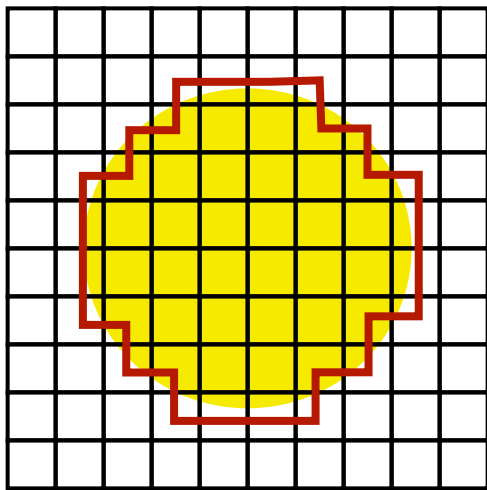


cannot be
achieved for disc-
like region on a
lattice

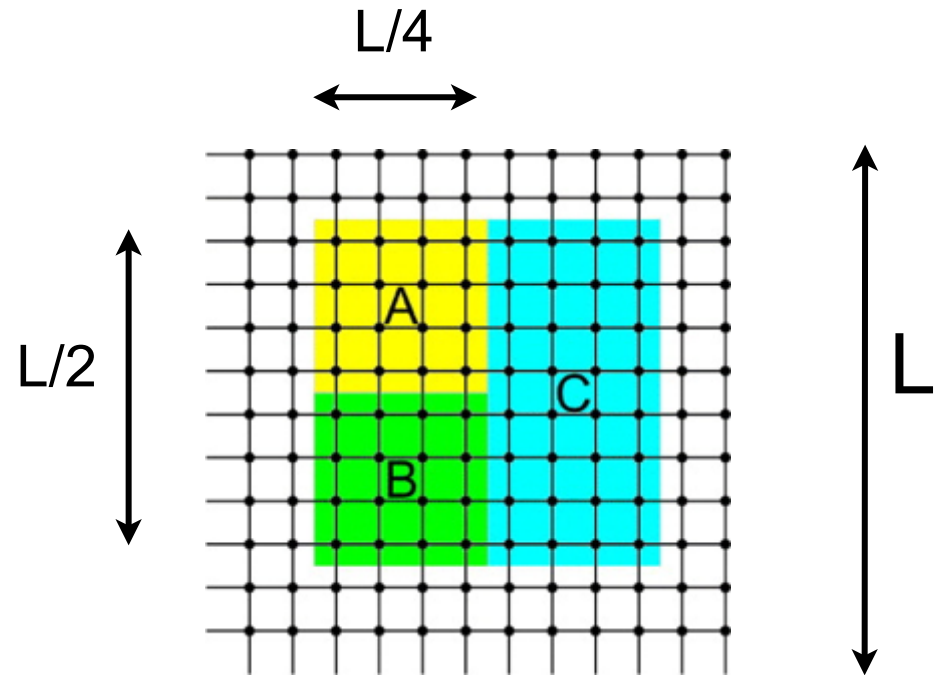


$$-\gamma = S_A + S_B + S_C \\ -S_{AB} - S_{AC} - S_{BC} + S_{ABC}$$

Smooth boundary?



cannot be
achieved for disc-
like region on a
lattice



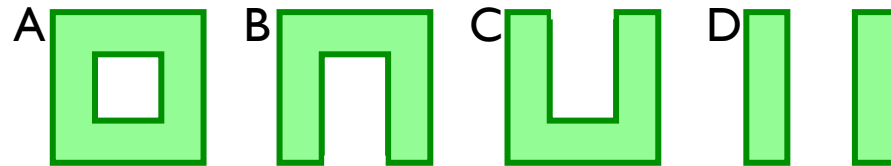
$$-\gamma = S_A + S_B + S_C$$

$$-S_{AB} - S_{AC} - S_{BC} + S_{ABC}$$

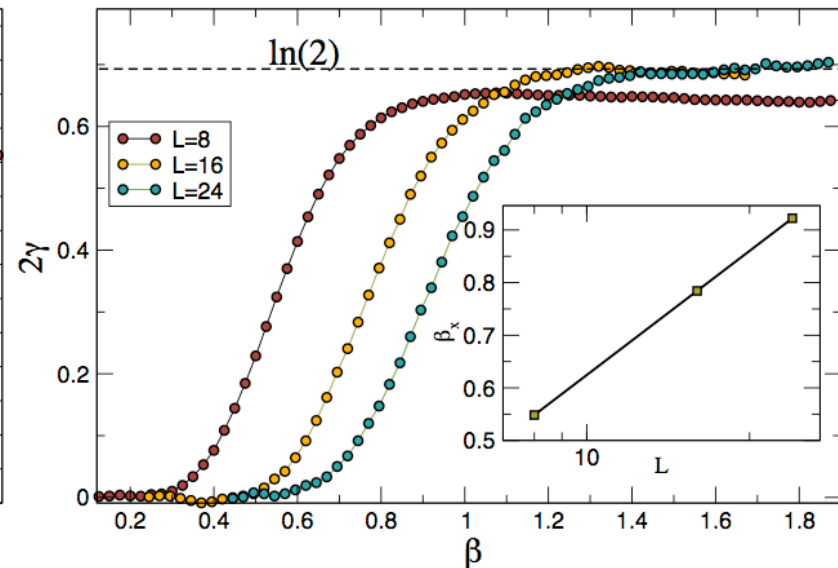
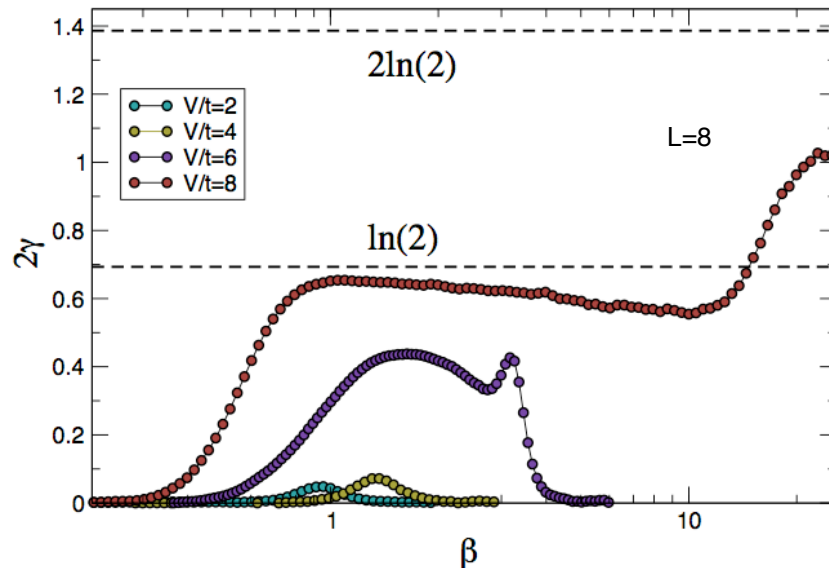
challenging due to cancellation of large
numbers, and smaller length scales

QMC results

Isakov, Hastings, RGM Nature Physics 7, 772 (2011)

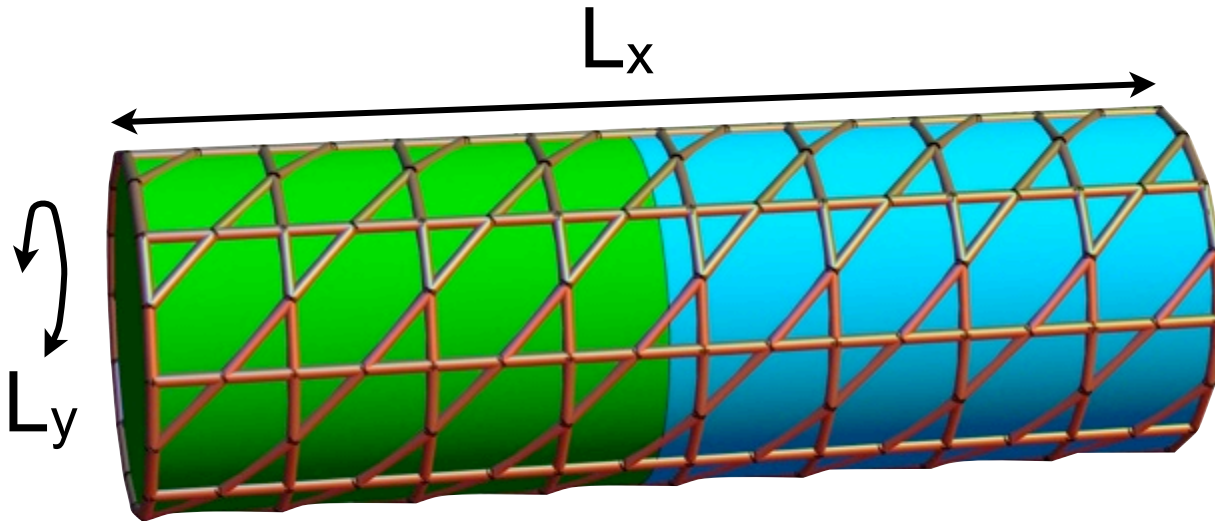


$$2\gamma = -S_n^A + S_n^B + S_n^C - S_n^D$$



heroic efforts get you halfway there

Cylinder



Easily
implemented
on lattice

- Only scales are circumference L_y , length L_x , and lattice spacing

$$S_\alpha \sim c_\alpha L_y - \gamma$$

$$L_x \gtrsim L_y \gg 1$$

$$+O(e^{-L_y/\xi_\alpha})$$

Cylinder



Easily
implemented
on lattice

- Only scales are circumference L_y , length L_x , and lattice spacing

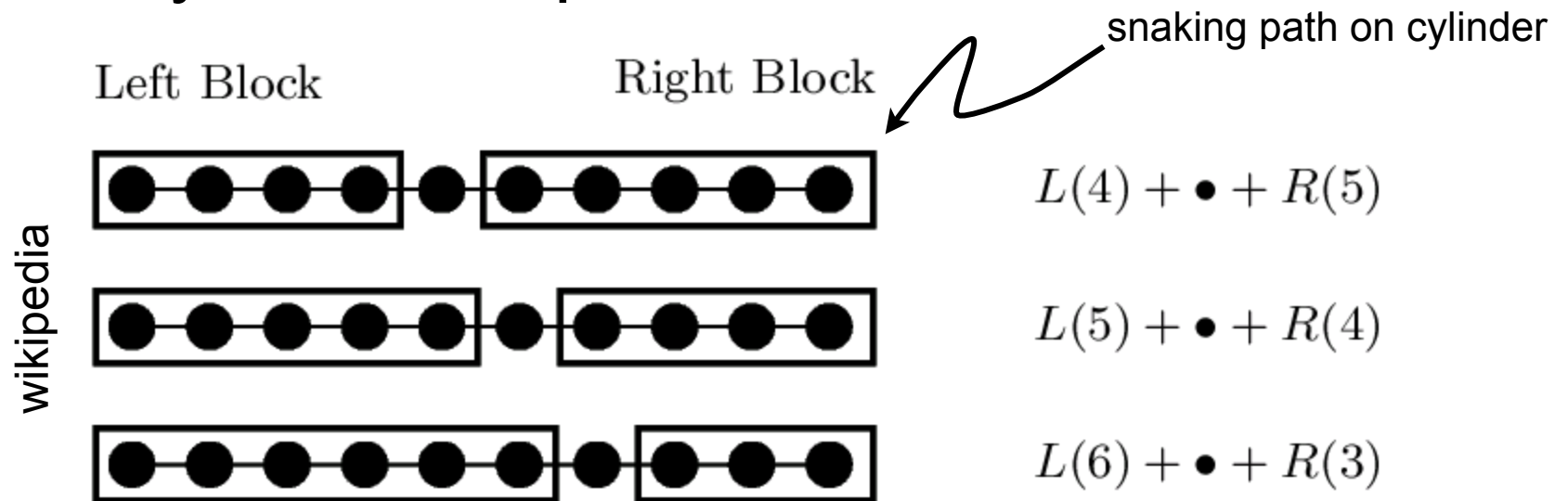
$$S_\alpha \sim c_\alpha L_y - \gamma$$

$$L_x \gtrsim L_y \gg 1$$

$$+O(e^{-L_y/\xi_\alpha})$$

DMRG

- Systems is split into “blocks”



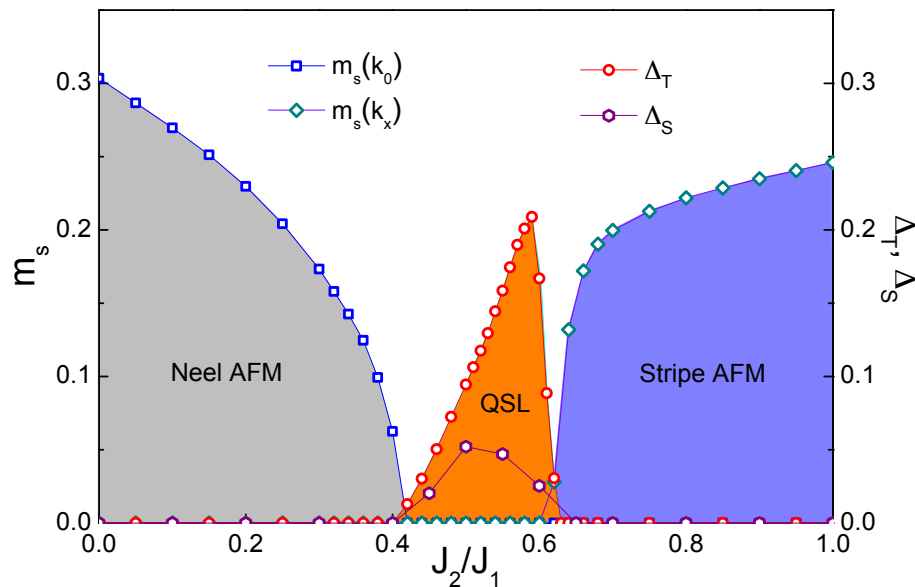
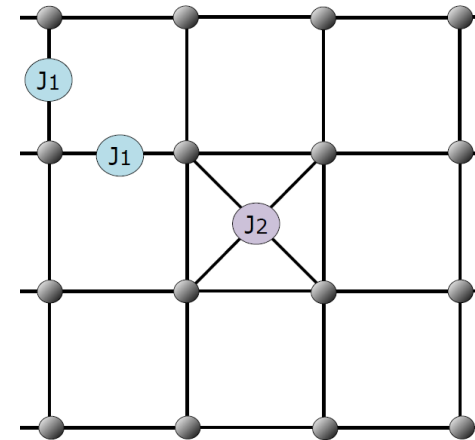
- Really a Schmidt decomposition

$$|\Psi\rangle = \sum_i c_i |\Psi\rangle_L \otimes |\Psi\rangle_R$$

Full entanglement spectrum
and all S_α readily available

Example 1: J_1 - J_2 model

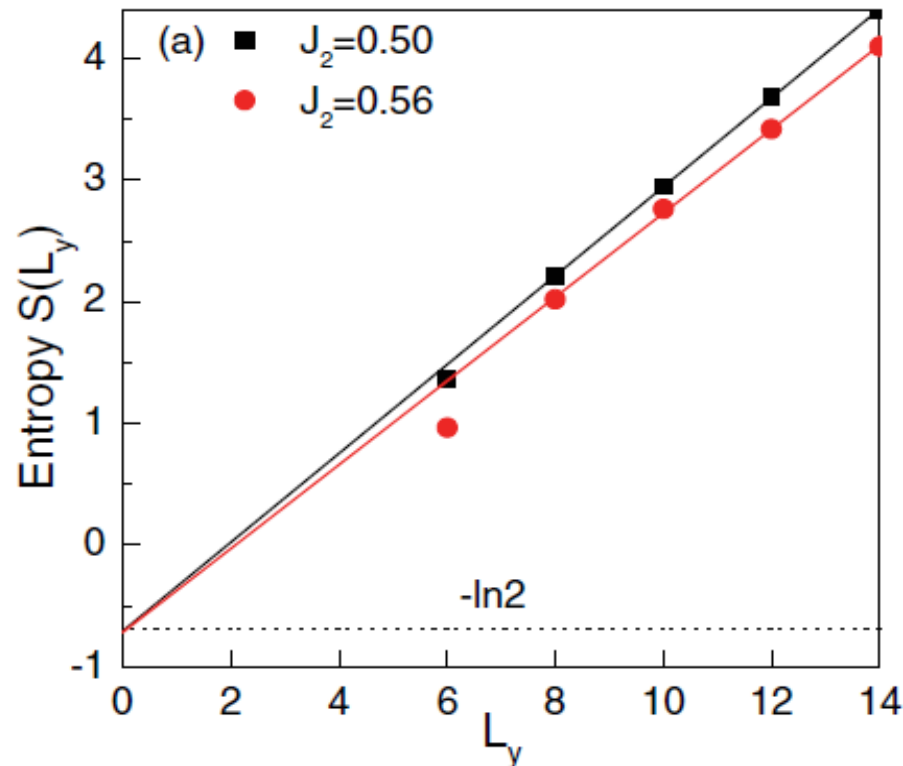
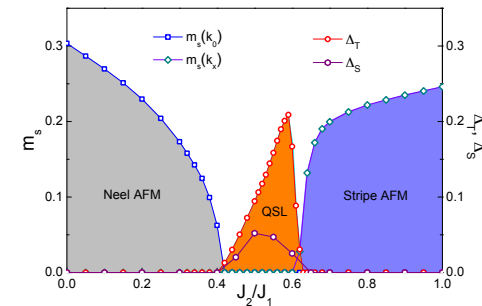
$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



decades of work shows that intermediate phase has a gap and no magnetic order

Example 1: J_1 - J_2 model

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



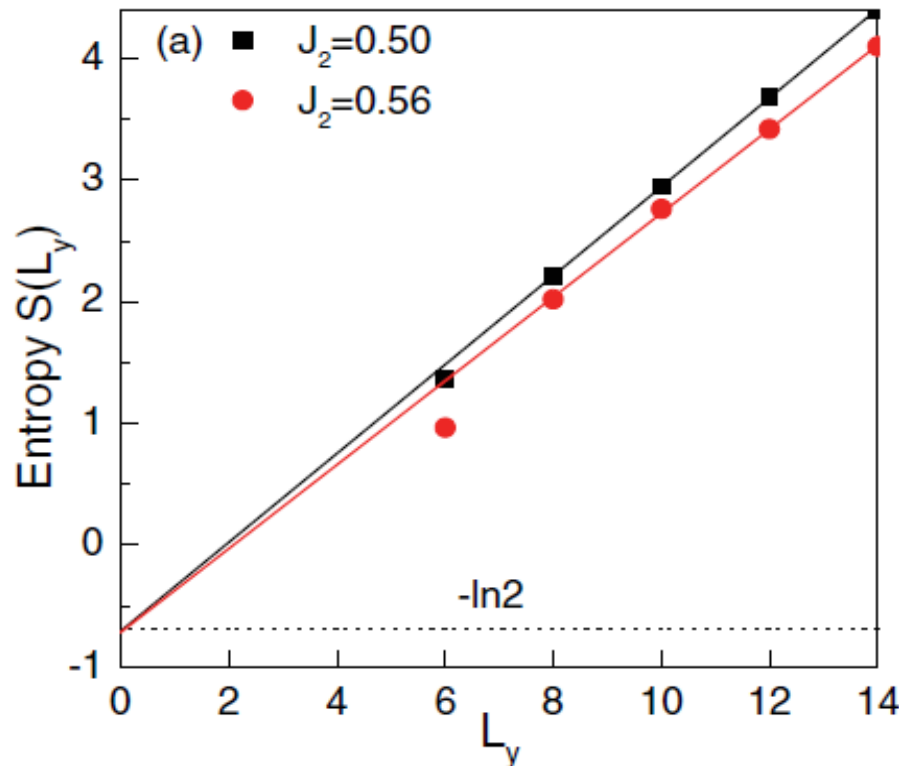
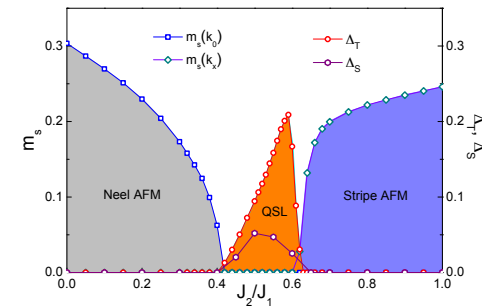
$$\gamma = 0.70 \pm 0.02 \quad J_2=0.50$$

$$= 0.72 \pm 0.04 \quad J_2=0.56$$

match to $\ln(2) = 0.69 \dots$

Example 1: J_1 - J_2 model

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



$$\gamma = 0.70 \pm 0.02 \quad J_2=0.50$$

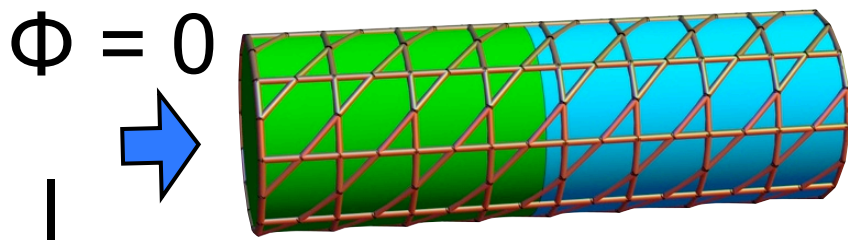
$$= 0.72 \pm 0.04 \quad J_2=0.56$$

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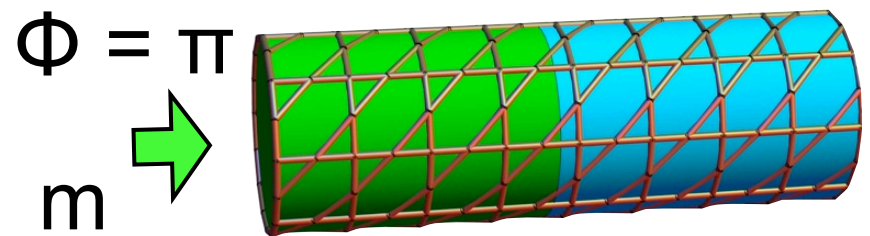
seems good...look more carefully

State dependence

- A basic characteristic of topological phases is ground state degeneracy
- For the Z_2 case (toric code), it is two-fold on the cylinder



$|0\rangle$



$|1\rangle$

State dependence

c.f. Yi Zhang
et al, 2011

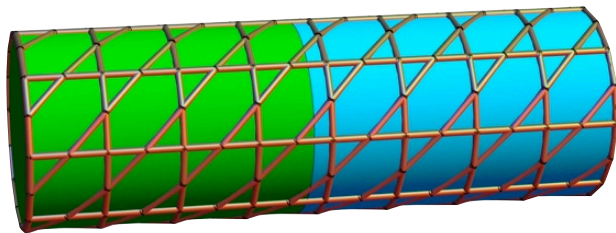
- The EE depends upon the state

$$|\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle \pm |1\rangle) \quad 0 \leq \gamma \leq \ln 2 \quad |0\rangle, |1\rangle$$

MES

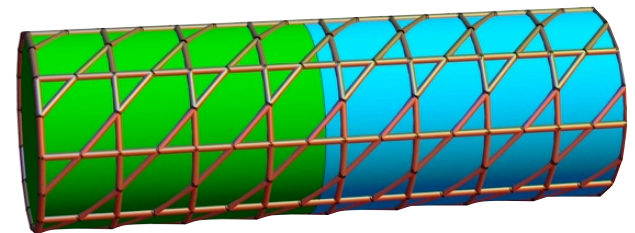
“minimally entangled states”,
“minimum entropy states”

$\Phi = 0$
→



$|0\rangle$

$\Phi = \pi$
→



$|1\rangle$

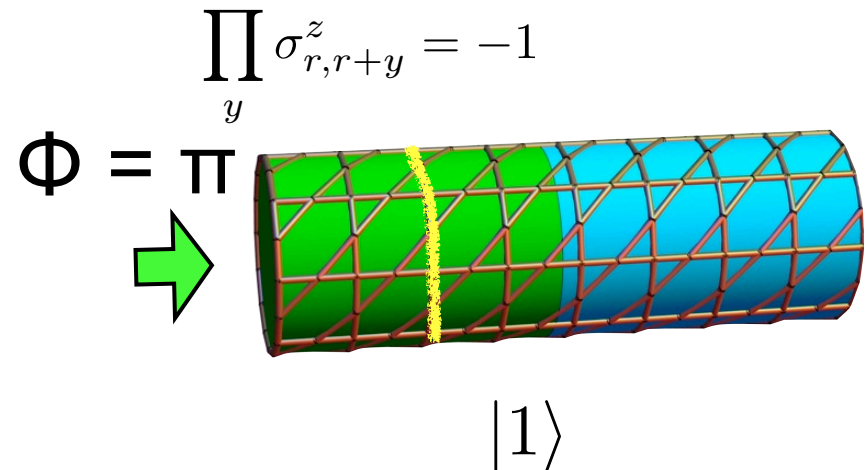
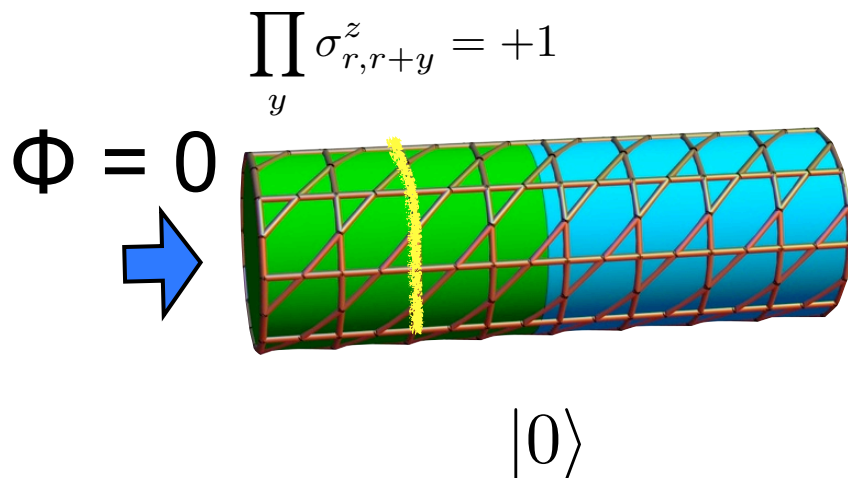
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State dependence

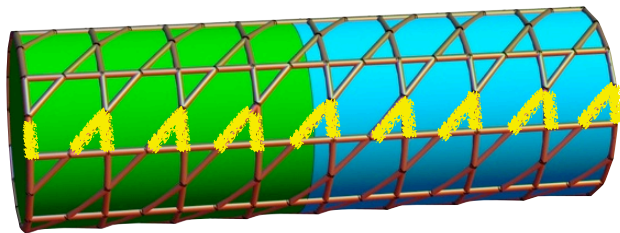
c.f. Yi Zhang
et al, 2011

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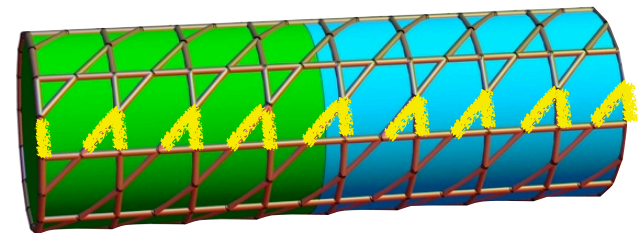
MES

$$\prod_x \sigma_{r,r+y}^x = +1$$



$|+\rangle$

$$\prod_x \sigma_{r,r+y}^x = -1$$



$|-\rangle$

definite parity of loops around cylinder

State dependence

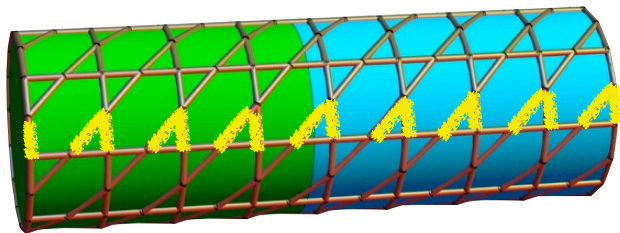
c.f. Yi Zhang
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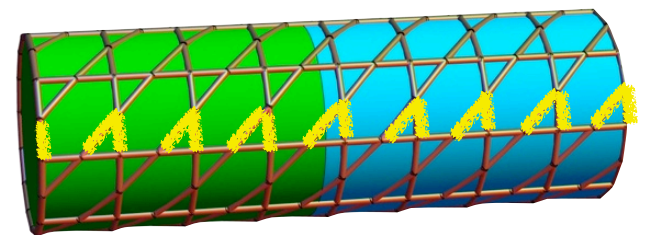
MES

$$\prod_x \sigma_{r,r+y}^x = +1$$



$|+\rangle$

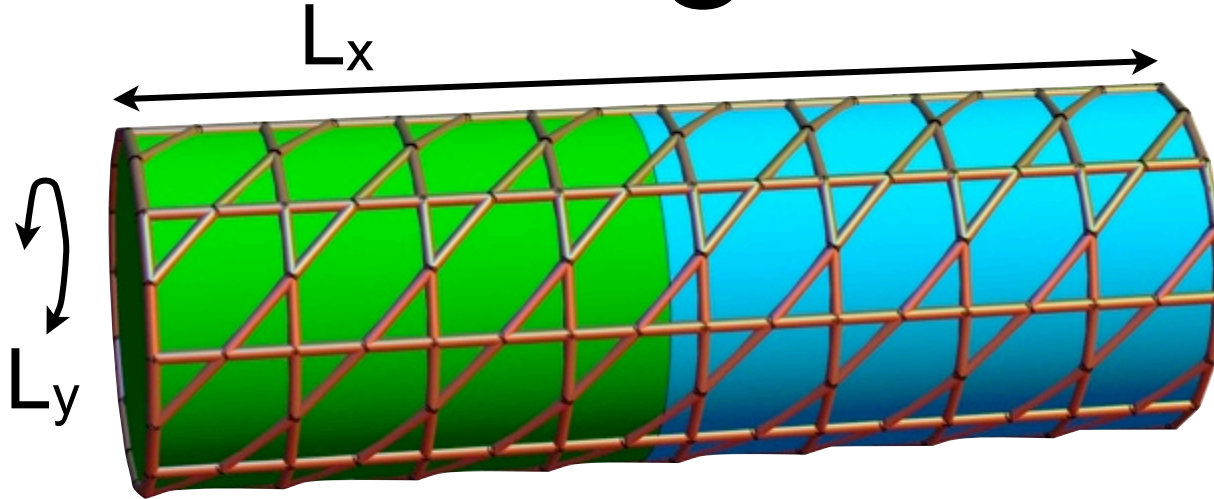
$$\prod_x \sigma_{r,r+y}^x = -1$$



$|-\rangle$

$$S(|\pm\rangle) = S(|0, 1\rangle) + \ln 2$$

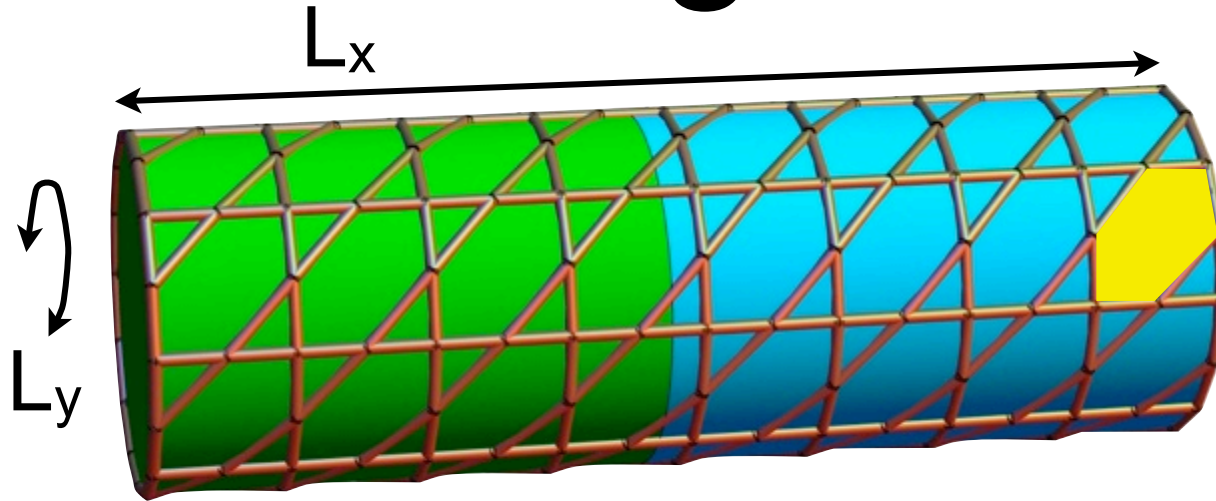
Quasi-degeneracy



- Hamiltonian

$$H_{\text{eff}} = -h (|0\rangle\langle 1| + |1\rangle\langle 0|) - h' (|0\rangle\langle 0| - |1\rangle\langle 1|)$$

Quasi-degeneracy



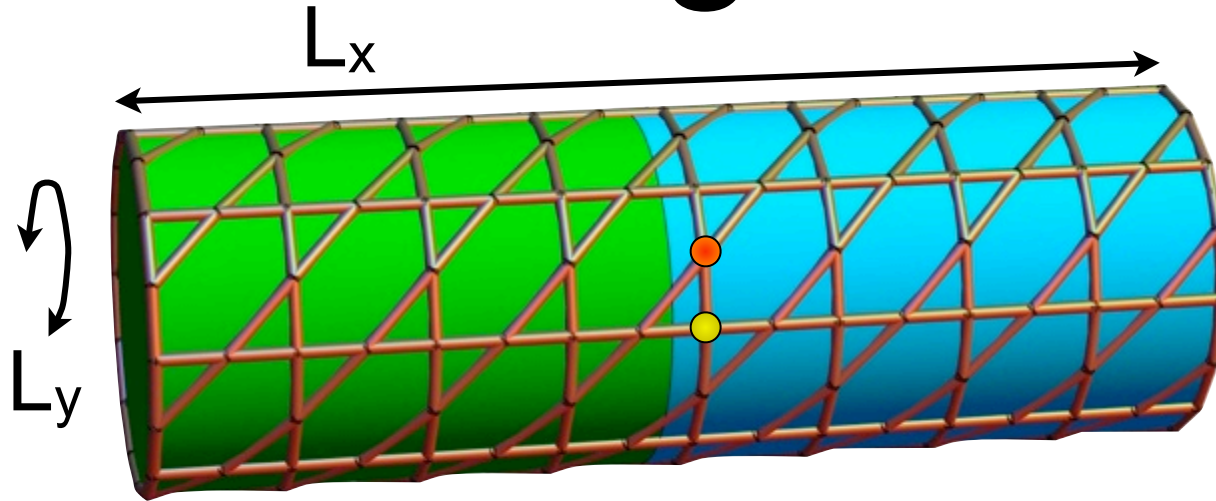
- Hamiltonian

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vison hopping

$$h \sim h_0 L_y e^{-L_x/\xi}$$

Quasi-degeneracy



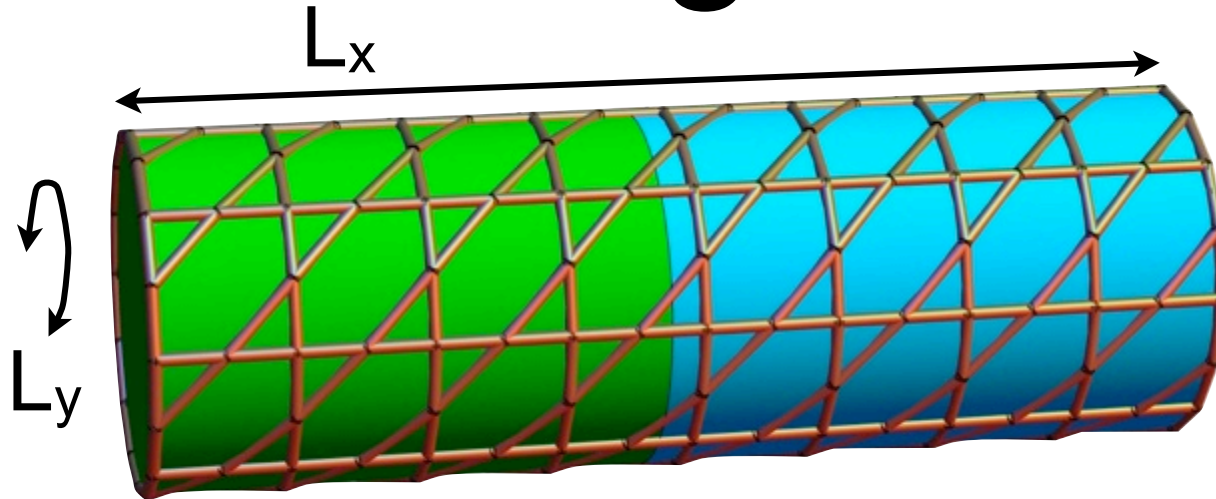
- Hamiltonian

$$H_{\text{eff}} = -h (|0\rangle\langle 1| + |1\rangle\langle 0|) - h' (|0\rangle\langle 0| - |1\rangle\langle 1|)$$

vison hopping $h \sim h_0 L_y e^{-L_x/\xi}$

spinon hopping $h' \sim h'_0 L_x e^{-L_y/\xi}$

Quasi-degeneracy



- Hamiltonian

GS is MES for L_x large

$$H_{\text{eff}} = -h (|0\rangle\langle 1| + |1\rangle\langle 0|) - h' (|0\rangle\langle 0| - |1\rangle\langle 1|)$$

vison hopping

$$h \sim h_0 L_y e^{-L_x/\xi}$$

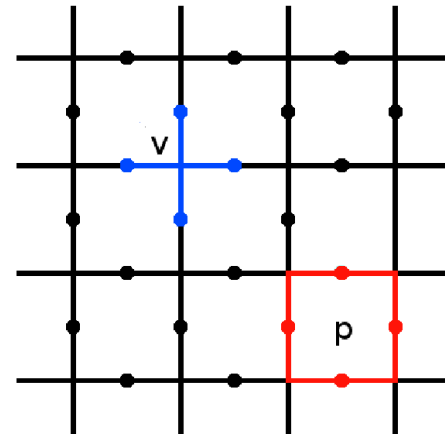
spinon hopping

$$h' \sim h'_0 L_x e^{-L_y/\xi}$$

Toric Code model

- Hamiltonian

$$H_{TC} = - \sum_s A_s - \sum_p B_p$$



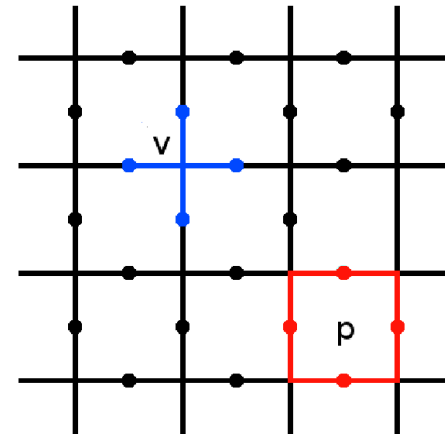
$$A_s = \prod_{\mu} \sigma_{s+\mu}^x$$

$$B_p = \prod_{\mu} \sigma_{p+\mu}^z$$

Toric Code model

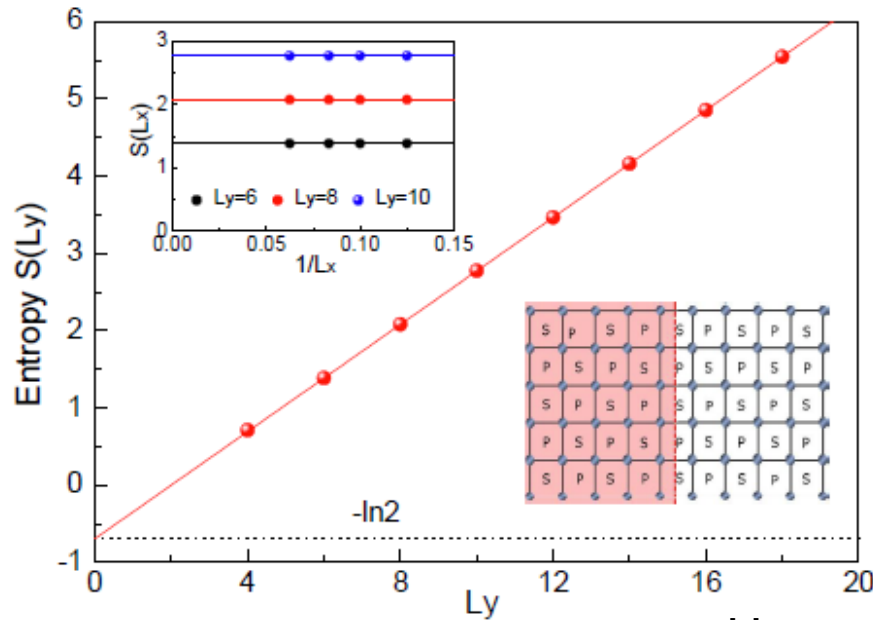
- Hamiltonian

$$H_{TC} = - \sum_s A_s - \sum_p B_p$$



$$A_s = \prod_{\mu} \sigma_{s+\mu}^x$$

$$B_p = \prod_{\mu} \sigma_{p+\mu}^z$$



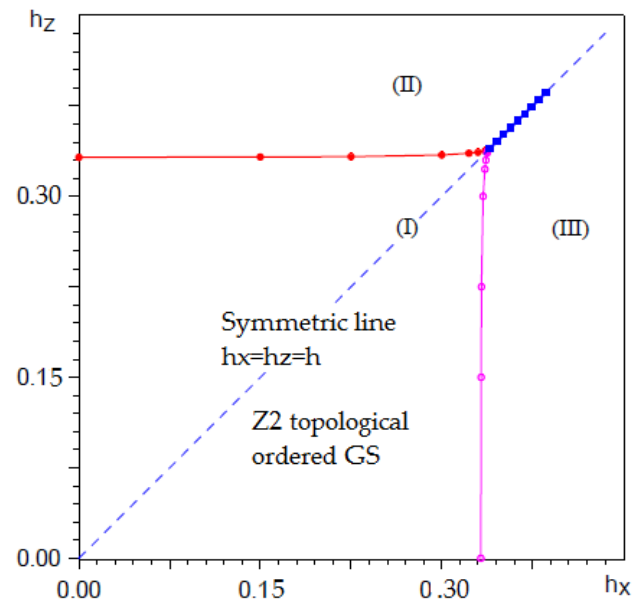
$$S = \frac{\ln 2}{2} L_y - \ln 2$$

Perturbed Toric Code

- Hamiltonian:

$$H = H_{TC} - \sum_i [h_x \sigma_i^x + h_z \sigma_i^z]$$

- Phase diagram:

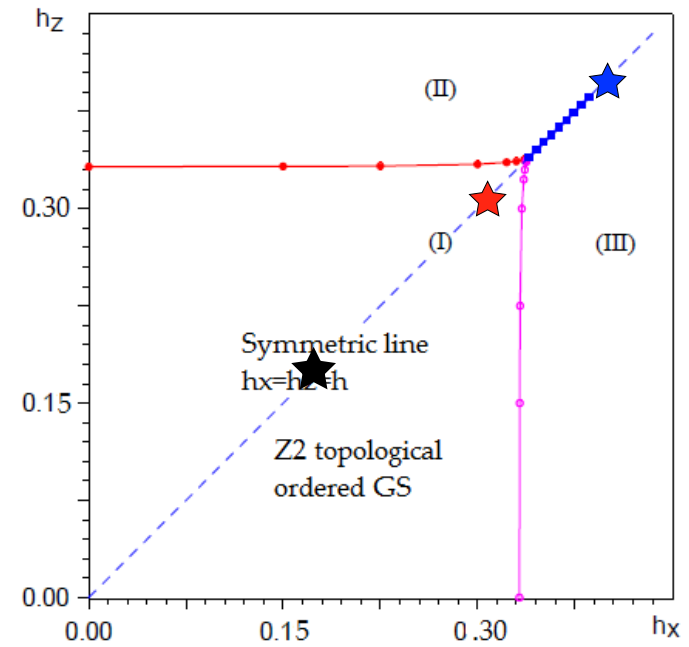
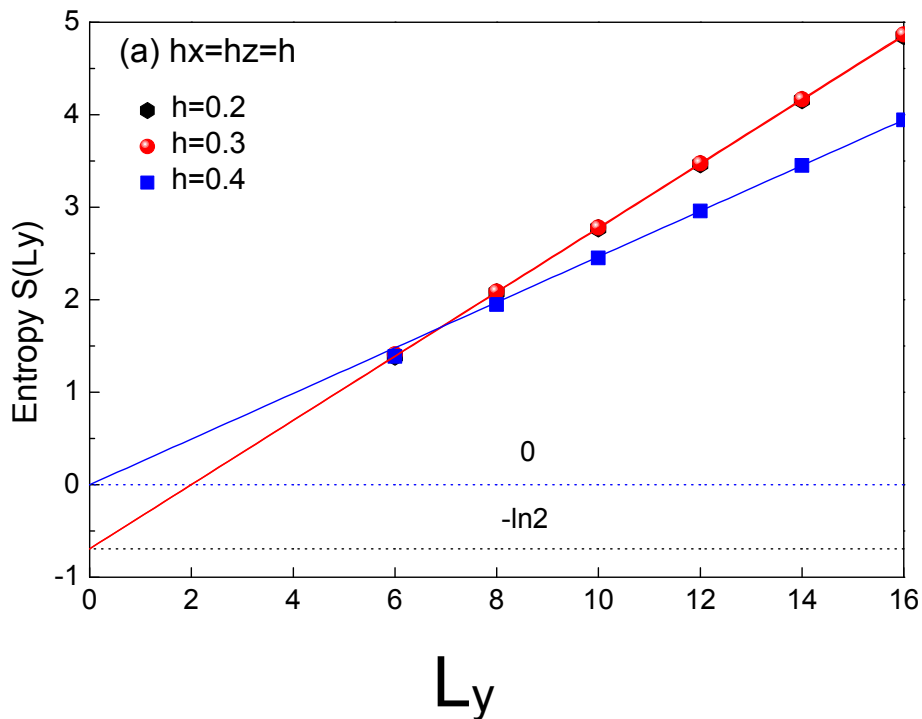


Tupitsyn *et al*,
2010

Perturbed Toric Code

- Hamiltonian:

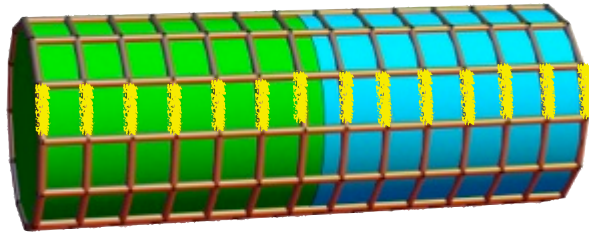
$$H = H_{TC} - \sum_i [h_x \sigma_i^x + h_z \sigma_i^z]$$



Perturbed Toric Code

- State dependence: $h_z = 0$

$$G = |0\rangle\langle 1| + |1\rangle\langle 0| = \prod_x \sigma_{i=(x,y)}^x \quad [G, H] = 0$$

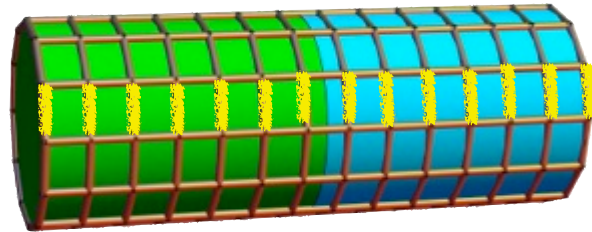


- The absolute ground state is a G eigenstate, $|\pm\rangle$, *not* a MES

Perturbed Toric Code

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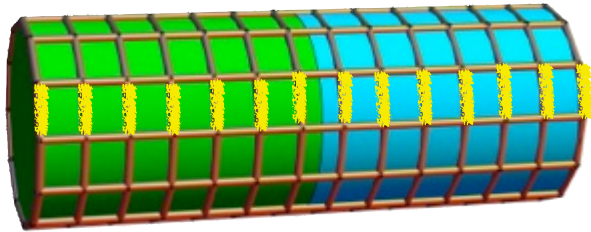
- The absolute ground state is a G eigenstate, $|\pm\rangle$, *not* a MES

$$H_{\text{eff}} = -h (|0\rangle\langle 1| + |1\rangle\langle 0|) - h' (|0\rangle\langle 0| - |1\rangle\langle 1|)$$

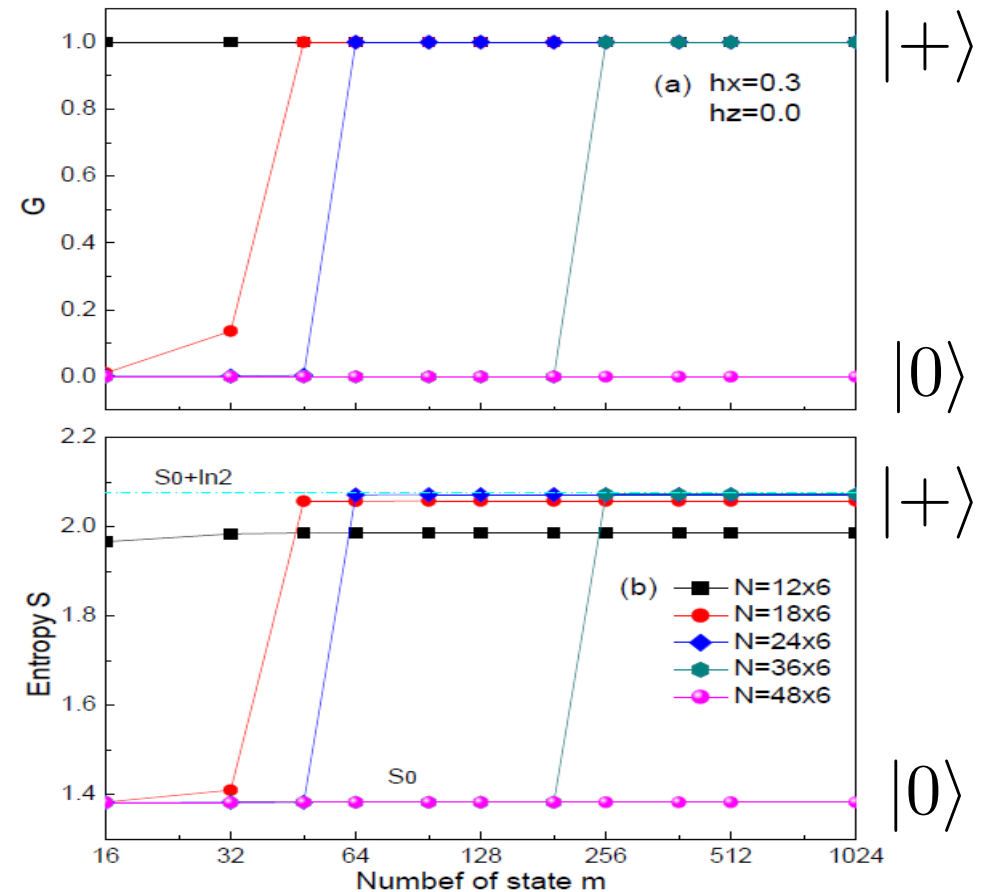
=0

Perturbed Toric Code

- State dependence: $h_z = 0$

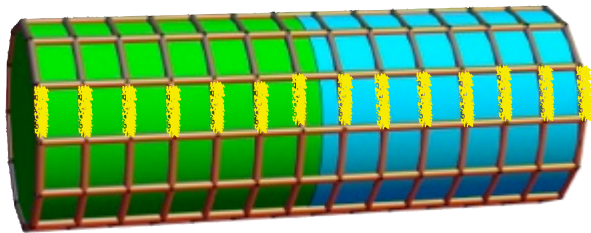


$$G|\pm\rangle = \pm|\pm\rangle$$



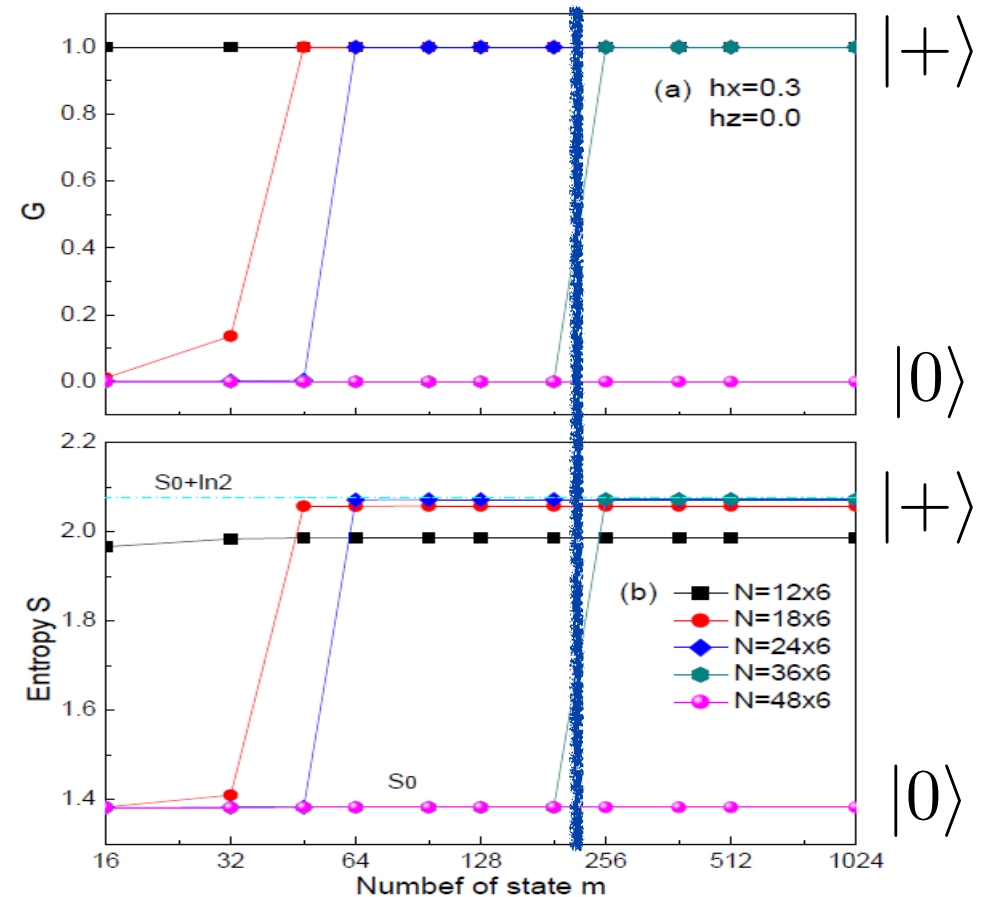
Perturbed Toric Code

- State dependence: $h_z = 0$ m_c



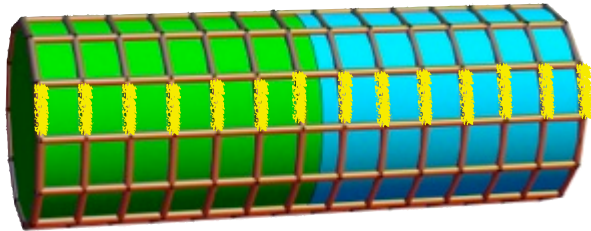
$$G|\pm\rangle = \pm|\pm\rangle$$

DMRG
favors MES

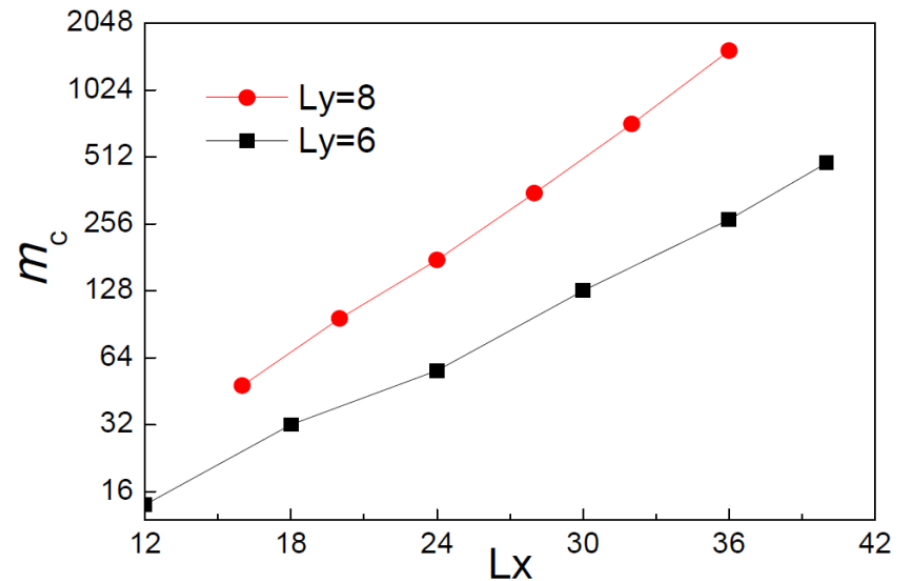


Perturbed Toric Code

- State dependence: $h_z = 0$



$$G|\pm\rangle = \pm|\pm\rangle$$

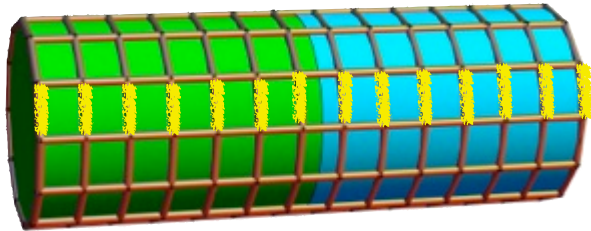


$$m_c \sim m_0 e^{cL_x}$$

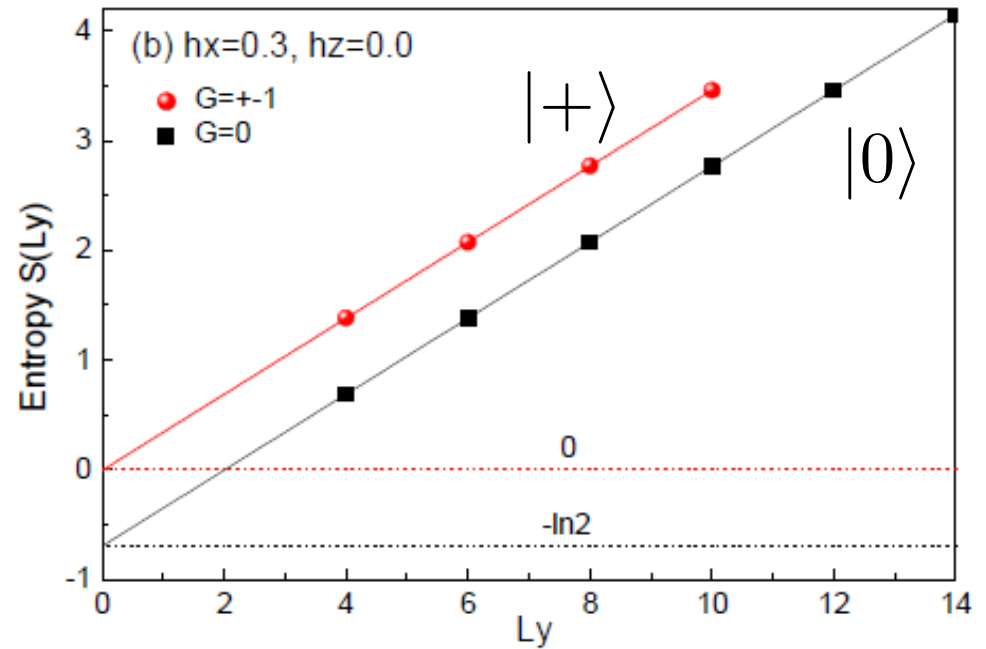
last qubit of entanglement takes exponential effort

Perturbed Toric Code

- State dependence: $h_z = 0$



$$G|\pm\rangle = \pm|\pm\rangle$$

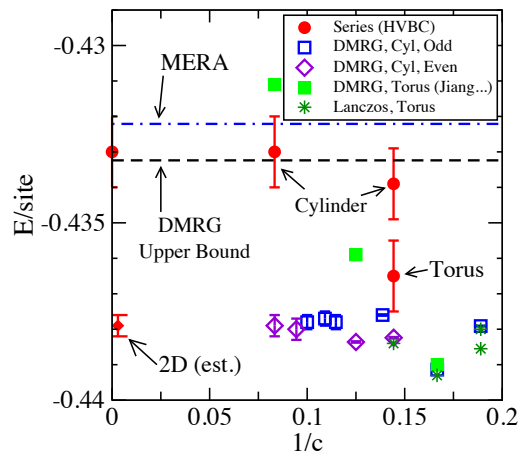
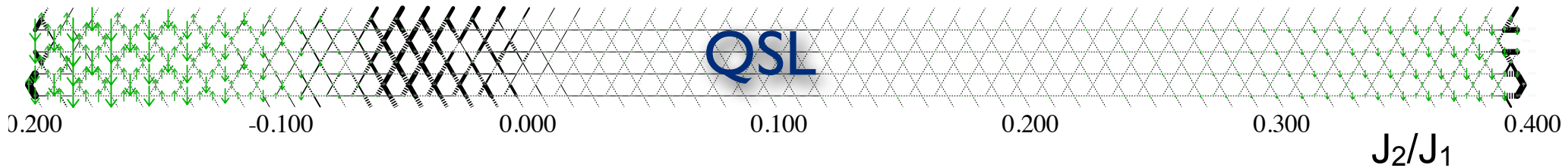
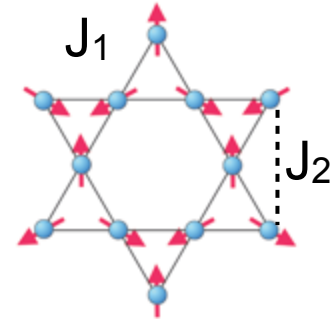


Kagome

- Hamiltonian

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

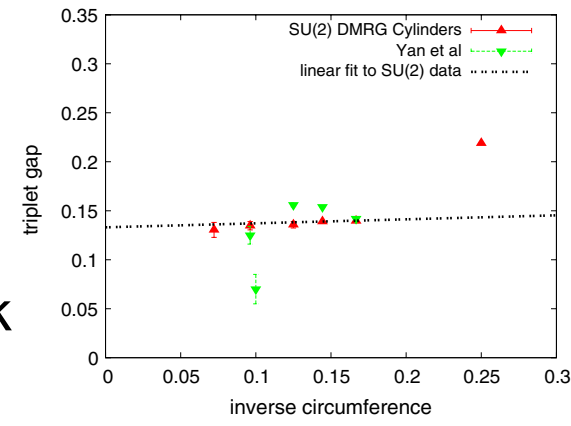
- Courtesy of Steve White:



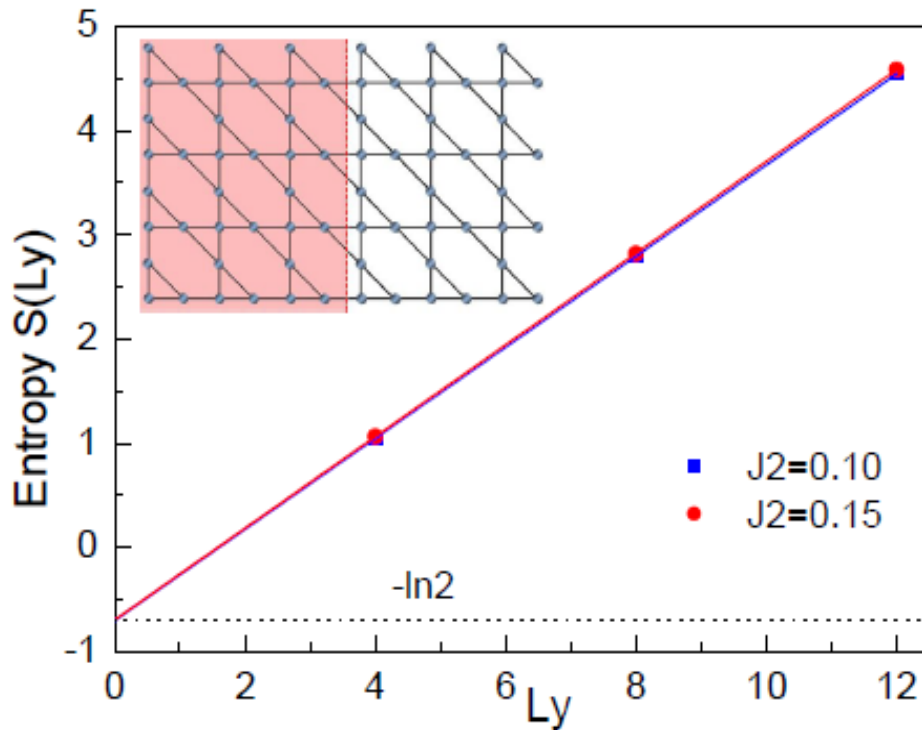
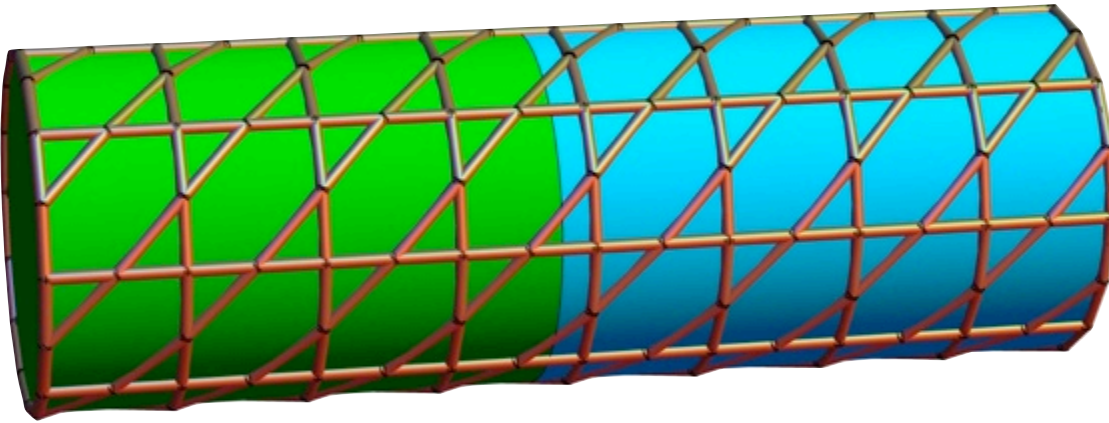
S. Yan *et al*, 2010

a Z_2 state?

S. Depenbrock *et al*, 2012



Kagome



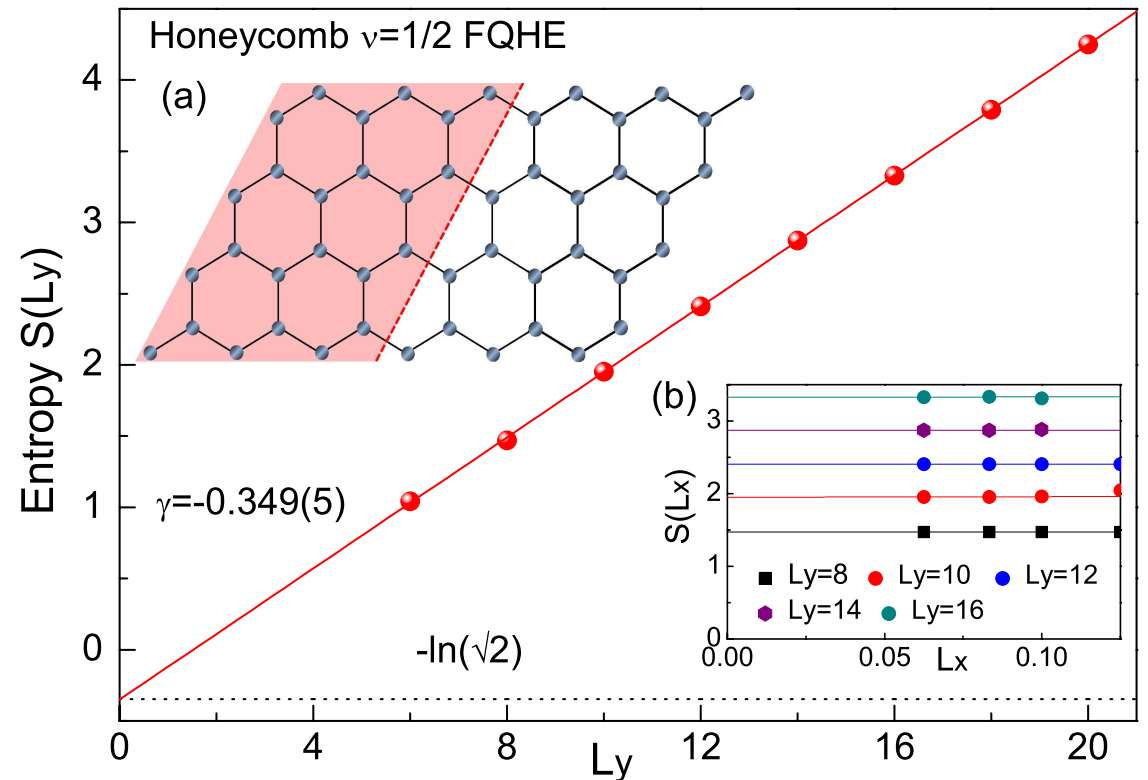
$$\gamma = \begin{cases} 0.698(8) & J_2 = 0.10 \\ 0.694(6) & J_2 = 0.15 \end{cases}$$

$$[\ln(2) = 0.693 \dots]$$

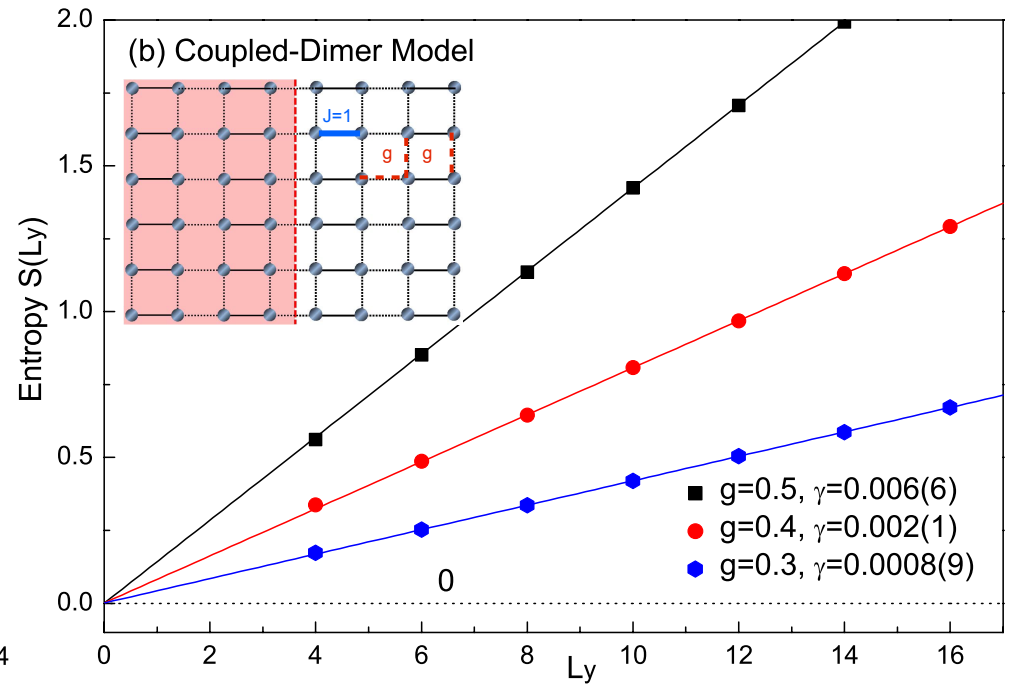
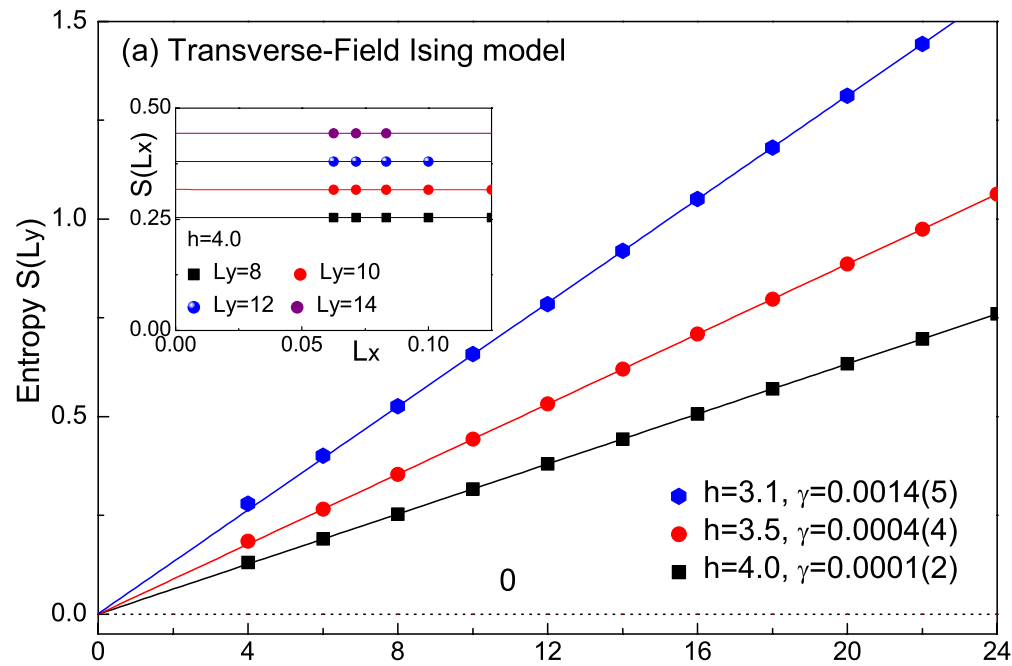
$\nu=1/2$ FQHE

$$H = -t' \sum_{\langle\langle rr' \rangle\rangle} \left[b_{r'}^\dagger b_r e^{i\phi_{r'r}} + \text{H.c.} \right]$$

$$- t \sum_{\langle rr' \rangle} \left[b_{r'}^\dagger b_r + \text{H.c.} \right] - t'' \sum_{\langle\langle\langle rr' \rangle\rangle\rangle} \left[b_{r'}^\dagger b_r + \text{H.c.} \right],$$



Not topological



Von Neumann vs. Renyi

strong
subadditivity

correspondence
to true entropy



dS_n/dn
 < 0

replica
field
theory

QMC

Both are expected to give universal TEE

Von Neumann vs. Renyi

strong subadditivity

correspondence to true entropy



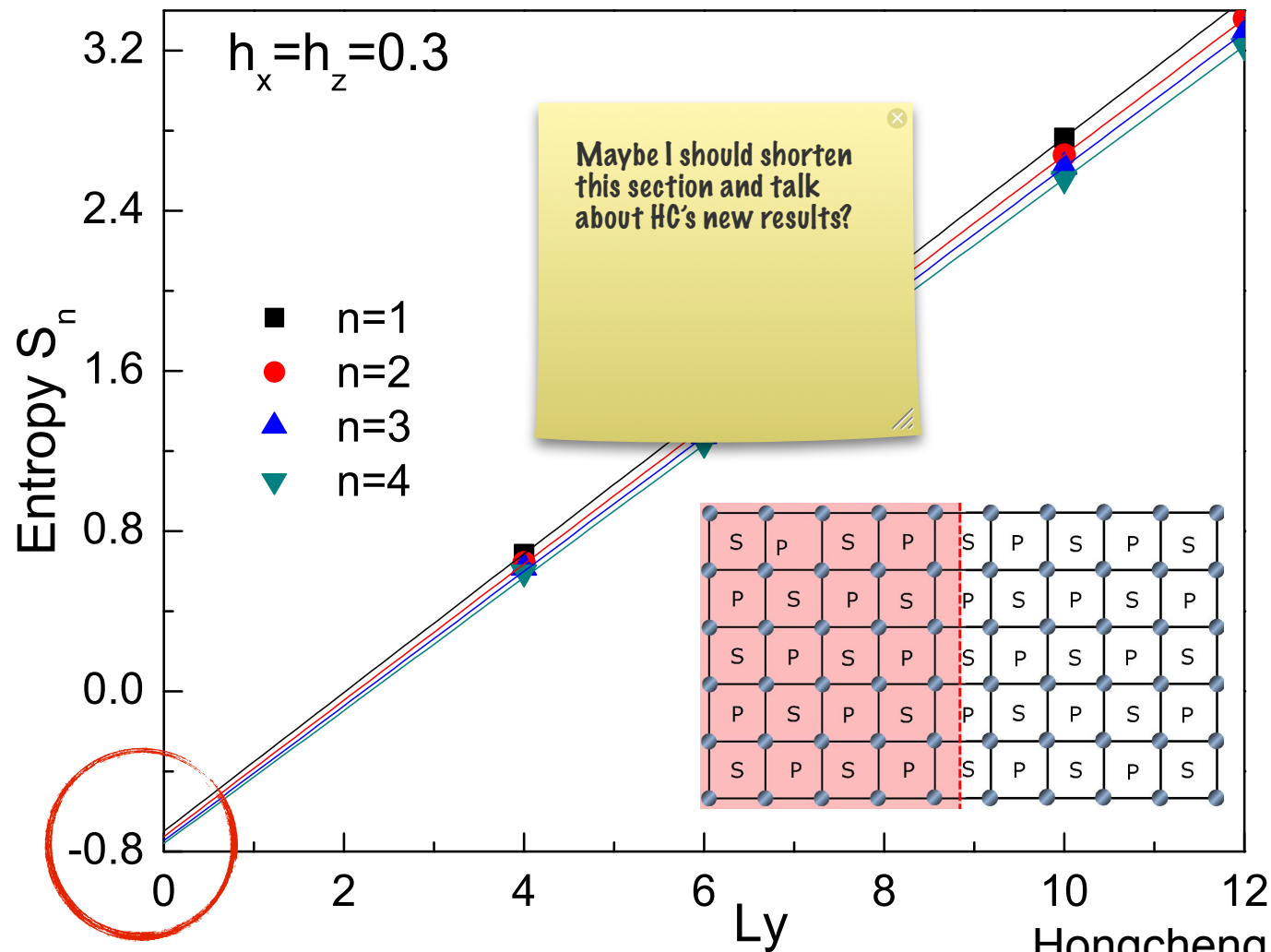
$dS_n/dn < 0$

replica field theory

QMC

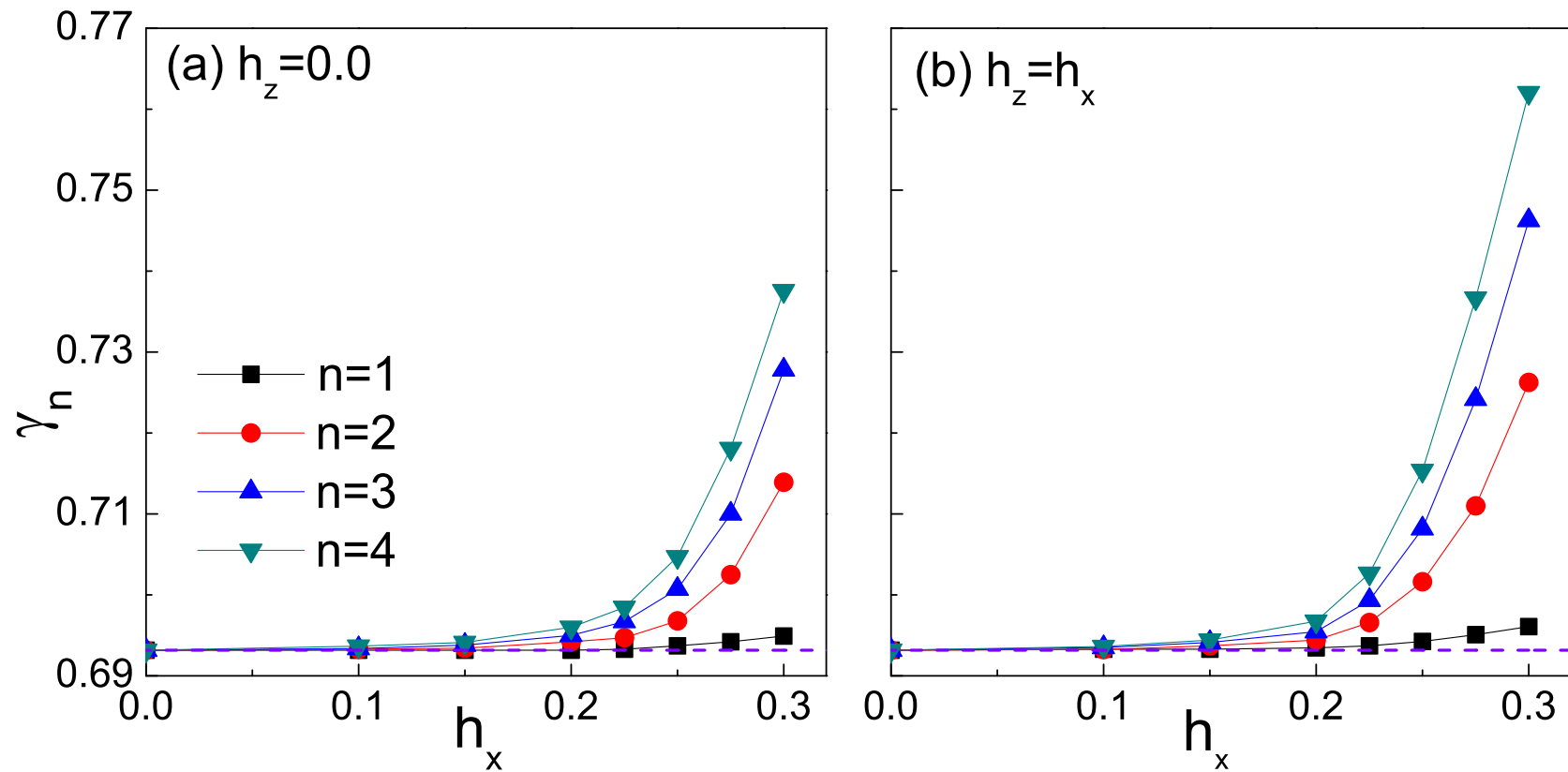
Numerical result: Renyi scales *much* worse

Trouble?



Trouble?

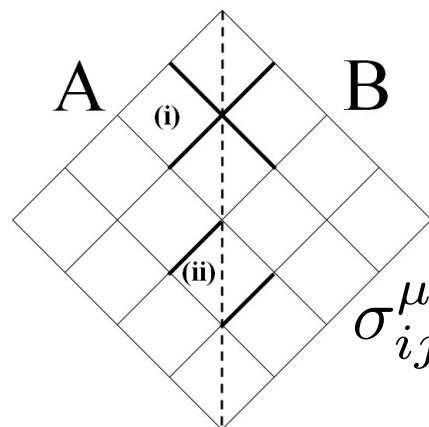
- Naively extrapolated TEE



Series Expansion

- We can check the DMRG, and get some insight, from numerical series expansion
- We use the linked cluster method, where the series can be extracted from a study of exact solutions on small clusters

clusters to $O(h^4)$



toric code
variables on
links

Series Expansion

- Entanglement entropy is *exactly* linear in L_y until clusters span cylinder width

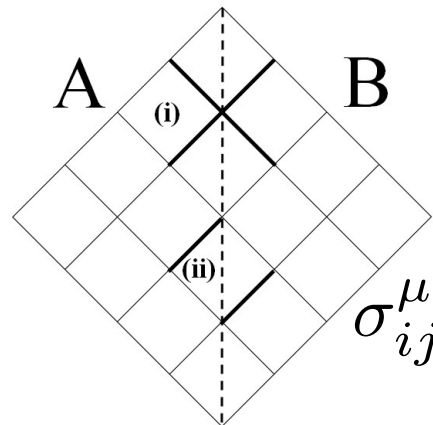
$$S_\alpha = c_\alpha L_y - \ln 2$$

line
entropy

$$c_\alpha = \frac{1}{2} \left(\ln 2 - \frac{9\alpha}{32} h^4 + \frac{3\alpha}{\alpha - 1} \frac{h^4}{128} \right)$$

$$h_x = h, h_z = 0$$

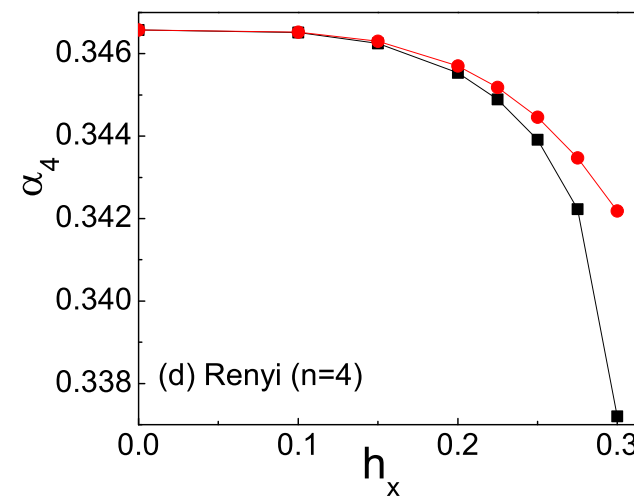
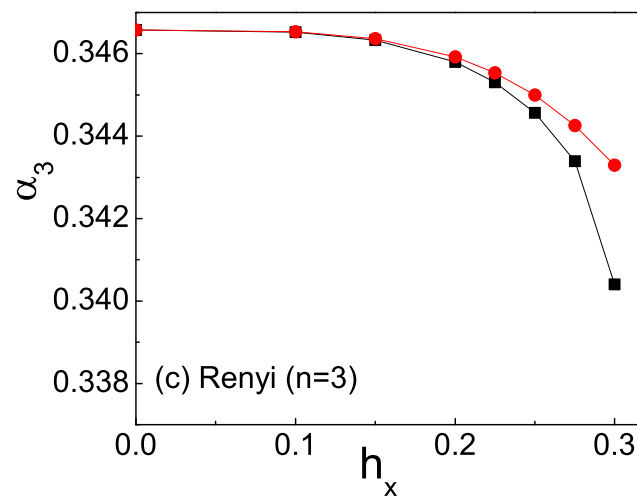
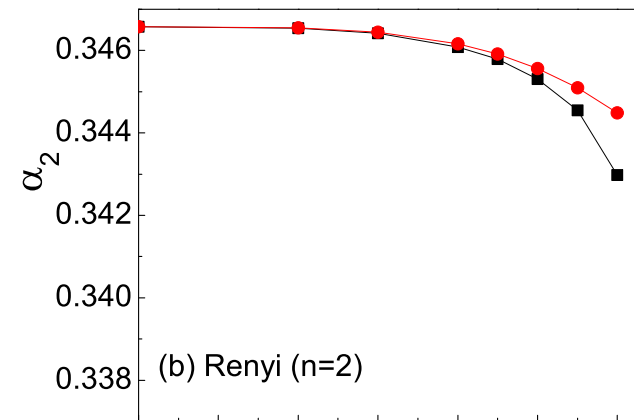
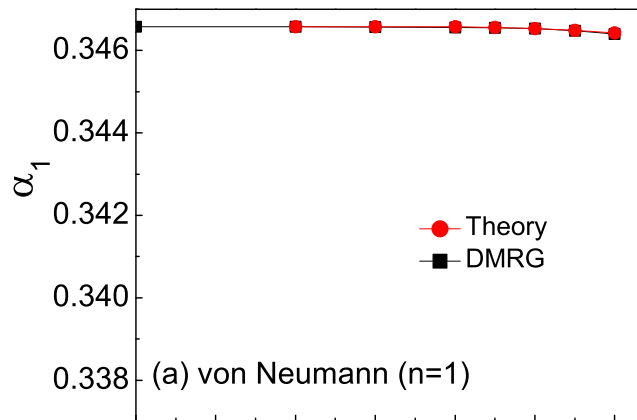
clusters to $O(h^4)$



toric code
variables on
links

Line Entropy

reasonable agreement for $O(h^4)$ expansion



$h_x = h, h_z = 0$

$h_c \approx 0.33$

TEE

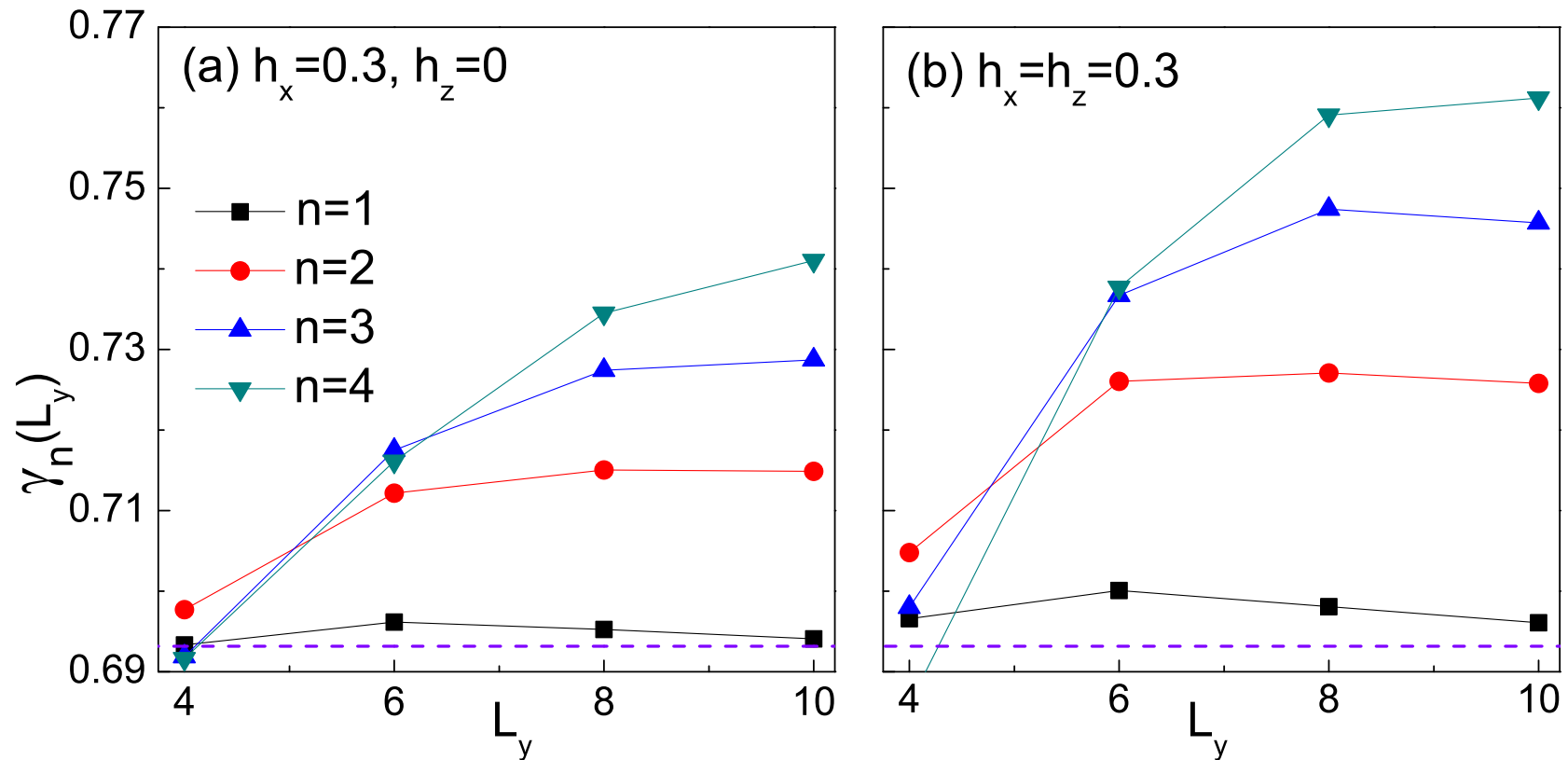
- TEE is *subdominant* term in an *asymptotic* large L_y expansion
- Reliable extraction is more difficult with increasing line entropy

$$c_\alpha = \frac{1}{2} \left(\ln 2 - \frac{9\alpha}{32} h^4 + \frac{3\alpha}{\alpha - 1} \frac{h^4}{128} \right)$$

large sensitivity of line entropy
with increasing Renyi index:
larger L_y needed to extract TEE?

TEE

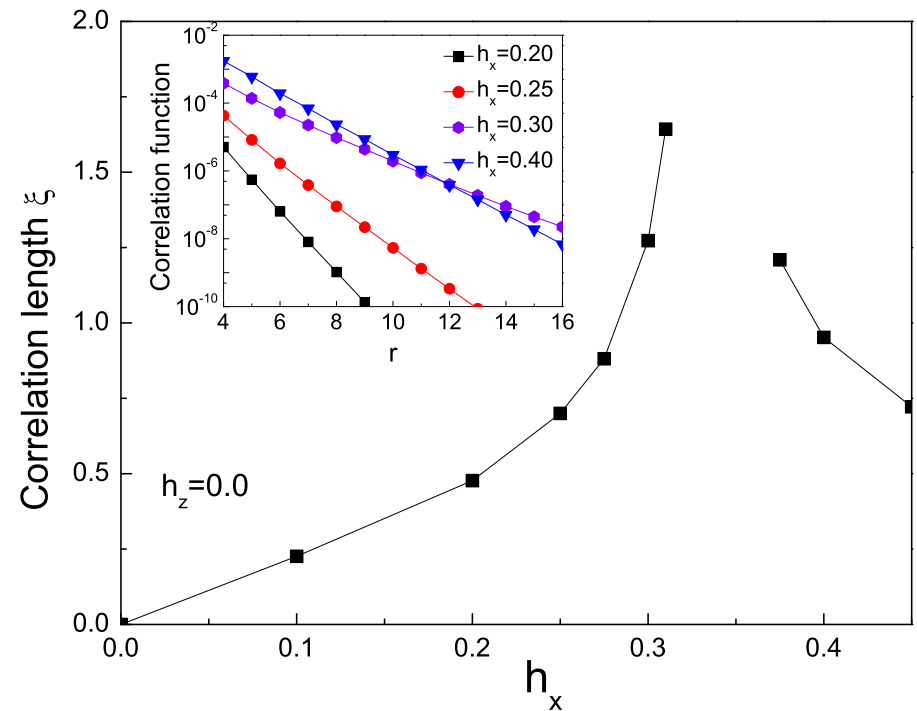
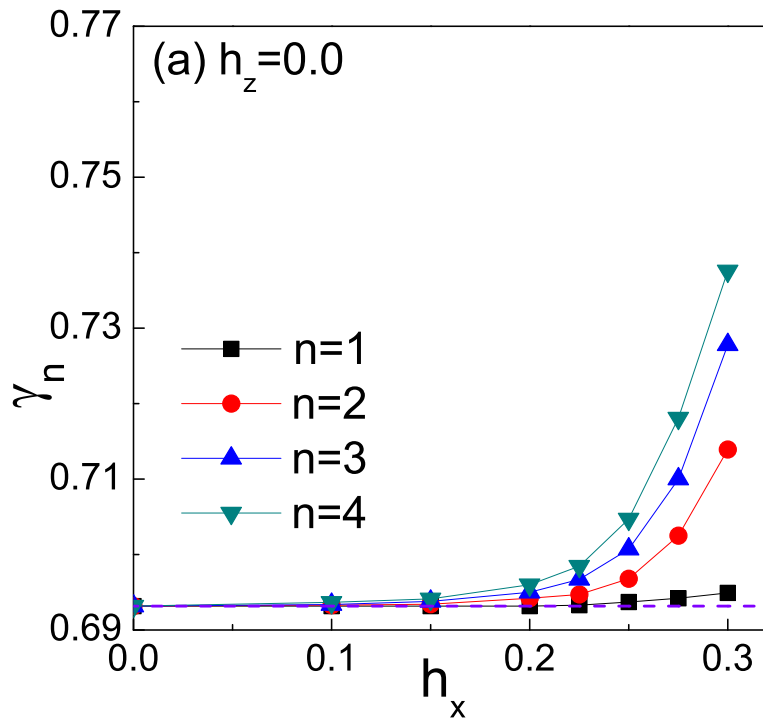
- Running two point fits at L_y and L_{y+2}



non-monotonic behavior: still far from converging for Renyi entropies

TEE

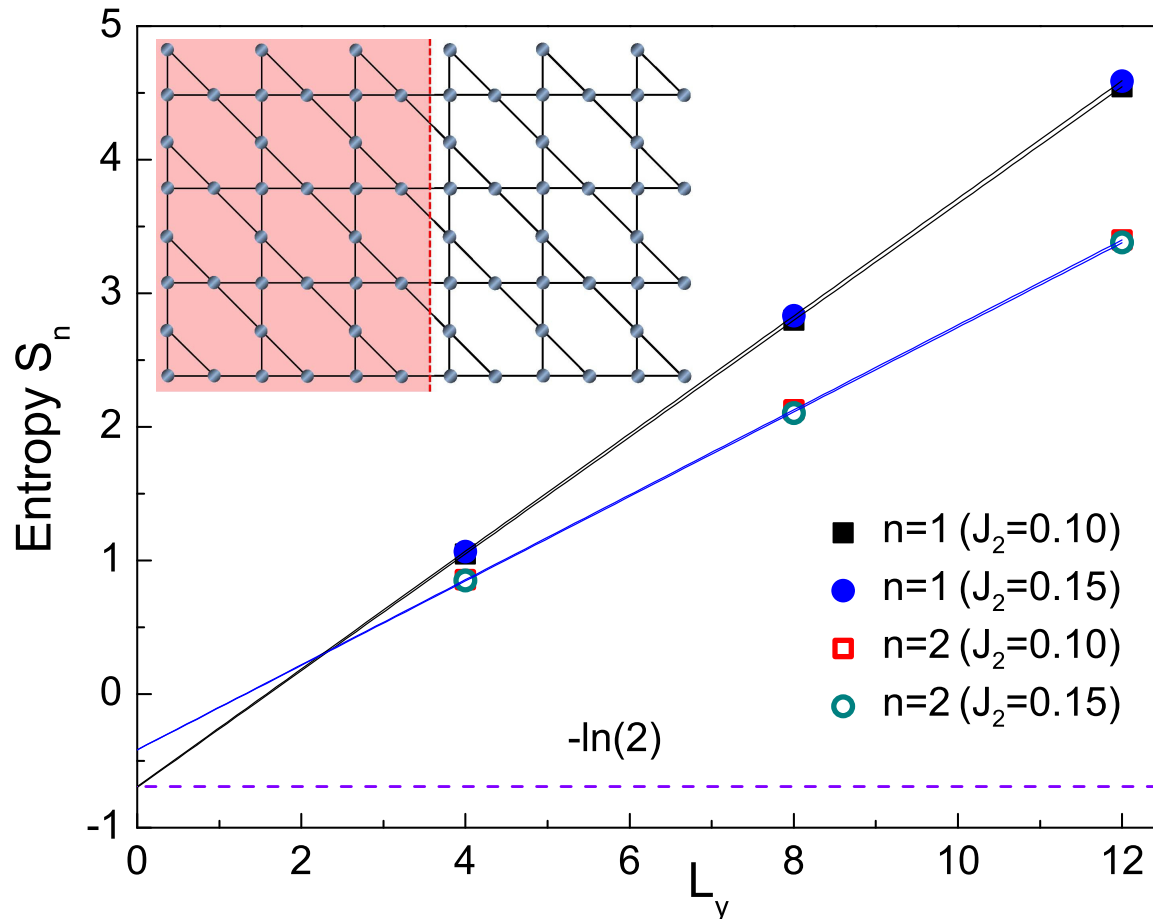
- Correlation length criteria?



S_{vN} determines TEE to $< 1\%$ for $L_y/\xi \approx 10$

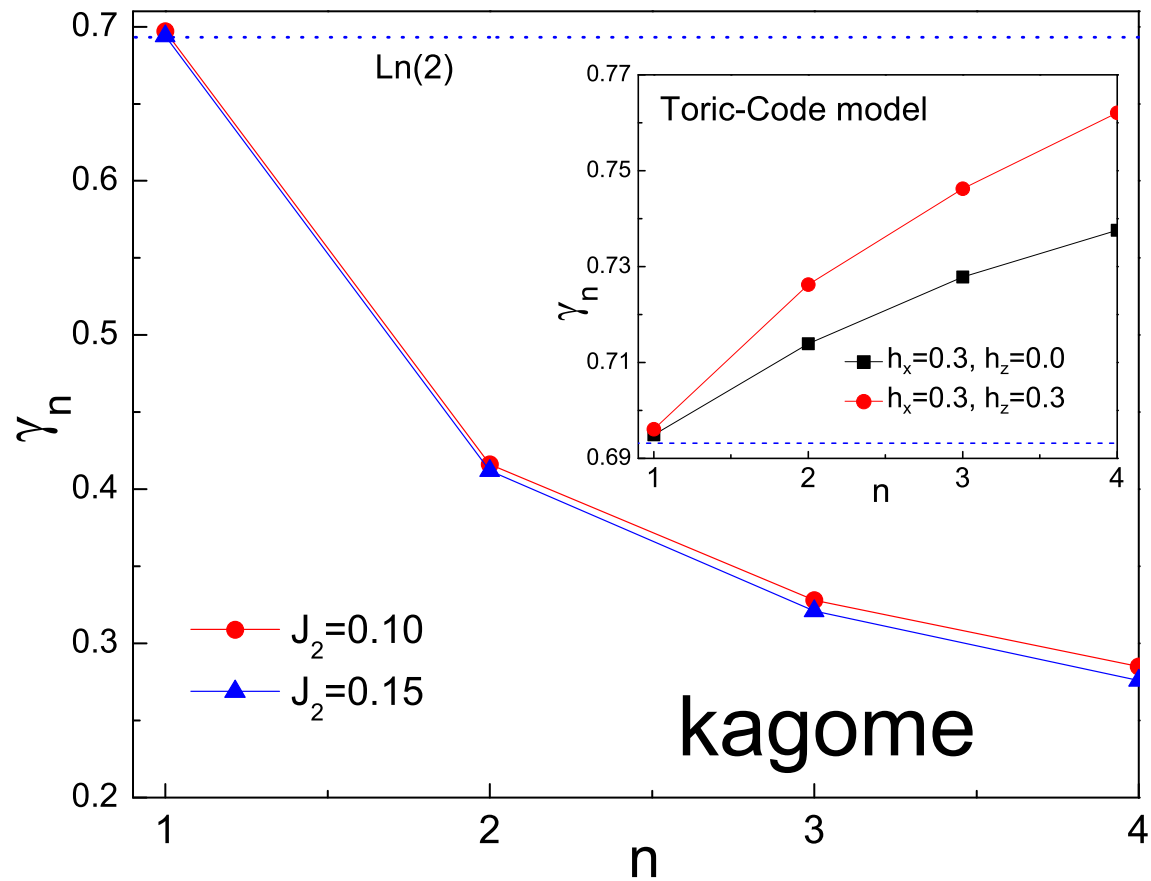
Kagome

- Problems even more severe



Kagome

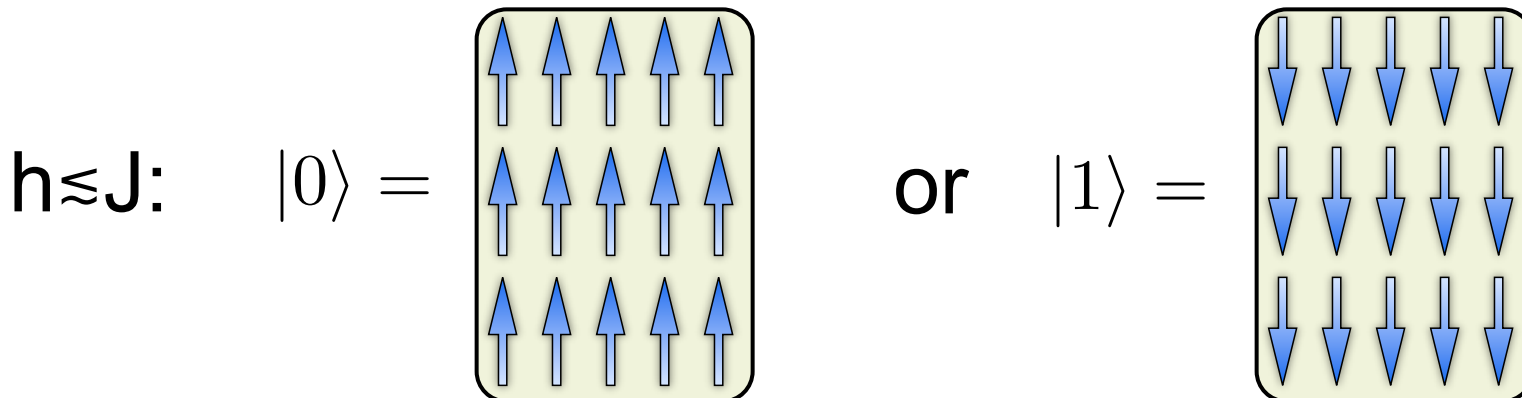
- Problems even more severe



more on MES

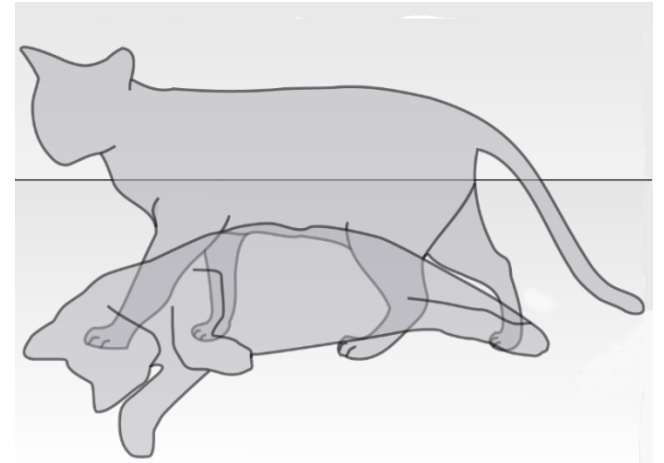
- Long-range entanglement can arise even in non-exotic systems
- Symmetry breaking

$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z - h \sum_i S_i^x$$



more on MES

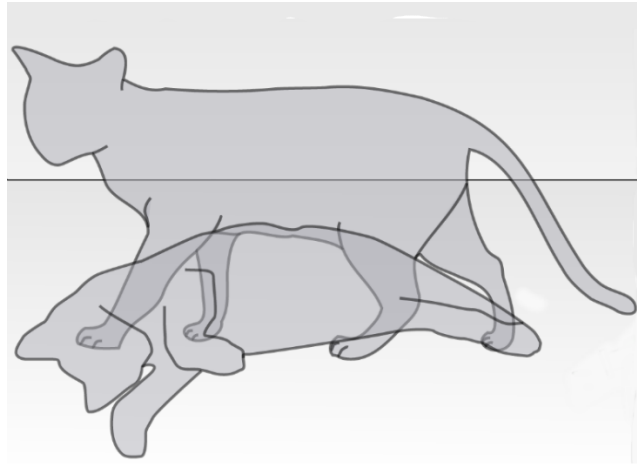
- Schrödinger cat



$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z - h \sum_i S_i^x$$

$h \approx J$: $|\pm\rangle = \frac{1}{\sqrt{2}} \left(\begin{array}{c} \uparrow \uparrow \uparrow \uparrow \uparrow \\ \uparrow \uparrow \uparrow \uparrow \uparrow \\ \uparrow \uparrow \uparrow \uparrow \uparrow \end{array} \pm \begin{array}{c} \downarrow \downarrow \downarrow \downarrow \downarrow \\ \downarrow \downarrow \downarrow \downarrow \downarrow \\ \downarrow \downarrow \downarrow \downarrow \downarrow \end{array} \right)$

Schrödinger cat



- Cat state is the global ground state
- BUT...undesirable
 - Not physical: decoherence collapses the cat into a symmetry broken state
 - Cannot directly measure local observables

Long-range entanglement

- The cat state has higher entanglement

$$S(|\pm\rangle) = S(|0\rangle, |1\rangle) + \ln 2$$

- To get it requires capturing entanglement between farthest pairs of spins in the system
- DMRG will avoid this state for *very long systems*, finding MES (physical!)

Long-range entanglement

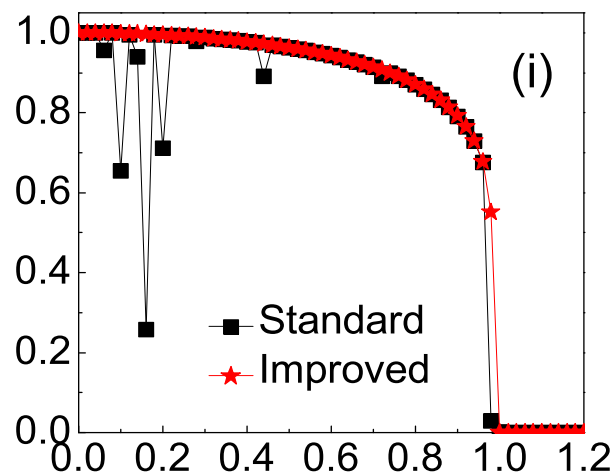
- The cat state has higher entanglement

$$S(|\pm\rangle) = S(|0\rangle, |1\rangle) + \ln 2$$

- To get it requires capturing entanglement between farthest pairs of spins in the system
- BUT, for shorter systems, or long simulations, the cat appears

Cat states

- The “best” simulations find a superposition (partial cat)
- local quantities, e.g. magnetization of Ising model, can be any value between $\pm m$

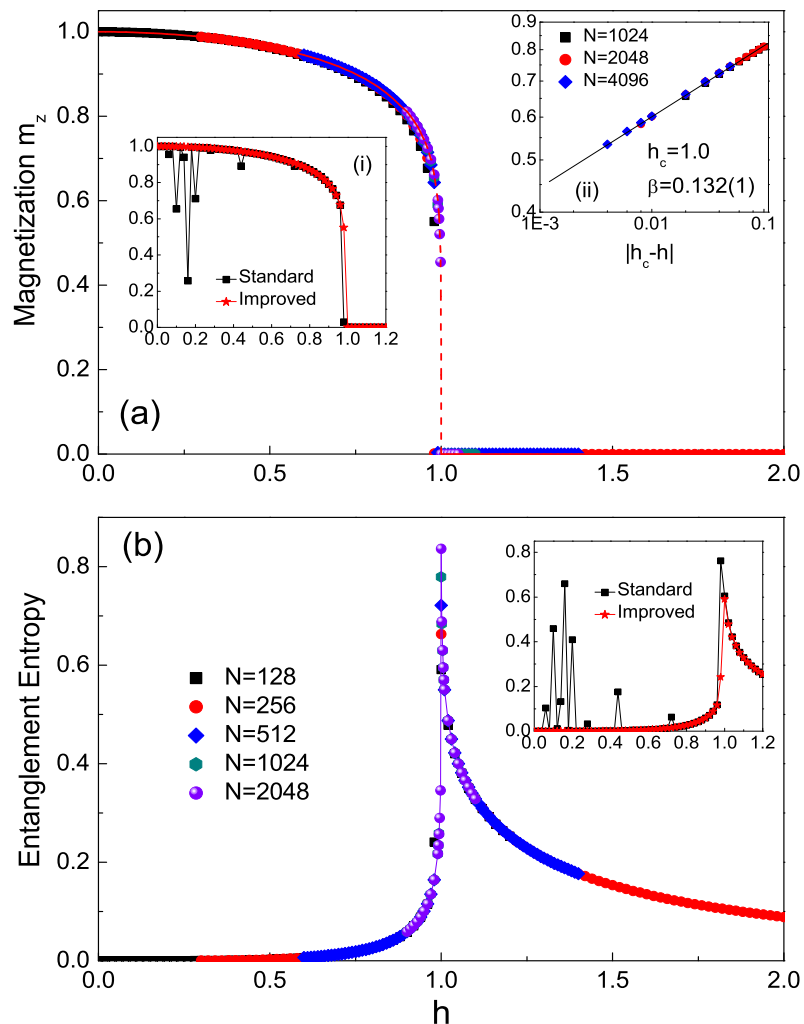


Collapse the cat



- It can be useful to select a MES by making small “observations” of the state
- This can be done in DMRG by introducing a “quench” - a short period of increased truncation error - followed by recovery

TFIM



- This procedure allows a *direct* measurement of order parameters, critical properties, etc
- One obtains a MES *without a priori* knowledge of broken symmetry, topological order, etc., even for “short” systems

Fin

- DMRG is remarkably efficient at obtaining TEE for realistic quantum spin models with short correlation lengths from the *von Neumann* entropy
- Empirically, the scaling limit occurs only in prohibitively large systems for the Renyi entropies
- Definitive identification of the kagome lattice QSL as a Z_2 topological phase. In the future we should use the methods to push connections to experiments on e.g. herbertsmithite
- MES are also useful for study of more conventional phases