Thermal Pure Quantum Matrix Product States

～Quantum Information meets Thermodynamics～

Iwaki, Shimizu, Hotta, arXiv:2005.06829

Atsushi Iwaki

Komaba, University of Tokyo (Hotta group)

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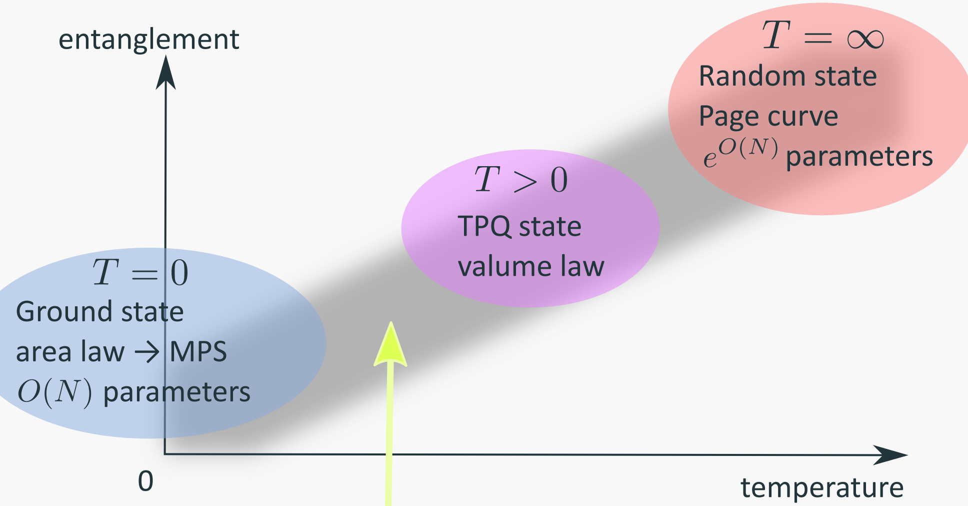
Quantum Many Body Pure state



Physical quantities like specific heat and susceptibility at low temperature include rich information about condenced matter physics.

Entanglement and Thermal Entropy

Gibbs state

$$\rho_\beta = \sum_n \frac{e^{-\beta E_n}}{Z} |n\rangle \langle n|$$

ensemble of exponentially many eigen states

Thermal entropy is von Neumann entropy.

$$S_{\rm th}(T) = -{\rm Tr}\rho_\beta \log \rho_\beta$$

TPQ state

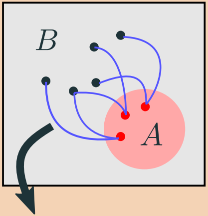
$$|\beta\rangle = e^{-\beta \hat{H}/2} |0\rangle$$

random state

Subsystems play the role of heat bath by entangling each other. TPQ state is locally equivalent to Gibbs state.

$$S_A = S_{\rm vN}(\rho_\beta^A) = N_A \times s_{\rm th}(T)$$

entanglement volume law



$$\rho_\beta^A = {\rm Tr}_B |\beta\rangle \langle\beta|$$

Numerical Application of TPQ states

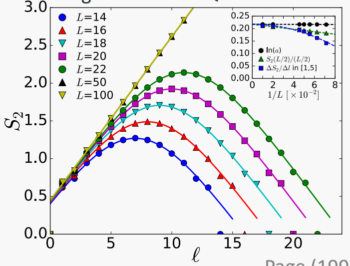
Specific construction of thermal typical states

Imada, Takahashi (1986) Hams, De Raedt (2000)
Iitaka, Ebisuzaki (2003) Machida, Iitaka, Miyashita (2005, 2012)
Sugiura, Shimizu (2012, 2013)

Random states		mTPQ states
$\|0\rangle = \sum_{\nu} z_\nu \|\nu\rangle$	$\xrightarrow{\text{operate Hamiltonian}}$	$\|k\rangle = (l - \hat{h})^k \|0\rangle$
(infinite temperature)		(finite temperature)

- ◎ Physical quantities are almost exactly evaluated with exponentially small error.
- ✕ The system size is restricted to $N \sim 30$.

Page curve of TPQ states



Page (1993)
Nakagawa, Watanabem Fujita, Sugiura (2018)

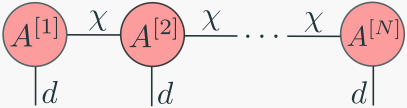
Matrix Product States

MPS and DMRG

Consider an 1D many body system where the size N and the local dimension d.

$$|\Psi\rangle = \sum_{\{i\}} \sum_{\{\alpha\}} A^{[1]i_1}_{\alpha_1} A^{[2]i_2}_{\alpha_1\alpha_2} \cdots A^{[N]i_N}_{\alpha_{N-1}} |i_1, \ldots, i_N\rangle$$

Fannes, Nachtergaele, Werner (1992)



The rank of matrices are called bond dimension χ.

◎ Represent a pure state by $O(Nd\chi^2)$ parameters.

Density matrix renormalization group (DMRG) calculate ground states with high accuracy.

White (1992, 1993)

DMRG is essentially a variational method of MPS.

Ostlund, Rommer (1995, 1997) Dukelsky, Martin-Delgado, Nishino, Sierra (1998)

Canonical Form of MPS

$$|\Psi\rangle = \sum_{\{i\}} \sum_{\{\alpha\}} \Gamma^{[1]i_1}_{\alpha_1} \lambda^{[1]}_{\alpha_1} \Gamma^{[2]i_2}_{\alpha_1\alpha_2} \lambda^{[2]}_{\alpha_2} \cdots \lambda^{[N-1]}_{\alpha_{N-1}} \Gamma^{[N]i_N}_{\alpha_{N-1}} |i_1, \ldots, i_N\rangle$$

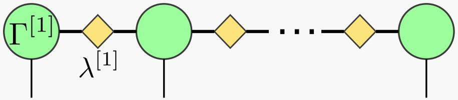
Vidal (2003)

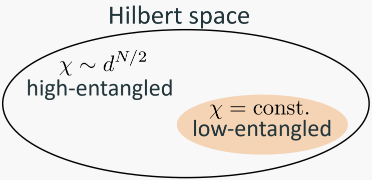
λs are Schmidt coefficients when we dividethe system at each bond.

$$S_m = -\sum_{\alpha=1}^{\chi} (\lambda^{[m]}_\alpha)^2 \log(\lambda^{[m]}_\alpha)^2 \le \log \chi$$

→ entanglement area law

We can truncate the bond dimension efficiently in canonical form.





TPQ - MPS method

Outline

TPQ states

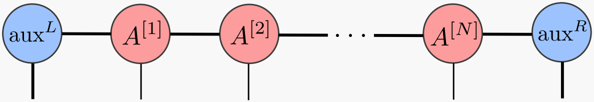
- ▷ Obey entanglement volume law.
- ▷ Need $e^{O(N)}$ parameters.

MPS representation

- ▷ Describe only low-entangled states.
- ▷ Need $O(N)$ parameters.

The key idea of our study

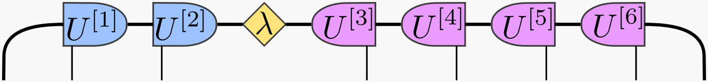
New MPS with auxiliary systems at both sides



TPQ - MPS method

- ▷ Volume law entanglement at low temperature
  → Extract thermal entropy
- ▷ Calculate thermodynamical quantities of large systems with lower computational cost.

Random MPS with Auxiliaries

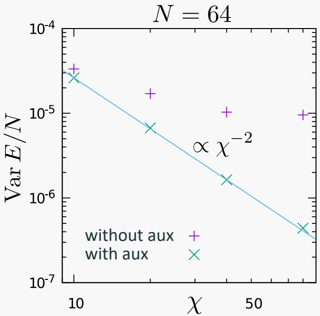


We prepare random MPS (RMPS) in canonical condition by using random unitary matrices. Garnerone, de Oliveira, Zanardi (2010)

In contrast to previous works, we attach auxiliary systems at both edges of the system and get following analytical result for all sites.

For 1-site local operator $\hat{O}$,

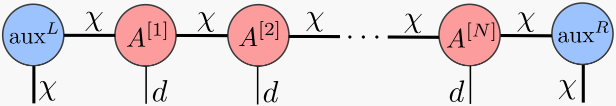
$$\overline{\left(\langle\Psi|\hat{O}|\Psi\rangle - \langle O\rangle_\infty\right)^2} = \frac{d-1}{\chi^2 d^2 - 1}\langle(\Delta\hat{O})^2\rangle_\infty$$



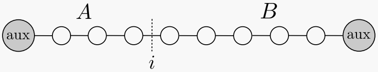
This result ensure typicality at infinite temperture.

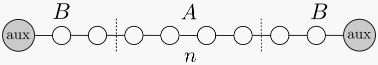
Auxiliaries at Finite Temperature

Auxiliary sytems with degrees of freedom χ



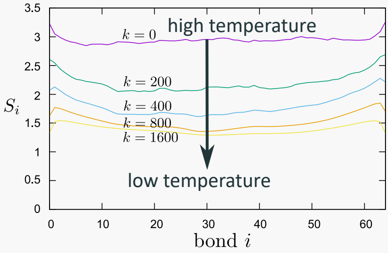
the subsystem from the edge ⟷ the subsystem at the center

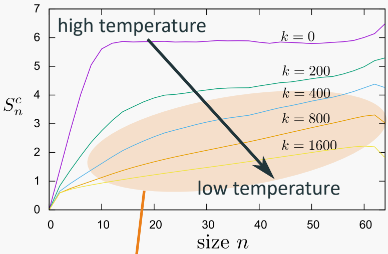




$S_i = S_{\mathrm{vN}}(\rho_A)$

$S_n^c = S_{\mathrm{vN}}(\rho_A)$



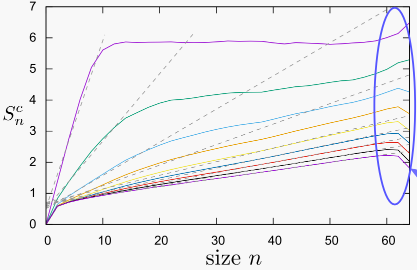


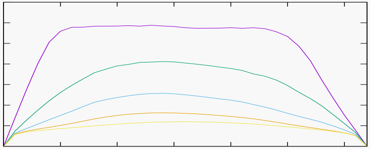
entanglement volume law

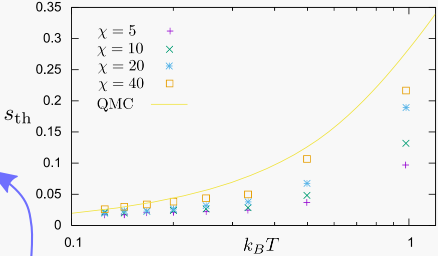
Thermal Entropy from Entanglement

$$S_n^c = n \times s_{\rm th}$$

entanglement volume law







The subsystem does not "feel" the edge for the existence of auxiliaries.

There has been no previous works on calculating thermal entropy from entanglement entropy.

Quantum information meets thermodynamics !!!

TPQ - MPS algorithm

1. Prepare an RMPS $|0^{\mathrm{MPS}}\rangle$ with auxiliary systems.

$A^{[m]i}_{\alpha\beta}$: independent Gaussian distribution

2. Operate $(l - \hat{h})$ to the state $|k-1^{\mathrm{MPS}}\rangle$.

$$|\tilde{k}^{\mathrm{MPS}}\rangle = (l - \hat{h})\,|k-1^{\mathrm{MPS}}\rangle$$

3. Truncate the increased bond dimension.

$$|\tilde{k}^{\mathrm{MPS}}\rangle \xrightarrow{\text{truncation}} |k^{\mathrm{MPS}}\rangle$$

4. Repeat 2. and 3. until enough low temperature.

microcanonical inverse temperture $\beta_k = \frac{2k}{N}\frac{1}{l-u_k}, \quad u_k = \frac{\langle k|\hat{h}|k\rangle}{\langle k|k\rangle}$

5. Calculate physical quantities at finite temperature by using the following formula.

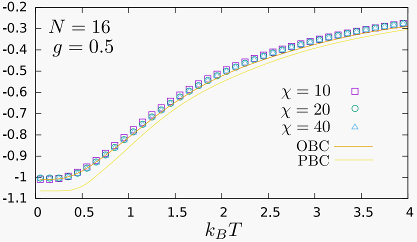
$$\langle O\rangle_{\beta,N} \propto e^{-\beta N l}\left\{\sum_k \frac{(N\beta)^{2k}}{(2k)!}\,\langle k|\hat{O}|k\rangle + \sum_k \frac{(N\beta)^{2k+1}}{(2k+1)!}\,\langle k|\hat{O}|k+1\rangle\right\}$$

Sugiura, Simizu (2013)

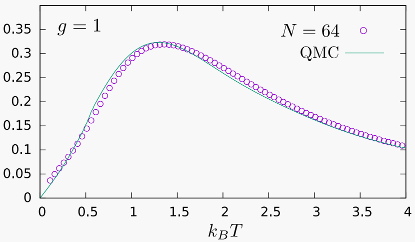
Demonstration : transverse Ising model

$$\hat{H} = -J \sum_{i=1}^{N-1} \hat{\sigma}_z^i \hat{\sigma}_z^{i+1} - g \sum_{i=1}^{N} \hat{\sigma}_x^i$$

Energy per site



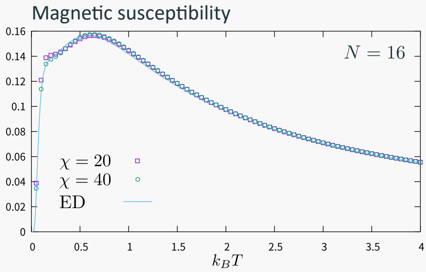
Specific heat

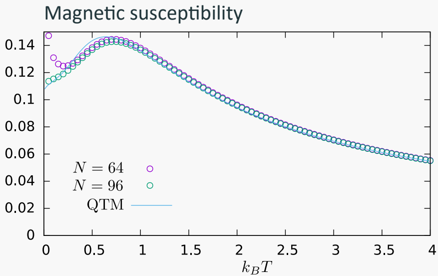


- ▷ We get sufficient exact values with the small bond dimension, $\chi = 10$ for $N = 16$ and $\chi = 40$ for $N = 64$.
- ▷ We take 10 samples for $N = 16$ and 5 samples for $N = 64$. The METTS method typically needs 100 sample for each temperture.

Demonstration : Heisenberg model

$$\hat{H} = J \sum_{i=1}^{N-1} \hat{\boldsymbol{s}}_i \cdot \hat{\boldsymbol{s}}_{i+1}$$





▷ Calculation time

$N = 16, \chi = 20, 10$ samples : about 15 minutes

$N = 64, \chi = 40, 5$ samples : about 8 hours

Summary

▷ By introducing new MPS with auxiliaries, we realized χ^{-2} scaling of random fluctuation in RMPS and entanglement volume law at low temperature. We succeeded in extracting thermal entropy from information of entanglement.

Quantum information meets thermodynamics !!!

▷ The TPQ - MPS method is useful for thermodynamical calculation for large systems. The METTS method well known as finite temperture MPS needs 100 samples for each data point. On the other hand, the TPQ - MPS method can obtain physical quantities for all temperature with 5 - 10 samples.