Tensor network methods in condensed matter physics

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Targets of tensor network methods

- Lattice models

Localized spin system:

\[ \mathcal{H} = \sum_{i,j} J_{ij} S_i S_j \]

*Spins located on a lattice:
  - square, triangular, cubic, …

We want to find novel states of the matter

- Quantum spin liquids
- Topological phases
- Valence Bond Solids
- ...

We want to investigate phase transition

- (Quantum) critical phenomena
- Topological phase transition
- ...

Targets of tensor network methods

- Lattice models

Itinerant electron systems: (Hubbard model)

\[ H = \sum_{\langle i,j \rangle, \sigma} t_{i,j} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \]

- creation operator of an electron.

We are interested in

- Super conductivity
- Non-equilibrium phenomena
- ...

A lot of interesting things occur in the Avogadro scale ~ 10

We need large scale calculations.
Numerical methods

- Numerical diagonalization
  - Exact and applicable for any systems, but
    - S=1/2 spin models ~ 40 sites
    - Hubbard model ~ 20 sites
  - We need careful extrapolation. (It is often very difficult.)

- Quantum Monte Carlo (QMC)
  - Within statistical error, solving problem “exactly”!
    - Easy calculation for
    - But, Interesting problems are usually suffer from the

- Dynamical Mean Field Theory (DMFT)
  - Kind of mean-field
    - Temporal quantum fluctuations are treated accurately through a few sites
  - Success in description of metal - insulator phase transition
Numerical methods

☑ Variational method

Assuming a wave-function ansatz with several parameters. Determining parameters so as to minimize the energy.

• Variational Monte Carlo
  Calculate energy using Monte Carlo sampling
  No sign problems.
  Larger system size than the diagonalization.

• Tensor network methods (including DMRG)
  Wave-function is represented by
  No sign problems.
  Very large system size (or infinite)
Tensor network method

G.S. wave function:  
\[ |\Psi\rangle = \sum_{\{m_i=\uparrow \downarrow\}} T_{m_1,m_2,\ldots,m_N} |m_1,m_2,\ldots,m_N\rangle \]

\( T \): N-rank tensor  
\( T_{m_1,m_2,\ldots,m_N} \)  
``Tensor network” decomposition

• Matrix Product State (MPS)  
\[ A_1[m_1]A_2[m_2]\cdots A_N[m_N] = A[m] \quad \text{Matrix for state } m \]

• General network  
\[ \text{Tr} X_1[m_1]X_2[m_2]X_3[m_3]X_4[m_4]X_5[m_5]Y \]
\( X,Y \): Tensors  
\( \text{Tr} \): Tensor network contraction

By choosing a “good” network, we can express G.S. wave function efficiently.

**ex.** MPS: # of elements = 2ND²  
D: dimension of the matrix A

Exponential → Linear

°If D does not depend on N…
Family of tensor network states

**MPS:** Work well in one-dimensional systems
DMRG, TEBD, ...

**PEPS, TPS:**
Two or higher dimensional systems
Generalization of MPS

**MERA:** Suitable for a scale invariant states

Renormalization
Quantum Entanglement

Reduced density matrix of the subsystem.

$$\rho_{\text{sub}} \equiv \text{Tr}_{\text{env}} |\Psi\rangle \langle \Psi|$$

Entanglement entropy

$$S_{\text{sub}} \equiv -\text{Tr}(\rho_{\text{sub}} \log \rho_{\text{sub}})$$

general states: $S_{\text{sub}} \sim L^d$ : Volume low

A lot of ground state

$$S_{\text{sub}} \sim L^{d-1}$$ : Area low

1-dimensional gapless system:

$$S_{\text{sub}} \sim \log L$$

Metallic system:

$$S_{\text{sub}} \sim L^{d-1} \log L$$
**Entanglement entropy of MPS and PEPS**

- **Entanglement entropy of MPS**
  Sub-system connected to the environment through only two bonds.
  For matrix dimension $D$:
  \[
  S_{\text{sub}} \leq 2 \log D
  \]
  In order to represent the entanglement entropy, we need exponentially large matrix dimension for two and higher dimensions.

- **Entanglement entropy of PEPS**
  For tensor dimension $D$:
  \[
  S_{\text{sub}} \leq L^{d-1} \log D
  \]
  For sufficiently large, but finite, $D$, a lot of ground states of very large (infinite) system can be represented by PEPS!
Advantage of tensor network method

☑ Efficient representation of the ground state

MPS (for d=1) and PEPS (for 2 > d) can represent the ground state wave-function for very large system efficiently.

Finite tensor-dimension

☑ Applicable to any system

No sign problems!

☑ Small bias

• Assumed wave-function contains large # of elements.
• The shapes of MPS and PEPS reflect only underlying lattice geometry.
Difficulties

1. High computational costs for contraction of the network

For PEPS:

Calculation of the entire tensor products need exponentially large costs

We use

But, still very high cost.

2D- PEPS: $O(D)$

MPS: $O(D)$

For two or higher dimensions, tensor dimensions are limited:

$D \sim 10$
Difficulties

2. Fermionic system with fermi surface (metal, semi-metal)

Entanglement entropy has a

\[ S_{\text{sub}} \sim L^{d-1} \log L \]

PEPS need

• Another tensor network states: branching MERA?
• Combination with variational Monte Carlo ?
• ....

Challenging problem!
Partition function representation

Partition function: \( Z = \text{Tr} \exp(-\beta \mathcal{H}) \)

\( Z \) can be represented by

Example: classical Ising model on the

\[
A_{i,j,k,l} = e^{(\sigma_i \sigma_j + \sigma_j \sigma_k + \sigma_k \sigma_l + \sigma_l \sigma_i)/T} \quad \sigma_i = \pm 1 = \uparrow, \downarrow
\]

*For quantum system:

Path integral representation \( \rightarrow \) \( 1+d \) dimensional tensor network

\[\begin{align*}
\sigma_i, \sigma_j, \sigma_k, \sigma_l & \in \{\uparrow, \downarrow\} \\
\end{align*}\]

from G. Evenbly and G. Vidal, arXiv:1412.0732
Contraction and renormalization

\[ Z = \text{Tr} \exp(-\beta \mathcal{H}) = \]

Contraction: exponentially large cost

\[ \text{Approximation: Using real space renormalization} \]

Tensor Renormalization Groupe (TRG)

M. Levin and C. P. Nave PRL (2007)
Improved renormalization method

Problems in TRG: TRG does not represent

Especially,

New renormalization methods: Tensor Network Renormalization (TNR)


Point

Insertion of disentangler

efficient renormalization of short range correlation

TNR can produce renormalization flow to the physical fixed point!
Summary

• Tensor network methods are efficient tools to investigate condensed matter physics

• As the ansatz of variational wave-functions

• As a tool for efficient Real space renormalization