Thermal tensor network renormalization group algorithms and applications

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Outline

• Motivation
• Linearized tensor renormalization group (LTRG) approach and applications
• Optimized decimation of tensor networks with super-orthogonalization (ODTNS) and implications
• Theory of tensor network contractor dynamics (NCD) and applications
• Concluding remarks
Quantum phase transition

In some cases, phase I and phase II cannot be distinguished by any local order parameter.

disordered quantum states vs. quantitative measure

Topological order
## Traditional quantum phases and topological phases

<table>
<thead>
<tr>
<th></th>
<th>traditional</th>
<th>topological</th>
</tr>
</thead>
<tbody>
<tr>
<td>Order parameter</td>
<td>local</td>
<td>nonlocal</td>
</tr>
<tr>
<td>Spontaneously symmetry breaking</td>
<td>yes</td>
<td>no</td>
</tr>
<tr>
<td>Mathematical description</td>
<td>group theory</td>
<td>tensor categories (quantum group)</td>
</tr>
<tr>
<td>Low-lying effective theory</td>
<td>Ginzburg-Landau field theory</td>
<td>doubled Chern-Simons theory, deconfined gauge theory</td>
</tr>
<tr>
<td>Underlying physics</td>
<td>spontaneous magnetization, condensation of particles</td>
<td>condensation of quasi-particles (e.g. gauged boson, fermion, anyon)</td>
</tr>
</tbody>
</table>
• **Topological phases** are unique states of matter incorporating long-range quantum entanglement, hosting exotic excitations with fractional quantum statistics.

• **Topological order** describes the property of a quantum state, not a Hamiltonian.

• **Topological entanglement entropy (TEE):**

For a bipartite system, A and B

\[ S(A) = -Tr[\rho_A \ln(\rho_A)] \]

entanglement entropy

\[ \rho_A = Tr(|0\rangle\langle 0|) \]
reduced density matrix

\[ S(A) = S(B) \]
duality property

\[ \ln 2D, \quad S(A) = \alpha L - \gamma + ... \]

L: length with smooth boundary;
\(\gamma\): the terms vanishing when \(L\)-\(\infty\);
\(\alpha\): non-universal coefficient, near the boundary

\[ \gamma = \ln(D) \]

\[ D = \sqrt{\sum_i d_i^2} \]
Total quantum dimension of the medium
Topological entanglement entropy (TEE, \(-\gamma\)) is a universal additive constant characterizing the long-range entanglement in the ground state.

<table>
<thead>
<tr>
<th>model</th>
<th>(\gamma)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\mathbb{Z}_2) spin liquid</td>
<td>(\text{Ln}2)</td>
</tr>
<tr>
<td>Kagome (J_1)-(J_2) model</td>
<td>0.698, 0.694</td>
</tr>
<tr>
<td>Toric-code model</td>
<td>0.693</td>
</tr>
<tr>
<td>Haldane model</td>
<td>0.349</td>
</tr>
<tr>
<td>Transverse-field Ising model</td>
<td>0.0014, 0.0004</td>
</tr>
<tr>
<td>Coupled spin-dimer model</td>
<td>0.006, 0.002</td>
</tr>
</tbody>
</table>
Gapped phases

• For the gapped systems without considering any symmetry

Short-range entanglement state: can be represented by direct product of states through local unitary transformations. Belong to the same phase

Long-range entanglement state: cannot be represented by direct product of states through local unitary transformations. Topological states

• For the gapped systems with consideration of symmetry

Short-range entanglement state: do not belong to the same phase. Symmetry protected topological phase

Long-range entanglement state: complicated. Symmetry enriched topological phase
Gapless quantum spin liquids

Algebraic Spin Liquids

- Stable gapless phase with no broken symmetries
- No free particle description
- Power-law correlations

Routes to gapless spin liquids

- Frustration
- Low spin
- Low coordination number

How to characterize?

<table>
<thead>
<tr>
<th>Material</th>
<th>Lattice</th>
<th>$\Theta_{cw}[K]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\kappa$(BEDT-TTF)$_2$Cu$_2$(CN)$_3$</td>
<td>anisotropic triangular</td>
<td>-375</td>
</tr>
<tr>
<td>ZnCu$_5$(OH)$_6$Cl$_2$ (herbertsmithite)</td>
<td>Kagome</td>
<td>-241</td>
</tr>
<tr>
<td>BaCu$_3$V$_2$O$_8$(OH)$_2$ (vesignieite)</td>
<td>Kagome</td>
<td></td>
</tr>
<tr>
<td>Na$_4$Ir$_3$O$_8$</td>
<td>Hyperkagome</td>
<td>-650</td>
</tr>
<tr>
<td>Cu-(1,3-benzenedicarboxylate)</td>
<td>Kagome</td>
<td>-33 [5]</td>
</tr>
<tr>
<td>Rb$_2$Cu$<em>3$SnF$</em>{12}$</td>
<td>Kagome</td>
<td>[6]</td>
</tr>
</tbody>
</table>
Geometrically frustrated magnets

**Herbertsmithite**, ZnCu₃(OH)₆Cl₂, spin-1/2 kagome lattice, with additional Dzyaloshinskii-Moriya interactions. It is thought that the ground-state is a spin liquid, with no onsite magnetization and no spin gap.


**Barlowite**: Cu₄FBr(OH)₆

Spin ½ perfect kagome motif

T.H. Han et al, PRL 113, 227203 (2014)

Kagome lattice: Z2 gap 0.13; energy per site in GS: -0.4386(5)

Inconclusive!

Gapped or Gapless?
Correlated Quantum Spin Systems

• Heisenberg Model:

\[ \hat{H}_{\text{Heisenberg}} = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \]

• Analytical methods such as mean-field theory, perturbation, bosonization, etc. are difficult to give reliable and accurate results for these models in D>1.

• Numerical means are always helpful.
Numerical approaches for quantum lattice systems

- Various quantum Monte Carlo simulations, powerful, but suffering from “negative sign problem”, cannot access to strongly correlated electrons away from the half-filling as well as quantum spin systems with frustrations.

- Exact diagonalization with Lanczos, Jacobi-Davidson algorithms, etc., are always effective for systems with small size. For large systems it depends on computer’s capacity.

- Numerical renormalization group methods are always useful and effective for low dimensional quantum lattice systems. DMRG, tensor network-based methods, ...
To understand the exotic quantum phases and experimental observations in correlated quantum magnets

**Thermal** tensor network states based approaches for quantum lattice systems

NEEDED!
(1) Linearized Tensor Renormalization Group (LTRG) Method

W. Li et al., PRL106, 127206 (2011)

**Target:** An effective algorithm to simulate the thermodynamics of low-dimensional quantum lattice models.

**Strategy:** First, transform the D-dimensional quantum lattice model to a (D + 1) dimensional classical tensor network by means of the Trotter-Suzuki decomposition; then, decimate linearly the tensors following the lines developed in the iTEBD scheme to obtain the thermodynamics of the original quantum many-body system. This algorithm is referred to as the linearized TRG (LTRG).

**Prototype:** The exactly solvable 1D quantum XY spin chain. The precision of the LTRG method is comparable with that of the transfer-matrix renormalization group (TMRG).

**Scalability:** The LTRG result with remarkable precision for a 2D spin-1/2 Heisenberg antiferromagnet on a honeycomb lattice can be obtained.
Consider the Hamiltonian of a 1D quantum many body model

\[ H = \sum_{i=1}^{N} h_{i,i+1} = H_1 + H_2, \]

\[ H_1 = \sum_{i=1}^{N/2} h_{2i-1,2i}, \quad H_2 = \sum_{i=1}^{N/2} h_{2i,2i+1}, \]

The partition function

\[ Z_N \approx Tr[e^{-\beta H_1/K} e^{-\beta H_2/K}]^K \]

\[ = \sum_{\{\sigma_j^i\}} \prod_{j=1}^{K} \langle \sigma_1^{2j-1} \sigma_N^{2j-1} | e^{-\beta H_1/K} | \sigma_1^{2j} \sigma_N^{2j} \rangle \]

\[ \times \langle \sigma_1^{2j} \sigma_N^{2j} | e^{-\beta H_2/K} | \sigma_1^{2j+1} \sigma_N^{2j+1} \rangle, \]
Transfer-Matrix Tensor Network

- **Trotter-Suzuki decomposition**: the partition function of 1d quantum system can be represented by a transfer-matrix tensor network.

\[ Z_N \approx \sum_{\{\sigma_i\}} \prod_{i=1}^{N/2} \prod_{j=1}^{K} V_{\sigma_{2i-1}^{2j-1} \sigma_{2i}^{2j} \sigma_{2i+1}^{2j+1} \sigma_{2i+1}^{2j+1} \sigma_{2i+1}^{2j+1} \sigma_{2i+1}^{2j+1} \sigma_{2i+1}^{2j+1}} \]

- Contract the tensor network to obtain the thermodynamic properties

\[ v_{\sigma_1 \sigma_4, \sigma_2 \sigma_3} \equiv \langle \sigma_1 \sigma_4 | \exp(-\beta h_{i,i+1} / K) | \sigma_2 \sigma_3 \rangle \]
Primary steps

Contraction of tensor network of transfer matrices

Decimate linearly the tensors layer by layer to obtain and trace a one-dimensional MPS

Computational cost: $O(D^6 D_c^3)$. 
Evaluation of Thermodynamic Quantities

- Normalize the tensors in order to avoid *divergence* during the RG process.
  linear decimation of 2d TN: $n_i$
  coarse-graining procedure of 1d MP: $m_j$

- Collect the *renormalization factors*, which determine the free energy:

$$ f = -\frac{1}{\beta L} \ln \left[ \prod_{i=1}^{2K-2} (n_i)^{\frac{L}{2}} \prod_{j=1}^{p} (m_j)^{\frac{L}{2p}} \right] $$

$$ = -\frac{1}{K\tau} \left( \sum_{i=1}^{2K-2} \frac{\ln n_i}{2} + \sum_{j=1}^{p} \frac{\ln m_j}{2j} \right). $$

$$ \beta = K\tau $$

- Other *thermodynamic quantities* can be evaluated by simple derivation.
Benchmark

1D XY spin chain

Free energy and relevant error w.r.t. exact solution vs $1/T$

Specific heat

LTRG method

- High precision
- Small computing tasks
- Readily coding
- Scalable
- No "negative sign" problem
Applications of LTRG method

(a) $S=1$ bond-alternating Heisenberg AF chain

Tomonaga-Luttinger Liquid in a Quasi-One-Dimensional $S = 1$ Antiferromagnet Observed by Specific Heat Measurements


Ground State
Field induced LRO
Luttinger liquid behavior

A Spin-1 Model Material: Ni(C$_2$H$_{24}$N$_4$)NO$_2$(ClO$_4$)$_2$, NTENP
LTRG fitting of susceptibility and magnetization in experiments

\[ \mathcal{H}_{\text{chain}} = J \sum_{i=1}^{L/2} (S_{2i-1} \cdot S_{2i} + \alpha S_{2i} \cdot S_{2i+1}) \]
\[ + \sum_{i=1}^{L} D(S_i^z)^2 - \sum_{i=1}^{L} \mu_B S_i \vec{g} \vec{H} , \]

Both magnetic curves can be well fitted, as well as the high-field curve.

\[ \alpha = 0.45, D/J = 0.25, J = 54.2 \text{K} \]
\[ g_x = 2.14, g_y = 2.27 \]
A TLL behavior is observed at low temperature in a longitudinal field.

An excitation gap exists in a transverse field.

LTRG results with high precision explain well the distinct experimental observation under transverse and longitudinal fields at very low temperatures.
(b) Spin-1/2 honeycomb Heisenberg ladder
Honeycomb Heisenberg spin ladder: Unusual ground state and thermodynamic properties

Yang Zhao¹, Wei Li¹, Bin Xi¹, Shi-Ju Ran¹, Yuan-Yuan Zhu², Bing-Wu Wang², Song Gao² and Gang Su¹(α)

\[
H = J_1 \sum_{i=1,2} \sum_i S_{i,l} \cdot S_{i+1,l} + J_2 \sum_i S_{2i-1,1} \cdot S_{2i-1,2} - g\mu_B h \sum_{i=1,2} \sum_i S_{i,l}^z,
\]

Three cases are considered:

(i) \(J_1, J_2 > 0\) [couplings all antiferromagnetic (AF)]
(ii) \(J_1 < 0, J_2 > 0\) [leg: ferromagnetic (F); rung: AF]
(iii) \(J_1 > 0, J_2 < 0\) [leg: AF; rung: F]
Spin gap vs $J_2/J_1$ differs at HC ladder and square ladder.
1/2 magnetization plateau in HC

Diluted dimer state on ½ plateau in HC

(a) $J_1 = 1.0$
- $J_2/J_1 = 0.6$
- $1.0$
- $1.5$

(b) $J_1 = -1.0$
- $J_2/J_1 = 0.6$
- $1.0$
- $1.6$
- $2.0$

(c) $J_1 = 1.0$
- $J_2/J_1 = 0.6$
- $-1.0$
- $-1.6$

$J_2:J_1 = 1.5$
Phase Diagram

Spin-1/2 two-leg honeycomb spin ladder
Specific heat

(HC: honeycomb; SQ: square)

HC: \( C(T) \sim \frac{1}{T^\alpha} e^{-\Delta/T}, \quad \alpha \approx 1 \)

SQ: \( \tilde{C}_{\text{mag}} \sim T^{-3/2} \exp(-\Delta/T) \)

Susceptibility

(HC: two kinds of low-lying excitations)

HC: \( \chi(T) \sim \frac{1}{T^\gamma} e^{-\Delta/T}, \quad \gamma \approx 6/5, \quad \gamma \approx 5/4. \)

SQ: \( \chi(T) = \alpha T^{-1/2} \exp(-\Delta/T) \)

Experimental data:
S. Gao et al., EJIC, (2013).
(2) Optimized decimation of tensor networks with super-orthogonalization (ODTNS) for two-dimensional quantum lattice models

S. J. Ran et al., PRB86, 134429 (2012)

Basic idea

- Transforming the 2D quantum model into a three-dimensional (3D) closed tensor network (TN) comprised of the tensor product density operator and a 3D brick-wall TN
- The network Tucker decomposition is proposed to obtain the optimal lower-dimensional approximation on the bond space by transforming the TN into a super-orthogonal form
- The free energy of the system can be calculated with the imaginary time evolution
- Hamiltonian: \( \hat{H} = \sum_{<ij>} \hat{H}_{ij} \)

- Trotter-Suzuki decomposition: \( \rho = \prod_{t=1}^{K+1} \prod_{<ij>} \hat{U}_{ij}^t, \quad \hat{U}_{ij}^t = e^{-\tau \hat{H}_{ij}} \)

- SVD: \( <ij | \hat{U}_{ij} | i' j' > = U_{ij}^{ij'}^{SVD} = \sum_s G_{ii',s}^L \lambda_s^0 G_{jj',s}^R \)

- Construct TPDO:

The density operator \( \rho \) at an inverse temperature \( \tau \) has the form of a TN:

\[
\rho_{...ii'jj'...} = \text{Tr}_G \left( \cdots \lambda_{g_2}^I \lambda_{g_3}^I T_{ii',g_1g_2g_3}^L \lambda_{g_1}^I T_{jj',g_1g_2g_3}^R \lambda_{g_2}^I \lambda_{g_3}^I \cdots \right),
\]
Evolution of 2D TPDO in imaginary time direction is equivalent to the linearized renormalization of the corresponding 3D classical model:

\[
\bar{T}^L_{ik,(g_1 g'_1)g_2g_3} = \sum_j G^L_{ij,g'_1} T^L_{jk,g_1g_2g_3}, \quad \bar{T}^R_{ik,(g_1 g'_1)g_2g_3} = \sum_j G^R_{ij,g'_1} T^R_{jk,g_1g_2g_3}
\]

\[
\bar{\lambda}^I_{g_1 g'_1} = \lambda^0_{g'_1} \lambda^I_{g_1}
\]

- Evolution enlarges the bond dimension of TPDO;
- Locating the optimal approximation of the local representation is crucial:
  Using network Tucker decomposition

Tucker decomposition

- Convincing and widely-used method for the optimal approximation of a single tensor;
- Applied to data compression, image processing, etc.
- Matrix singular value decomposition: $M = U D V^T$
- Keep the $D_c$ largest singular values and corresponding singular vectors to obtain the optimal lower-dimensional approximation.
- Form of Tucker decomposition of the tensor $A$:
  $$A = S \times_1 U^{(1)} \times_2 U^{(2)} \cdots \times_N U^{(N)}$$
- Properties of the core tensor $S$:
  (a) All-orthogonal: $\langle S_{i_n=\alpha}, S_{i_n=\beta} \rangle = 0$ when $\alpha \neq \beta$
  (b) Ordering: $\|S_{i_n=1}\| \geq \|S_{i_n=2}\| \geq \cdots \geq \|S_{i_n=I_n}\| \geq 0$

- $||S_i||$ contains the information of the weight distribution of the tensor $S$ for the $i$th mode, similar to higher-order singular values of matrix.

- The optimal lower-dimensional approximation can be obtained by keeping the first $D_c$ dimension of the core tensor and the corresponding space of $U$, while the cost function $f=||A-A'||$ is minimized (tensor $A'$ is the approximation of $A$).

- Algorithms: Higher-order SVD (HOSVD), Higher-order Orthogonal Iteration (HOOI), etc.

```
procedure HOOI($X, R_1, R_2, \ldots, R_N$)

procedure HOSVD($X, R_1, R_2, \ldots, R_N$)
    for $n = 1, \ldots, N$ do
        $A^{(n)} \leftarrow R_n$ leading left singular vectors of $X^{(n)}$
    end for
    $\mathcal{G} \leftarrow X \times_1 A^{(1)T} \times_2 A^{(2)T} \cdots \times_N A^{(N)T}$
    return $\mathcal{G}, A^{(1)}, A^{(2)}, \ldots, A^{(N)}$
end procedure
```
```
Superorthogonal form of tensor networks

- Network reduced matrix (NRM): 

\[
\mathcal{M}_{g_i g'_i} = \sum_{p} \sum_{g_1 g_2 \cdots g_n} T_{p, g_1 g_2 \cdots g_i \cdots g_n} T_{p, g_1 g_2 \cdots g'_i \cdots g_n} (\lambda_{g_1} \lambda_{g_2} \cdots \lambda_{g_{i-1}} \lambda_{g_{i+1}} \cdots \lambda_{g_n})^2 \lambda_{g_i} \lambda_{g'_i}
\]

- The conditions of the super-orthogonal form:

(a) Ordering: all \(\lambda\)'s on the geometrical bonds \((g_{1'}, g_{2'}, \ldots)\) are positive-defined, normalized and the elements of each \(\lambda\) are in descending order.

(b) Orthogonality: for any tensor \(T\) in the TN and any geometrical bond \(g_i\) of \(T\), the NRM \(M\) is diagonal and equals to the square of the corresponding \(\lambda\):

\[
\mathcal{M}_{g_i g'_i} = \lambda_i^2 \delta_{g_i g'_i}
\]

- Remarks:

1. The analyses of the optimal dimension deduction of the spaces are analogous to those of the Tucker decomposition;
2. Instead of the conditions of the core tensor in the Tucker decomposition, these two conditions are non-local for the TN.
Network Tucker Decomposition

- The network Tucker decomposition (NTD) for the TPDO of the Heisenberg model on the honeycomb lattice.

- The key step: find the transformation matrix for each geometrical bond:

1. Calculate the eigenvalues $\chi^{L(R)}$ and eigenvectors $U^{L(R)}$ of the matrix

\[
\overline{M}_{bc}^{L(R)} = (\lambda_b^L \lambda_c^R)^{-1} M_{bc}^{L(R)}
\]

in which $M^{L(R)}$ is the NRM;

2. Calculate the left (right) singular vectors $P(Q)$ that are the intermediate matrix defined as

\[
W_{ac} = \sum_b (\chi^L)_a^{1/2} U_{ba}^L \lambda_b^L U_{bc}^R (\chi^R)_c^{1/2}
\]

3. Find the transformation matrices by

\[
X_{ab}^{L} = \sum_c P_{ca} (\chi^L)_c^{-1/2} U_{bc}^L,
\]

\[
X_{ab}^{R} = \sum_c Q_{ca} (\chi^R)_c^{-1/2} U_{bc}^R
\]
(4) Transform the tensors and obtain the new $\lambda$ on the geometrical bond

$$
\tilde{T}_{p,gbc}^L = \sum_a T_{p,abc}^L(X^L)_{ag}^{-1}; \quad \tilde{T}_{p,gbc}^R = \sum_a T_{p,abc}^R(X^R)_{ag}^{-1};
$$

$$
\tilde{\lambda}_g^l \delta_{gg'} = \sum_a X_{ga}^L \lambda_a^l X_{ag'}^R = \sum_{af} P_{ag} W_{af} Q_{fg'}.
$$

- The convergence of the NTD is tested on the honeycomb and square TN’s, whose elements are **randomly initialized** with Gaussian distribution $N(0,1)$.

$$
\zeta = (|\chi^L - \mathcal{V}| + |\chi^R - \mathcal{V}|) / (2 \mathcal{L}) \quad \sigma^{L(R)} = \sum_{ab}|M_{ab}^{L(R)} - (\lambda_a^S)^2 \delta_{ab}| \quad \mu(t) = \sum_{S=I,II,III} (|\lambda^S(t-3) - \lambda^S(t)| / |\lambda^S(t)|) / 3
$$

- The factors that describe the convergence of the NTD decay **exponentially** with the iteration step;
- The error of the eigenvalue decomposition is around $10^{-15}$.
- **Truncation** of the bond dimension: keep the $D_c$ largest elements of $\lambda$ and the corresponding space of the geometrical bond after transforming the TN into super-orthogonal form.

- **Error** can be estimated as
  \[
  \varepsilon = \sqrt{\sum_{a=D_c+1}^{D} (\lambda_a^S)^2} / \sqrt{\sum_{a=1}^{D} (\lambda_a^S)^2}
  \]

- **Normalization factor**: normalize $\lambda$ by
  \[
  r_q^S = \sqrt{\sum_{a=1}^{D_c} (\lambda_a^S)^2}
  \]
  where $S=(I, \ II, \ III)$.

- **Free energy**:
  \[
  f(\beta) = \frac{1}{2\beta} \left( \sum_{q=1}^{K} \sum_{S=I,II,III} \ln r_q^S + 2 \ln \bar{r} \right)
  \]

- **Ground state energy**:
  \[
  e_0 = \lim_{K \to \infty} \lim_{\tau \to 0} \frac{1}{2\tau} \ln \left( \prod_{S=I,II,III} r^S \right)
  \]
Spin-1/2 Anisotropic Heisenberg Antiferromagnet on Honeycomb lattice

- Local Hamiltonian:

$$\hat{H}_{ij} = \delta (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y) + \hat{S}_i^z \hat{S}_j^z + (\hat{S}_i^z - \hat{S}_j^z)h_s/3$$

- Comparison to QMC calculations:

  - The energy difference with different $\beta$ and $D_c$.
  - When $\delta=0.5$, the difference $\Delta E$ is about $10^{-5}$ away from the critical point; near the critical point, $\Delta E \sim 10^{-3}$.
  - When $\delta=1$, $\Delta E$ is about $10^{-2}$ to $10^{-3}$ for different $\beta$.
  - $\Delta E$ becomes smaller when $D_c$ is increased.
  - Trotter errors are within $10^{-4}$. 

![Graphs showing energy difference $\Delta E$ and Trotter errors](image-url)
- The staggered magnetization and specific heat: great agreement with the QMC calculations.

- A thermodynamic phase transition from antiferromagnetic to paramagnetic phase occurs.

- The critical point can be determined by the divergent peak of specific heat.

**ODTNS method**

- Calculate both thermodynamic and ground state properties of 2D quantum spin models
- High precision and efficiency, small tasks
- No “negative sign” problem
- Applicable to 2D quantum frustrated spin systems
Application of ODTNS method

PHYSICAL REVIEW B 89, 054426 (2014)

Featureless quantum spin liquid, $\frac{1}{3}$-magnetization plateau state, and exotic thermodynamic properties of the spin-$\frac{1}{2}$ frustrated Heisenberg antiferromagnet on an infinite Husimi lattice

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\[ H = J \sum_{<ij>} [(S_i^x S_j^x + S_i^y S_j^y) + \delta S_i^z S_j^z] - h \sum_i S_i^z, \]

Husimi lattice
ODTNS results

- Ground state energy: $e_0 = -0.4343(1)$;
- Correlation length: $\xi = 1.09(2)$

Kagome lattice: energy per site in GS $e_0 = -0.4386(5)$

Magnetization and susceptibility

FIG. 2. (Color online) The calculated energy per site $e_0$ and the correlation length $\xi$ versus inverse bond dimension $1/D$ of the tree tensor network (up to $D = 100$) for $\delta = 1$. It is shown that $e_0$ decreases and $\xi$ increases with enhancing $D$, and $e_0$ converges faster than $\xi$. The solid lines are polynomial fittings, where $e_0$ is extrapolated to be $-0.4344(1)$ in the infinite-$D$ limit.
- Ground state: gapless quantum spin liquid (QSL)
- 1/3 magnetization plateau (up-up-down spin state)
- Susceptibility has two peaks at low T in QSL regime
- Specific heat has even three peaks, power-law decay
(3) Theory of NCD and algorithm

Theory of network contractor dynamics for exploring thermodynamic properties of two-dimensional quantum lattice models

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Contraction: by rank-1 decomposition in multilinear algebra, be realized through a contraction of a local tensor cluster with vectors on its boundary.
Algorithm: an imaginary-time-sweep algorithm for implementation in practical numerical simulations.
Exponents: The quasi entanglement entropy $S$, Lyapunov exponent $\lambda_{Lyap}$, and loop character $\lambda_{loop}$, to determine the thermodynamic phase transitions of both classical and quantum systems.

Features

- Thermodynamics for 2D quantum lattice models
- Accurate, efficient, small tasks, flexible
- No “sign” problem
- Applicable to 2D frustrated spin systems
By means of rank-1 decomposition, the infinite tensor network can be well approximated by an optimized tree-like tensor network, transforming the contraction (decimation and observables) of an infinite tensor network into a contraction of finite-size cell tensor network.
Main idea

Approximate the infinite contraction of the TN for the partition function and observables with a finite contraction of a local tensor cluster and vectors on its boundary.

1. **Evolve** the TPDO along the imaginary time.
2. Obtain the **TN of partition function** $Z$ by tracing the physical bonds of the TPDO.
3. Transform TN to ensure there is only one inequivalent $T$ (cell tensor).
   - Get the contractors by calculating the **fixed point** of the nonlinear mappings defined by the cell tensor.
4. **Making local contraction of the cell tensor and contractors**: Calculate truncation matrices if needed through the cell tensor and the contractors.
   - Calculate partition function and observables if needed.
Construction of finite temperature TNS

------ Tensor product density operator

- Trotter-Suzuki decomposition:

\[ \hat{U}_{ij} = \exp(-\tau \hat{H}_{ij}) \quad U_{i'j'}^{ij} = \langle ij | \hat{U}_{ij} | i' j' \rangle \]

\[ \rho \sim [\prod_{i,j} \hat{U}_{ij}]^{K+1} = \prod_{q=1}^{K+1} \prod_{i,j} \hat{U}_{ij}^q \]

\[ U_{i'j'}^{ij} = \sum_g G_{ii',g}^L \lambda_g^0 G_{jj',g}^R \]

- Evolution

\[ A'_{pp', \tilde{g}_1 g_2 g_3} = \sum_{p''} A_{pp'', \tilde{g}_1 g_2 g_3} G_{p_i' p_i', g_1}^L \]

\[ B_{pp', \tilde{g}_1 g_2 g_3} = \sum_{p''} B_{pp'', \tilde{g}_1 g_2 g_3} G_{p_i' p_i', g_1}^R \]

Translational invariance
NCD on the prototype model -------

*Spin $\frac{1}{2}$ Heisenberg antiferromagnet on honeycomb lattice*

- Obtain TN of $Z$ by tracing over physical bonds

\[
A_{g_1 g_2 g_3} = \sum_p A_{pp, g_1 g_2 g_3}, \quad B_{g_1 g_2 g_3} = \sum_p B_{p p, g_1 g_2 g_3}, \quad Z = Tr_G(\prod_{i \in A} A^i \prod_{j \in B} B^j)
\]

- Transform TN so that it consists of one inequivalent tensor (cell tensor):

\[
T_{g_1 g_2 g_3 g_4}^{\text{cell}} = \sum_{g_5} A_{g_1 g_2 g_5} B_{g_3 g_4 g_5}
\]

- Permutation invariance in each index pair:

\[
T_{g_1 g_2 g_3 g_4}^{\text{cell}} = T_{g_3 g_2 g_1 g_4}^{\text{cell}} = T_{g_1 g_4 g_3 g_2}^{\text{cell}}
\]
• Define the mappings by $\mathcal{T}_{\text{cell}}$:

$$
T_i(i = 1, ..., D): \prod_{a \neq i} V^a \rightarrow V^j \text{ as } \sum_{\{g_{a \neq i}\}} T_{\text{cell}}^{g_{1}g_{2}g_{3}g_{4}} \prod_{a \neq i} x_{g_{a}}^{a} = \Gamma x_{g_{j}}^{r_{a}}
$$

$D$: the order of $\mathcal{T}_{\text{cell}}$; $X^{\alpha_{a}}$: a unit-norm vector on bond $a$; $V^{a}$: the vector space of corresponding bond; $\Gamma$: positive real number.

Here, bonds $i$ and $j$ form an **index pair**!

• A compact form of the mappings:

$$\{x'\} = \mathcal{T}(\{x\})$$

• Fixed point conditions:

$$\mathcal{T}(\{\tilde{x}\}) = \tilde{\Gamma}\{\tilde{x}\}$$
Using the permutation invariance, one can have:

$$\mathcal{T}_i(\{x^{\alpha_{a\neq i}}\}) = \Gamma x^\alpha_i$$

It’s the self-consistent condition for **rank-1 decomposition**

$$T^{cell} \approx \tilde{T} = \prod_{\alpha_a} \tilde{x}^{\alpha_a}$$

which is the solution of

$$\min_{\text{rank}(\tilde{T})=1} |T^{cell} - \tilde{T}|$$

**Note:**
A tensor is rank-1 means that it can be decomposed as the direct product of several vectors.

The tensor norm is defined as

$$|T| = \sqrt{\sum_{g_1g_2\ldots} T_{g_1g_2\ldots} \overline{T}_{g_1g_2\ldots}}.$$
- **Defective TN**: destruct the loops of the TN by replacing minimal number of cell tensors with the rank-1 tensors.

- The TN marked by the shaded area has no loop and can be contracted as readily as a tree TN with contractors on the boundary.

\[
Z \approx \tilde{\Gamma}^{N-1} Tr_G (T_{\text{cell}} \tilde{T}) = \tilde{\Gamma}^{N-1} Tr_G (T_{\text{cell}} \prod_{a} \tilde{x}^{a} ) = \tilde{\Gamma}^{N}
\]

- **Solid circles**: rank-1 tensor.
- **Dashed circles**: fixed point conditions.
• **Observables** (The TN of $<O>$ is the same as the TN of $Z$ except for the tensors that share the physical bonds with the operator $O$):

$$
\langle \hat{O}_i \rangle = \sum_{p_i p_i, g_1 g_2 g_5} A_{p_i p_i, g_1 g_2 g_5} B_{p_j p_j, g_3 g_4 g_6} O_{p_i p_i} x^{\alpha_1} x^{\alpha_2} x^{\alpha_3} x^{\alpha_4} / Z
$$

• **Lyapunov exponent**: describe convergence property

$$
I^{lya} = \lim_{\Theta \to \infty} \sum_{\Theta = 1} \{ \ln \sum_{a=1}^D \left| \mathcal{T}^{\theta} (\{x_0\}) - \mathcal{T} [\mathcal{T}^{\theta-1} (\{x_0\}) + \varepsilon^a] \right| / \mathcal{D} \left| \varepsilon^a \right| \}
$$

$\varepsilon^a$: the infinitesimal random vector to exert a perturbation on $x^{\alpha_a}$

The mapping $T^\theta = T [T (\ldots)]$
Quasi-entanglement entropy

• Contractor: it is the dominant eigenstate of $M(\gamma)$ and can be written in the form of matrix product states.

Quasi-entanglement entropy:

$$S = -\sum_i (\mu_i^{b(d),\gamma})^2 \ln[(\mu_i^{b(d),\gamma})^2]$$

$\mu$ is the singular value spectrum of $x$.

• The entanglement of the dominant eigenstate.
Loop character

• Recall that the defective TN formed by $T^{\text{cell}(\gamma)}$’s contains no loop of $T^{\text{cell}(\gamma)}$, but contains loops of $T^{\text{cell}(\gamma' \leq \gamma-1)}$;

• If the cell tensor converges as $\gamma$ increases, effects of larger loops can be ignored.

• Loop character:

$$I^{\text{loop}}(\gamma) = 1 - (x^{\alpha_{b(d)},\gamma+1})^T x^{\alpha_{b(d)},\gamma}$$

$I^{\text{loop}}$ controls the error brought by the destruction of loops.
Truncation principle

- **General strategy**: Use the environment of the enlarged bond to obtain the non-local optimal truncations.

- **Denote the enlarged \( \tilde{g} \) bond as**

\[
Z = \sum_{g\tilde{g}} \delta_{g\tilde{g}} M_{g\tilde{g}} = Tr(M) \quad \text{SVD: } M = P\Lambda Q
\]

Rewrite: \( \tilde{M} = \sqrt{\Lambda} P^T Q \sqrt{\Lambda} \quad \text{SVD again: } \tilde{M} = \tilde{P}\Lambda \tilde{Q} \)

- **Truncation matrices (isometries)** obtained by \( M \):

\[
\tilde{P} = P\Lambda^{-1/2} \tilde{P} \sqrt{\Lambda}, \quad \tilde{Q} = Q\Lambda^{-1/2} \tilde{Q} \sqrt{\Lambda}
\]
• Calculation of truncation matrices with NCD

• Construct bilayer TN of Z (at targeted temperature $\tilde{\beta}$) as

$$Z(\tilde{\beta}) = Tr[\hat{\rho}(\tilde{\beta})] = Tr[\hat{\rho}(\beta)\hat{\rho}(\tilde{\beta} - \beta)]$$

$$T_{\text{cell}}^{\text{cell}} = \sum_{\xi_5} A_{\xi_1\xi_2\xi_3\xi_4}, A_{\xi_1\xi_2\xi_3\xi_4} = \sum_{pp'} A_{pp',g_1g_2g_5} \tilde{A}_{p'p,g_1g_2g_5}, B_{\xi_1\xi_2\xi_3\xi_4} = \sum_{pp'} B_{pp',g_3g_4g_5} \tilde{B}_{p'p,g_3g_4g_5}.$$ 

The tensors without tilde are in the TPDO at $\beta$ and those with tilde are in the TPDO at $\tilde{\beta} - \beta$.

• Result of M employing NCD with cell tensor size $\gamma=1$:

$$\frac{M_{g_jg_j'}}{\tilde{\Gamma}^N} = \left\{ \frac{\sum_{g''} x_j^g x_j^{g''}}{\sum_{\xi_\alpha\xi_\beta\xi_\delta\xi_\gamma} A_i^{\xi_\alpha\xi_\beta\xi_\delta\xi_\gamma} B_j^{\xi_\alpha\xi_\beta\xi_\delta\xi_\gamma}, x^a x^b x^a x^b / \tilde{\Gamma} \right\}$$
Imaginary-time-sweep algorithm

- Flow chart of imaginary-time-sweep algorithm (ITSA)

- Remark: sweep along the imaginary time is introduced to avoid error accumulation.
Error control

Error

- Trotter-Suzuki decomposition
- Dimension truncation
- Defects

Quantity

- Trotter slice $\tau$

\[ \varepsilon = \left( \sum_{a=\chi+1}^{\bar{\chi}} \Lambda_a \right) / \left( \sum_{a=1}^{\bar{\chi}} \Lambda_a \right) \]

\[ I_{\text{loop}}(\gamma) = 1 - (\mathbf{x}^{\alpha_{b(d)}, \gamma+1})^T \mathbf{x}^{\alpha_{b(d)}, \gamma} \]
Benchmark

- Model: 2D Ising model on square lattice
- The error of free energy is compared with the exact solution.
• **Model:** Heisenberg XXZ model.

- Energy, magnetization per site and specific heat at finite temperatures. A phase transition occurs.
Determination of $T_c$ with three quantities

- Model: 2D Ising model on square lattice ($T_c=2.27$, exact solution).

- The singular behavior of quasi-entanglement entropy, loop character and Lyapunov exponent near the critical temperature.

- Origination: the non-locality of the state near $T_c$. 
• Model: 2D anisotropic Heisenberg model on honeycomb lattice.

• The critical temperature is given by QMC with specific heat $T_c = 0.345$. 

![Graph showing critical temperature and specific heat](image-url)
Thermodynamics of a 2D frustrated Heisenberg model by NCD

• Accurate results of energy, magnetization, magnetic susceptibility, specific heat, correlations, spin gap have been obtained.

• Down to temperature $T \approx 10^{-2}J$ ($\beta \approx 10^{2}$) ($J$ the coupling constant, $\beta$ the inverse temperature), the results, including specific heat (differential of energy) and susceptibility (differential of magnetization), are very stable and reliable.

• This work will be accomplished soon.
Concluding remarks

(1) Three algorithms (including LTRG, ODTNS, NCD) are proposed to simulate efficiently and accurately the thermodynamics of low-dimensional quantum (frustrated) spin lattice systems;

(2) Successful applications of these methods to some intriguing 1D and 2D quantum Heisenberg models have been done, and some are in progress. Comparisons to experimental results are possible.

(3) There are large rooms to extend them to other quantum systems.
Thank you for attention!