## 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 Finite-temperature entanglement spectrum
- 3.2 disorder operator

## ➢ 1.1 Motivation

□ Strong Correlated systems:

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

"Exponential wall"



Quantum Monte Carlo (QMC)

Negative sign problem

Tensor Network (TN)

capture the entanglement structure

"Wheat and chessboard" problem

### Basic terminology



Manybody wavefunction



# of parameters:  $d^N$ Exponential wall!

- Typical Tensor Network
- ✓ Matrix Product State (MPS)



✓ Projected Entangled-Pair State (PEPS)



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

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,  $~S_E \sim {
m const.}$ 

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

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

Then, for 2D gapped systems,

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

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







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)



Czarnik, et al. 2017



### 1.1 Path-Integral Thermal Tensor Network

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

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

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

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

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

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

## > 1.1 Path-Integral Thermal Tensor Network

Trotter

$$Z = Tr(e^{-\beta H})$$

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

1+1D Tensor Network

β

au

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:

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

□ Main Procedure:



### 1.2 Basic Idea of SETTN

Taylor Expansion of Partition Function:

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

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



(a)  $H = - \Phi - \Phi$ 

(b)  $Z = \omega_0 Tr$ 

+  $\omega_n Tr$ 

+  $\omega_1 Tr \left[ - \phi \right]$ 

 $\hat{P} \in \left\{ \hat{I}, \hat{S}_x, \hat{S}_y, \hat{S}_z \right\}$ 

2**T** 

#### $+S^x S^x II + S^y S^y II + S^z S^z II$

 $IIS^{x}S^{x} + IIS^{y}S^{y} + IIS^{z}S^{z}$  $= +IS^{x}S^{x}I + IS^{y}S^{y}I + IS^{z}S^{z}I$ 

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

## 1.2 Basic Idea of SETTN

E.g. N= 4 Heisenberg chain

## 1.2 Efficient contraction of H<sup>n</sup>



 $H^n$ 

will have bond dimension

 $D^n$ 

Η

 $H^2$ 

 $H^3$ 

Bond dimension scales exponentially and will quickly become unaffordable.

## 1.2 Efficient contraction of H<sup>n</sup>

#### Canonical form:



### 1.2 Expansion cutoff

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

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

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

which is most prominent around  $n=eta L|e_{
m g}|$ 



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

Then partition function is dominant by weight around

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

# 1.2 Performance of SETTN

• L=14 XY chain

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



## > 1.2 Summary of SETTN



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

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



## > 1.3 Reduce numbers of truncation steps

logarithmic scaling of entanglement entropy

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



### 1.3 Performance of XTRG



1 order of magnitude better than Linear scheme and also SETTN

## ▶ 1.3 More data of XTRG

Extraction of central charge

✓ Long Heisenberg chain

 $10^{0}$ αT<sup>η</sup>, α=0.667, η=0.996 × XTRG, D\* = 150  $T^{\mu}, \mu = -2.01$ O D\* = 250 L = 300ు><sup>10-2</sup> • o<sup>></sup> 0.2 10<sup>-4</sup> 0 10<sup>-2</sup> 10<sup>0</sup>  $10^{2}$ 10<sup>-2</sup> 10<sup>-1</sup> 10<sup>0</sup> 10<sup>1</sup> 10<sup>2</sup> т  $\alpha = \frac{\pi c}{3v}$  $c_V = \alpha T^{\eta}$ 



## 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





## ▶ 1.4 Basic Idea of ∂TRG



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

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

internal energy

specific heat



accurate estimate of transition temperature ~1%

## ➢ Summary of ∂TRG



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Nov. 2, 2022

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### 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



## > 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
- $\checkmark$  single-site resolution

Current Experimental Scope



"Long-range" Antiferromagnet



# 2.1 Ultra-cold Fermions in optical lattice

0.3

0.2

0.1

0.0

2

 $(-1)^{i} C_{d}$ 





Doping

Long-range Antiferromagnet

Spin Removal

**↑**+

♠





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



Efficient & accurate numerical simulations! (XTRG is promising!)

Greiner's group (Harvard), Nature 2017

d (sites)

8

## 2.1 Spin correlation under half-filling



Greiner, Nature 2017

# 2.1 Spin correlation under 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

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





Greiner, Nature 2017



#### ✓ 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 compounds:

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



Spin Liquid?













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

## 2.2 Motivation from theoretical studies



• 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)
- --- Mishmash, Phys. Rev. Lett. 111, 157203 (2015)

Nodal gapless spin liquid

#### • DMRG Results:

2-leg ladder: U(1) gapless
 Mishmash, PRB 91, 235140 (2015)

#### (preserve TRS)

(break TRS)

Finite DMRG: gapped
 infinite DMRG: chiral spin liquid
 Shirakawa, PRB 96, 205130 (2017)
 Szasz, PRX 10, 021042 (2020)

### 2.2 Model and Main Results (Phase diagram)



## 2.2 Phase diagram





## 2.2 Chiral Spin Liquid: TRS-breaking

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



## 2.2 CSL: On the need for long cylinder



- 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





semion sector of CSL



thus, 4-fold degeneracy

block diagonal with conserved charge Q and total spin S



5 min break; will be back at 3 pm

#### 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

Serlin et al., Science 2020

• QAH at 3/4-filling



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

### 2.3 Magic-Angle Twisted Bilayer Graphene



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



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



- ✓ 3-peak structure
- $\checkmark\,$  centered at the honeycomb lattice

Projecting onto these Wannier basis:

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

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

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

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



Cluster charge



- $Q_{\bigcirc} = \sum_{i \in \bigcirc} \hat{n}_i / 3$
- Hopping Assisted interaction



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

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

### 2.3 Ground-state phase diagram

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



## 2.3 Magic-angle twisted bilayer graphene



## 2.3 Identify QAH

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

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



## 2.3 Identify QAH

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

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





## 2.3 Identify QAH

- ✓ Spontaneous time-reversal symmetry breaking
- ✓ Loop current
- ✓ non-zero Chern number
- Flux Insertion (Laughlin's thought experiment)



### 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



## > 2.3 Exciton proliferation regime

✓ Finite-T phase diagram



### Spectral function



Mean-field estimation of Tc ~ 100 K

Obtained Tc ~ 10 K



Exciton corrects the spectrum!

### 2.3 Thermodynamic signature of exciton





