Minimally entangled typical thermal states with auxiliary matrix-product-state bases

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**Motivation:** Finite temperature problems for frustrated or Fermionic systems

**Example 1:** Hubbard model

[Image: Mazurenko, Nature 22362, 2017]

**Example 2:** Heisenberg model on triangular lattice
Outline

- Review the finite-temperature algorithms
  - Purification
    - Minimally entangled typical thermal states (METTS)
- METTS with auxiliary MPS
- Benchmark on XXZ model on triangular lattice
Purification is equivalent to the density matrix

\[
\rho_{T=\infty} = \mathbf{1}
\]

Bases on auxiliary sites are arbitrary

\[
\text{Tr}[e^{-\beta \hat{H}/2} \hat{O} e^{-\beta \hat{H}/2}]
\]

\[
= \text{Tr}[\hat{U}^\dagger e^{-\beta \hat{H}/2} \hat{O} e^{-\beta \hat{H}/2} \hat{U}]
\]

- Represent a mixed state by a pure state with enlarged Hilbert space

\[
\text{purification } \Psi(T = \infty)
\]

- Imaginary time evolution on a purified MPS

\[
e^{-\beta \hat{H} / 2}
\]

\[
= \Psi(T = 2/\beta)
\]
Purification is equivalent to the density matrix evolved from identity

\[
\text{singlet} = \begin{pmatrix}
0 & \frac{1}{\sqrt{2}} \\
-\frac{1}{\sqrt{2}} & 0
\end{pmatrix}
\]

(The same number of auxiliary sites are always enough)
Sample the state \( |i\rangle \) with probability \( \propto \langle i | e^{-\beta \hat{H}} | i\rangle / Z \)

Given an arbitrary product state \( |i\rangle \)

1. Time evolution, \( |\phi_i\rangle = e^{-\beta \hat{H}} / 2 |i\rangle \)

2. **Collapse** \( |\phi_i\rangle \) to \( |i'\rangle \) with probability \( q_{i \rightarrow i'} = \frac{|\langle i' | \phi_i \rangle|^2}{\langle \phi_i | \phi_i \rangle} \)

### Detail balance

\[
q_{i \rightarrow i'} = \frac{|\langle i' | \phi_i \rangle|^2}{\langle \phi_i | \phi_i \rangle} = \frac{\langle i' | e^{-\beta \hat{H}} | i' \rangle}{\langle i | e^{-\beta \hat{H}} | i \rangle} \\
P_i = \langle i | e^{-\beta \hat{H}} | i \rangle / Z
\]
METTS – “diagram” representation

\[ \text{Tr}(e^{-\beta \hat{H}}) = \sum_{ij} \langle i | e^{-\beta \hat{H}/2} | j \rangle \langle j | e^{-\beta \hat{H}} | i \rangle \]

\[ e^{-\beta \hat{H}/2} \]

METTS: sample \( |i\rangle \) and \( |j\rangle \) iteratively.

1. Time evolution, \( |\phi_i\rangle = e^{-\beta \hat{H}/2} |i\rangle \)

2. Collapse \( |\phi_i\rangle \) to \( |i'\rangle \) with probability

\[ q_{i \rightarrow i'} = \frac{|\langle i' | \phi_i \rangle|^2}{\langle \phi_i | \phi_i \rangle} \]

= probability weight
• Measure in the ensemble \( \{ |\phi_i\rangle \} \)

\[
\langle O \rangle_\beta = \sum_i \frac{\langle \phi_i | \hat{O} | \phi_i \rangle}{Z} \\
= \sum_i \frac{\langle \phi_i | \hat{O} | \phi_i \rangle}{\langle i | e^{-\beta \hat{H}} | i \rangle} \cdot \frac{\langle i | e^{-\beta \hat{H}} | i \rangle}{Z} \\
\equiv \sum_i \mathcal{O}_i P_i, \quad \mathcal{O}_i \equiv \frac{\langle \phi_i | \hat{O} | \phi_i \rangle}{\langle \phi_i | \phi_i \rangle} = \text{Monte Carlo sum}
\]
METTS – original scheme

Collapse $|\phi_i\rangle$ to $|i'\rangle$ with probability $q_{i\rightarrow i'} = \frac{|\langle i'|\phi_i\rangle|^2}{\langle \phi_i|\phi_i\rangle}$

Algorithm: collapse site by site

collapse the first site

\[ q_{i_1} \propto |i_1\rangle \quad \langle \phi_{i'} | \quad |\phi_{i'}\rangle \]

collapse the second site

\[ q_{i_2} \propto |i_2\rangle \quad \langle \phi_{i'} | \quad |\phi_{i'}\rangle \]

\[ q_{i'i\rightarrow i} = q_{i_1} q_{i_2} \cdots q_{i_N}; \quad |i\rangle = |i_1 i_2 \cdots i_N\rangle \]
Collapsing probability

\[ q_{i' \rightarrow i} = \frac{\left| \langle i | \phi_{i'} \rangle \right|^2}{\langle \phi_{i'} | \phi_{i'} \rangle} \]
Comparison between purification and METTS

Required bond dimensions

- $T \to \infty$
  - purification: 1
  - METTS: $1 \times$ lot of samplings

- $T \to 0$
  - purification: $D^2$
  - METTS: $D$ (1 sampling)

$\rho_\infty = \begin{array}{c}
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\end{array}$

$\rho_0 = \begin{array}{c}
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\end{array}$

Purification is more efficient at high and intermediate temperature, while METTS is more efficient at low temperature.
Quantum number and autocorrelation in METTS

- If $|i\rangle$ and $\hat{H}$ conserve quantum number, the simulation will be stuck in the corresponding quantum number sector.

- For high T or small off-diagonal Hamiltonian, METTS algorithm will be stuck.

\[ e^{-\beta \hat{H}/2} |i\rangle = |i'\rangle \quad \text{collapse} \]
Good:
- Reduce autocorrelation time.
- Grand canonical ensemble.

Bad:
- Require MPS with no quantum number.

We want:
- Use quantum number conserving MPS
- Reduce the autocorrelation

Key idea:
- Remain some sites **uncollapsed**

\[ e^{-\beta \hat{H}/2} \]

MPS with auxiliary indices (auxiliary MPS, or AMPS)
The uncollapsed sites play roles as “presuming” the partition function.
Auxiliary sites induce the quantum number fluctuation

- The whole AMPS still has good quantum number
- The quantum number can change in each step by $N_{aux} \Delta Q$

$L=64$ Heisenberg chain at $\beta=2$

Starting from all down spins


- Collapsing algorithm

$$q_{i_n} \propto |i_n\rangle \langle \phi_{i'} |$$
contract both the physical and auxiliary indices

$$q_{i' \rightarrow i} = \sum_{i_1} |i_1\rangle \langle i_{i'} |$$

$$= \frac{|\langle i | \phi_{i'} \rangle|^2}{\langle \phi_{i'} | \phi_{i'} \rangle}$$
Grand canonical METTS

- Measure:

\[ \mathcal{O}_i = \frac{\langle \phi_i | \hat{\mathcal{O}} | \phi_i \rangle}{\langle \phi_i | \phi_i \rangle} = \]

contract both the physical the auxiliary sites
Benchmark on triangular lattice, XXZ model, \( J_z=0.8 \)

\[
H = J \sum_{\langle ij \rangle} \left( S_i^x S_j^x + S_i^y S_j^y \right) + J_z \sum_{\langle ij \rangle} S_i^z S_j^z - B \sum_i S_i^z
\]

- Sign problem in the quantum Monte Carlo
- We consider \( B=0, J_z=0.8 \)
Benchmark: 12x3 triangular lattice, XXZ model, $J_z=0.8$

\[ \beta = 16 \]

AMPS-METTS outperforms $S_z-S_x$ METTS and purification at low temperature
Benchmark: 12x3 triangular lattice, XXZ model, Jz=0.8

$\beta=4$

![Graph showing error of energy vs. CPU time for different $N_{aux}$ values.](image)

![Graph showing $m$ vs. $N_{aux}$.](image)

![Graph showing $\tau_{autocorr}$ vs. $N_{aux}$.](image)
Benchmark: 12x3 triangular lattice, XXZ model, $J_z=0.8$

$\beta=0.2$

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**Panel (a):** Error of energy vs. CPU time for different $N_{aux}$ values.

- $N_{aux} = 2$
- $N_{aux} = 4$
- $N_{aux} = 8$
- $N_{aux} = 16$

**Panel (d):** $m$ vs. $N_{aux}$

**Panel (e):** $\tau_{autocorr}$ vs. $N_{aux}$
Heisenberg model on triangular lattice

Lei Chen, PRB 99, 140404(R) (2019)
Effects of auxiliary indices:

- Induce quantum number fluctuation
- Reduce autocorrelation time
- Narrow the probability distribution
Benchmark: 12x3 triangular lattice, XXZ model, $J_z=0.8$

$\beta=16$

$\langle S_i \cdot S_j \rangle$
METTS with AMPS bases

- Simulate grand canonical ensemble
- Increasing $N_{aux}$:
  1) Narrow distribution
  2) reduce autocorrelation time
  3) increase bond dimension
- Works better than $S_z - S_x$ basis at low temperature
- Easy to be extend to SU(2)
Approach the path-integral Monte Carlo

\[ \text{Tr} e^{-\beta \hat{H}} = \text{Tr}(e^{-\tau \hat{H}} \cdots e^{-\beta \hat{H}}) \]

\[ \hat{1} = \sum_i |i\rangle\langle i| \]

Can update the configuration by collapsing

- Sign problem will come back
- Completely flexible in choosing bases

New hope?
Example of possible bases:

- Local rotation
Discussion

Example of possible bases:

- Local rotation

- Multiple-site bases
  [Alet, et. al. PRL 117, 197203 (2016)]

For example, singlet-triplet basis is shown to be sign-problem free for J1-J2 model on two-leg ladder for J1=J2 (and some other region).
Discussion

Example of possible bases:

- Local rotation

- Multiple-site bases
  [Alet, et. al. PRL 117, 197203 (2016)]

- MPS bases

- MERA-like bases
Example of possible bases:

- Local rotation

- Multiple-site bases
  [Alet, et. al. PRL 117, 197203 (2016)]

- MPS bases

- MERA-like bases

- Rotation of single particle basis

→ New hope???