Thermal Tensor Network Approach for Quantum Many-Body systems

Bin-Bin Chen

Oct. 19, 2022

Outline

1. Finite-T tensor network methods

- 1.1 Tensor network basis
- 1.2 Series-expansion thermal tensor network
- 1.3 Exponential tensor renormalization group
- 1.4 Differentiable tensor renormalization group

2. Application 1

- 2.1 Square-lattice Hubbard model
- 2.2 Triangular-lattice Hubbard model
- 2.3 Magic-angle twisted bilayer graphene model

3. Application 2

- 3.1 Quantum entanglement and disorder operator
- 3.2 topological disorder operator

➢ 1.1 Motivation

❑ Strong Correlated systems:

- High-T superconductivity in cuprate
- Quantum spin liquid
- Magic-angle twisted bilayer graphene
- …

“Exponential wall”

“Wheat and chessboard” problem

- **Quantum Monte Carlo (QMC)**

  Negative sign problem

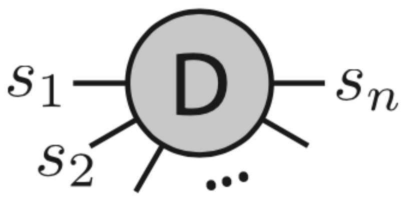
- **Tensor Network (TN)**

  capture the entanglement structure

➢ 1.1 Tensor network basis

❑ Basic terminology

- Rank-n Tensor

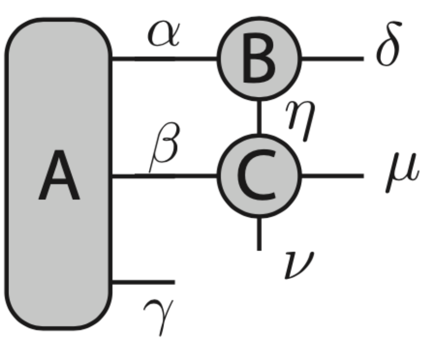


$$D_{s_1,\ s_2,\ldots,\ s_n}$$

[special cases]

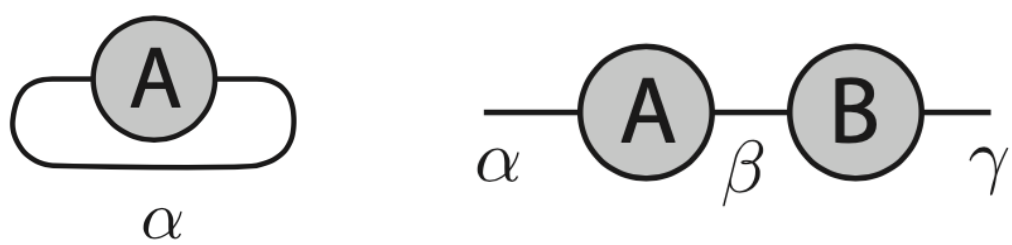
scalar vector matrix

- Contraction



$$\sum_{\alpha,\beta,\eta} A_{\alpha,\beta,\gamma} B_{\alpha,\delta,\eta} C_{\beta,\eta,\mu,\nu}$$

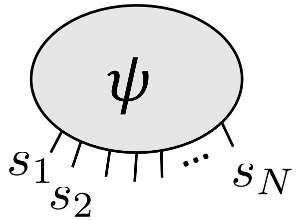
[special cases]



trace matrix product

➢ 1.1 Tensor network basis

❑ Manybody wavefunction

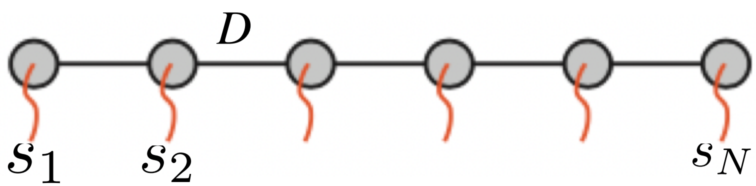


\# of parameters: d^N

Exponential wall!

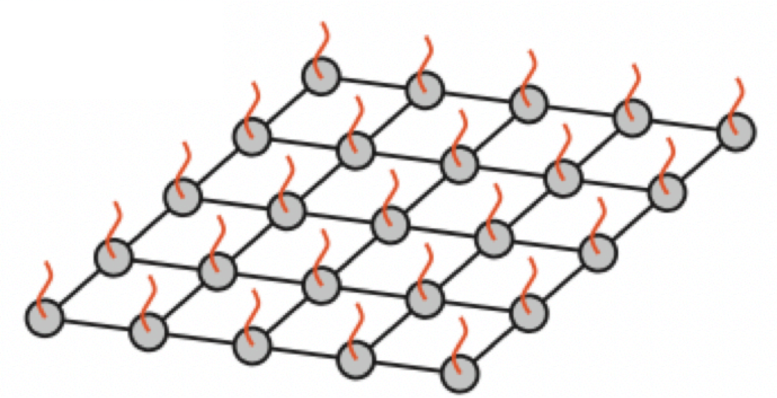
❑ Typical Tensor Network

✓ Matrix Product State (MPS)



$\sim N \times (dD^2)$

✓ Projected Entangled-Pair State (PEPS)

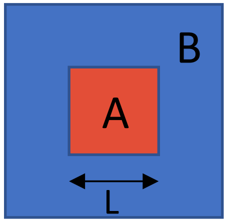


$\sim N \times (dD^4)$

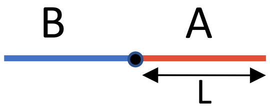
1.1 Tensor network basis

✓ Remarkable fact: For Hamiltonians with local interactions, the ground state entanglement entropy is governed by an "area law"(Eisert2010).

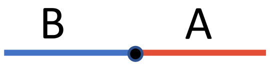
E.g., for 2D gapped systems, $S_E \sim L$



E.g., for 1D gapped systems, $S_E \sim \text{const.}$



E.g., for 1D gapless systems, $S_E \sim \ln L$



For a bond with dimension D, entanglement entropy $S_E = -\text{Tr}\rho_A \ln \rho_A \leq \ln D$

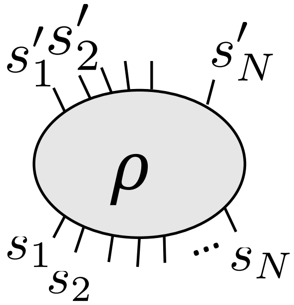
Then, for 2D gapped systems, $D \geq e^{S_E} \sim e^L$

for 1D gapped systems, $D \geq e^{S_E} \sim \text{const.}$ (independent of system size)

for 1D gapless systems, $D \geq e^{S_E} \sim L^\alpha$ (polynomial resources)

➢ 1.1 Tensor network basis

❑ Density operator

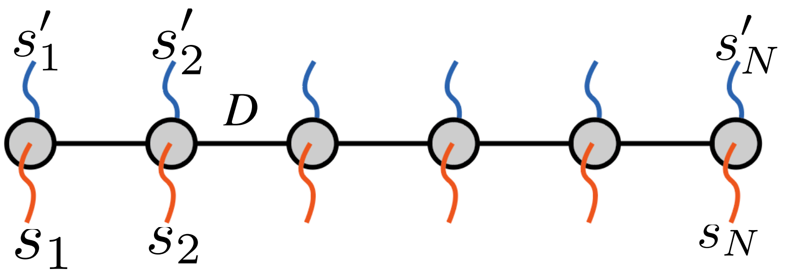


# of parameters: d^{2N}

Exponential wall!

❑ Typical Tensor Network

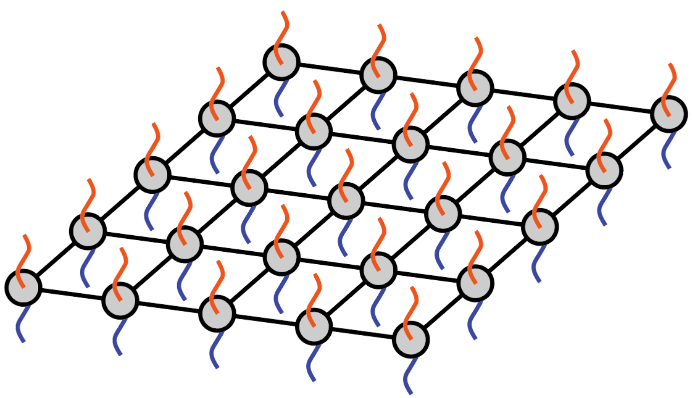
✓ Matrix Product Operator (MPO)



$\sim N \times (d^2 D^2)$

W. Li, et al. 2011; Dong, et al. 2017

✓ Projected Entangled-Pair Operator (PEPO)



$\sim N \times (d^2 D^4)$

Czarnik, et al. 2017

1.1 Path-Integral Thermal Tensor Network

Partition function for Hamiltonian with local interactions $H = \sum_i h_{i,i+1} = \sum_i S_i \cdot S_{i+1}$

$$Z = \mathrm{Tr}\ e^{-\beta H} = \mathrm{Tr}\ e^{-\beta \sum_i h_{i,i+1}}$$

$$= \sum_{\vec{\sigma}^1} \langle \vec{\sigma}^1 | e^{-\beta \sum_i h_{i,i+1}} | \vec{\sigma}^1 \rangle \qquad |\vec{\sigma}\rangle := |\sigma_1, \sigma_2, \cdots, \sigma_N\rangle$$

$$= \sum_{\vec{\sigma}^1, \vec{\sigma}^2, \cdots, \vec{\sigma}^M} \langle \vec{\sigma}^1 | e^{-\frac{\beta}{M} \sum_i h_{i,i+1}} | \vec{\sigma}^M \rangle \cdots \langle \vec{\sigma}^3 | e^{-\frac{\beta}{M} \sum_i h_{i,i+1}} | \vec{\sigma}^2 \rangle \langle \vec{\sigma}^2 | e^{-\frac{\beta}{M} \sum_i h_{i,i+1}} | \vec{\sigma}^1 \rangle$$

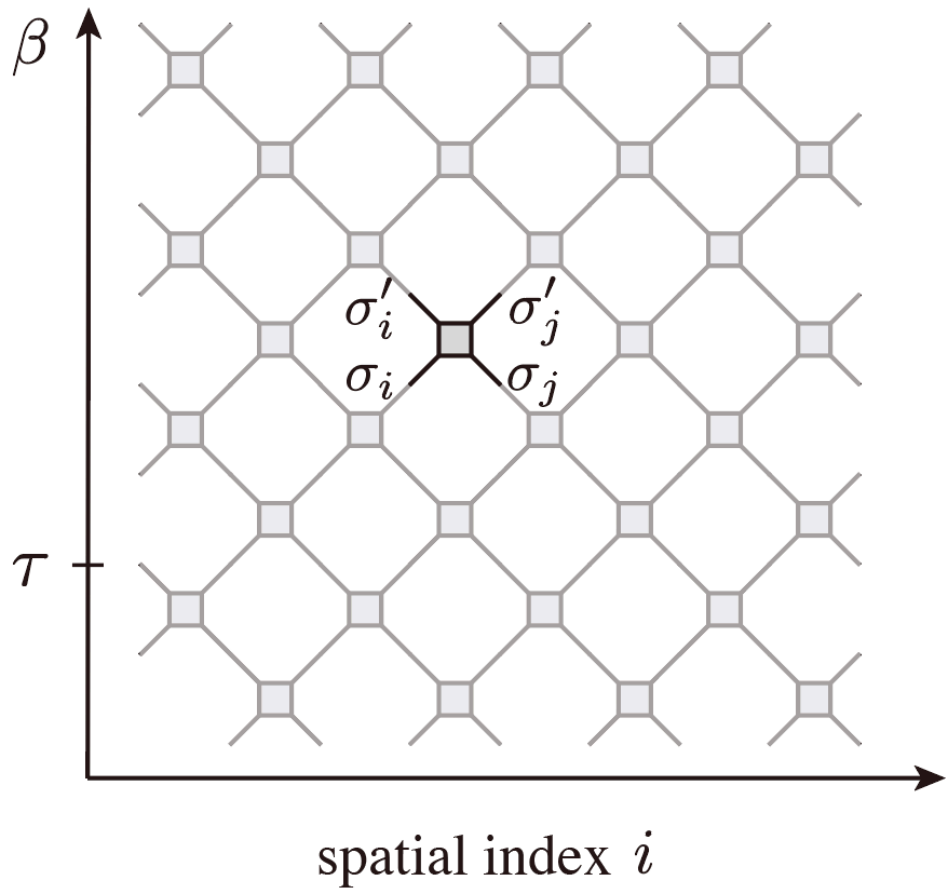
$$= \sum_{\vec{\sigma}^j} \prod_{j=1}^{M} \langle \vec{\sigma}^{j+1} | e^{-\tau \sum_i h_{i,i+1}} | \vec{\sigma}^j \rangle$$

$$= \sum_{\{\sigma_i^j\}} \prod_{i=1}^{N} \prod_{j=1}^{M} \langle \sigma_i^{j+1} \sigma_{i+1}^{j+1} | e^{-\tau h_{i,i+1}} | \sigma_i^j \sigma_{i+1}^j \rangle + O(\tau^2)$$

➢ 1.1 Path-Integral Thermal Tensor Network

$$Z = Tr(e^{-\beta H}) \xrightarrow{\text{Trotter}} Z \approx \sum_{\{\sigma_i^j\}} \prod_{i=1}^{N} \prod_{j=1}^{M} \langle \sigma_i^{j+1} \sigma_{i+1}^{j+1} | e^{-\tau h_{i,i+1}} | \sigma_i^j \sigma_{i+1}^j \rangle$$

- 1+1D Tensor Network



- Efficient contraction

Wang and Xiang, 1997

Li, et al. 2011

Dong, et al. 2017

Series-Expansion Thermal Tensor Network (SETTN)

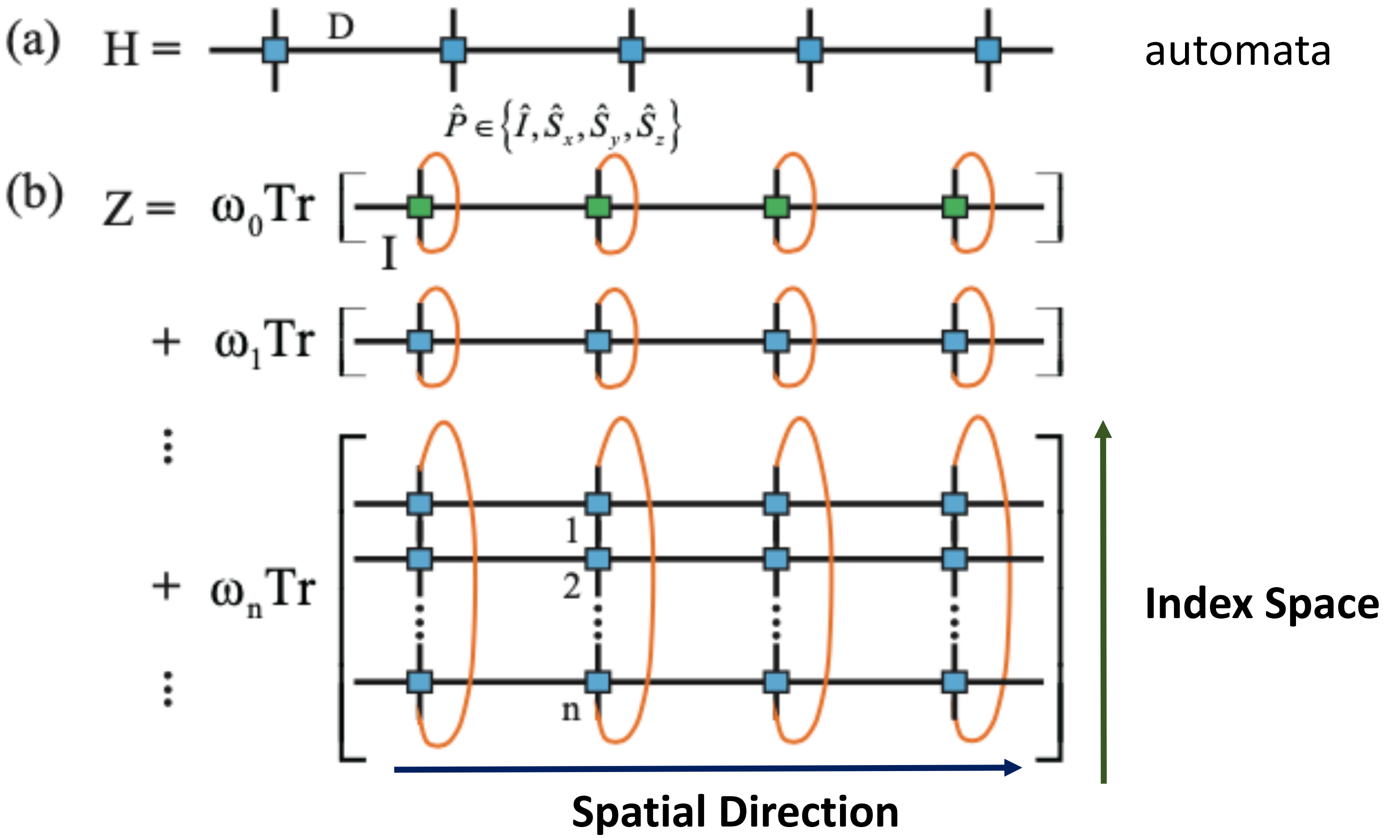
BC, Yun-Jing Liu, Ziyu Chen, Wei Li, ***PRB(R)*** 95, 161104

1.2 Basic Idea of SETTN

- Taylor Expansion of Partition Function:

$$Z(\beta) = \mathrm{Tr}(e^{-\beta H}) \simeq \sum_{n=0}^{N_c} \frac{(-\beta)^n}{n!} \mathrm{Tr}(H^n)$$

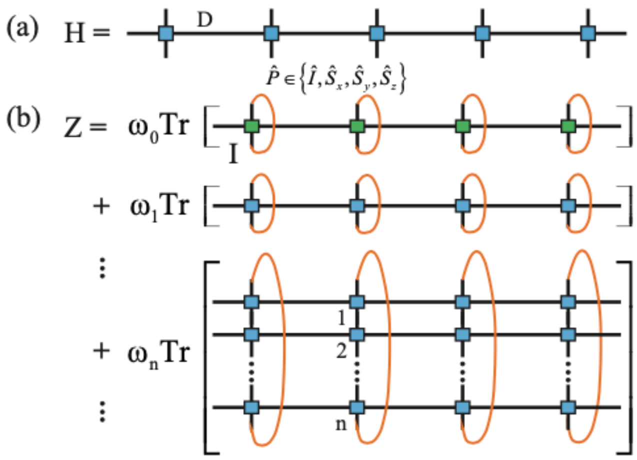
- Main Procedure:



➤ 1.2 Basic Idea of SETTN

❑ Taylor Expansion of Partition Function:

$$Z(\beta) = \mathrm{Tr}(e^{-\beta H}) \simeq \sum_{n=0}^{N_c} \frac{(-\beta)^n}{n!} \mathrm{Tr}(H^n)$$

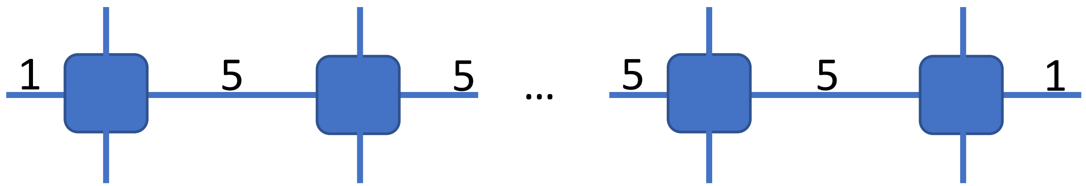


❑ MPO of Hamiltonian: (e.g Heisenberg chain)

$$H = \sum_{i=1}^{N-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z)$$

$$= \begin{bmatrix} I & S^x & S^y & S^z & 0 \end{bmatrix} \underbrace{\begin{bmatrix} I & S^x & S^y & S^z & 0 \\ 0 & 0 & 0 & 0 & S^x \\ 0 & 0 & 0 & 0 & S^y \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & I \end{bmatrix} \cdots \begin{bmatrix} I & S^x & S^y & S^z & 0 \\ 0 & 0 & 0 & 0 & S^x \\ 0 & 0 & 0 & 0 & S^y \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & I \end{bmatrix}}_{N-2} \begin{bmatrix} 0 \\ S^x \\ S^y \\ S^z \\ I \end{bmatrix}$$

=



1.2 Basic Idea of SETTN

E.g. N= 4 Heisenberg chain

$$[I \quad S^x \quad S^y \quad S^z \quad 0]\begin{bmatrix} I & S^x & S^y & S^z & 0 \\ 0 & 0 & 0 & 0 & S^x \\ 0 & 0 & 0 & 0 & S^y \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & I \end{bmatrix}\begin{bmatrix} I & S^x & S^y & S^z & 0 \\ 0 & 0 & 0 & 0 & S^x \\ 0 & 0 & 0 & 0 & S^y \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & I \end{bmatrix}\begin{bmatrix} 0 \\ S^x \\ S^y \\ S^z \\ I \end{bmatrix}$$

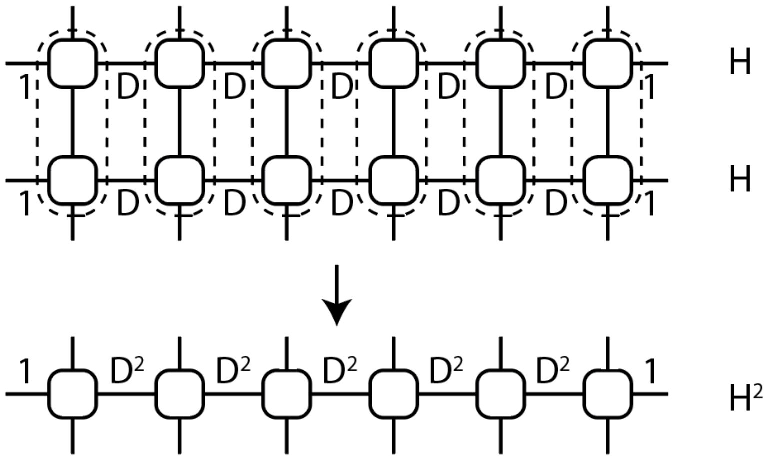
$$= \quad [I \quad S^x \quad S^y \quad S^z \quad 0]\begin{bmatrix} I & S^x & S^y & S^z & 0 \\ 0 & 0 & 0 & 0 & S^x \\ 0 & 0 & 0 & 0 & S^y \\ 0 & 0 & 0 & 0 & S^z \\ 0 & 0 & 0 & 0 & I \end{bmatrix}\begin{bmatrix} S^x S^x + S^y S^y + S^z S^z \\ S^x I \\ S^y I \\ S^z I \\ II \end{bmatrix}$$

$$= \quad [I \quad S^x \quad S^y \quad S^z \quad 0]\begin{bmatrix} IS^x S^x + IS^y S^y + IS^z S^z + S^x S^x I + S^y S^y I + S^z S^z I \\ S^x II \\ S^y II \\ S^z II \\ II \end{bmatrix}$$

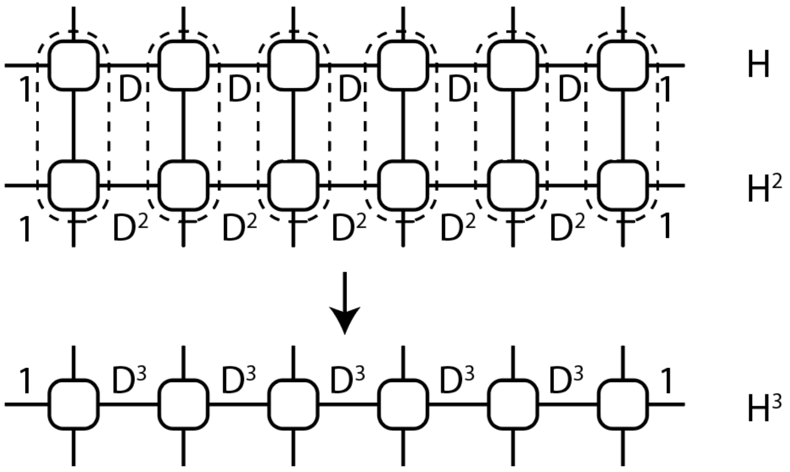
$$\begin{aligned} = \quad & IIS^x S^x + IIS^y S^y + IIS^z S^z \\ & + IS^x S^x I + IS^y S^y I + IS^z S^z I \\ & + S^x S^x II + S^y S^y II + S^z S^z II \end{aligned}$$

1.2 Efficient contraction of H^n

Construction of H^2



Construction of H^3

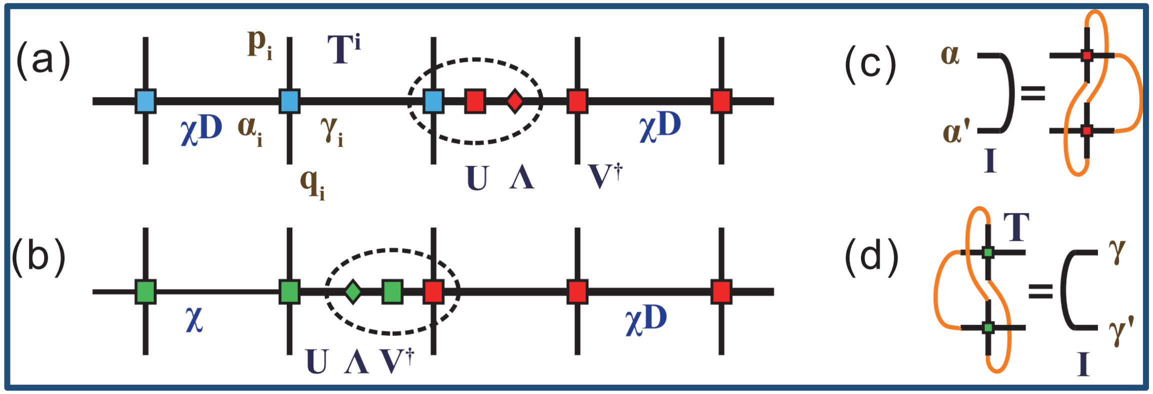


Similarly, H^n will have bond dimension D^n

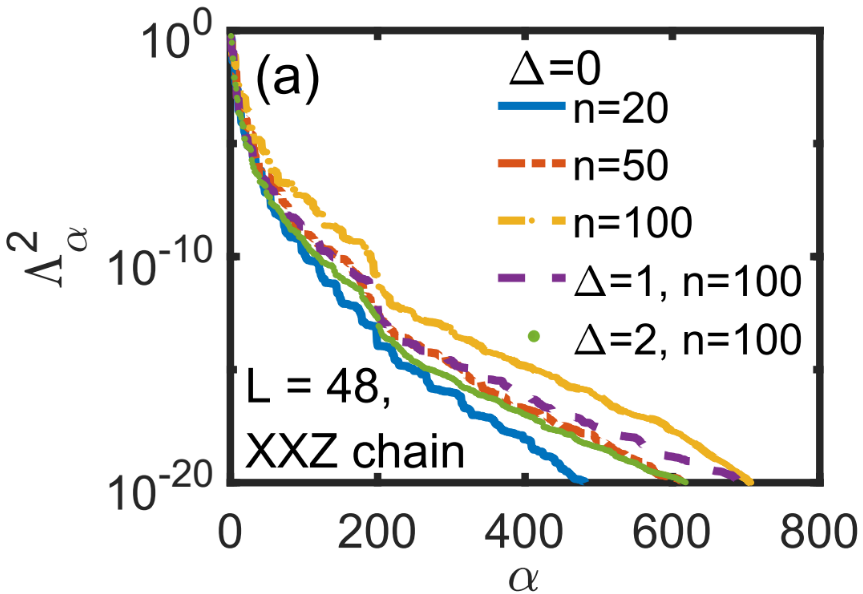
Bond dimension scales exponentially and will quickly become unaffordable.

➢ 1.2 Efficient contraction of H^n

❑ Canonical form:

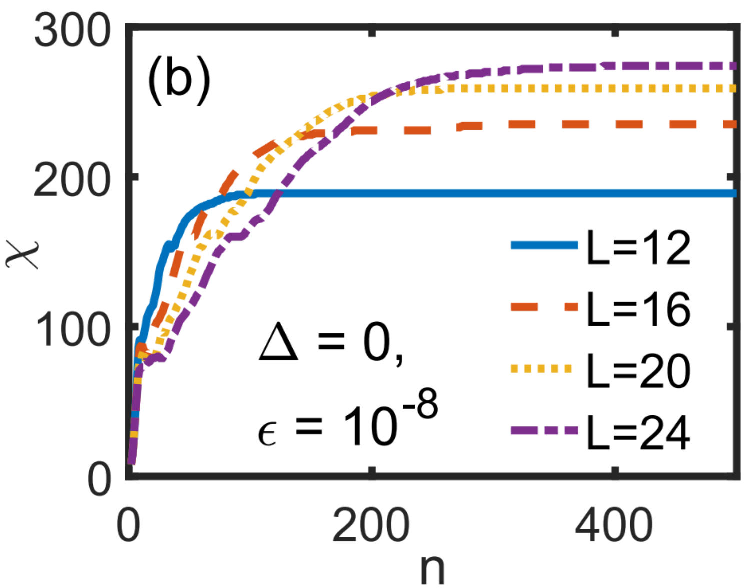


❑ "Entanglement" spectrum



Decay rapidly

❑ Required bond dimension



saturate with n

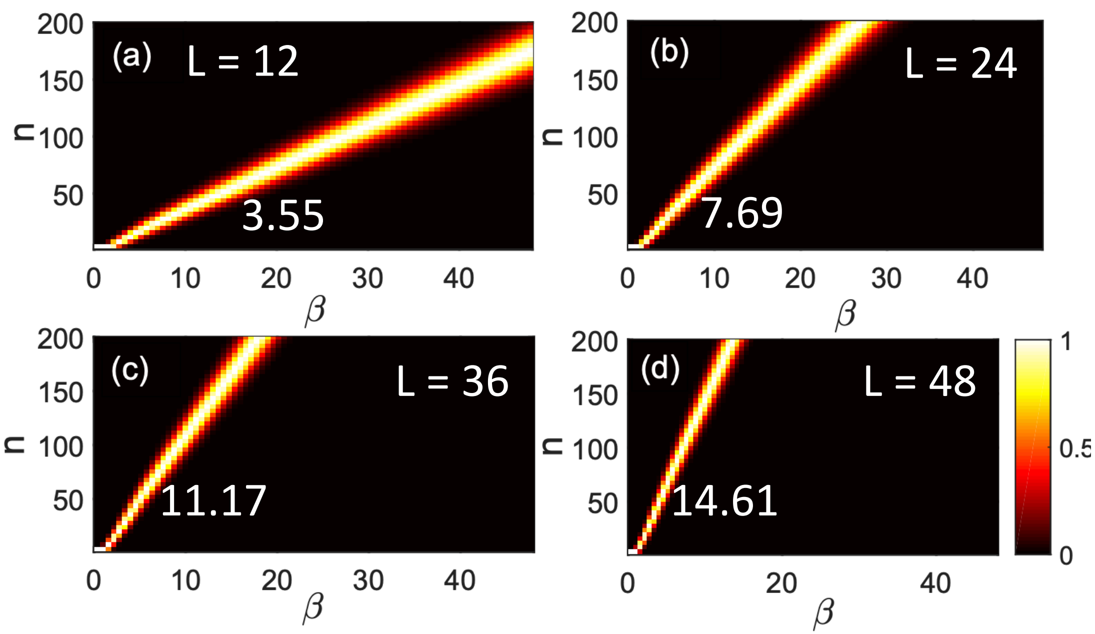
➢ 1.2 Expansion cutoff

$$Z(\beta) = \mathrm{Tr}(e^{-\beta H}) \simeq \sum_{n=0}^{N_c} \frac{(-\beta)^n}{n!} \mathrm{Tr}(H^n)$$

For large n, we have $\mathrm{Tr}(H^n) \propto (E_{\mathrm{ln}})^n = (e_{\mathrm{ln}} L)^n$

Partition function is sum of $\kappa(n) = \frac{(-\beta L e_{\mathrm{ln}})^n}{n!} = \frac{(\beta L |e_{\mathrm{g}}|)^n}{n!}$

which is most prominent around $n = \beta L |e_{\mathrm{g}}|$



E.g., XY chain: $e_{\mathrm{g}} = -1/\pi$

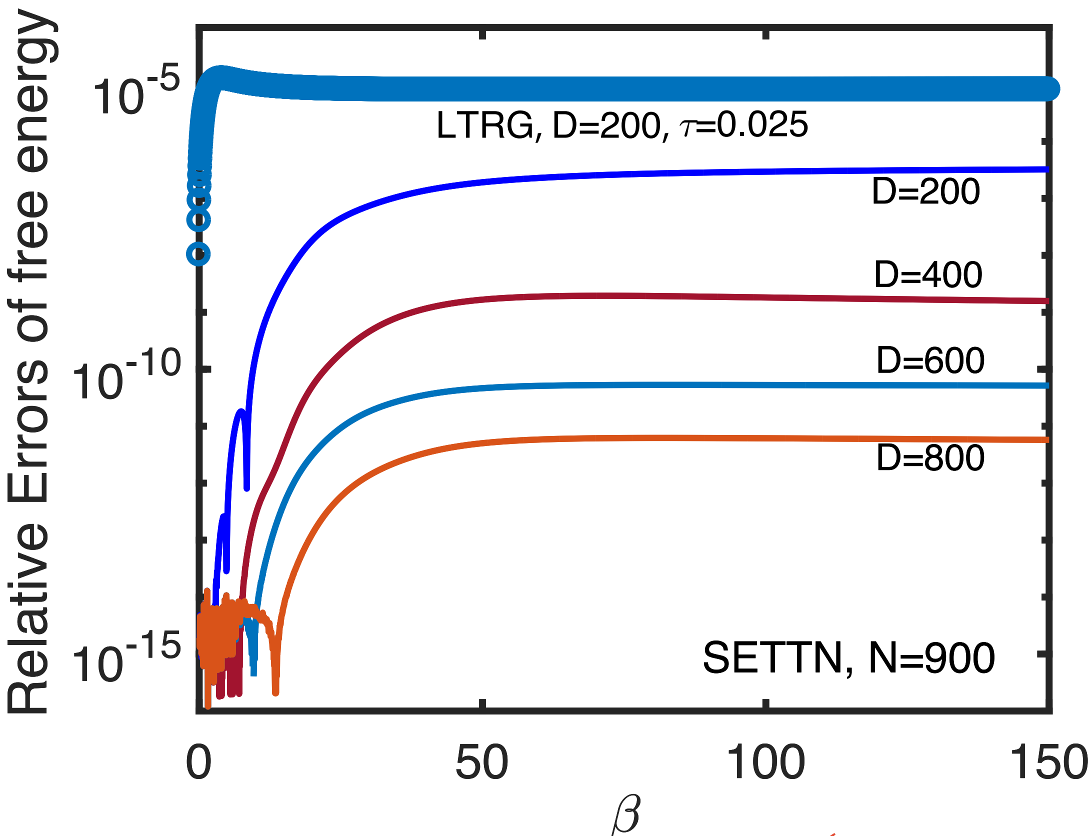
Then partition function is dominant by weight around

$$n = \beta L / \pi$$

1.2 Performance of SETTN

- L=14 XY chain

$$H = J\sum_{\langle i,j\rangle}(S_i^x S_j^x + S_i^y S_j^y)$$



✓ Extremely accurate at high-T

✓ SETTN outperform Trotter

1.2 Summary of SETTN

Trotter-error free ✅

Continuous Time ✅

Long-Range Couplings ✅

The problem is still very challenging for 2D system at Low *T*.

Exponential Tensor Renormalization Group (XTRG)

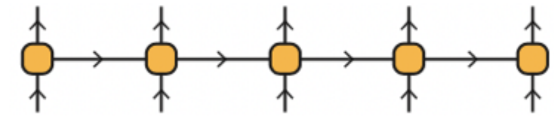
[1] **BC**, L. Chen, Z. Chen, W. Li, A. Weichselbaum. ***PRX** 8, 031082*

[2] L. Chen, D.-W. Qu, H. Li, **BC**, S.-S. Gong, J. von Delft, A. Weichselbaum, W. Li. ***PRB(R)** 99, 140404*

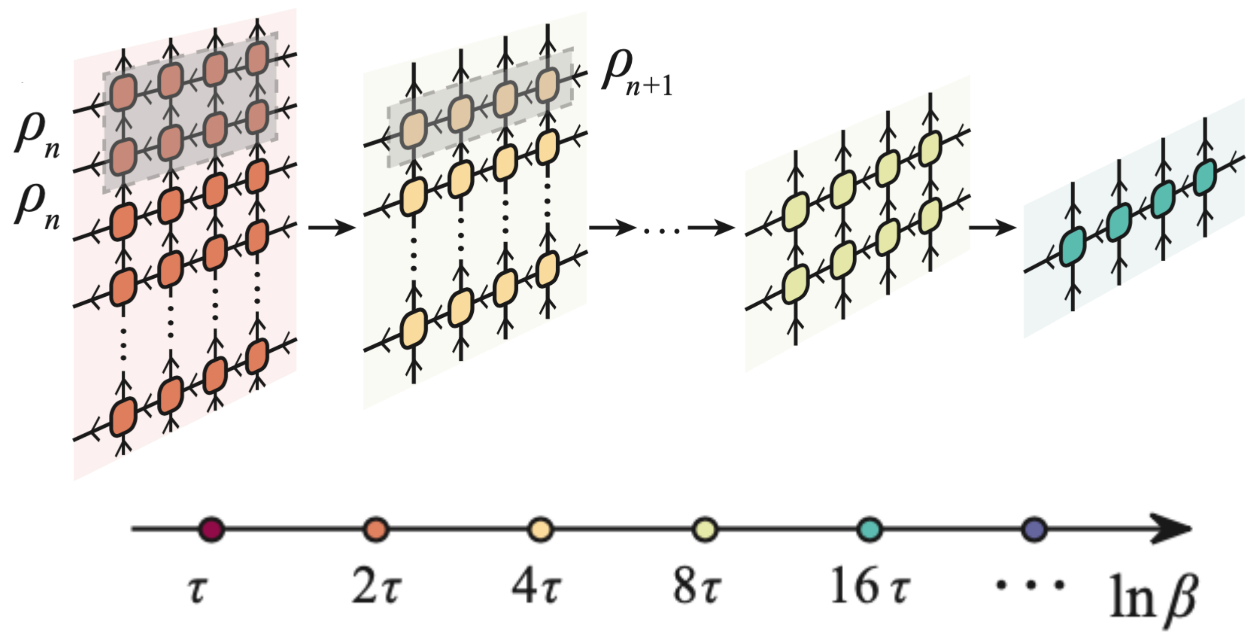
[3] H. Li, **BC**, Z. Chen, J. von Delft, A. Weichselbaum, W. Li. ***PRB(R)** 100, 045110*

➢ 1.3 Basic Idea of XTRG

1) SETTN initialization at high Temperature

$\rho_0 \equiv \rho(\tau)$ 

2) Exponential evolution $\rho_n \cdot \rho_n \rightarrow \rho_{n+1}$

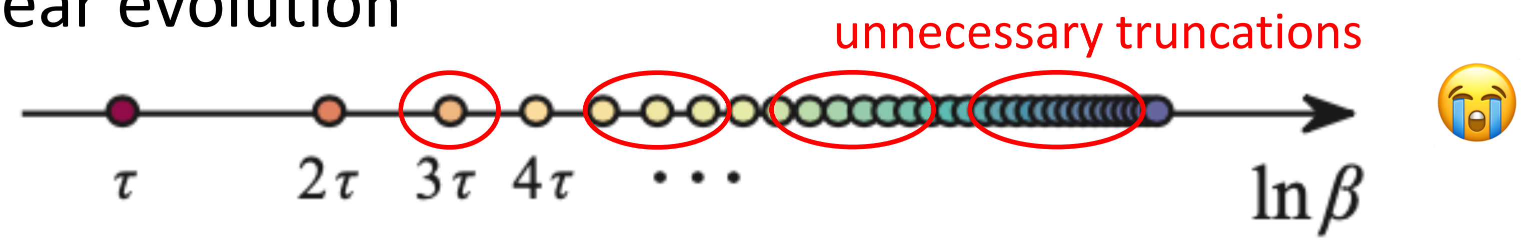


➢ 1.3 Reduce numbers of truncation steps

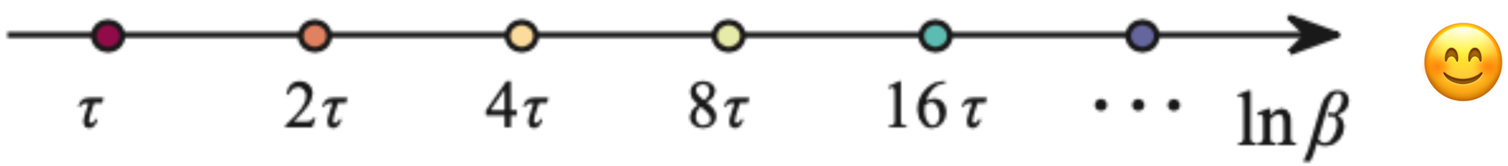
- logarithmic scaling of entanglement entropy

$$S_E \sim (c/3)\ln\beta$$

- Linear evolution



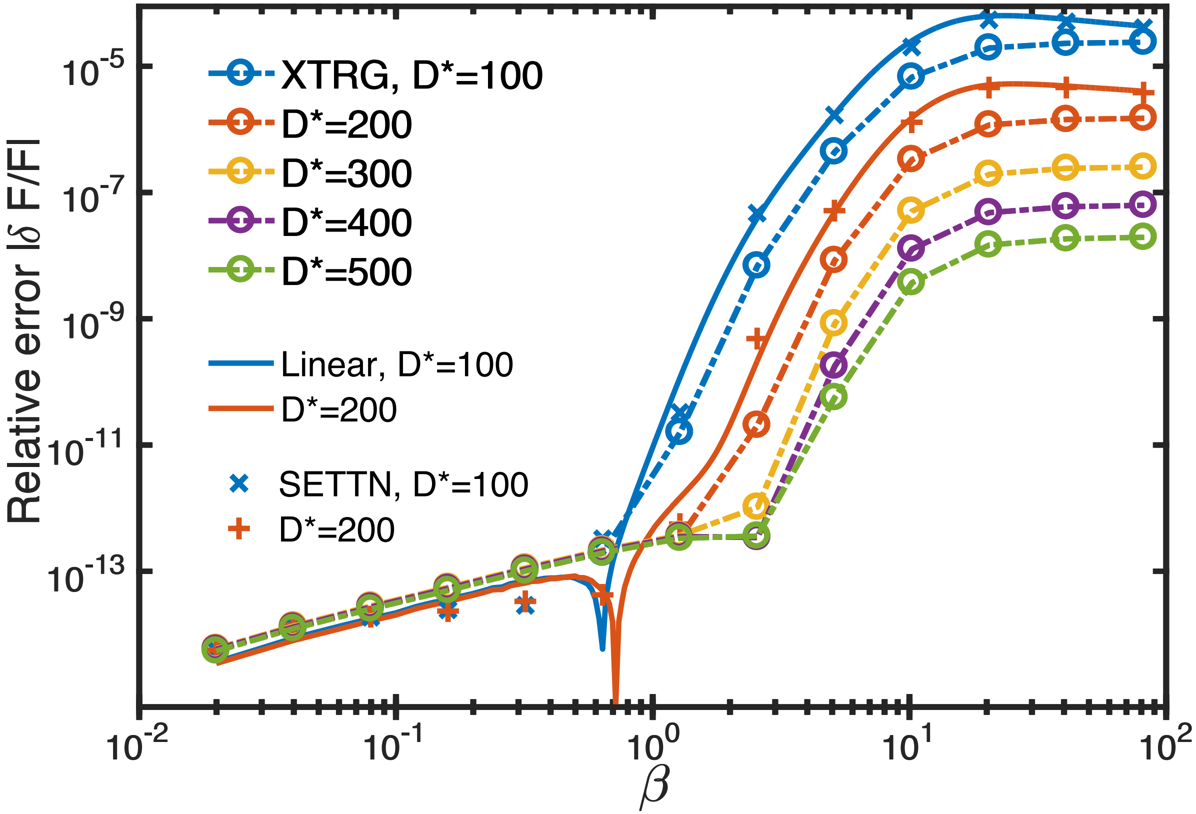
- Exponential evolution



➢ 1.3 Performance of XTRG

❑ *L*=18 Heisenberg chain

$$H = J\sum_{i,j}(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z)$$

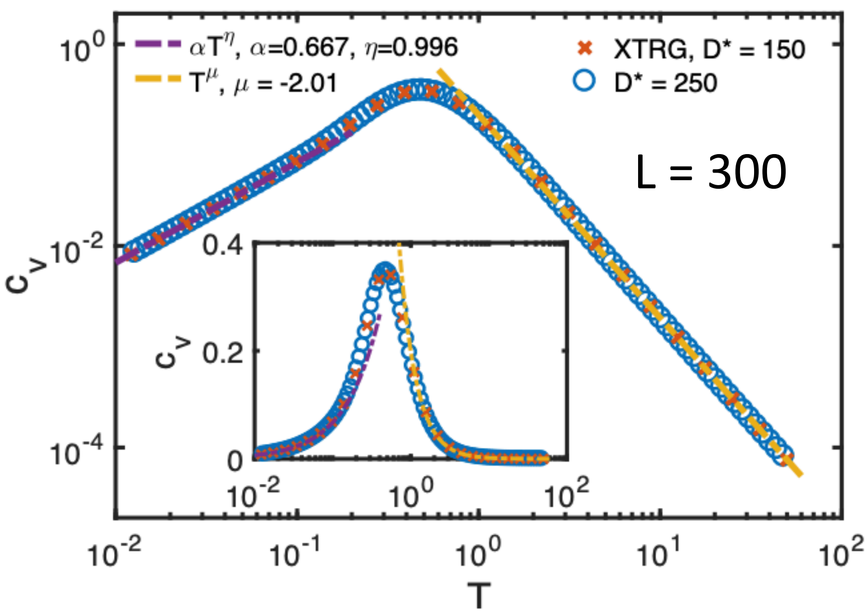


1 order of magnitude better than Linear scheme and also SETTN

1.3 More data of XTRG

✓ Long Heisenberg chain

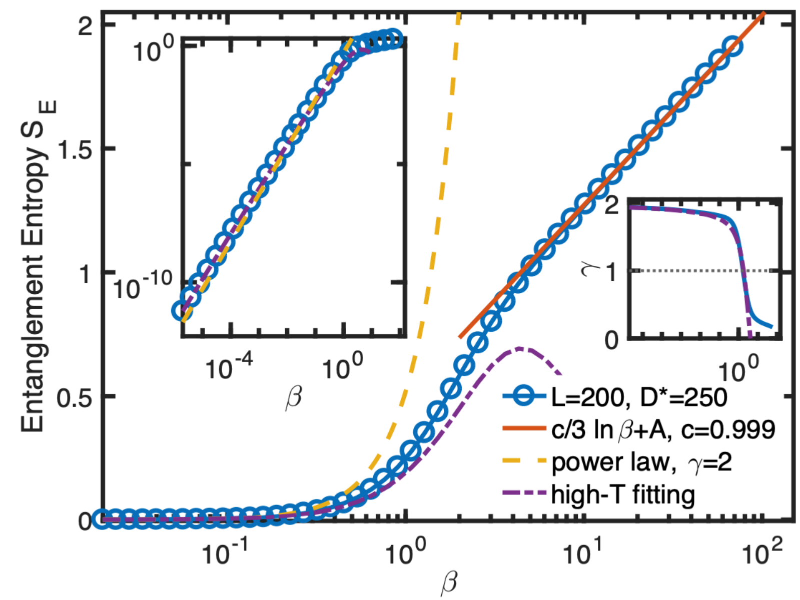
Extraction of central charge



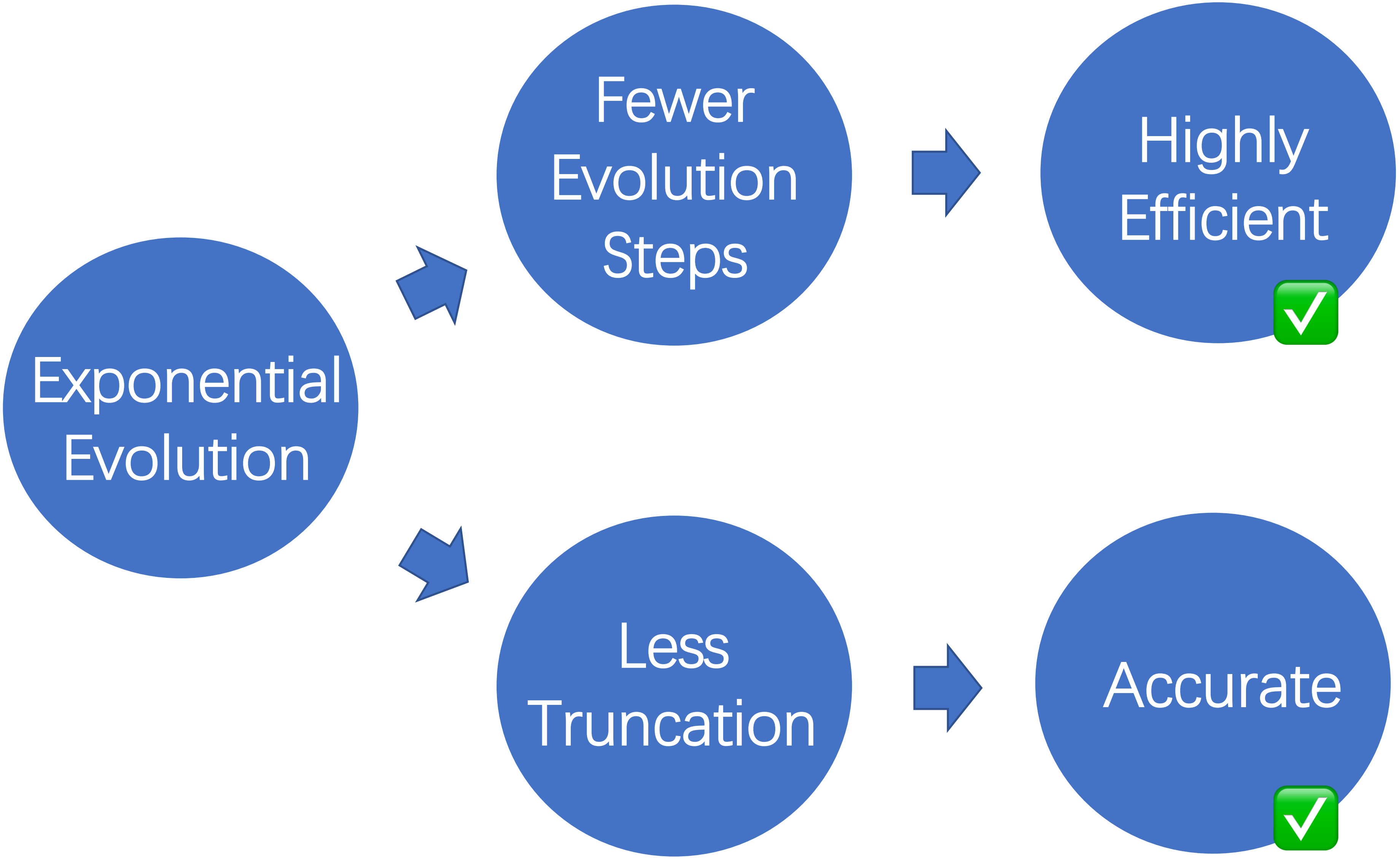
$$c_V = \alpha T^\eta \qquad \alpha = \frac{\pi c}{3v}$$

logarithmic scaling of entanglement entropy

$$S_E \sim (c/3)\ln\beta$$



➢ 1.3 Summary of XTRG

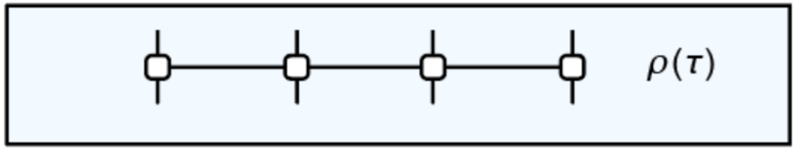


Differentiable Tensor Renormalization Group (∂TRG)

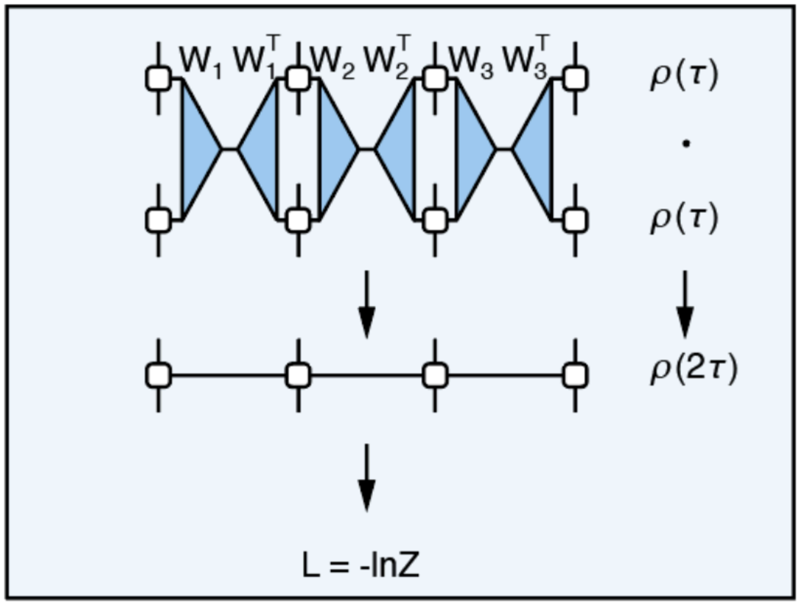
BC, Y. Gao, Y.-B. Guo, Y. Liu, H.-H. Zhao, H.-J. Liao, L. Wang, T. Xiang, W. Li, Z. Y. Xie. ***PRB(R)*** *101, 220409*

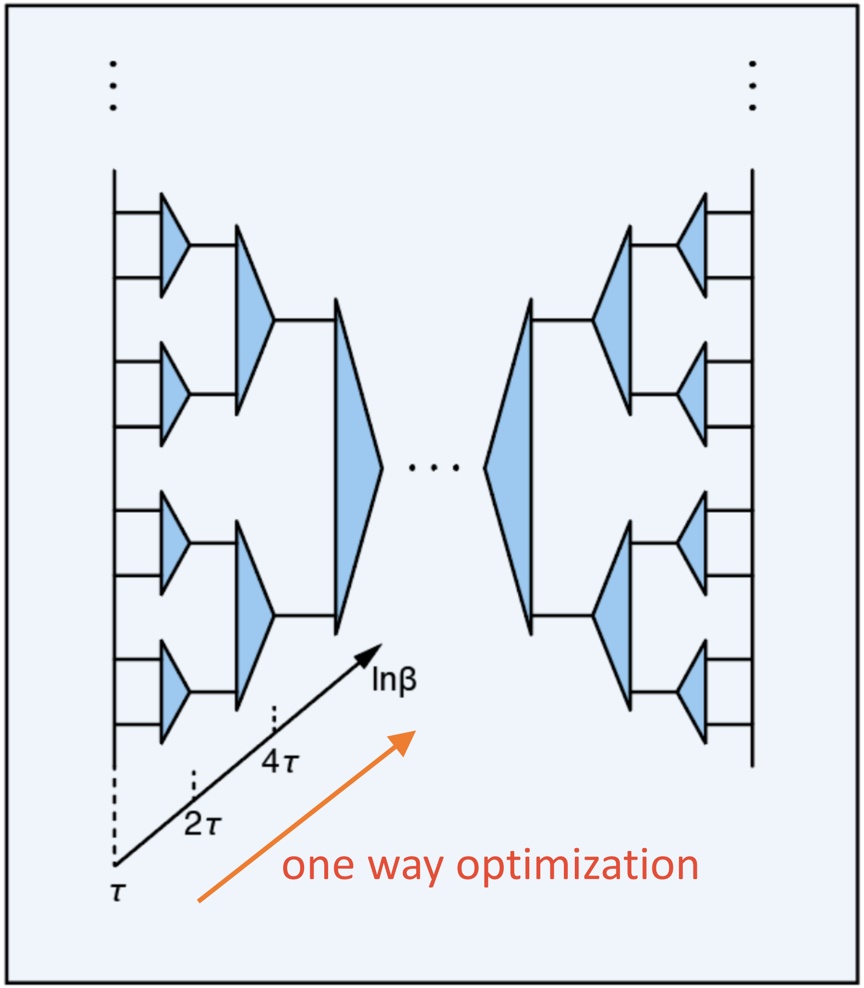
➢ 1.4 Basic Idea of ∂TRG

1） SETTN initialization at high temperature



2） Forward TRG





3) Backward optimization

By using Automatic Differentiation,
We can calculate environment

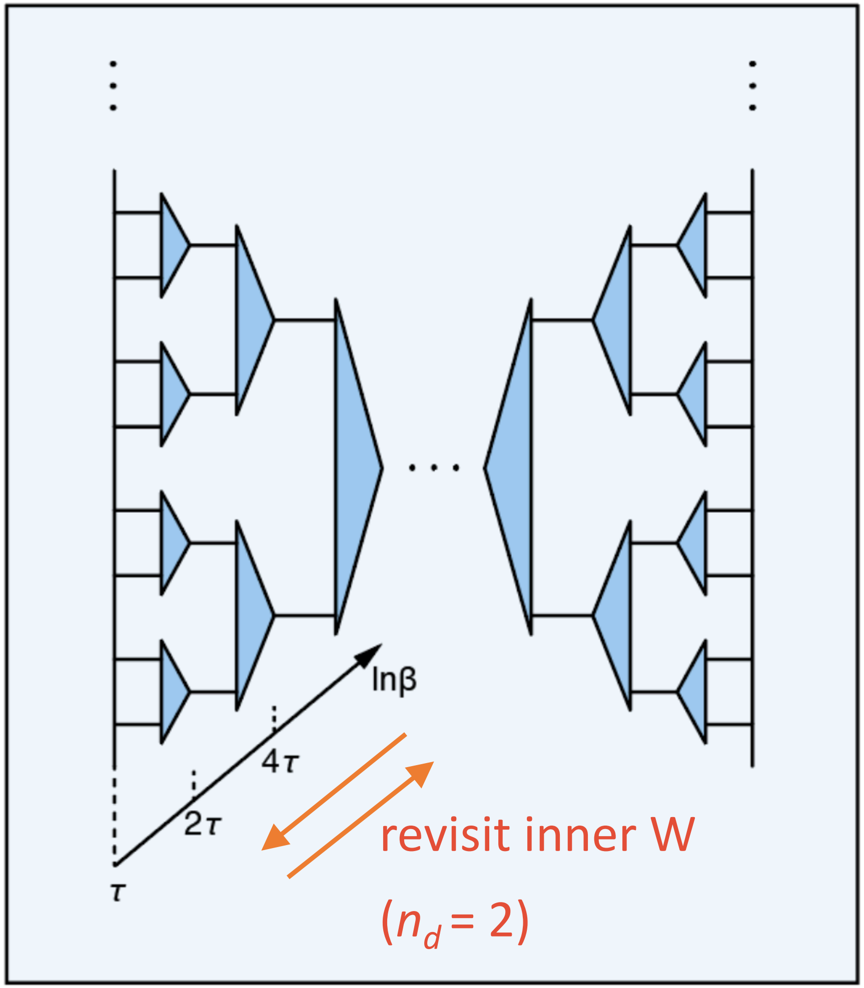
$$\frac{\partial \mathcal{L}}{\partial W_i}$$

and update W_i

4) Repeat forward and backward for all

$$W_i$$

within optimization depth n_d



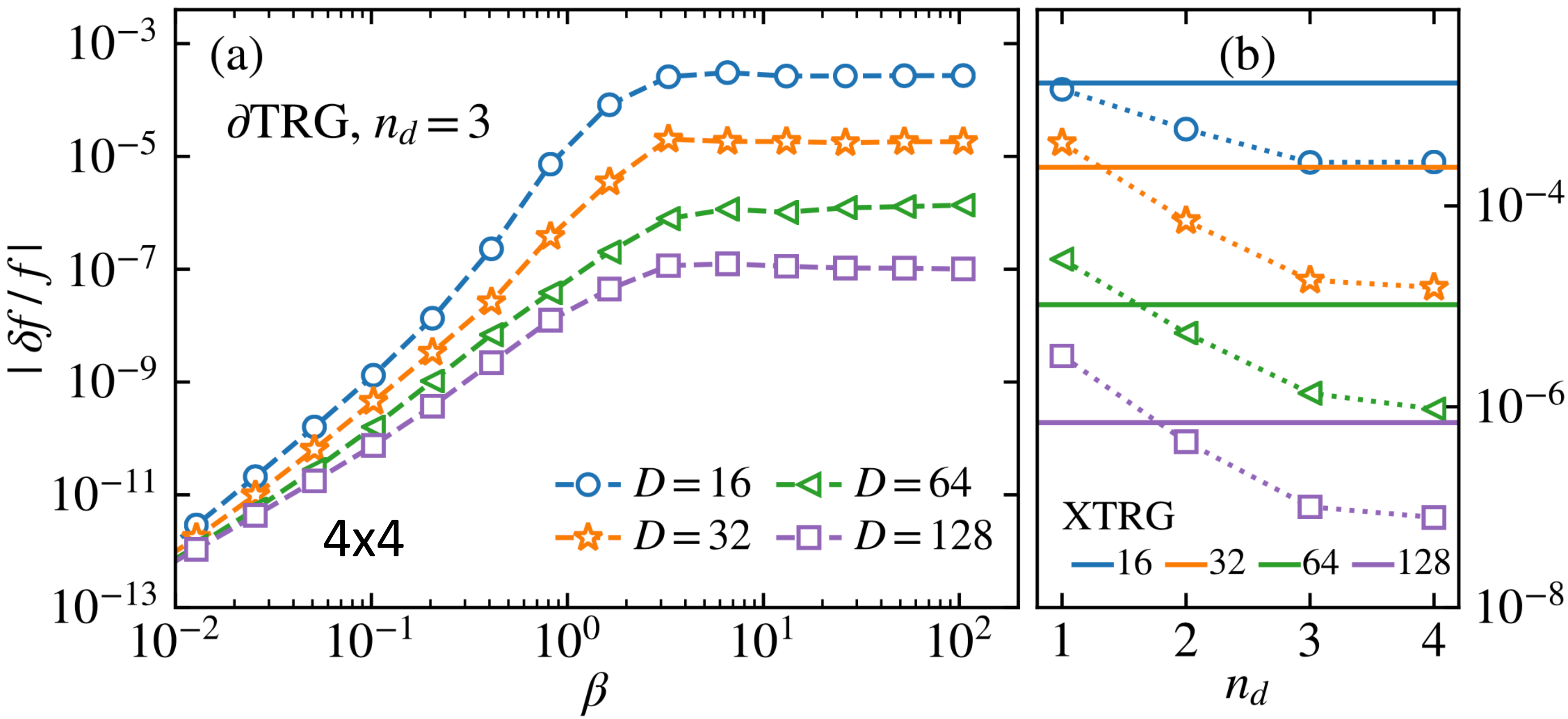
Deep optimization in thermal tensor network

➢ 1.4 2D transverse-field Ising model

$$H = J\sum_{i,j} S_i^z S_j^z + h\sum_i S_i^x$$

with J=-1, h = h_c = 1.522

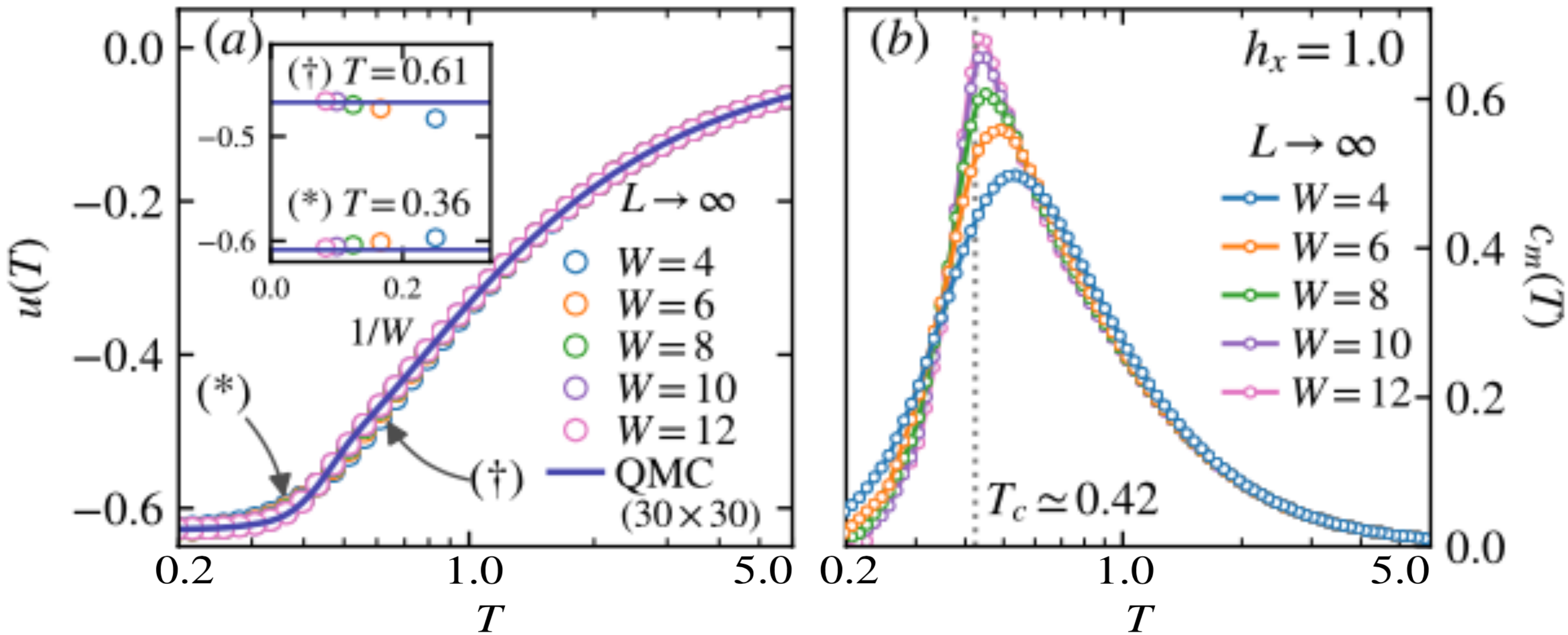
- relative error of free energy



➢ 1.4 transverse-field Ising model

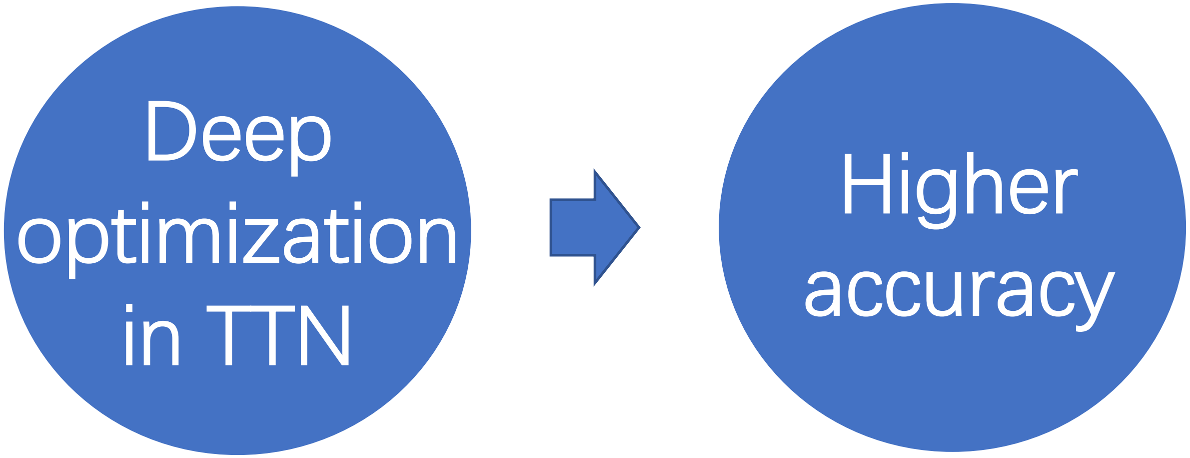
$$H = J\sum_{i,j} S_i^z S_j^z + h\sum_i S_i^x$$ with J=-1, h = 1 T_c = 0.42

- internal energy
- specific heat



accurate estimate of transition temperature ~1%

Summary of ∂TRG



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❑ 2. Application 1

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- 2.3 Magic-angle twisted bilayer graphene model

❑ 3. Application 2

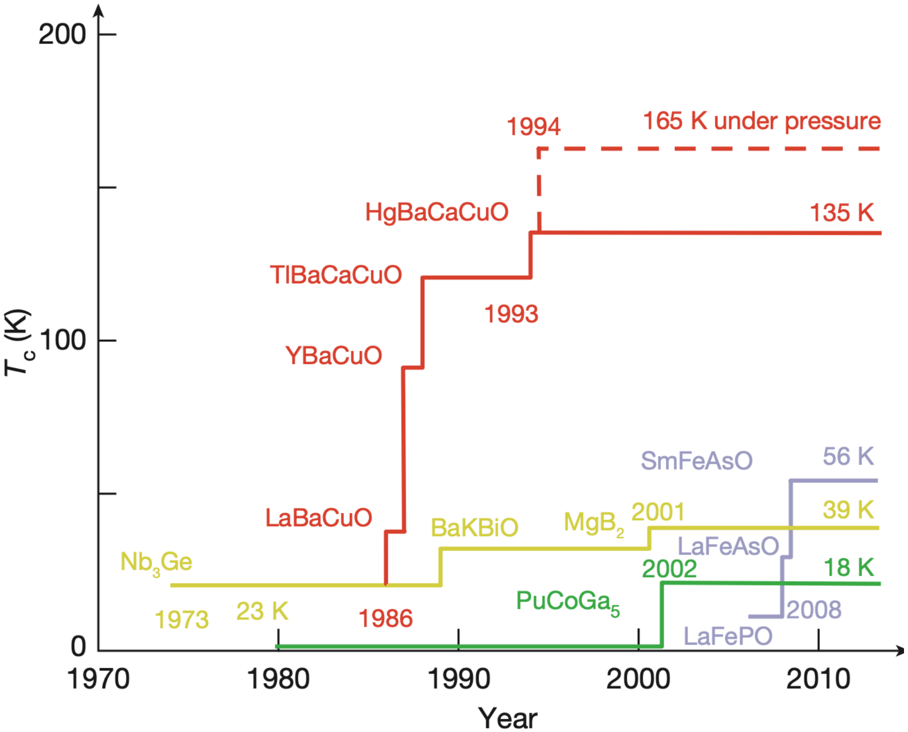
- 3.1 Quantum entanglement and disorder operator
- 3.2 topological disorder operator

XTRG study of Finite-T square-lattice Hubbard model

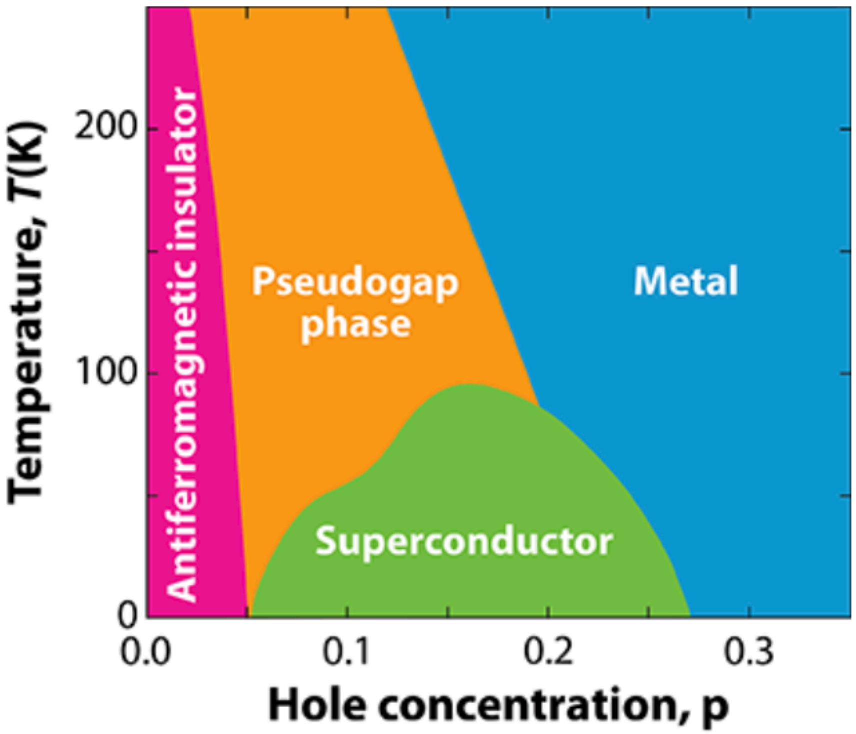
BC, C. Chen, Z. Chen, J. Cui, Y. Zhai, A. Weichselbaum, J. von Delft, Z. Y. Meng, and W. Li. **PRB** 103, L041107

➢ 2.1 High-Tc Superconductivity

- race of highest Tc



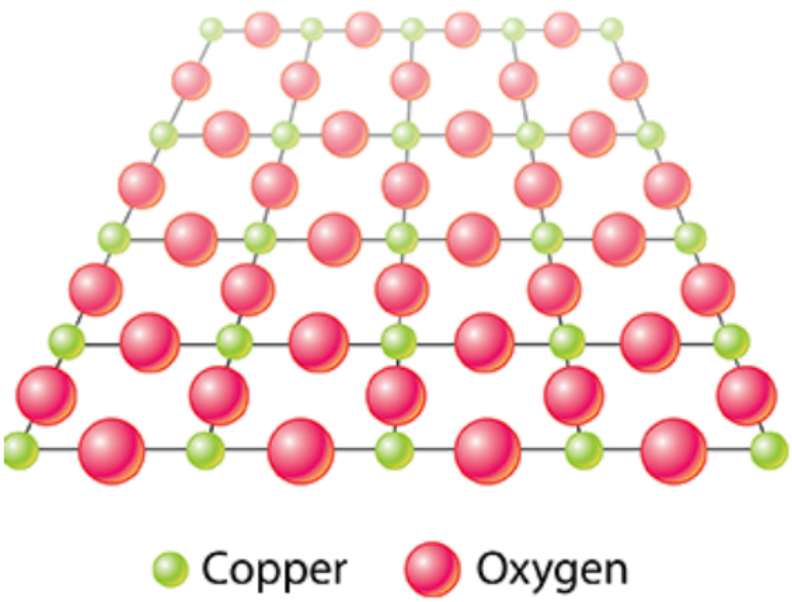
Keimer B, et al. Nature2015



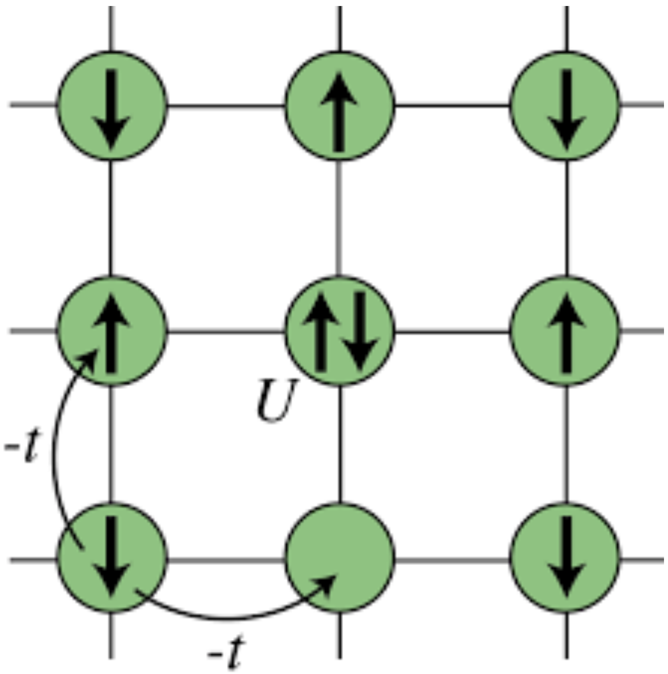
APS/Carin Cain

➢ 2.1 Mechanism of High-Tc ?

- Copper oxide plane



- Single-band Hubbard model

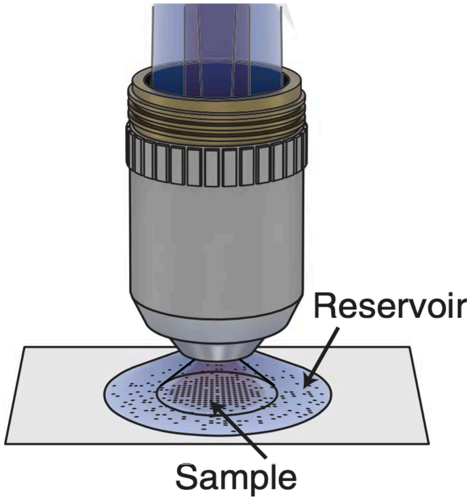


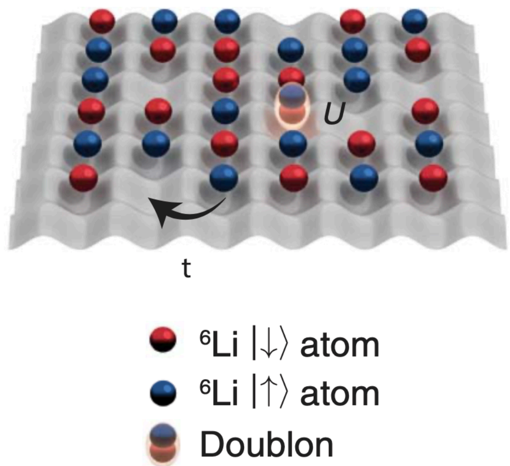
$$H = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

➢ 2.1 Correlated matter: Ultra-cold Fermions

- Realization of Fermi-Hubbard Model

Greiner's group, *Nature* 2017



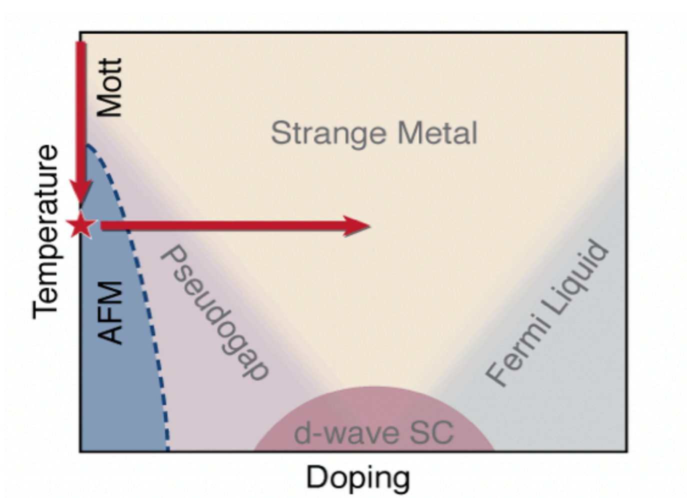


✓ trap fermions in optical lattice

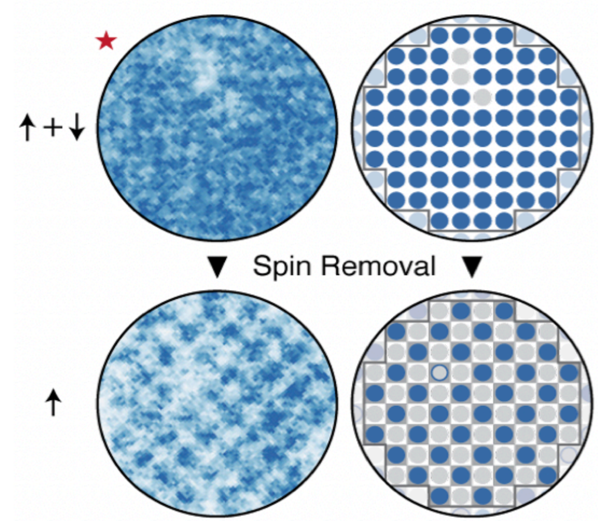
✓ tunable interactions

✓ single-site resolution

- Current Experimental Scope

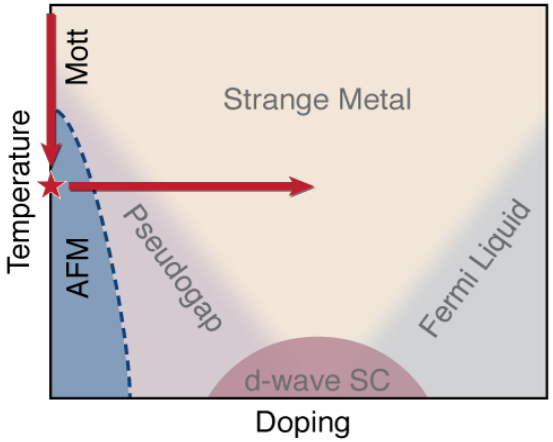


- "Long-range" Antiferromagnet

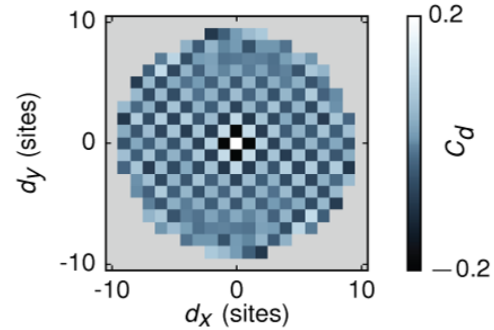


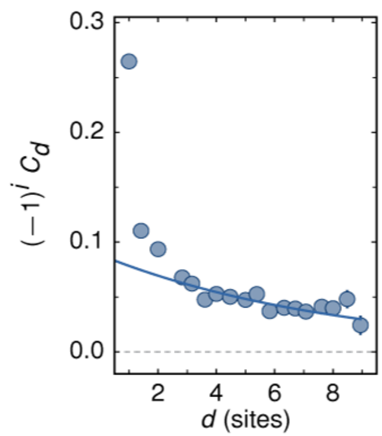
➢ 2.1 Ultra-cold Fermions in optical lattice

The Hubbard Model

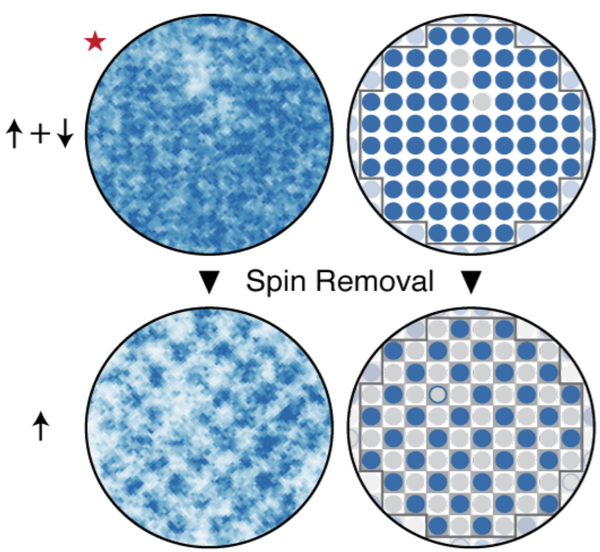


Spin Correlation Function





Long-range Antiferromagnet



- fitting & analysis on the raw experimental data
- Determination of temperature and model parameters

calls for

Efficient & accurate numerical simulations!

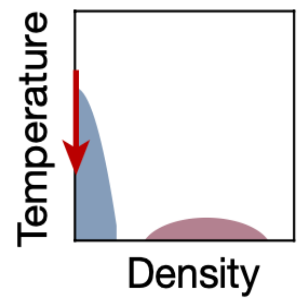
(XTRG is promising!)

Greiner's group (Harvard), *Nature* 2017

➢ 2.1 Spin correlation under half-filling

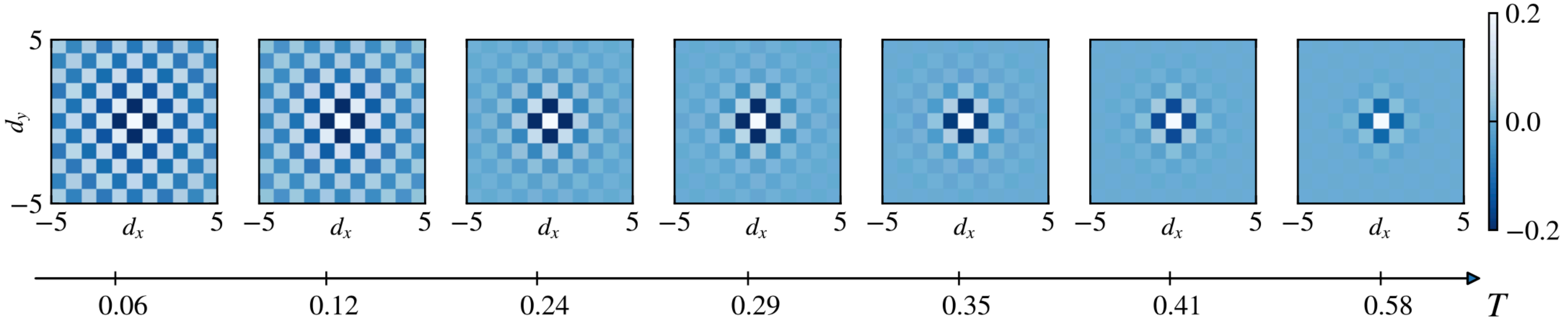
- Definition

$$C_S(d) \equiv \frac{1}{N_d} \sum_{|i-j|=d} \frac{\langle \hat{S}_i \cdot \hat{S}_j \rangle}{S(S+1)}$$

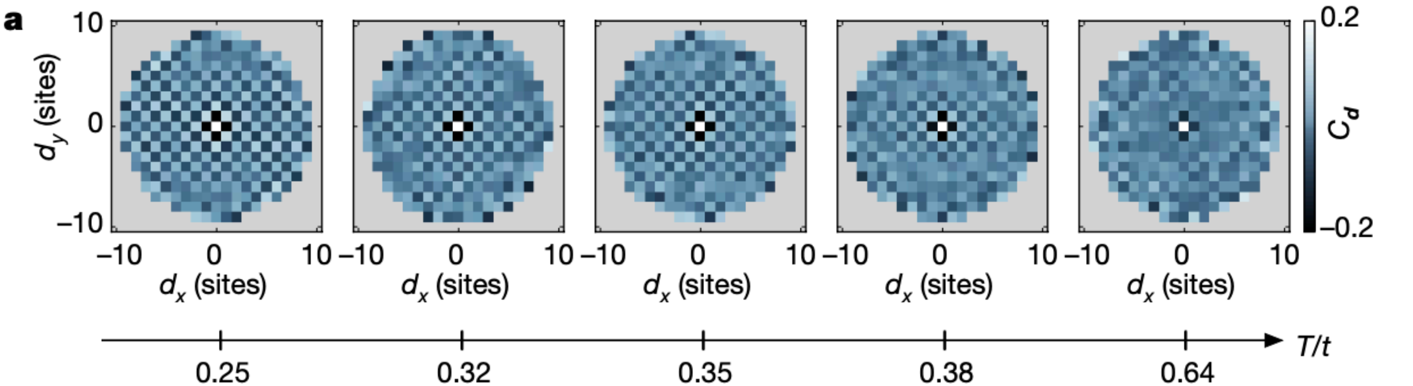


U = 7.2,
L = 6, 8
half-filling

- XTRG results

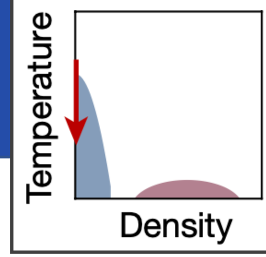


- Experiments



Greiner, *Nature* 2017

➢ 2.1 Spin correlation under half-filling



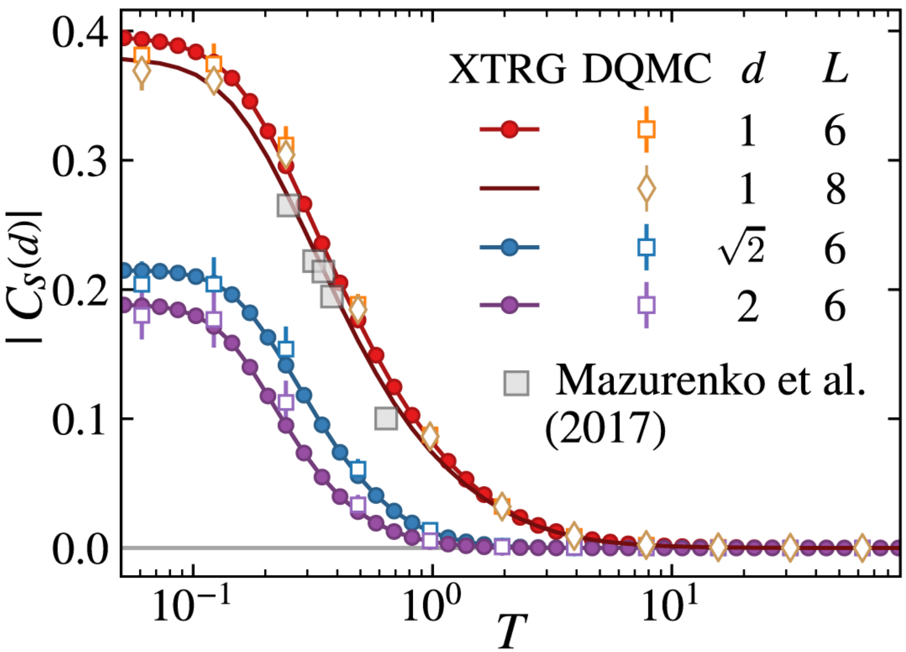
U = 7.2,
L = 6,
half-filling

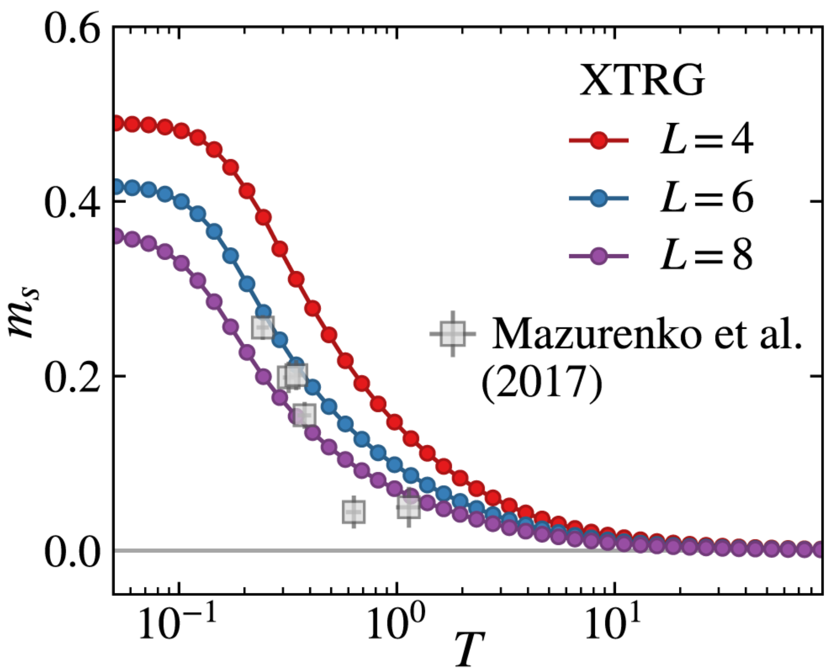
- spin correlation function

$$C_S(d) \equiv \frac{1}{N_d} \sum_{|i-j|=d} \frac{\langle \hat{S}_i \cdot \hat{S}_j \rangle}{S(S+1)}$$

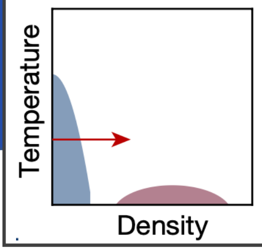
- spontaneous magnetization

$$m_s \equiv \sqrt{S(\pi,\pi) - S(0)}$$



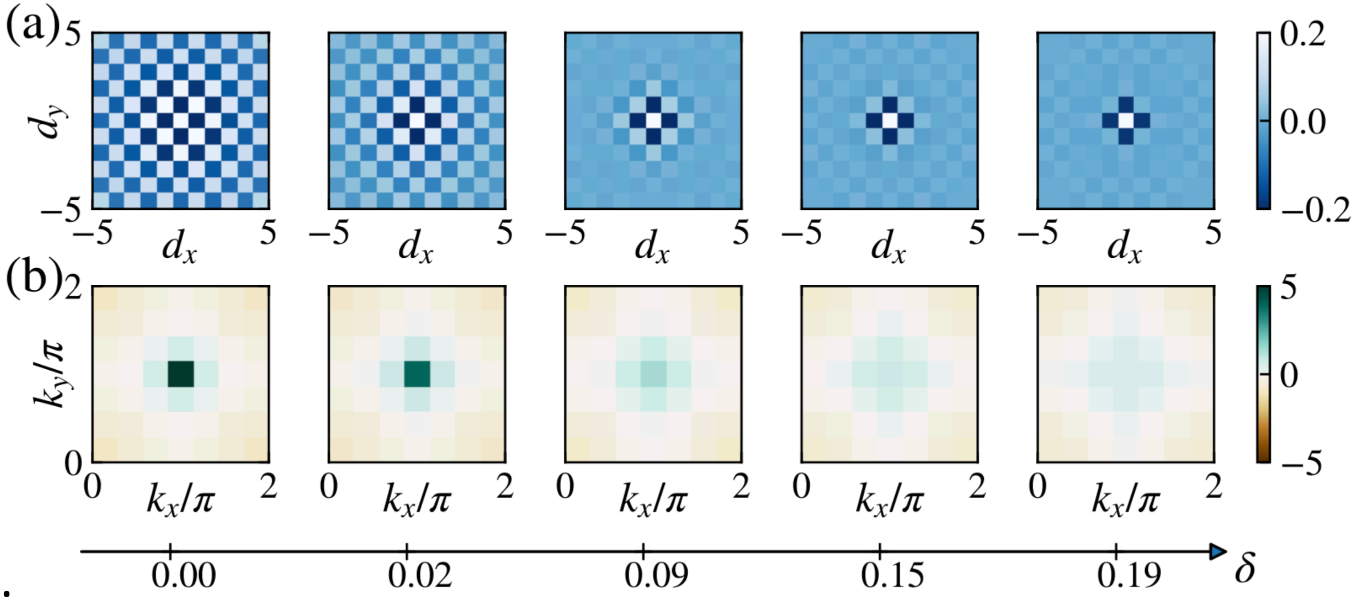


➢ 2.1 Spin correlation upon doping

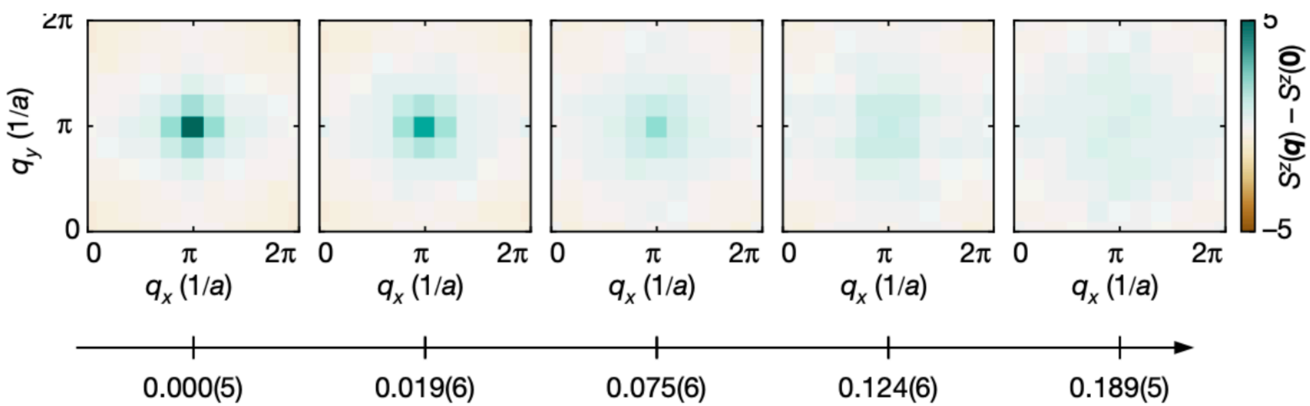


U = 7.2,
L = 6,
doping

- spin correlation function:
- structure factor:

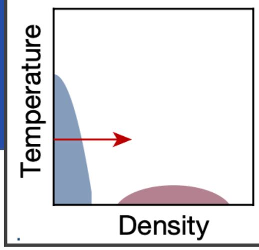


- Experimental results:



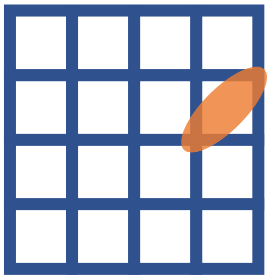
Greiner, *Nature* 2017

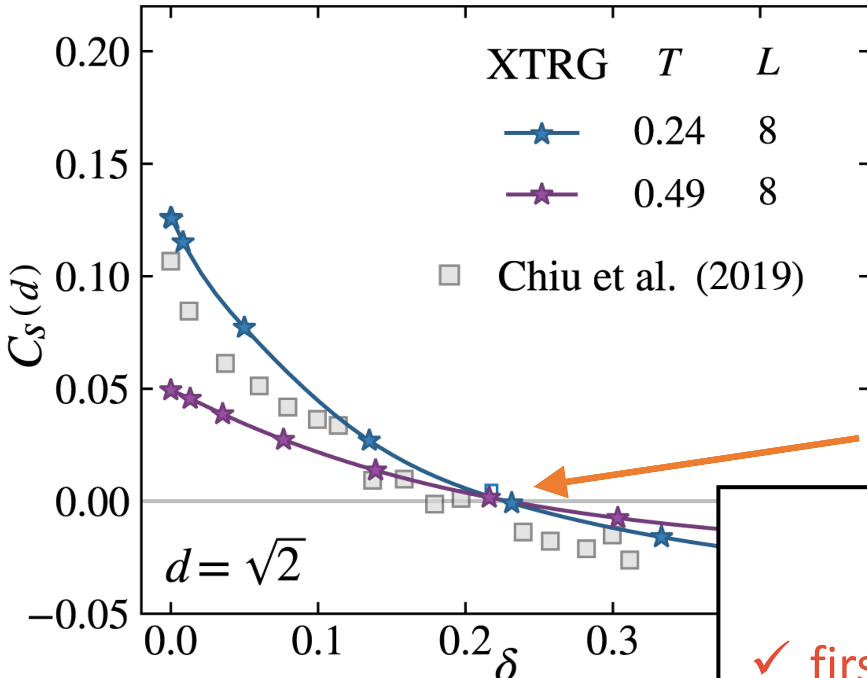
➢ 2.1 Sign-reversal behavior



U = 7.2,
L = 6,
doping

- longer-ranged spin correlation function





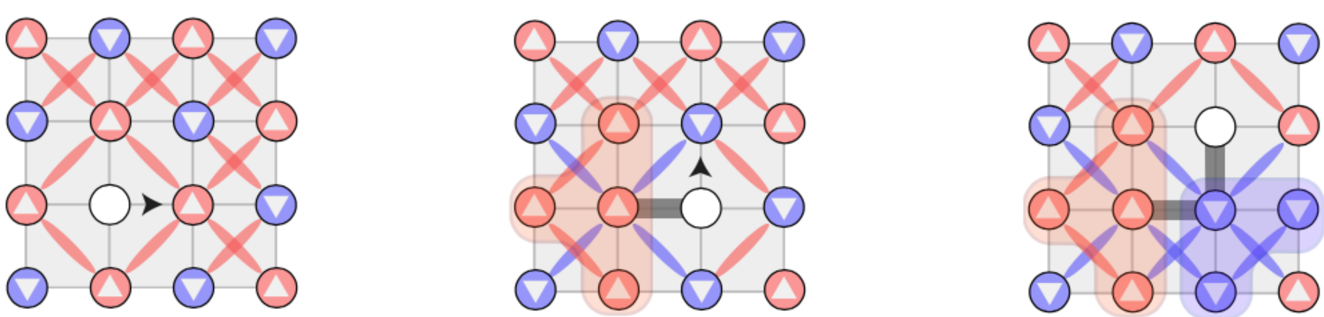
$\delta_c = 20\%$

✓ high-quality data

↓

✓ first quantitative agreement with ultra-cold fermion

✓ consistent with magnetic polaron



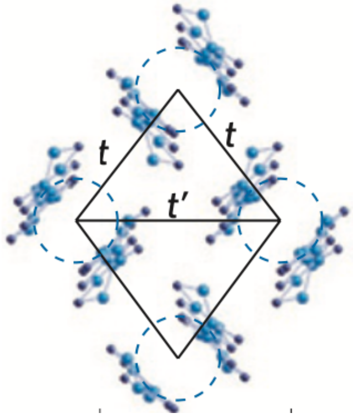
DMRG study of triangular-lattice Hubbard model

BC, Z. Chen, S.-S. Gong, D. N. Sheng, W. Li, and A. Weichselbaum, **PRB** 106, 094420 (Editors' Suggestion)

➢ 2.2 Motivation from experiments

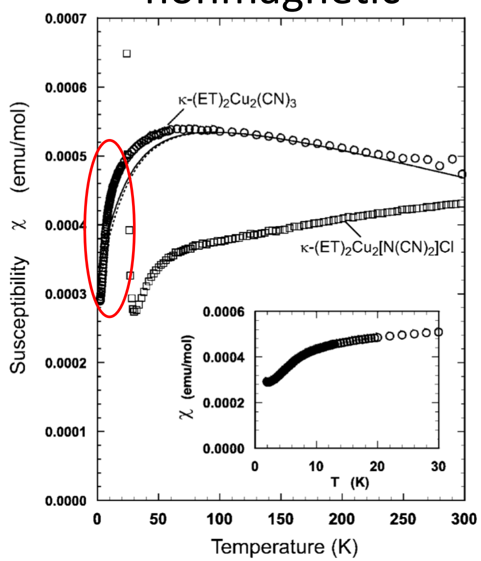
✓ Organic salt compound:

$$\kappa - (\mathrm{BEDT})_2(\mathrm{Cu})_2(\mathrm{CN})_3$$



Spin Liquid?

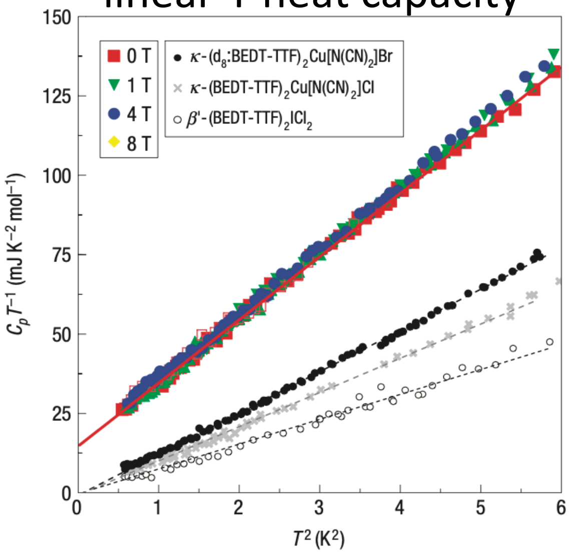
nonmagnetic



Shimizu et al, PRL 91, 107001 (2003)

Gapless?

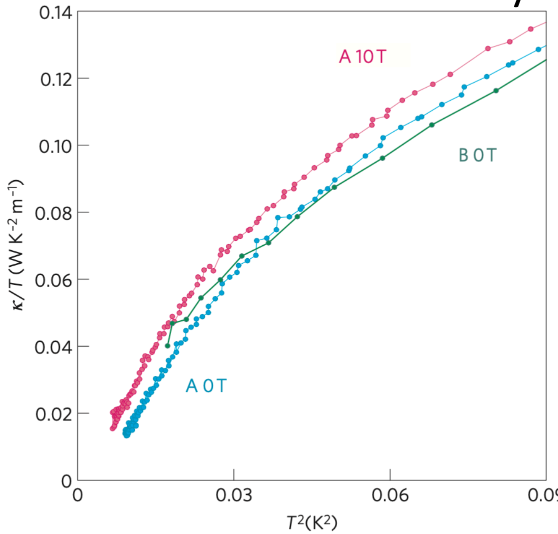
linear-T heat capacity



Yamashita et al, Nat. Phys. 4, 459 (2008)

Gapped?

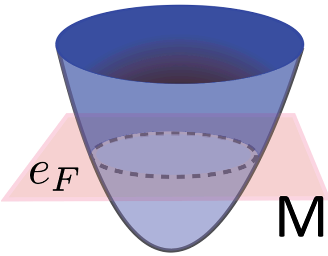
vanished conductivity

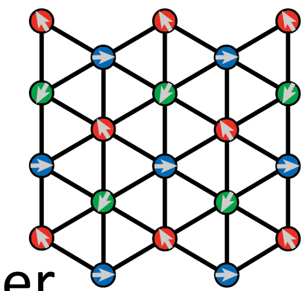


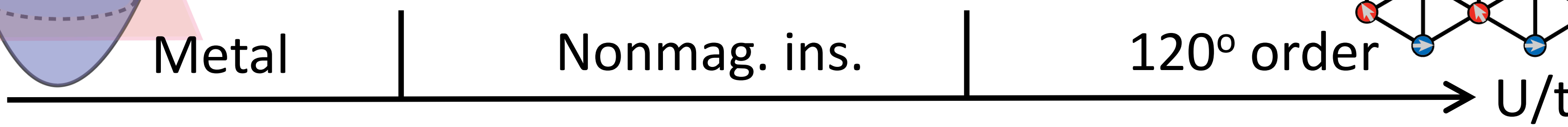
Yamashita et al, Nat. Phys. 5, 44 (2008)

➢ 2.2 Motivation from theoretical studies

$$H = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$







○ Nonmagnetic insulator candidates:

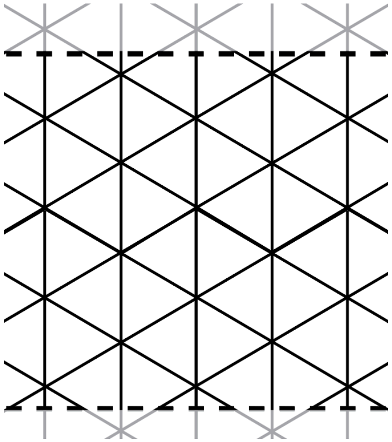
- U(1) spin liquid with spinon Fermi surface --- Motrunich, Phys. Rev. B 72, 045105 (2005)
- Gapped Z2 spin liquid --- Zhu, Phys. Rev. B 92, 041105 (2015)
- Nodal gapless spin liquid --- Mishmash, Phys. Rev. Lett. 111, 157203 (2015)
- …….

○ DMRG Results:

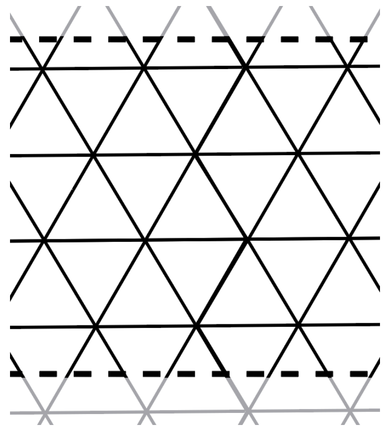
- 2-leg ladder: U(1) gapless
  Mishmash, PRB 91, 235140 (2015)
- Finite DMRG: gapped
  Shirakawa, PRB 96, 205130 (2017)
- infinite DMRG: chiral spin liquid
  Szasz, PRX 10, 021042 (2020)

➢ 2.2 Model and Main Results (Phase diagram)

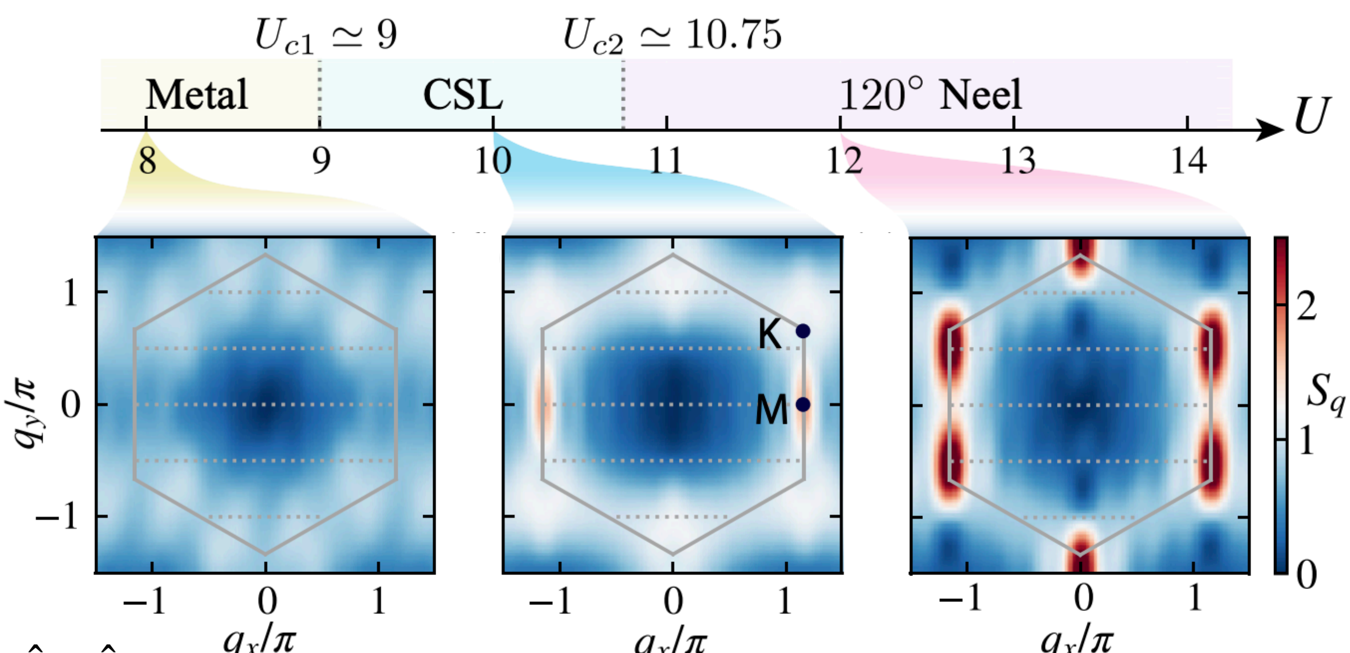
YC:



XC:



$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

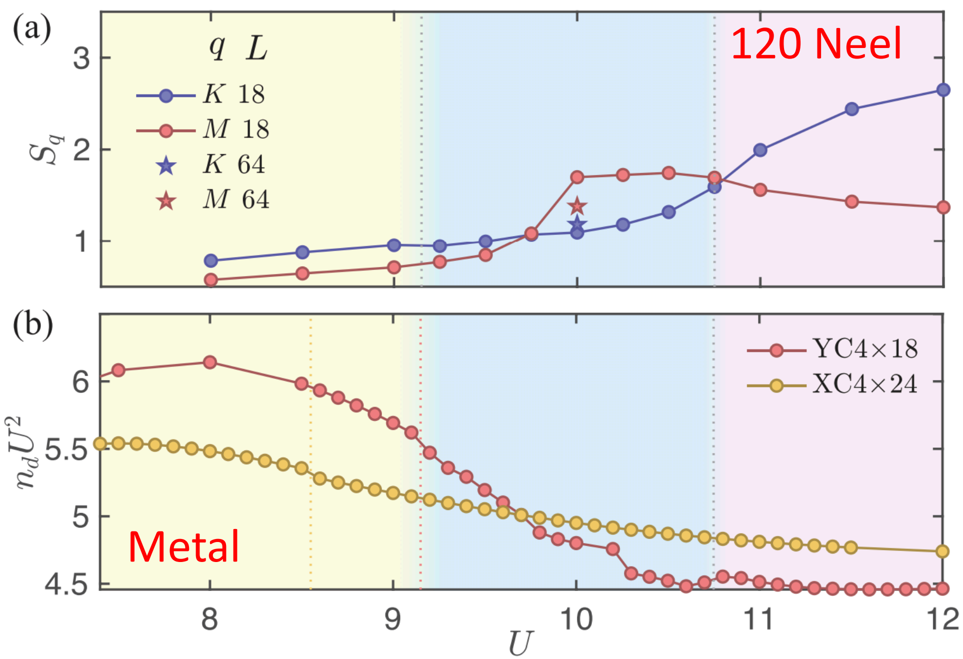


$S_q \equiv \sum_j e^{iq\cdot R_{0j}} \langle \hat{S}_j \cdot \hat{S}_0 \rangle$

➢ 2.2 Phase diagram

✓ static spin structure factor

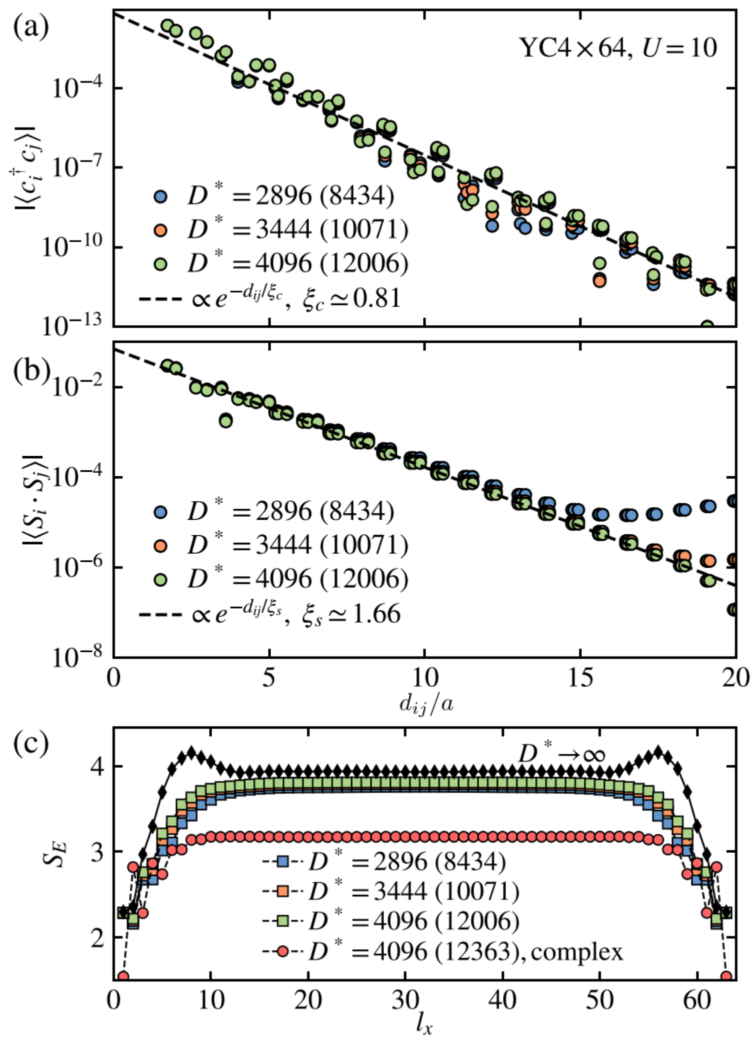
$$S_q \equiv \sum_j e^{iq\cdot R_{0j}} \langle \hat{S}_j \cdot \hat{S}_0 \rangle$$



✓ double occupancy

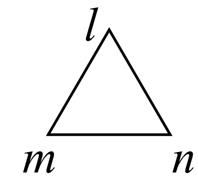
$$n_d \equiv \langle \psi | \hat{n}_{0\uparrow} \hat{n}_{0\downarrow} | \psi \rangle$$

Gapped

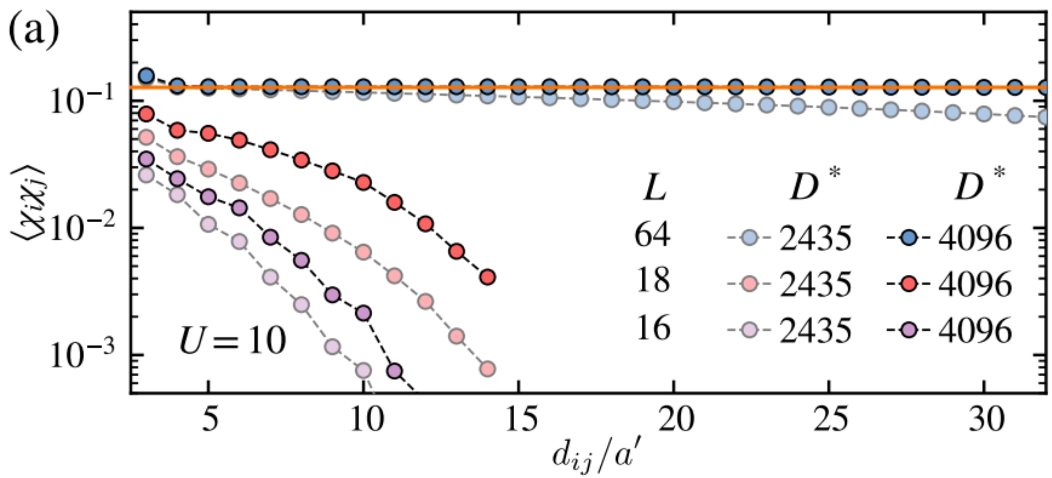


➢ 2.2 Chiral Spin Liquid: TRS-breaking

✓ chiral correlation/order: $\langle \chi_i \chi_j \rangle$ and $\langle \chi_i \rangle$ with $\chi_i = \sigma_l \times \sigma_m \cdot \sigma_n$

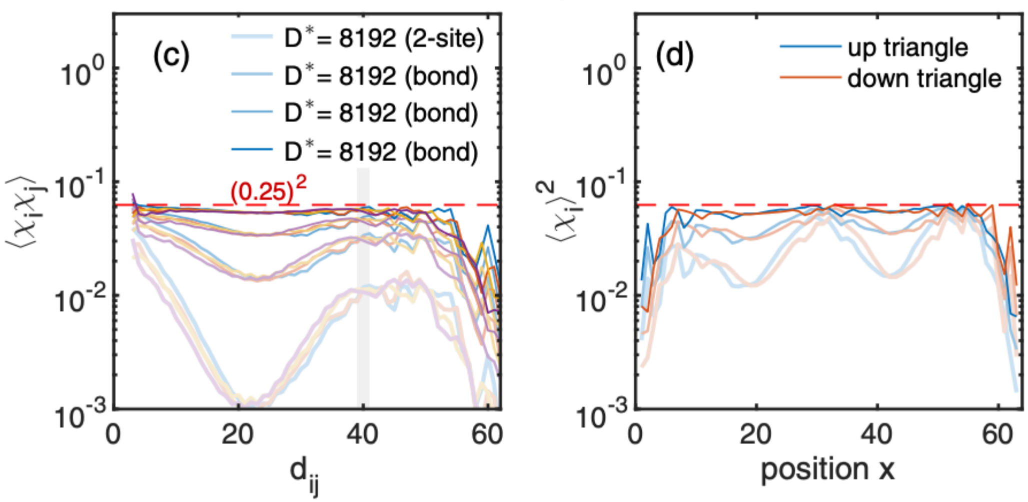


YC4 Data:



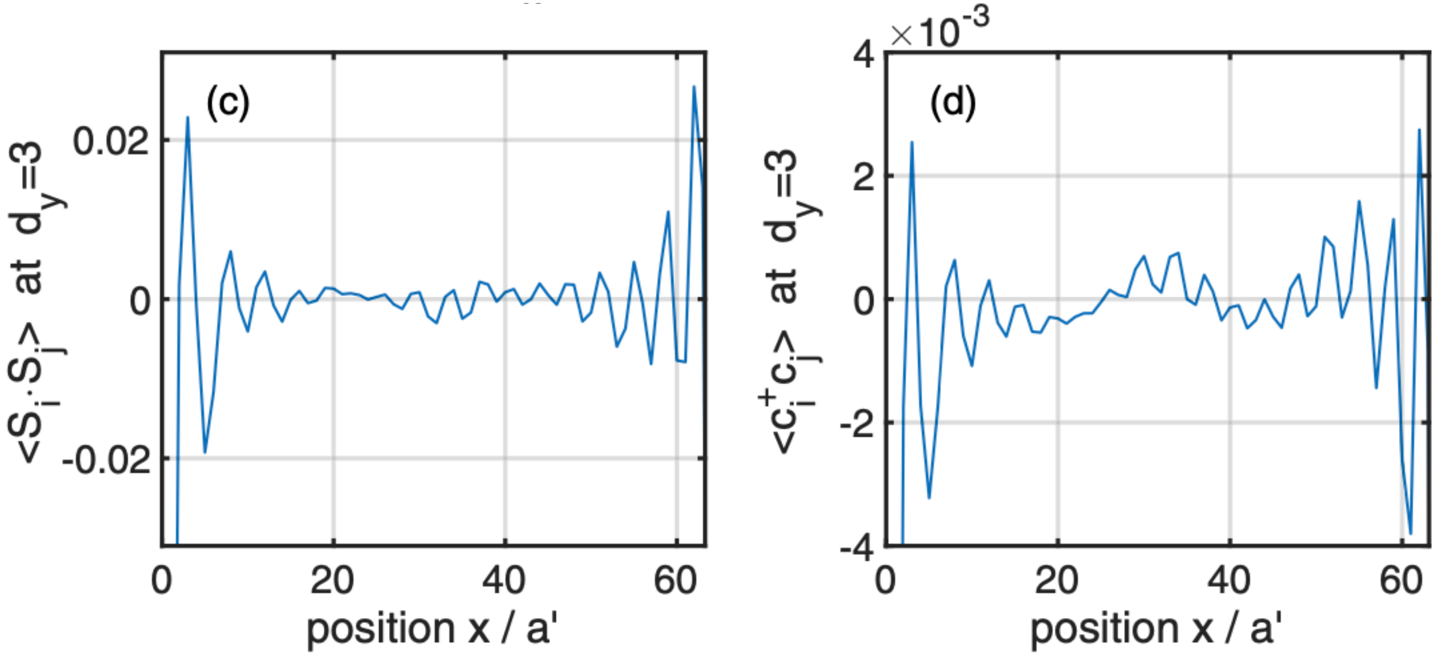
YC6 Data:

(L=64)



2.2 CSL: On the need for long cylinder

- spin correlation
- charge correlation



✓ Strong boundary oscillation (slow decay ~20 columns)

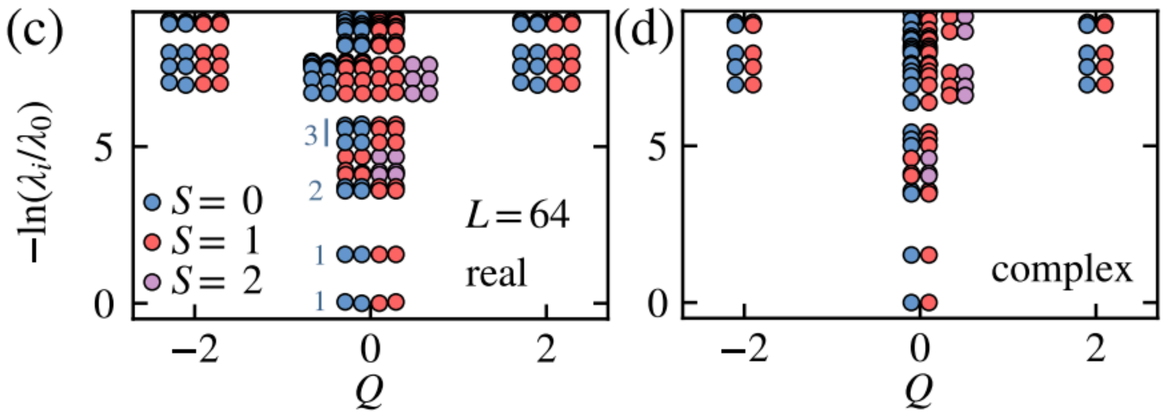
✓ L > 40 is needed.

We note that, L = 8 in [Shirakawa, PRB 96, 205130 (2017)]

➢ 2.2 Chiral Spin Liquid: chiral edge mode

✓ Entanglement spectrum: SU(2) level-1 WZW CFT (1,1,2,3,5,...)

8-fold degeneracy



4-fold degeneracy

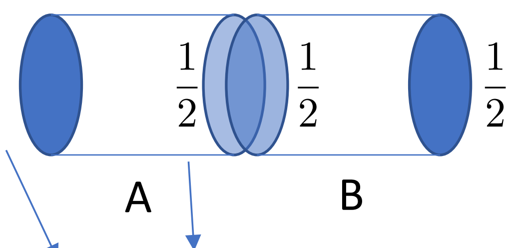
---

block diagonal with conserved charge Q and total spin S

$$\rho^A = \begin{bmatrix} (Q_1, S_1) & & & \\ & (Q_2, S_2) & & \\ & & \cdots & \\ & & & (Q_i, S_i) \end{bmatrix}$$

semion sector of CSL

spinon $\frac{1}{2}$



$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$$

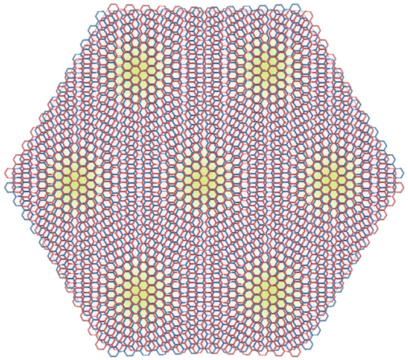
thus, 4-fold degeneracy

Ground state of twisted bilayer graphene model

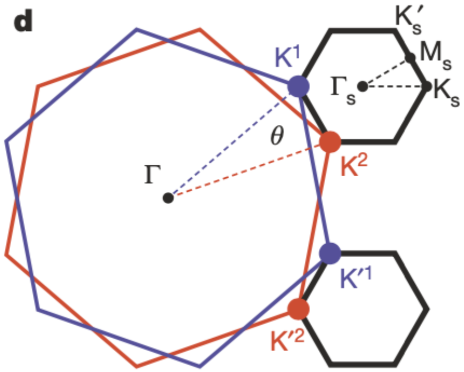
BC, Y. D. Liao, Z.Chen, O. Vafek, J. Kang, W. Li, and Z. Y. Meng. Nat. Commun. 12, 5480 (2021)

➢ 2.3 Magic-Angle Twisted Bilayer Graphene

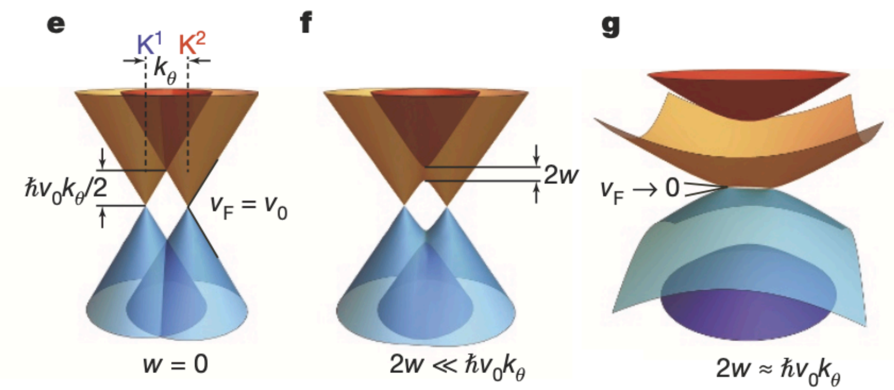
- Twisted Bilayer Graphene (TBG)



Moire pattern



- Narrow band at magic angle

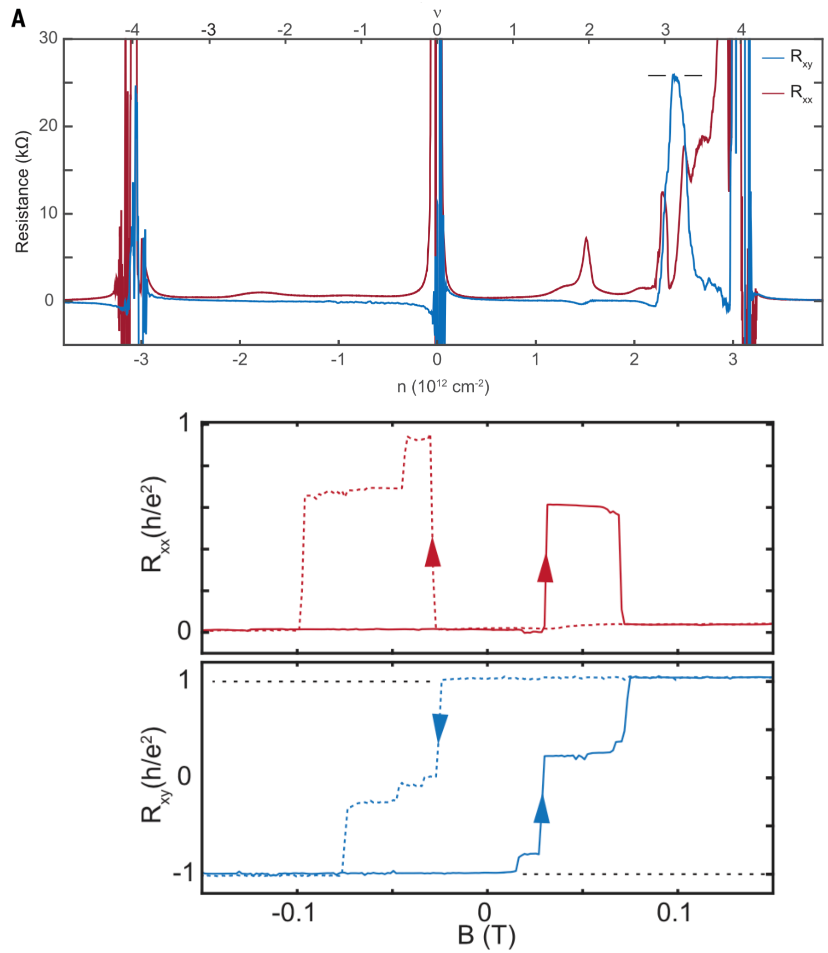


New playground for strongly correlated states

Cao, Nature 556, 43 (2018)
Cao, Nature 556, 80 (2018)

- QAH at 3/4-filling

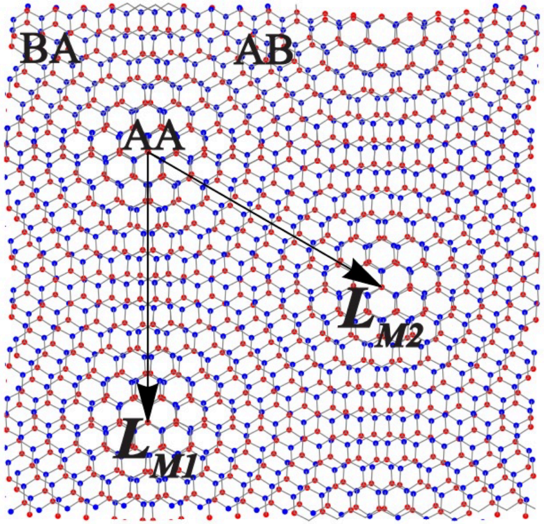
Chern number C=1



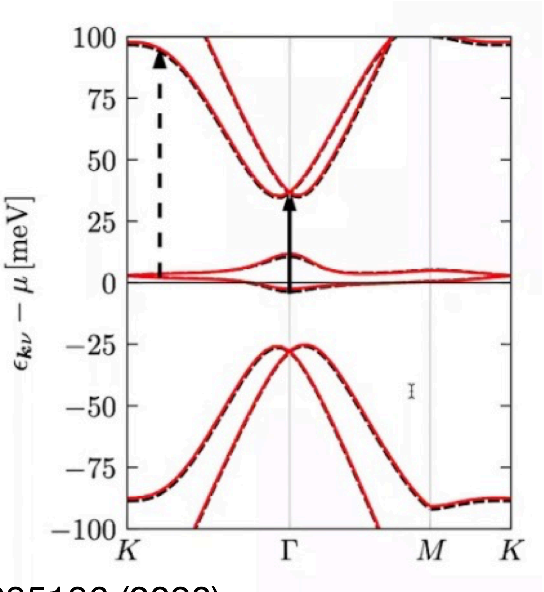
Serlin et al., Science 2020

➢ 2.3 Magic-Angle Twisted Bilayer Graphene

✓ Moire Lattice



✓ flat bands



8 narrow bands:

2 valleys
x
2 spins
x
2 bands

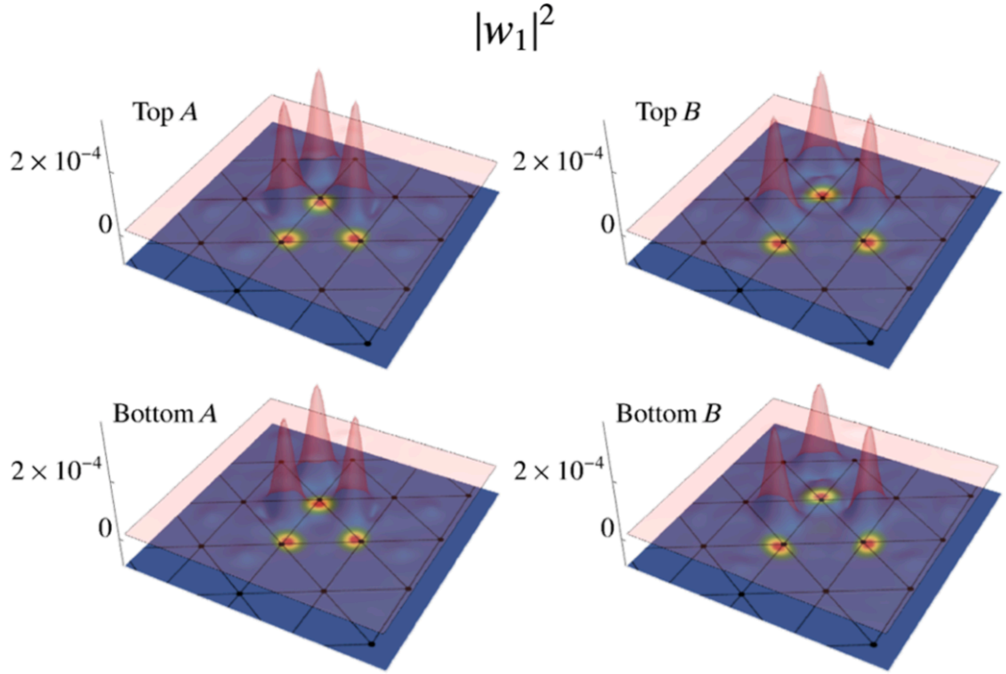
•Yi Zhang et al, Phys. Rev. B 102, 035136 (2020)

✓ Coulomb interactions between electrons in narrow bands:

$$U = \frac{1}{2} \sum_{r,r'} \sum_{\sigma,\sigma'} \rho_\sigma(r)\ V(r-r')\ \rho_{\sigma'}(r')$$

➢ 2.3 Real-space effective model

✓ localized wannier function



✓ 3-peak structure

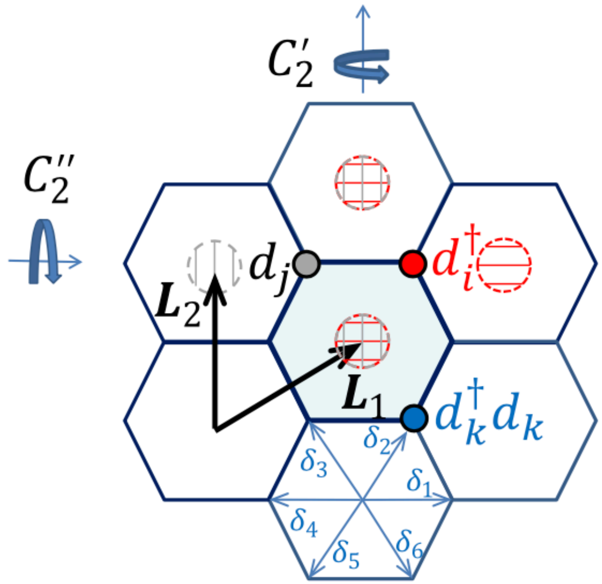
✓ centered at the honeycomb lattice

Projecting onto these Wannier basis:

$$c_\sigma(r) = \frac{1}{3}\sum_R \sum_{p=1}^{6} \sum_{j=\pm1} w_{R+\delta_p,j}(r)\ d_{j,\sigma}(R+\delta_p)$$

J. Kang, O. Vafek, PRX 8, 031088 (2018)

$$U = \frac{1}{2}\sum_{r,r'}\sum_{\sigma,\sigma'} \rho_\sigma(r)\ V(r-r')\ \rho_{\sigma'}(r')$$



$$U = \frac{V_0}{2}\sum_R \left(\sum_{j,\sigma} O_{j\sigma}(R)\right)^2$$

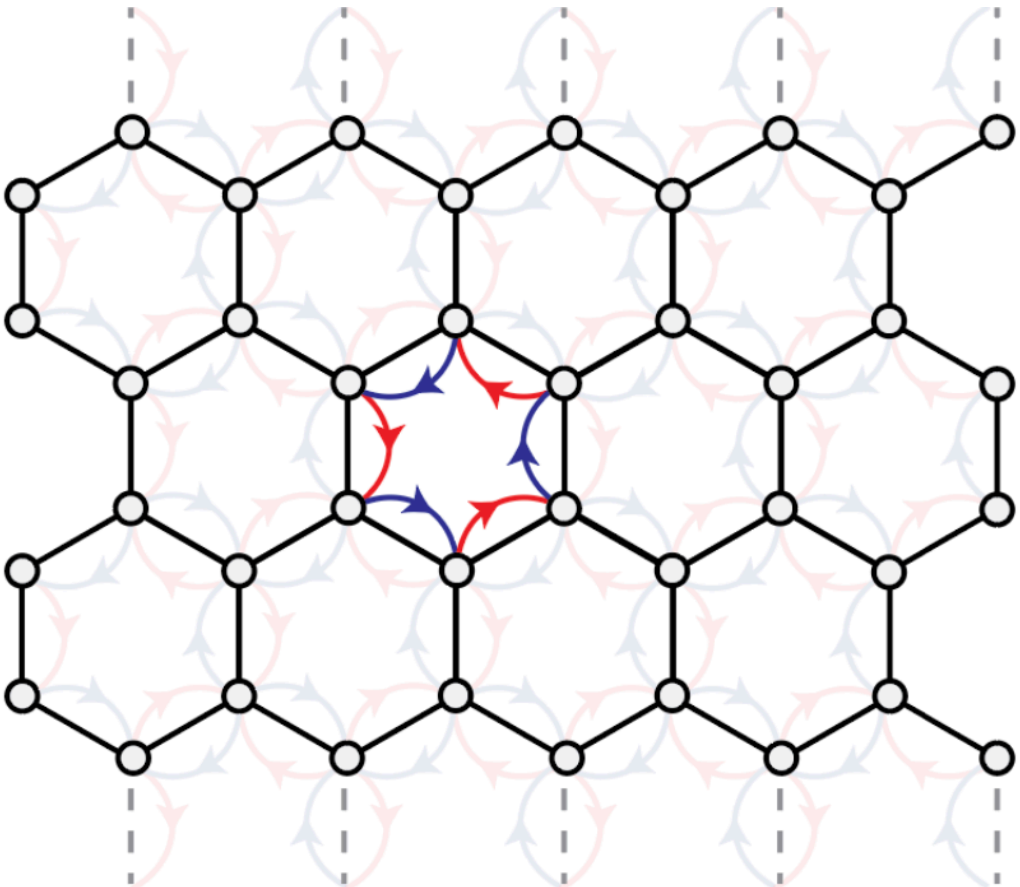
With $O_{j,\sigma}(R) = Q_{j,\sigma}(R) + \alpha T_{j,\sigma}(R)$

J. Kang, O. Vafek, PRL 122, 246401 (2019)

➢ 2.3 TBG Model

- Hubbard-like Model

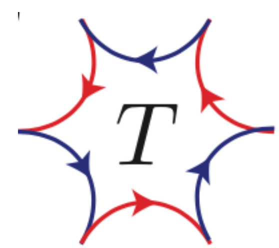
$$H = U_0 \sum_{\hexagon} (Q_{\hexagon} + \alpha T_{\hexagon} - 1)^2,$$



- Cluster charge

$$Q_{\hexagon} = \sum_{i\in\hexagon} \hat{n}_i/3$$

- Hopping Assisted interaction

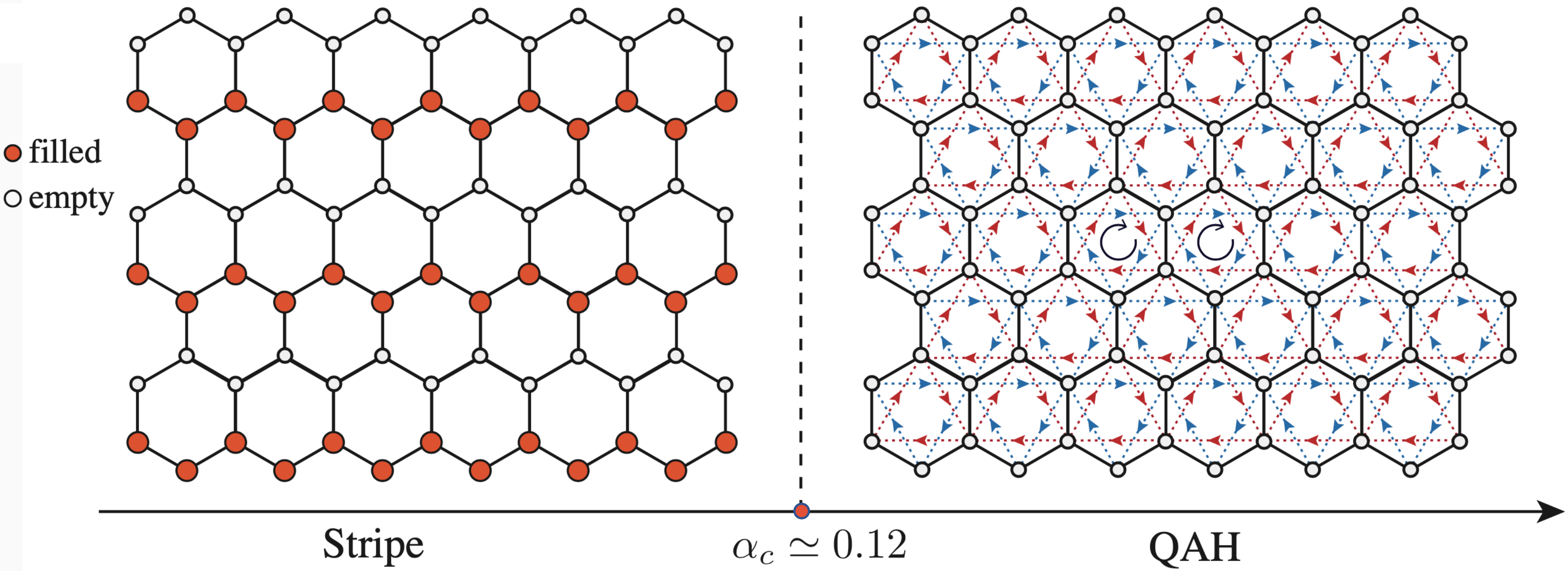


$$T_{\hexagon} = \sum_{j\in\hexagon}[(-1)^j c^\dagger_{j+1} c_j + h.c.]$$

J. Kang, O. Vafek, **PRL** 122, 246401 (2019)

2.3 Ground-state phase diagram

- TBG Model $H = U_0 \sum_{\hexagon} (Q_{\hexagon} + \alpha T_{\hexagon} - 1)^2,$



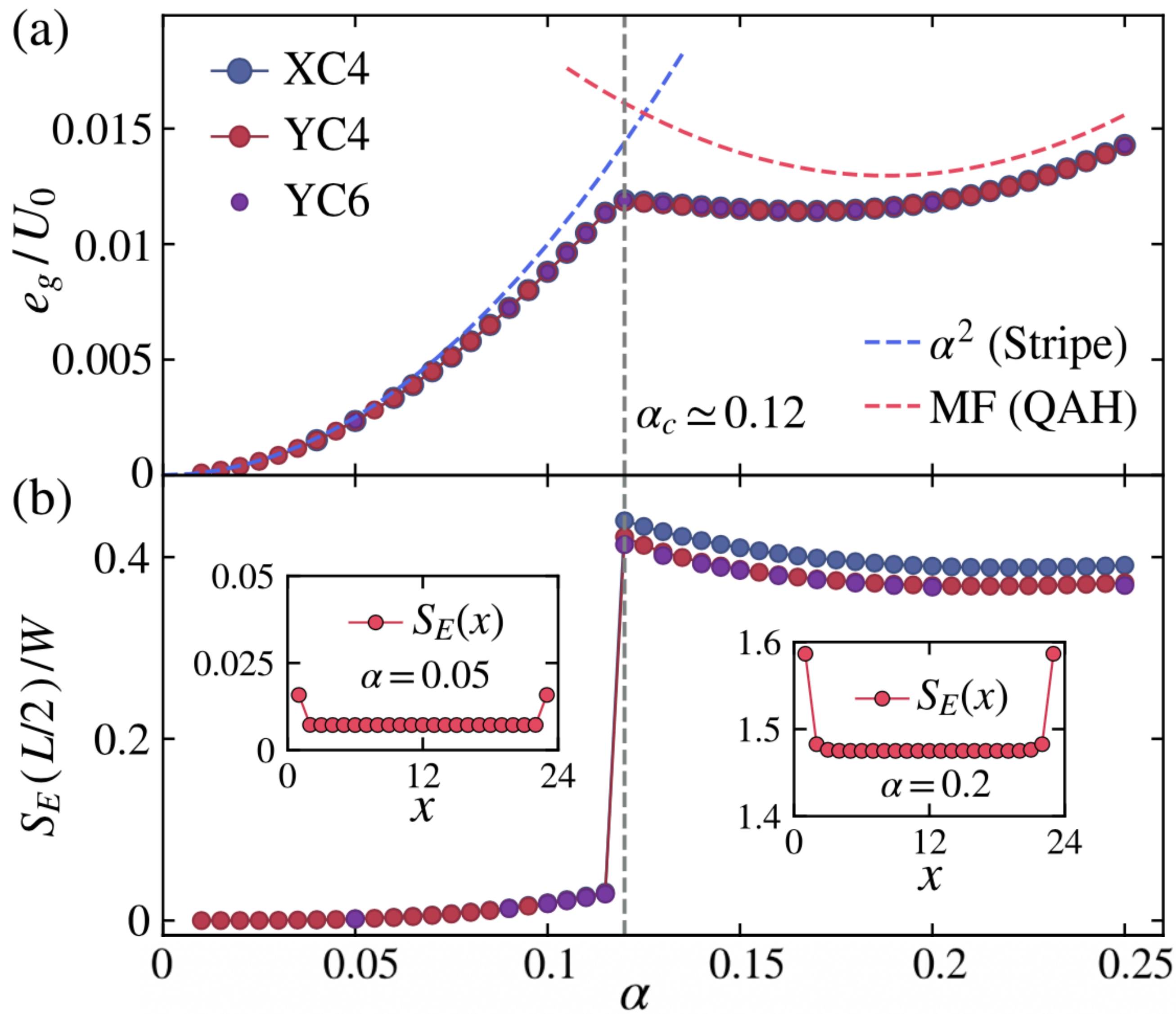
➢ 2.3 Magic-angle twisted bilayer graphene

- Ground-state energy

first-order transition

- Entanglement entropy

Both Gapped

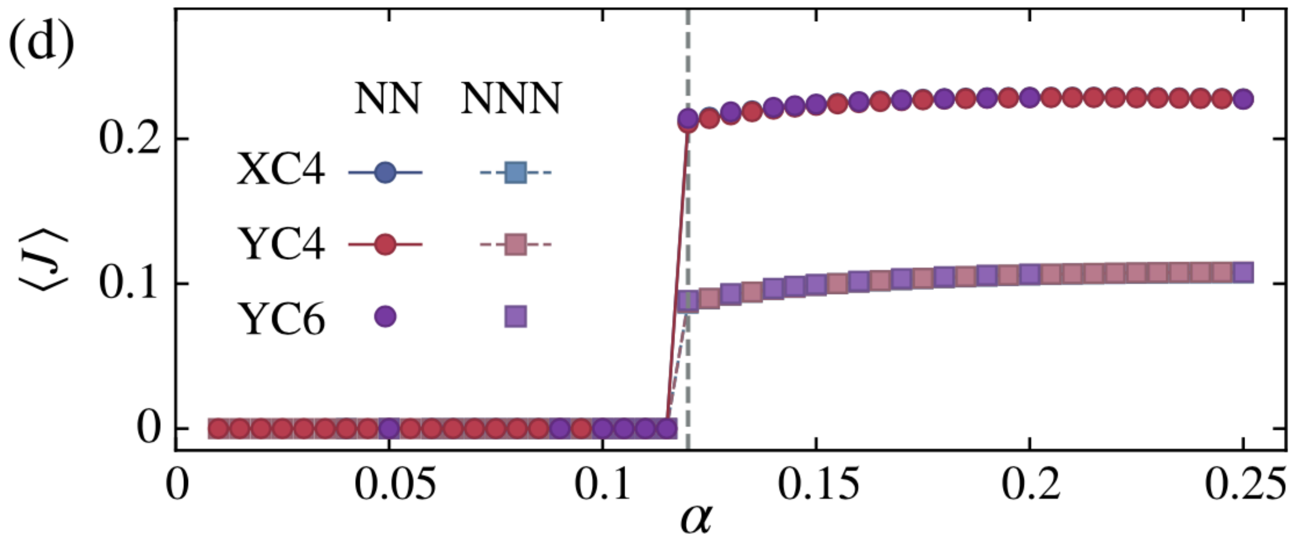


➢ 2.3 Identify QAH

- ❑ Spontaneous time-reversal symmetry (TRS) breaking?
- ❑ Loop current?
- ❑ non-zero Chern number?

✓ Spontaneous TRS breaking

- current operator $J \equiv \mathrm{i}(c_i^\dagger c_j - c_j^\dagger c_i)$



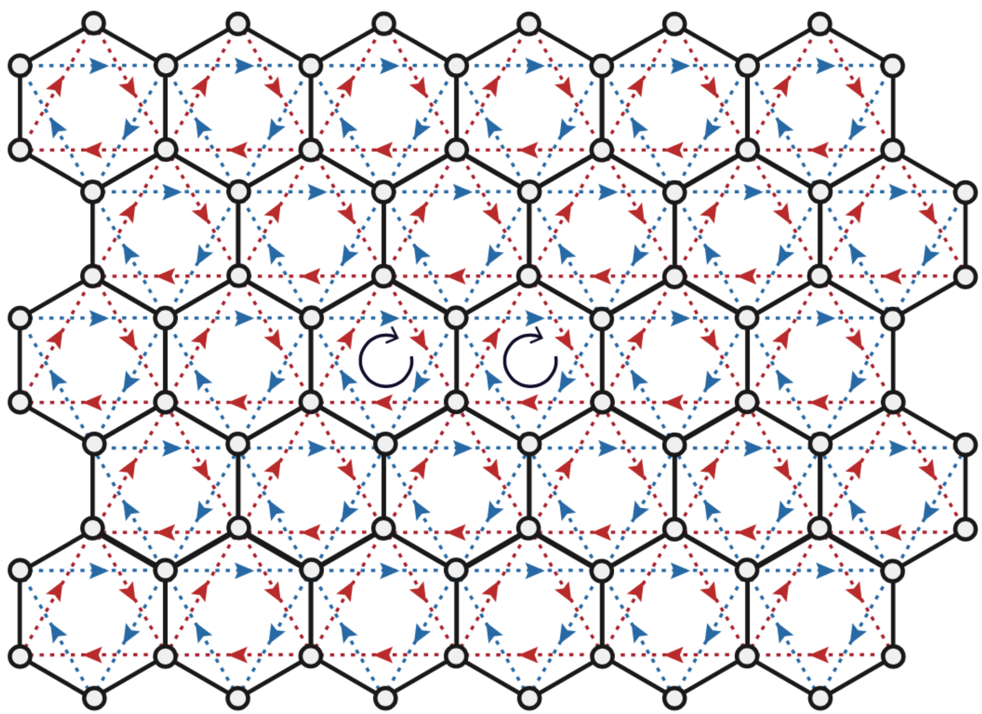
➢ 2.3 Identify QAH

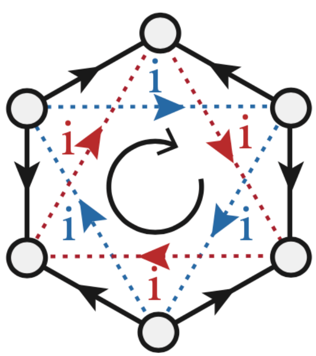
✓ Spontaneous time-reversal symmetry breaking

❑ Loop current?

❑ non-zero Chern number?

✓ Loop current $J \equiv \mathrm{i}(c_i^\dagger c_j - c_j^\dagger c_i)$





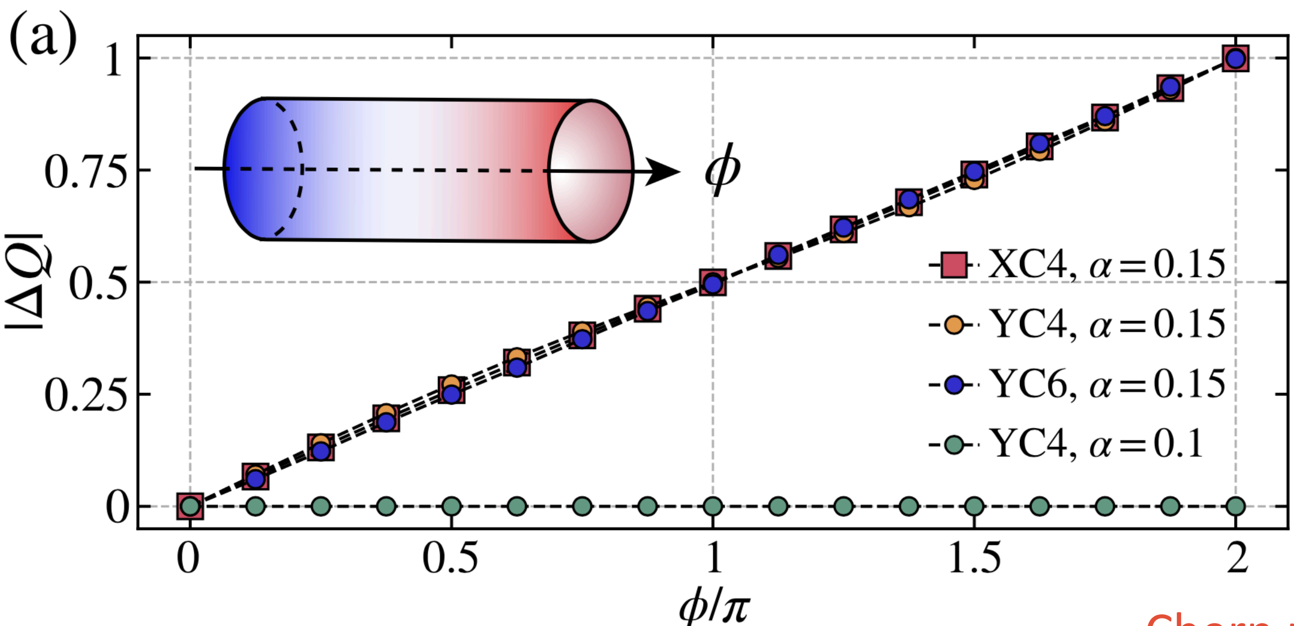
➢ 2.3 Identify QAH

✓ Spontaneous time-reversal symmetry breaking
✓ Loop current
✓ non-zero Chern number

✓QAH

- Flux Insertion (Laughlin's thought experiment)

$$c_{\mathbf{i}} \equiv c_{\mathbf{i}+\mathbf{W}} \rightarrow c_{\mathbf{i}} \equiv e^{i\phi} c_{\mathbf{i}+\mathbf{W}}$$

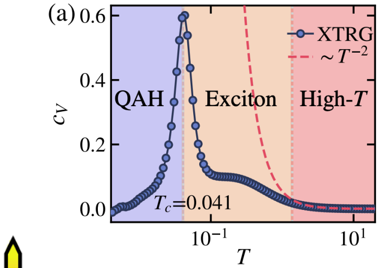


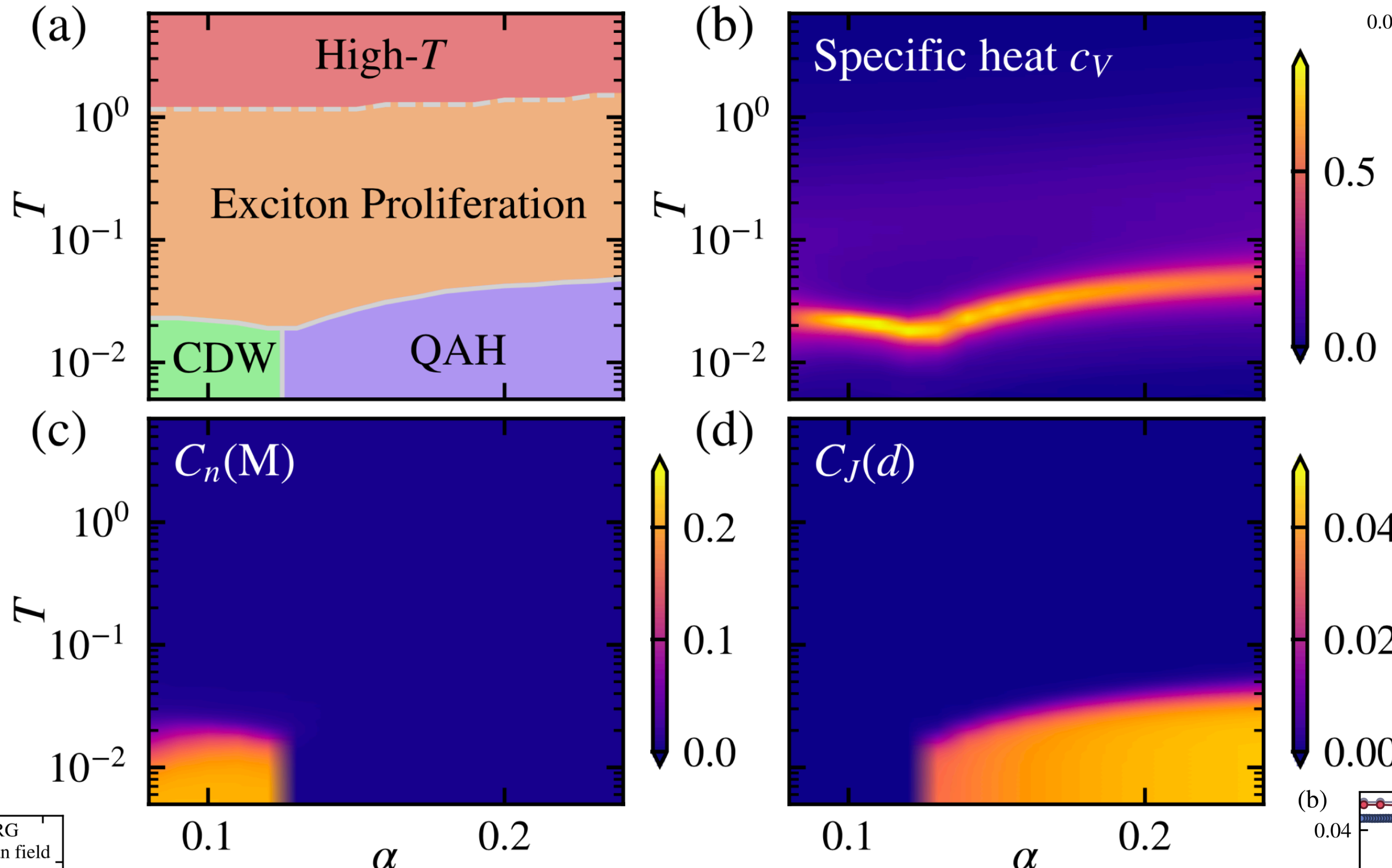
Chern number = 1

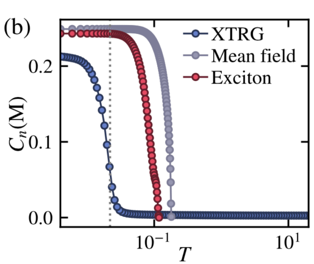
Thermodynamics of twisted bilayer graphene model

X. Lin, **BC***, Wei Li, Zi Yang Meng*, and Tao Shi*, Phys. Rev. Lett. **128**, 157201

2.3 Finite-T phase diagram

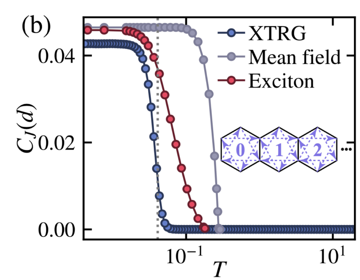






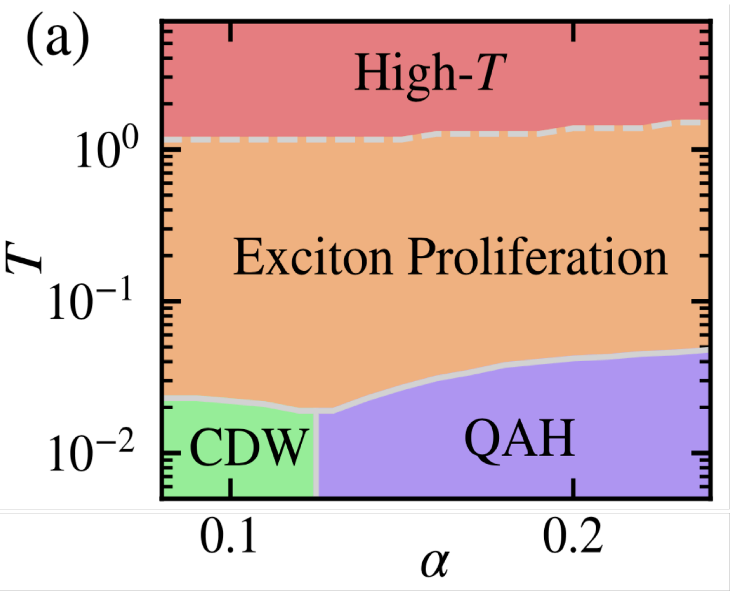
$$C_n(k) \equiv \frac{1}{N}\sum_i e^{-ik\cdot r_{0i}}\left(\langle \hat{n}_i \hat{n}_0\rangle - \langle \hat{n}_i\rangle\langle \hat{n}_0\rangle\right)$$

$$C_J(d) = \langle J_0 J_d \rangle$$



➢ 2.3 Exciton proliferation regime

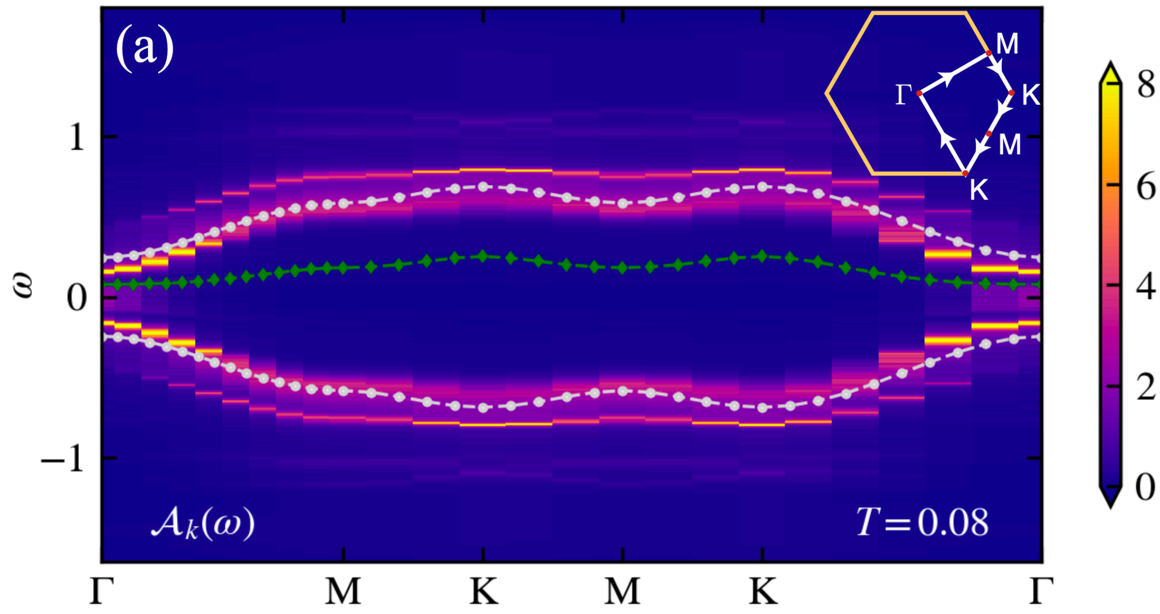
✓ Finite-T phase diagram

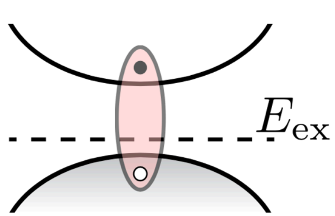


Mean-field estimation of Tc ~ 100 K

Obtained Tc ~ 10 K

✓ Spectral function

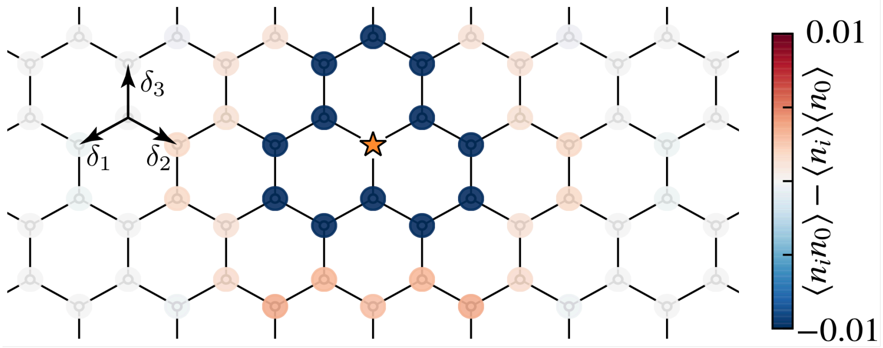




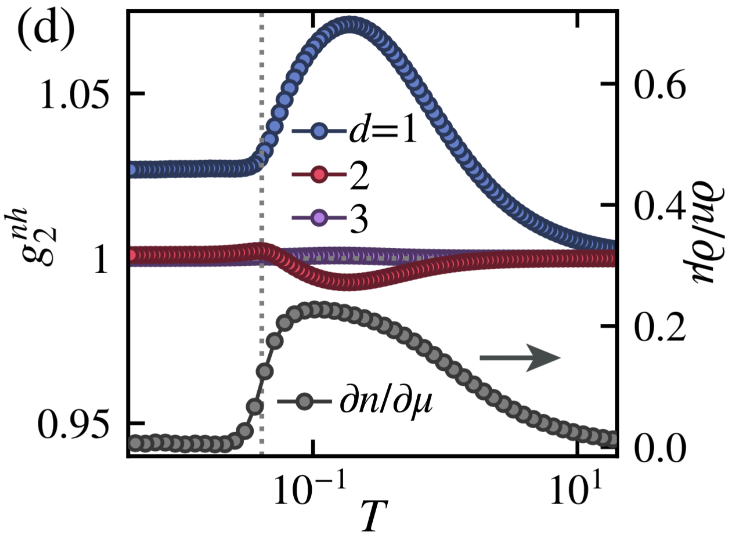
Exciton corrects the spectrum!

➢ 2.3 Thermodynamic signature of exciton

✓ Microscopic characteristic



✓ Charge compressibility



Thermal Tensor Network Approach for Quantum Many-Body systems

Bin-Bin Chen

Nov. 9, 2022

Outline

❑ 1. Finite-T tensor network methods

- 1.1 Tensor network basis
- 1.2 Series-expansion thermal tensor network
- 1.3 Exponential tensor renormalization group
- 1.4 Differentiable tensor renormalization group

❑ 2. Application 1

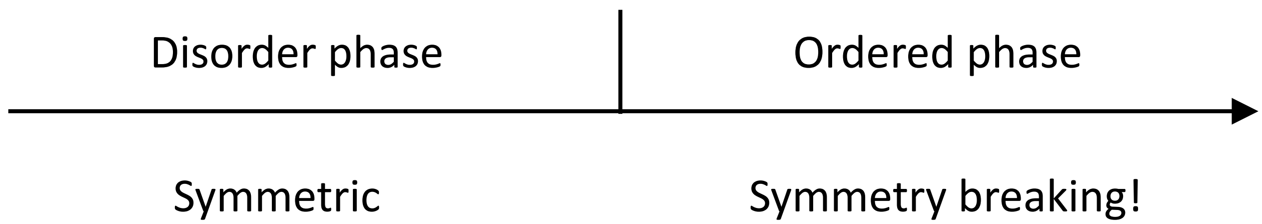
- 2.1 Square-lattice Hubbard model
- 2.2 Triangular-lattice Hubbard model
- 2.3 Magic-angle twisted bilayer graphene model

❑ 3. Application 2

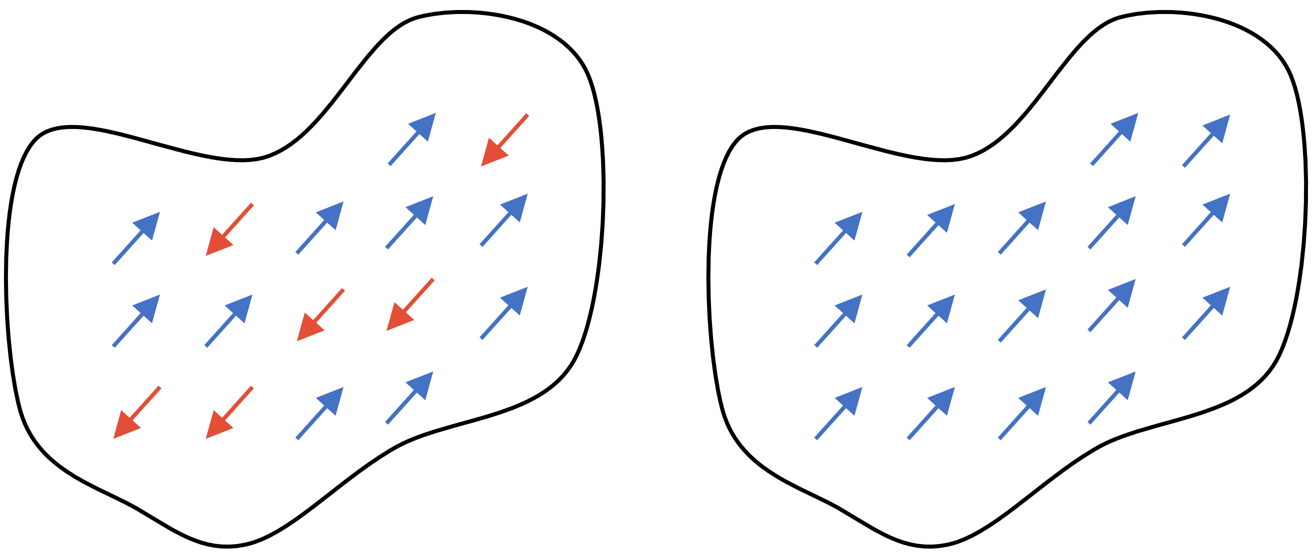
- 3.1 Quantum entanglement and disorder operator
- 3.2 topological disorder operator

➢ 3.1 Entanglement and Disorder Operator

- ✓ **Landau paradigm for phase transition:**



- ✓ E.g. Ferromagnetic phase transition



3.1 Entanglement and Disorder Operator

✓ **Landau paradigm for phase transition:**

Disorder phase	Ordered phase
Symmetric	Symmetry breaking!

✓ **Order parameter** (e.g. Magnetization for FM)

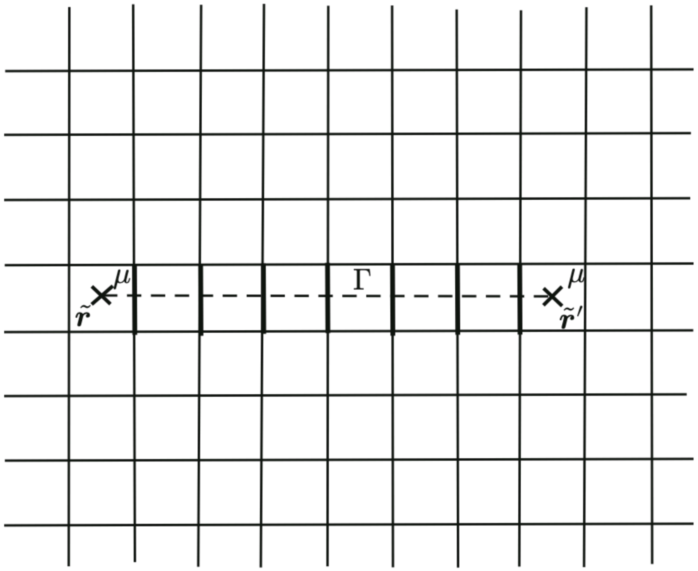
Short-range correlation (Exponential decay of correlation)	Long-range correlation of local order parameter

✓ **Disorder operator to characterize symmetric phase** Kadanoff and Ceva, 1971

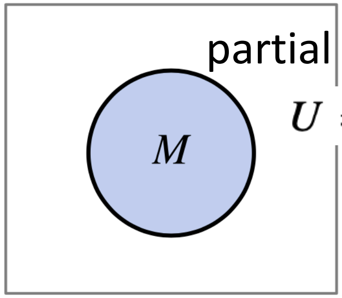
non-vanishing expectation	vanishing expectation

3.1 Entanglement and Disorder Operator

✓ **Disorder operator to characterize symmetric phase**



Classical 2D FM Ising model
[Kadanoff and Ceva, 1971]



partial transformation

$U = \prod_{\mathbf{r}} U_{\mathbf{r}}$

✓ **Modified 2D FM Ising model with defect**

changing the coupling constant J to have an antiferromagnetic sign

✓ **Disorder operator (variable)**

$$\langle \mu(\tilde{\boldsymbol{r}})\mu(\tilde{\boldsymbol{r}}')\rangle = \frac{Z[\Gamma]}{Z} \equiv \exp(-\Delta F[\Gamma]/T)$$

$$\langle \mu(\tilde{\boldsymbol{r}})\mu(\tilde{\boldsymbol{r}}')\rangle = \begin{cases} \text{const.} \times \dfrac{e^{-\kappa|\tilde{\boldsymbol{r}}-\tilde{\boldsymbol{r}}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|^{1/2}}, & T < T_c \\ \dfrac{\text{const.}}{|\boldsymbol{r}-\boldsymbol{r}'|^{1/4}}, & T = T_c \\ |\langle \mu \rangle|^2 + O(e^{-\kappa'|\tilde{\boldsymbol{r}}-\tilde{\boldsymbol{r}}'|}), & T > T_c \end{cases}$$

✓ **non-vanishing expectation in symmetry-preserving phase**

➢ 3.1 Entanglement and Disorder Operator

✓ Disorder operator and entanglement

E.g. Bose Hubbard Model $X_M(\theta) = \prod_{\mathbf{r}\in M} e^{i\theta n_{\mathbf{r}}}$ [Y. C. Wang, et al. PRB **104**, L081109 (2021)]

Superfluid | 3D XY transition | Mott Insulator → U/t

$|\langle X_M(\theta)\rangle| \sim e^{-b(\theta)l\,\ln l}$

$U_c = 16.74$

$|\langle X_M(\theta)\rangle| \sim e^{-a_1(\theta)l}$

"area" law

$$\ln|\langle X_M(\theta)\rangle| = -a_1 l + s\,\ln l + a_0$$

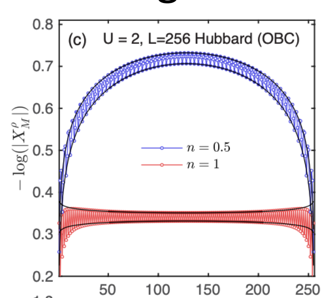
logarithmic correction
from corner correction

E.g. Free and interacting fermion systems [W. Jiang, **BC**, et al. arXiv: 2209.07103 (2022)]

✓ non-interacting fermion

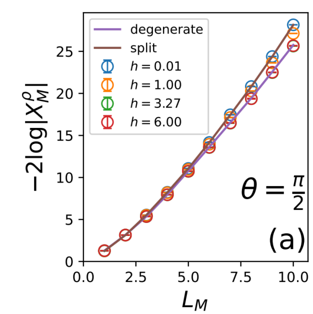
$$S_2 = -2\log\left|X_M^{\rho}\left(\frac{\pi}{2}\right)\right|,$$
$$S_3 = -\log\left|X_M^{\rho}\left(\frac{2\pi}{3}\right)\right|.$$

✓ interacting fermion in 1D



$$-\log|X_M^{\rho}(\tfrac{\pi}{2})| = \frac{K_\rho}{4}\log L_M + \text{const}$$

✓ interacting fermion in 2D



scale as $L_M \log L_M$

3.1 Entanglement and Disorder Operator

✓ **Topological entanglement entropy** [Kitaev and Preskill, PRL 96, 110404 (2006)]

For a disk in the plane, the von Neumann Entanglement entropy

$$S(\rho) = \alpha L - \gamma + \cdots$$

where

$$\gamma = \log \mathcal{D} \quad \text{with} \quad \mathcal{D} = \sqrt{\sum_a d_a^2}$$

Total quantum dimension

Summing over all superselection sectors (anyon types)

Disorder operator to detect topological order?

Topological Disorder Parameter

BC, Hong-Hao Tu, Zi Yang Meng, Meng Cheng, PRB **106**, 094415 (2022)

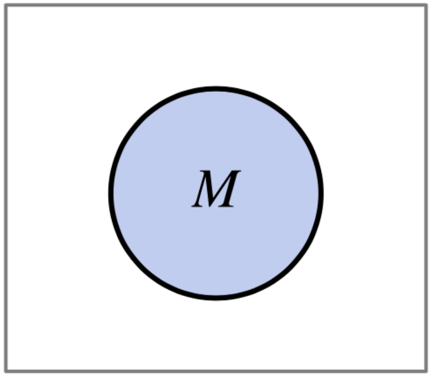
➢ 3.2 Topological Disorder Parameter

✓ **Topological disorder parameter (TDP)**

(Constant correction that appears in the ground-state expectation value of a partial symmetry transformation applied to a connected spatial region M.)

$$\ln|\langle U_M(g)\rangle| = -\alpha|\partial M| + \gamma_g + \cdots$$

$$\gamma_g = \ln d_g$$



✓ **Useful properties of symmetry defect** [M. Barkeshli, P. Bonderson, M. Cheng, and Z. Wang, PRB 100, 115147 (2019)]

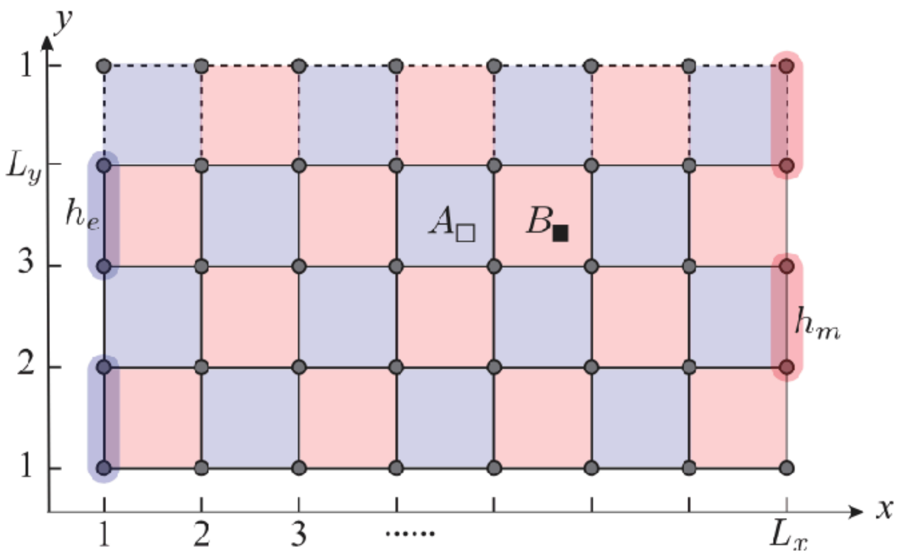
1. Total quantum dimension of *g* defects defined as $\mathcal{D}_g = \sqrt{\sum_{a_g \in \mathcal{C}_g} d_{a_g}^2}$, one can prove $\mathcal{D}_g = \mathcal{D}$

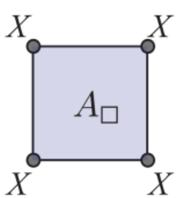
2. the number of *g*-defect types is the same as the number of *g*-invariant anyons.

3. if all anyons are Abelian, then all *g* defects must have the same quantum dimensions.

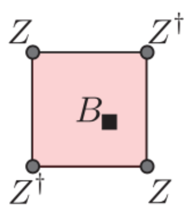
3.2 Topological Disorder Parameter

✓ Z_N toric code model





$$A_\square = X_1 X_2 X_3 X_4$$



$$B_\blacksquare = Z_1 Z_2^\dagger Z_3 Z_4^\dagger$$

- At each site, there is a **Z_N Spin:**

$$|n\rangle \quad (n = 0, 1, \cdots, N-1)$$

- Clock operator **Z**, and shift operator **X**:

$$Z|n\rangle = \omega^n |n\rangle, \;\; X|n\rangle = |[n+1]_N\rangle$$

- Hamiltonian

$$H = -\sum_\square (A_\square + \text{H.c.}) - \sum_\blacksquare (B_\blacksquare + \text{H.c.}) - \sum_{\mathbf{r}} (h_x X_{\mathbf{r}} + h_z Z_{\mathbf{r}} + \text{H.c.}),$$

➢ 3.2 Topological Disorder Parameter

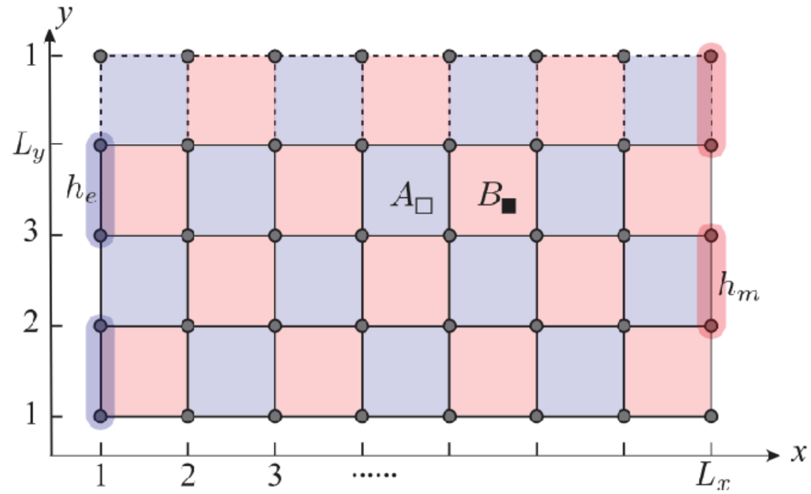
✓ **exactly solvable limit (h=0):**

Ground state: $A_\square = B_\blacksquare = 1$ for all squares

e excitation: $A_\square = \omega$

m excitation: $B_\blacksquare = \omega$

N^2 topological distinct excitation: $e^a m^b$



✓ **charge conjugation symmetry:** $U = \prod_{\mathbf{r}} U_{\mathbf{r}}$ $\quad U_{\mathbf{r}}|n\rangle_{\mathbf{r}} = |N-n\rangle_{\mathbf{r}}$

$$U_{\mathbf{r}} X_{\mathbf{r}} U_{\mathbf{r}}^\dagger = X_{\mathbf{r}}^\dagger \qquad UA_\square U^\dagger = A_\square^\dagger = A_\square^{N-1}$$

$$U_{\mathbf{r}} Z_{\mathbf{r}} U_{\mathbf{r}}^\dagger = Z_{\mathbf{r}}^\dagger \quad \Rightarrow \quad UB_\blacksquare U^\dagger = B_\blacksquare^\dagger = B_\blacksquare^{N-1}$$

under the action of U, excitations transform as $C : e^a m^b \to e^{N-a} m^{N-b}$

1) For odd N, no anyon is invariant. $d_{\sigma_C} = N$ $\Rightarrow$ $\mathrm{TDP} = \ln N$

2) For even N, 4 C-invariant anyons: $d_{a_C} = \frac{N}{2}$ $\Rightarrow$ $\mathrm{TDP} = \ln \frac{N}{2}$

$1,\ e^{N/2},\ m^{N/2},\ e^{N/2} m^{N/2}$

➢ 3.2 Topological Disorder Parameter

✓ **DMRG calculations for Z3 toric code at h>0:**

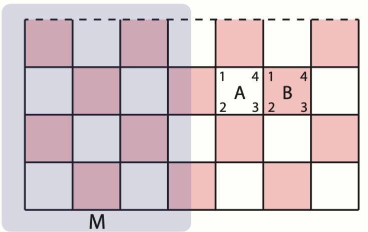
✓ Ground-state energy:

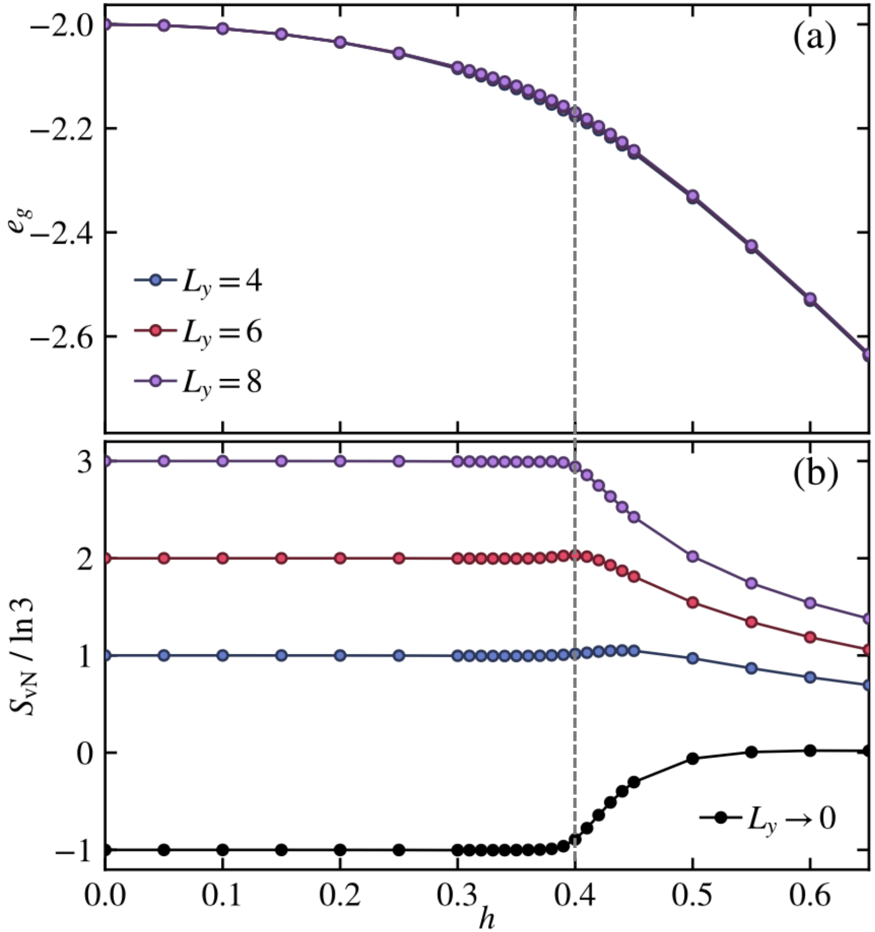
$$\frac{1}{L_x L_y}\langle\psi_{gs}|H|\psi_{gs}\rangle$$

$(L_x = 16 \text{ fixed})$

✓ Entanglement (von Neumann) entropy:

$$S_{vN} = -\mathrm{tr}(\rho_A \ln \rho_A)$$





$$S^{vN} = \alpha|\partial M| - \gamma$$

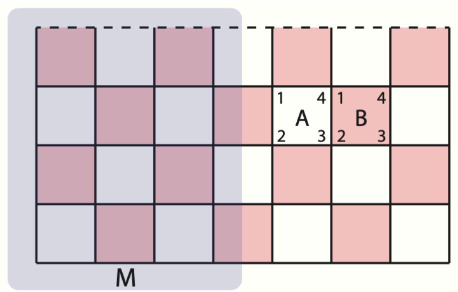
- First-order transition at h=0.4
- TEE = ln3 for h<0.4

[Schulz et al New J. Phys. 14 025005 (2012)]

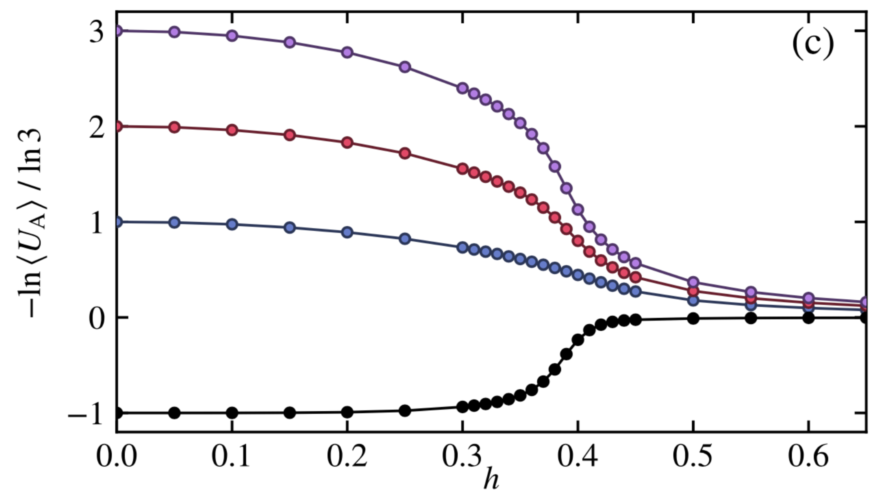
➢ 3.2 Topological Disorder Parameter

✓ DMRG calculations for the h>0 cases:

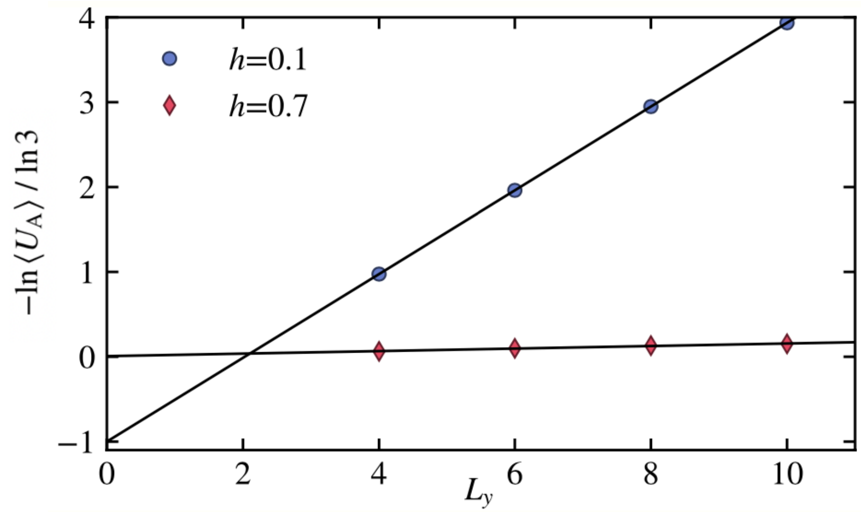
✓ Disorder operator:



$$U_{\mathrm{A}} = \Pi_{\mathbf{r}\in\mathrm{A}} C_{\mathbf{r}}$$



$$-\ln|\langle U_{\mathrm{A}}\rangle| = \alpha' L_y - \ln 3$$



- TDP = ln3 for h<0.4