QIEP international workshop

Purity of thermal mixed quantum states

A. Iwaki, C. Hotta, arXiv:2202.07207

Atsushi Iwaki

University of Tokyo

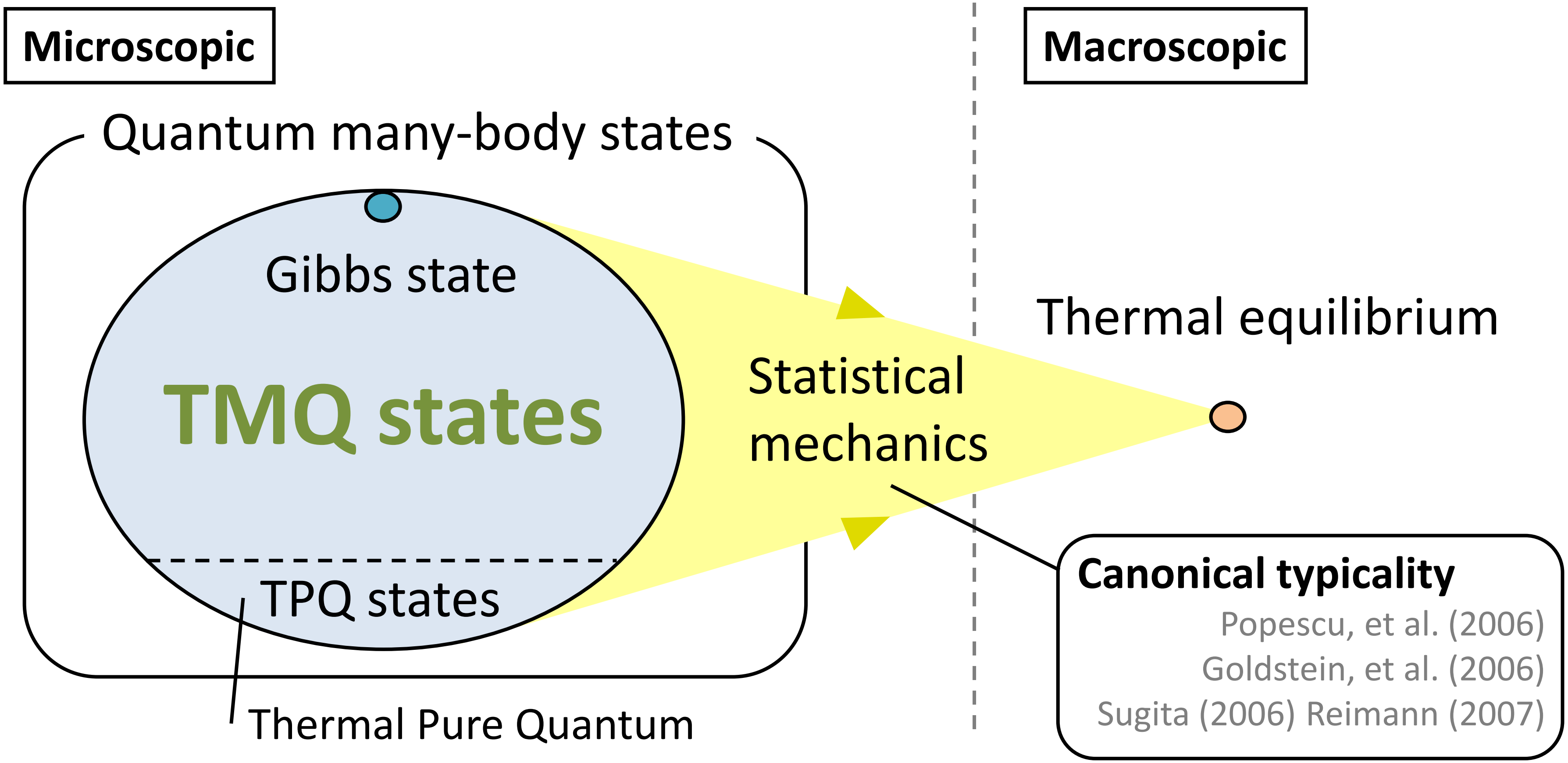
Collaborator: Chisa Hotta

Contents

Contents

TMQ (Thermal Mixed Quantum) states

Microscopic descriptions of thermal equilibrium



There are many different microscopic expressions, which all give the same macroscopic properties = Local observables / local density matrix are the same.

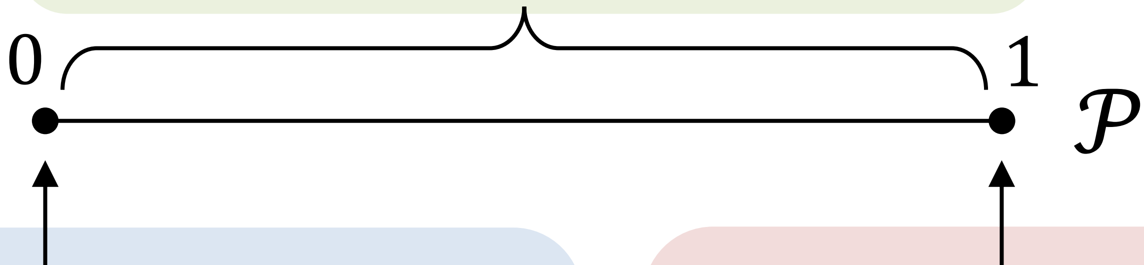
Purity distinguishes TMQ states

(Thermal Mixed Quantum)

$\mathcal{P} = \mathbf{Tr}\left(\boldsymbol{\rho}^2\right)$ → How many states classically mixed ?

TMQ states

- Classical mixture of TPQ states
- Subsystem of a TPQ state
- **Finite temperature methods** … etc.



Gibbs state

$$\rho_\beta^{\mathrm{G}} = \frac{e^{-\beta \hat{H}}}{Z(\beta)} = \sum_n \frac{e^{-\beta E_n}}{Z(\beta)} |n\rangle\langle n|$$

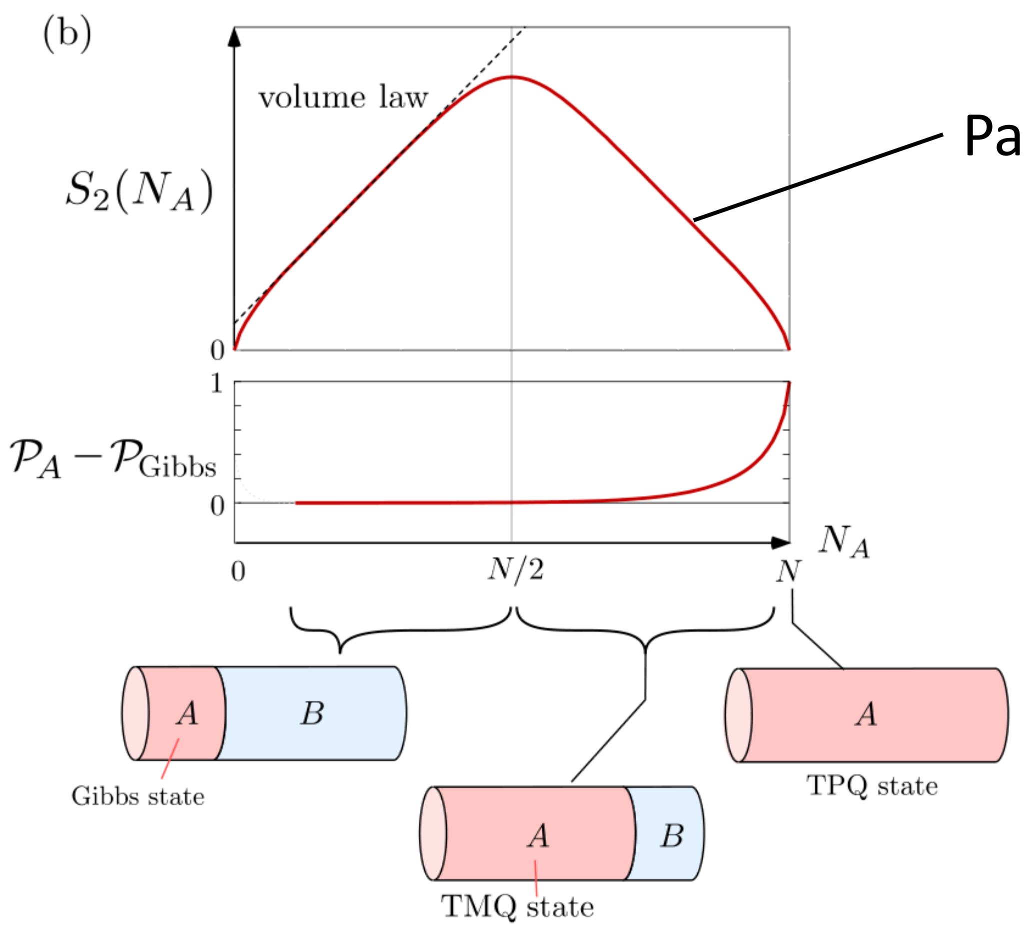
Mixture of exponentially large number of pure states

TPQ (Thermal Pure Quantum) states $|\beta\rangle = e^{-\beta \hat{H}/2} \underline{|0\rangle}$

Maximally entangled (entanglement volume law)

TMQ state as subsystem of TPQ state

(Thermal Pure Quantum)



Page curve of TPQ state

Nakagawa et al. (2018)

Rényi-2 entropy

$$S_2 = -\log \mathrm{Tr}(\rho^2)$$
$$= -\log \mathcal{P}$$
$$\downarrow$$

Purity $\mathcal{P} = e^{-S_2}$

When we regard $\boldsymbol{A = system}$, $\boldsymbol{B = bath}$, the wave function in A takes the form of classical mixture of the pure states.

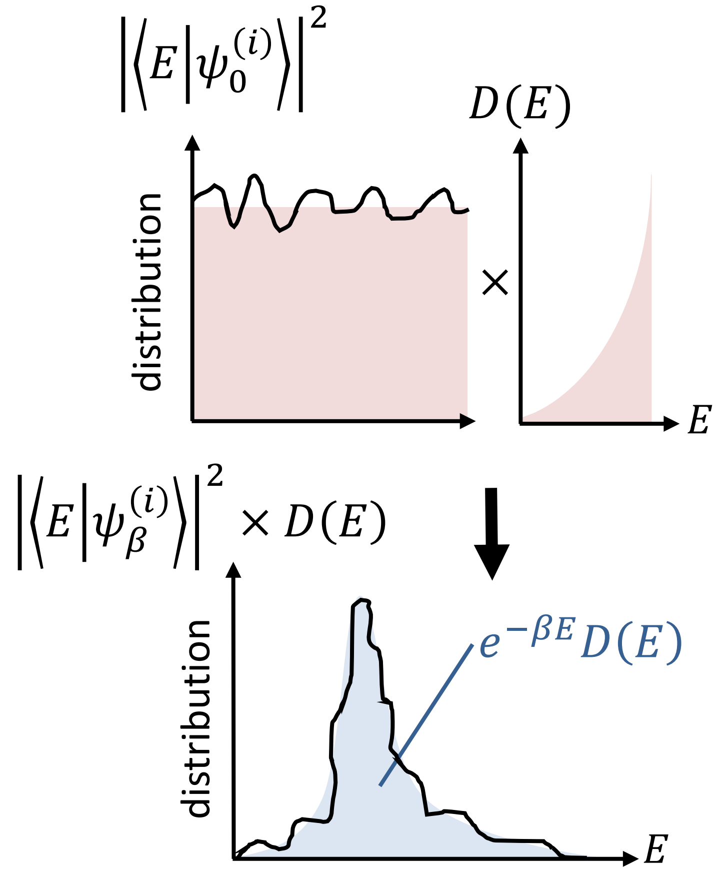
The degrees of **classical mixture** = degree of **entanglement** between A and B.

Contents

- Introduction
- Random sampling methods
- MPS-based samplings
- Demonstration
- Summary

Random sampling methods

1. Prepare initial states $\left|\psi_0^{(i)}\right\rangle$ satisfying
   $$\overline{|\psi_0\rangle\langle\psi_0|} = c\hat{I}.$$
2. Perform imaginary time evolution.
   $$\left|\psi_\beta^{(i)}\right\rangle = e^{-\beta\hat{H}/2}\left|\psi_0^{(i)}\right\rangle$$
3. Calculate physical quantities by average.
   $$\langle\hat{O}\rangle_{\beta,M}^{\mathrm{samp}} = \frac{\sum_{i=1}^{M}\left\langle\psi_\beta^{(i)}\middle|\hat{O}\middle|\psi_\beta^{(i)}\right\rangle}{\sum_{j=1}^{M}\left\langle\psi_\beta^{(j)}\middle|\psi_\beta^{(j)}\right\rangle} \xrightarrow{M\to\infty} \langle\hat{O}\rangle_\beta$$
   $$Z_M^{\mathrm{samp}} = \frac{1}{M}\sum_{i=1}^{M}\left\langle\psi_\beta^{(i)}\middle|\psi_\beta^{(i)}\right\rangle$$



We take finite M samples.

The norm $\left\langle\psi_\beta^{(i)}\middle|\psi_\beta^{(i)}\right\rangle$ has fluctuation.

E.g. : **TPQ method,**
finite temperature Lanczos method

The larger the fluctuation, the large the number of samples required.

“The required number of samples” decides the purity of the TMQ state.

Sample efficiency

Goto, Kaneko, Danshita (2021)

- Sample average can be rewritten in the form of **weighted** avereage..

$$\langle \hat{O} \rangle_{\beta,M}^{\mathrm{samp}} = \frac{\sum_{i=1}^{M} \left\langle \psi_\beta^{(i)} \middle| \hat{O} \middle| \psi_\beta^{(i)} \right\rangle}{\sum_{j=1}^{M} \left\langle \psi_\beta^{(j)} \middle| \psi_\beta^{(j)} \right\rangle} = \sum_{i=1}^{M} \boldsymbol{w_{i,M}} \frac{\left\langle \psi_\beta^{(i)} \middle| \hat{O} \middle| \psi_\beta^{(i)} \right\rangle}{\left\langle \psi_\beta^{(i)} \middle| \psi_\beta^{(i)} \right\rangle}$$

$$\boldsymbol{w_{i,M}} = \frac{\left\langle \psi_\beta^{(i)} \middle| \psi_\beta^{(i)} \right\rangle}{\sum_{j=1}^{M} \left\langle \psi_\beta^{(j)} \middle| \psi_\beta^{(j)} \right\rangle} = \frac{1}{M} \frac{\left\langle \psi_\beta^{(i)} \middle| \psi_\beta^{(i)} \right\rangle}{Z_M^{\mathrm{samp}}}$$

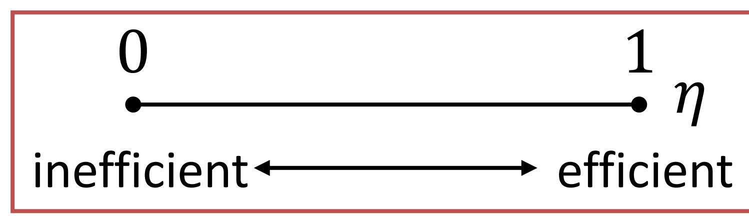
If weights distribute uniformly, the method is efficient.

- Introduce Shannon entropy of **weights**.

$$S_M = -\sum_{i=1}^{M} \boldsymbol{w_{i,M}} \log \boldsymbol{w_{i,M}}$$

- Define **sample efficiency**.

$$\boldsymbol{\eta = e^{S_M}/M}$$



Meaning of sample efficiency

NFPF represents fluctuation of norm.

(Normalized Fluctuation of Partition Function)

$$\boldsymbol{\delta z^2 = \frac{\mathrm{Var}(\langle \psi_\beta | \psi_\beta \rangle)}{\left(\overline{\langle \psi_\beta | \psi_\beta \rangle}\right)^2}}$$

$$\overline{\langle \psi_\beta | \psi_\beta \rangle} = cZ(\beta)$$

$$\langle \hat{O} \rangle^{\mathrm{samp}}_{\beta,M} = \sum_{i=1}^{M} w_{i,M} \frac{\langle \psi_\beta^{(i)} | \hat{O} | \psi_\beta^{(i)} \rangle}{\langle \psi_\beta^{(i)} | \psi_\beta^{(i)} \rangle}$$

$$w_{i,M} = \frac{\langle \psi_\beta^{(i)} | \psi_\beta^{(i)} \rangle}{\sum_{j=1}^{M} \langle \psi_\beta^{(j)} | \psi_\beta^{(j)} \rangle} = \frac{1}{M} \frac{\langle \psi_\beta^{(i)} | \psi_\beta^{(i)} \rangle}{Z_M^{\mathrm{samp}}}$$

We expand sample efficiency η by fluctuation of norm.

$$y^{(i)} = \langle \psi_\beta^{(i)} | \psi_\beta^{(i)} \rangle, \qquad y_0 = \overline{y^{(i)}}, \qquad \delta y^{(i)} = y^{(i)} - y_0$$

$$w_{i,M} = \frac{1}{M}\left(1 + \frac{\delta y^{(i)}}{y_0}\right) + \mathcal{O}\left(\frac{1}{M^2}\right)$$

$$\frac{\overline{e^{S_M}}}{M} = 1 - \frac{1}{2y_0^2}\overline{\delta y^2} + \mathcal{O}\left(\frac{1}{M}\right) + \mathcal{O}\left(\overline{\delta^3}\right)$$

We take the limit $M \to \infty$.

$$\boldsymbol{\eta = 1 - \frac{\delta z^2}{2} + \mathcal{O}\left(\overline{\delta^3}\right) = \exp\left(-\frac{\delta z^2}{2}\right) + \mathcal{O}\left(\overline{\delta^3}\right)}$$

NFPF of TPQ states

(Thermal Pure Quantum)

$$\delta z^2 = \mathrm{Var}(\langle\psi_\beta|\psi_\beta\rangle)/\left(\overline{\langle\psi_\beta|\psi_\beta\rangle}\right)^2$$

TPQ state

$$|\psi_0\rangle = \sum_r a_r|r\rangle \to |\psi_\beta\rangle = e^{-\beta\hat{H}/2}|\psi_0\rangle$$

Complex Gaussian distribution

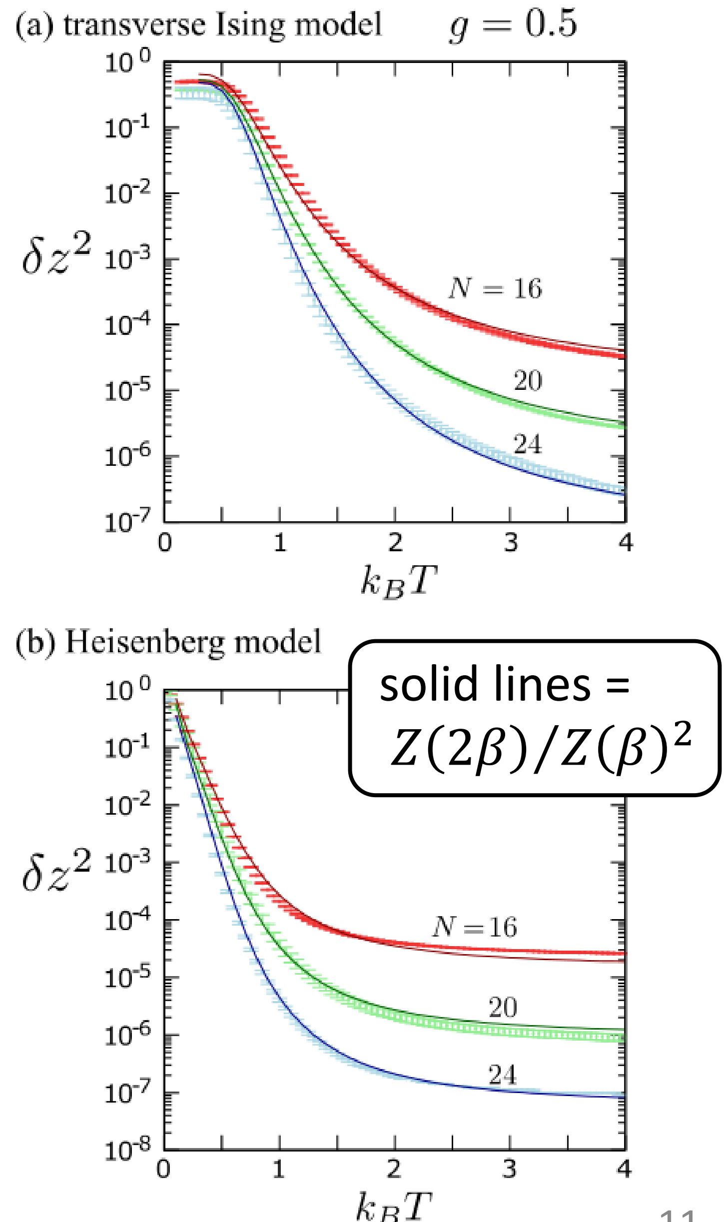
$$\delta z_{\mathrm{TPQ}}^2 = \frac{Z(2\beta)}{Z(\beta)^2} = e^{-Ns_{\mathrm{th}}(\tilde{\beta})}$$

$$\left(\beta \leq \exists\tilde{\beta} \leq 2\beta\right)$$

We can calculate this quantity by any finite temperature methods !!!

$$\eta \simeq 1 - \frac{1}{2}e^{-Ns_{\mathrm{th}}(\tilde{\beta})} \xrightarrow{N\to\infty} 1$$

The TPQ method is very efficient.



solid lines = $Z(2\beta)/Z(\beta)^2$

Fluctuation of physical quantities

$$\left\langle \left(\hat{O} - \langle \hat{O} \rangle_\beta\right)^2 \right\rangle_\beta = \overline{\left\langle \psi_\beta \middle| \left(\hat{O} - \langle \psi_\beta | \hat{O} | \psi_\beta \rangle\right)^2 \middle| \psi_\beta \right\rangle} + \overline{\left(\langle \boldsymbol{\psi}_{\boldsymbol{\beta}} | \hat{\boldsymbol{O}} | \boldsymbol{\psi}_{\boldsymbol{\beta}} \rangle - \langle \hat{\boldsymbol{O}} \rangle_{\boldsymbol{\beta}}\right)^{\mathbf{2}}}$$

Fluctuation = Quantum fluctuation + **Random fluctuation**

(if we assume $\rho_\beta^{\mathrm{G}} = \overline{|\psi_\beta\rangle\langle\psi_\beta|}$)

To improve **sample efficiency** of random sampling method, we need to decrease **random fluctuations**.

Q. What quantifies **random fluctuations** ?

→ A. **NFPF** !!!

Random fluctuation

- We want to evaluate the random fluctuations of physical quantities. For this purpose, we introduce an assumption.

$$\mathrm{Var}(\langle\psi_\beta|\hat{O}|\psi_\beta\rangle) \leq (\mathrm{const.}) \times \|\hat{O}\|^2 \mathrm{Var}(\langle\psi_\beta|\psi_\beta\rangle)$$

Assuming above inequality, we obtain

$$\overline{\left(\langle\hat{O}\rangle_{\beta,M}^{\mathrm{samp}} - \langle\hat{O}\rangle_\beta\right)^2} \leq (\mathrm{const.}) \times \|\hat{O}\|^2 \frac{\delta z^2}{M}.$$

  - **Random fluctuations are suppressed by the NFPF.**
  - **"The required number of samples" is proportional to the NFPF.**

- Counter examples to the assumption can be constructed by explicitly using **the information of energy eigenstates**. But we usually do not have the knowledge of energy eigenstates.

Purity of random sampling methods

$$\langle \hat{O} \rangle_{\beta,M}^{\text{samp}} = \sum_{i=1}^{M} w_{i,M} \frac{\langle \psi_\beta^{(i)} | \hat{O} | \psi_\beta^{(i)} \rangle}{\langle \psi_\beta^{(i)} | \psi_\beta^{(i)} \rangle} \Rightarrow \rho(M) = \sum_{i=1}^{M} w_{i,M} \frac{|\psi_\beta^{(i)}\rangle \langle \psi_\beta^{(i)}|}{\langle \psi_\beta^{(i)} | \psi_\beta^{(i)} \rangle}$$

$$w_{i,M} = \frac{\langle \psi_\beta^{(i)} | \psi_\beta^{(i)} \rangle}{\sum_{j=1}^{M} \langle \psi_\beta^{(j)} | \psi_\beta^{(j)} \rangle} = \frac{1}{M} \frac{\langle \psi_\beta^{(i)} | \psi_\beta^{(i)} \rangle}{Z_M^{\text{samp}}}$$

$$\text{Tr}[\rho(M)^2] = \sum_{i=1}^{M} w_{i,M}^2 + \sum_{i \neq j}^{M} \frac{\left| \langle \psi_\beta^{(i)} | \psi_\beta^{(j)} \rangle \right|^2}{y^{(i)} y^{(j)}} w_{i,M} w_{j,M}$$

$$\frac{1}{M}\left[1 + \left(1 - \frac{1}{M}\right) \delta z^2\right] + \mathcal{O}(\overline{\delta^3})$$

$e^{-\Theta(N)}$ → **neglected**

We take **"the required number of samples" N_{samp}** as $M = N_{\text{samp}}$.

$$\mathcal{P}_{\text{rand}} = \frac{1}{N_{\text{samp}}}\left[1 + \left(1 - \frac{1}{N_{\text{samp}}}\right) \delta z^2\right]$$

What is “the required number of samples” ?

$$\left\langle \left(\hat{O} - \langle \hat{O} \rangle_\beta \right)^2 \right\rangle_\beta = \overline{\left\langle \psi_\beta \middle| \left(\hat{O} - \langle \psi_\beta | \hat{O} | \psi_\beta \rangle\right)^2 \middle| \psi_\beta \right\rangle} + \overline{\left(\langle \psi_\beta | \hat{O} | \psi_\beta \rangle - \langle \hat{O} \rangle_\beta \right)^2}$$

Fluctuation = Quantum fluctuation + **Random fluctuation**

The TPQ state maximizes the quantum fluctuation and suppresses the random fluctuation. N_{samp} can be defined as the number of samples required to obtain physical quantities the same degrees of accuracy as the TPQ state.

$$N_{\mathrm{samp}} = \frac{\delta z^2}{\delta z_{\mathrm{TPQ}}^2}$$

All quantities can be calculated !

$$\delta z_{\mathrm{TPQ}}^2 = \frac{Z(2\beta)}{Z(\beta)^2}$$

⇨

$$\mathcal{P}_{\mathrm{rand}} = \frac{\delta z_{\mathrm{TPQ}}^2}{\delta z^2} \left(1 + \delta z^2 - \delta z_{\mathrm{TPQ}}^2\right)$$

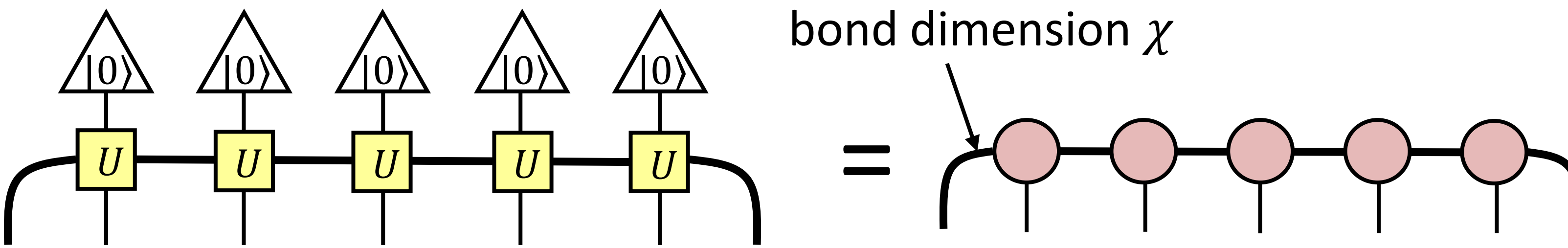
Contents

Initial random MPS

- **TPQ-MPS** : random MPS (RMPS) **with auxiliaries at both edges**

  Garnerone et al. (2010)

  Iwaki, Shimizu, Hotta (2021)

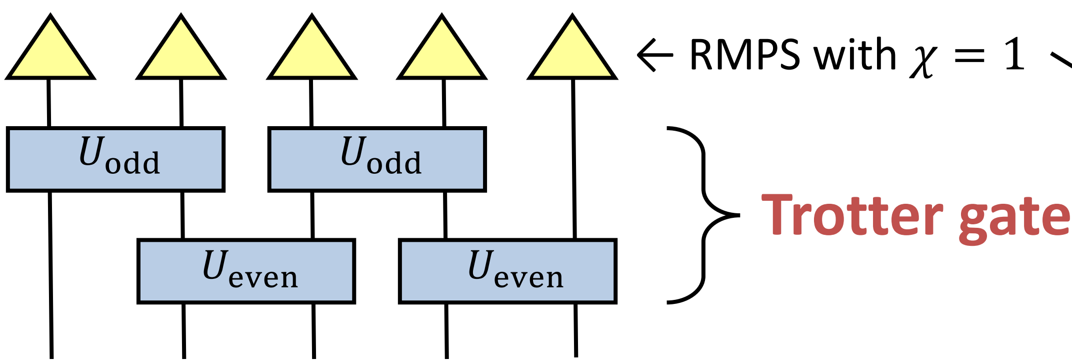


larger χ → larger entanglement → higher efficiency

- **RPMPS+T** (Random Phase MPS with Trotter gate) :

  local random phase + **quasi time evolution by Trotter Hamiltonian**

  Goto, Kaneko, Danshita (2021)



Sample efficiency

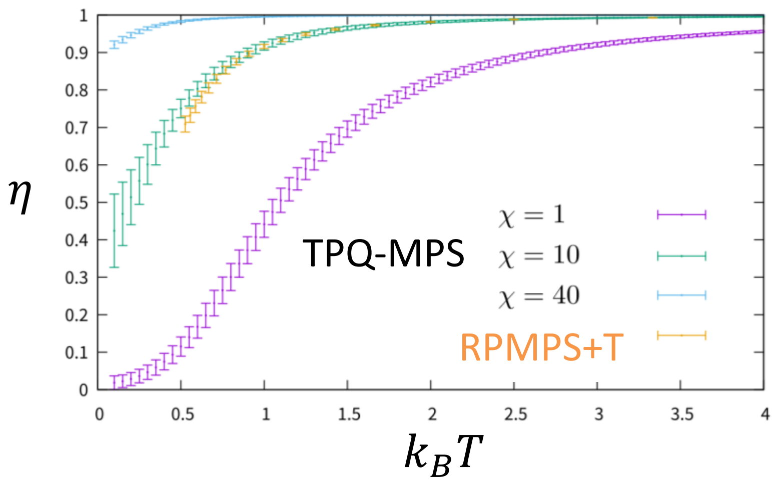
η_S
0.013 ± 0.003
0.218 ± 0.022

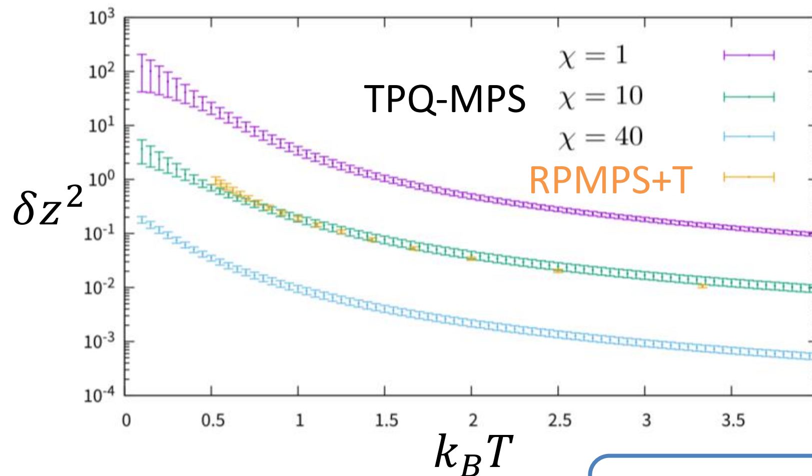
This method is better than the purification method in some cases.

Contents

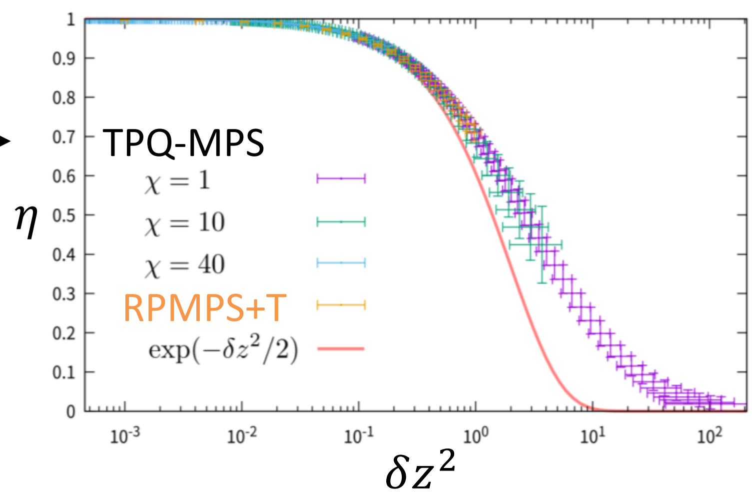
Sample efficiency and NFPF

- **TPQ-MPS vs RPMPS+T (Heisenberg chain with $N = 64$)**
- RPMPS+T is same efficiency as TPQ-MPS with $\chi = 10$.





$\delta z^2 \propto N_{\mathrm{samp}}$



- Mostly consistent with analytical result.

$$\eta = \exp\left(-\frac{\delta z^2}{2}\right) + \mathcal{O}\left(\overline{\delta^3}\right)$$

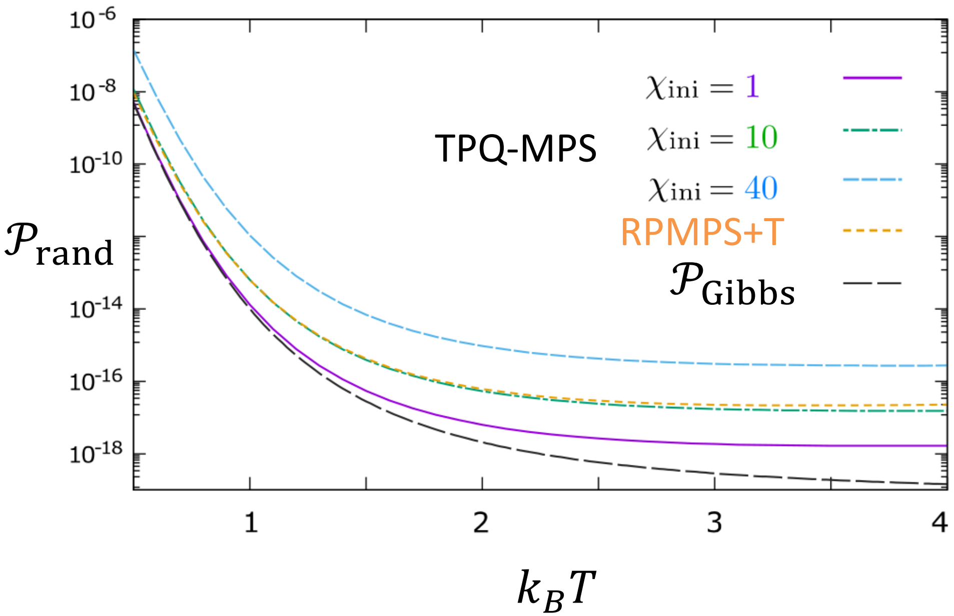
Purity of random samplings

- We calculate the purity of random samplings by

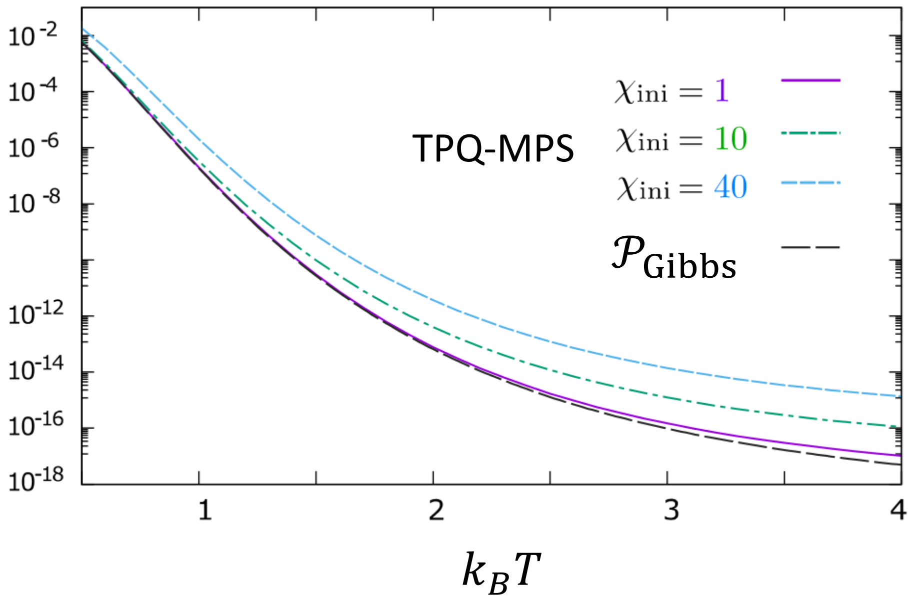
$$\mathcal{P}_{\mathrm{rand}} = \frac{\delta z_{\mathrm{TPQ}}^2}{\delta z^2}\left(1 + \delta z^2 - \delta z_{\mathrm{TPQ}}^2\right), \qquad \delta z_{\mathrm{TPQ}}^2 = \frac{Z(2\beta)}{Z(\beta)^2}.$$

- The larger the number of samples required, the closer the purity approaches that of the Gibbs state.

Heisenberg chain



transverse Ising chain with $g = 0.5$



Contents

What is useful about NFPF and purity ?

- **Trace estimation**

  Our theory can be applied to **general quantum mixed states**.

  Suppose that we want a quantum mixed state that follows the distribution defined by the positive operator $\hat{F}$.The quantum mixed state is obtained by

$$|\psi_F\rangle = \hat{F}^{1/2}|\psi_0\rangle.$$

  NFPF and purity of $|\psi_F\rangle$ can be evaluated in the same manner.

- **Quantum computing**

  Quantum algorithm for imaginary time evolution:

  - proposal Motta et al. (2020)
  - application to calculate thermal properties on IBM computer. Sun et al. (2021)

  Our formula can evaluate their efficiency / purity.

Summary

- There are many microscopic representations corresponding to a thermal equilibrium = TMQ states. Finite temperature methods generate some kind of TMQ states. The purity of TMQ states reveal how they are classically mixed.
- We obtained the analytical formula of efficiency of random sampling method using NFPF (Normalized Fluctuation of Partition Function).

$$\eta = \exp\left(-\frac{\delta z^2}{2}\right) + \mathcal{O}\left(\overline{\delta^3}\right)$$

- Random fluctuations of physical quantities are suppressed by the NFPF.

$$\overline{\left(\langle \hat{O} \rangle_{\beta,M}^{\mathrm{samp}} - \langle \hat{O} \rangle_{\beta}\right)^2} \leq (\mathrm{const.}) \times \|\hat{O}\|^2 \frac{\delta z^2}{M}$$

  The required number of samples is proportional to the NFPF.
- We define the purity of random samplings as computable quantity.

$$\mathcal{P}_{\mathrm{rand}} = \frac{\delta z_{\mathrm{TPQ}}^2}{\delta z^2}\left(1 + \delta z^2 - \delta z_{\mathrm{TPQ}}^2\right)$$