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

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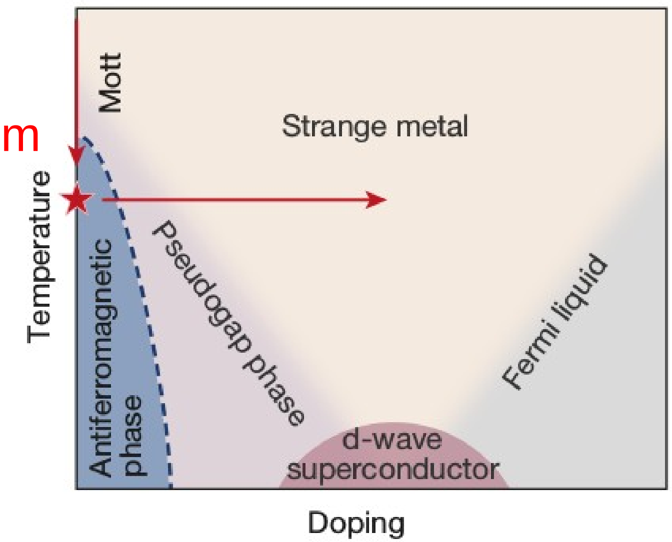
Motivation: Finite temperature problems for frustrated or Fermionic systems

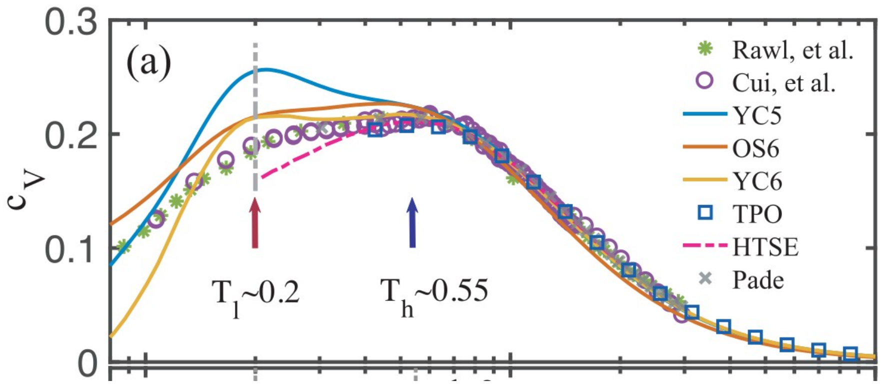
Example1: Hubbard model

[Mazurenko, Nature 22362, 2017]

cold atom



Example2: Heisenberg model on triangular lattice



High T: QMC

sign problem

???

Need to improve the method at low temperature

high entanglement

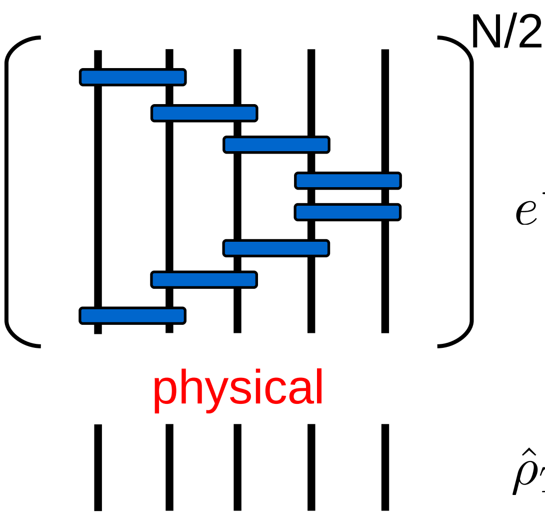
T=0: tensor network

Outline

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

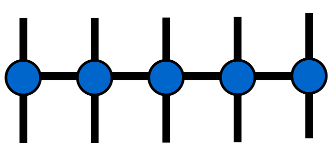
Purification [Verstraete, PRL. (2004), Zwolak, PRL. (2004), Feiguin, PRB (2005)]

Purification is equivalent to the density matrix



$$e^{-\beta \hat{H}/2}$$

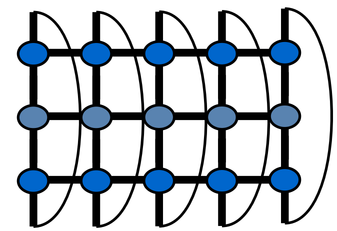
$$\hat{\rho}_{T=\infty} = \hat{1}$$



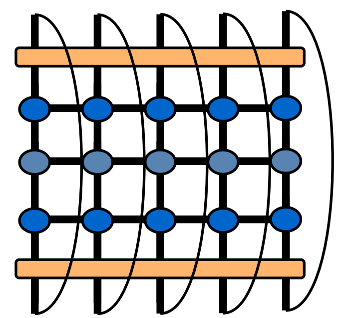
Bases on auxiliary sites are arbitrary

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

=



=



$\hat{U}^\dagger$

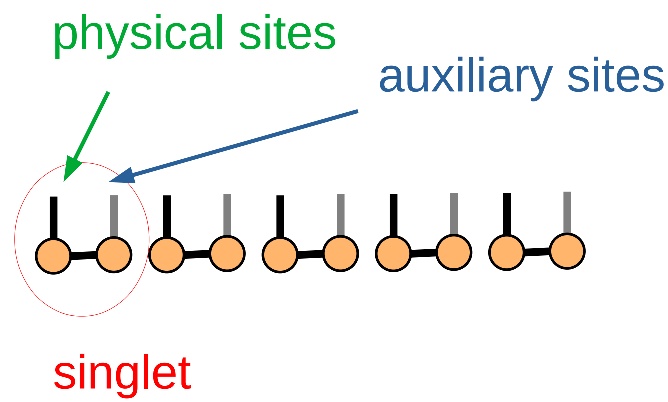
$\hat{U}$

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

Purification [Verstraete, PRL. (2004), Zwolak, PRL. (2004), Feiguin, PRB (2005)]

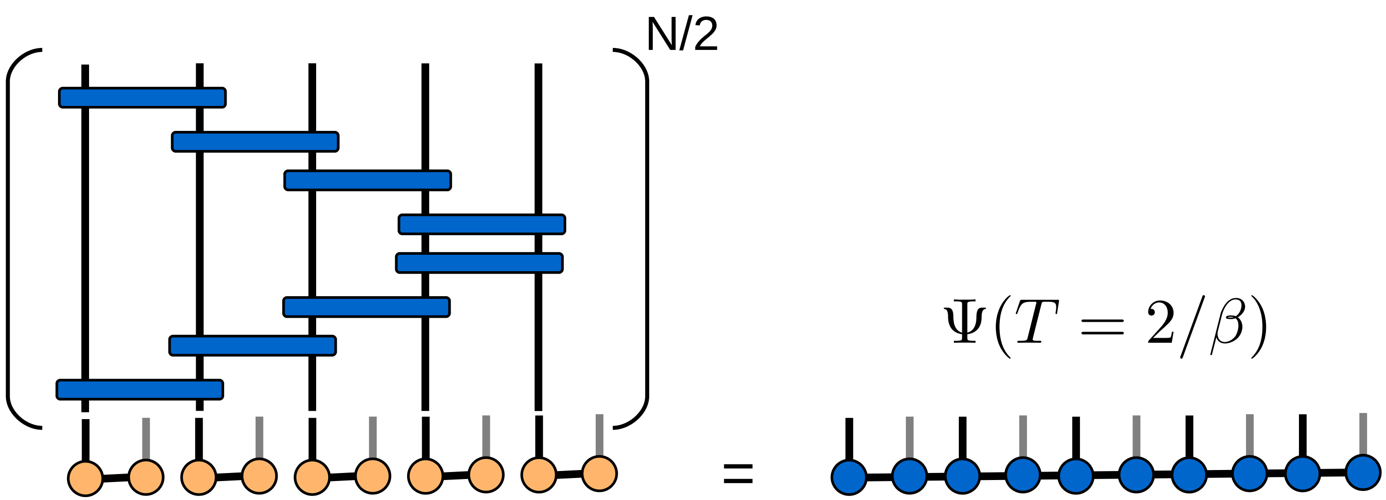
- Represent a mixed state by a pure state with enlarged Hilbert space

purification $\Psi(T=\infty)$



- Imaginary time evolution on a purified MPS

$e^{-\beta\hat{H}/2}$

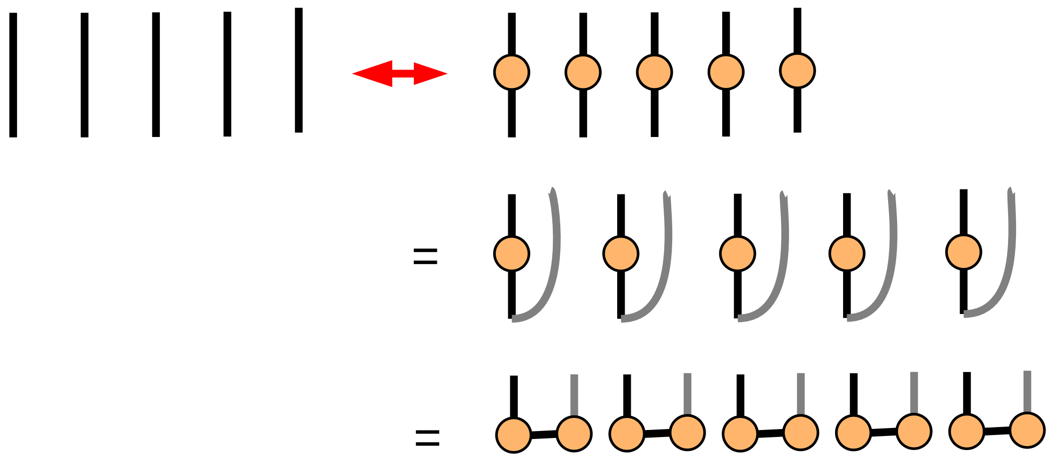


$\Psi(T=2/\beta)$

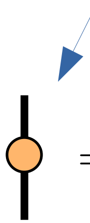
Purification [Verstraete, PRL. (2004), Zwolak, PRL. (2004), Feiguin, PRB (2005)]

Purification is equivalent to the density matrix evolved from identity

unitary transformation



unitary

singlet 

$$= \begin{array}{cc} \uparrow\uparrow & \uparrow\downarrow \\ \left(\begin{array}{c} 0 \\ -\frac{1}{\sqrt{2}} \end{array} \right. & \left. \begin{array}{c} \frac{1}{\sqrt{2}} \\ 0 \end{array} \right) \\ \downarrow\uparrow & \downarrow\downarrow \end{array}$$

(The same number of auxiliary sites are always enough)

METTS – original scheme

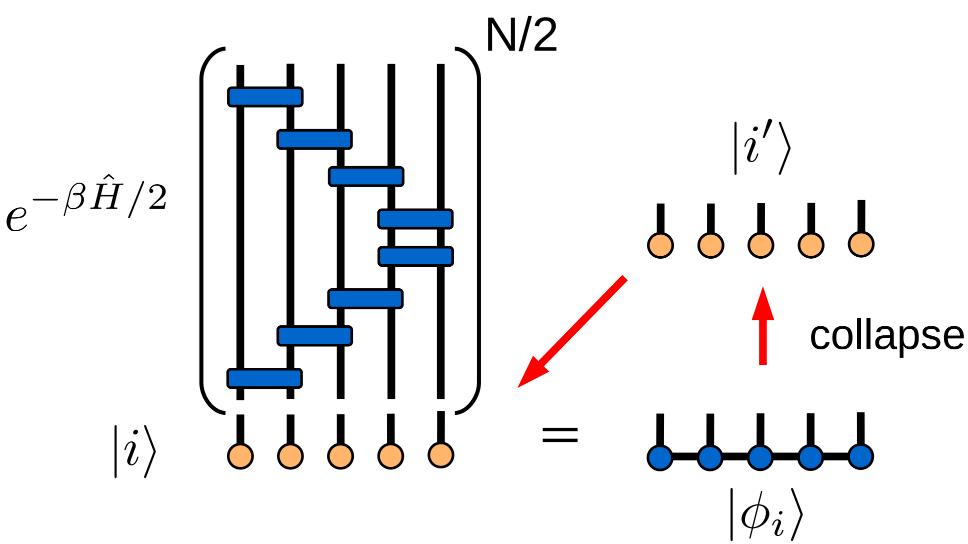
[Stoudenmire, New J. Phys. (2010), White, PRL. (2009)]

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 $q_{i\to i'} = \dfrac{|\langle i'|\phi_i\rangle|^2}{\langle\phi_i|\phi_i\rangle}$



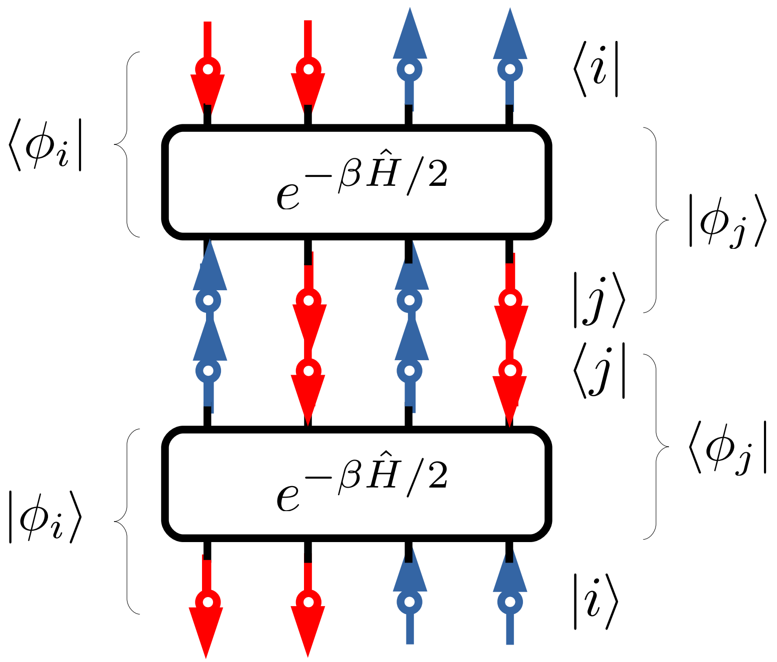
Detail balance

$$\frac{q_{i\to i'}}{q_{i'\to i}} = \frac{\dfrac{\left|\langle i'|\phi_i\rangle\right|^2}{\langle\phi_i|\phi_i\rangle}}{\dfrac{|\langle i|\phi_{i'}\rangle|^2}{\langle\phi_i'|\phi_i'\rangle}} = \frac{\langle i'|e^{-\beta\hat{H}}|i'\rangle}{\langle i|e^{-\beta\hat{H}}|i\rangle}$$

$$P_i = \langle i|e^{-\beta\hat{H}}|i\rangle/Z$$

METTS – "diagram" representation

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



= probability weight

METTS: sample $|i\rangle$ and $|j\rangle$ iteratively.

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

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

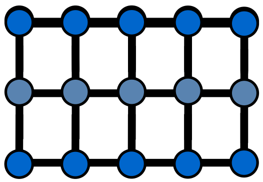
METTS – original scheme

[Stoudenmire, New J. Phys. (2010), White, PRL. (2009)]

- Measure in the ensemble $\{|\phi_i\rangle\}$

$$
\begin{aligned}
\langle \mathcal{O} \rangle_\beta &= \sum_i \frac{\langle \phi_i | \hat{\mathcal{O}} | \phi_i \rangle}{Z} \\
&= \sum_i \frac{\langle \phi_i | \hat{\mathcal{O}} | \phi_i \rangle}{\langle i | e^{-\beta \hat{H}} | i \rangle} \frac{\langle i | e^{-\beta \hat{H}} | i \rangle}{Z} \\
&\equiv \sum_i \mathcal{O}_i P_i, \qquad \mathcal{O}_i \equiv \frac{\langle \phi_i | \hat{\mathcal{O}} | \phi_i \rangle}{\langle \phi_i | \phi_i \rangle} \\
&\approx \frac{1}{M} \sum_k^M \mathcal{O}_i^{(k)}
\end{aligned}
$$

=



Monte Carlo sum

METTS – original scheme

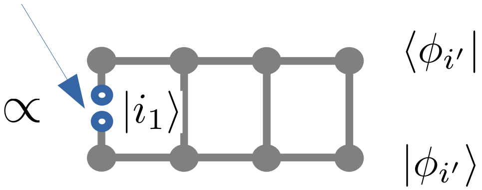
[Stoudenmire, New J. Phys. (2010), White, PRL. (2009)]

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

Algorithm: collapse site by site

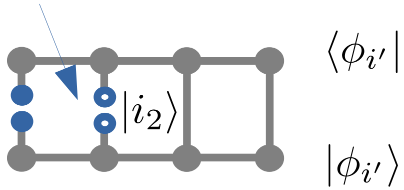
collapse the first site

$q_{i_1} \propto$



collapse the second site

$q_{i_2} \propto$



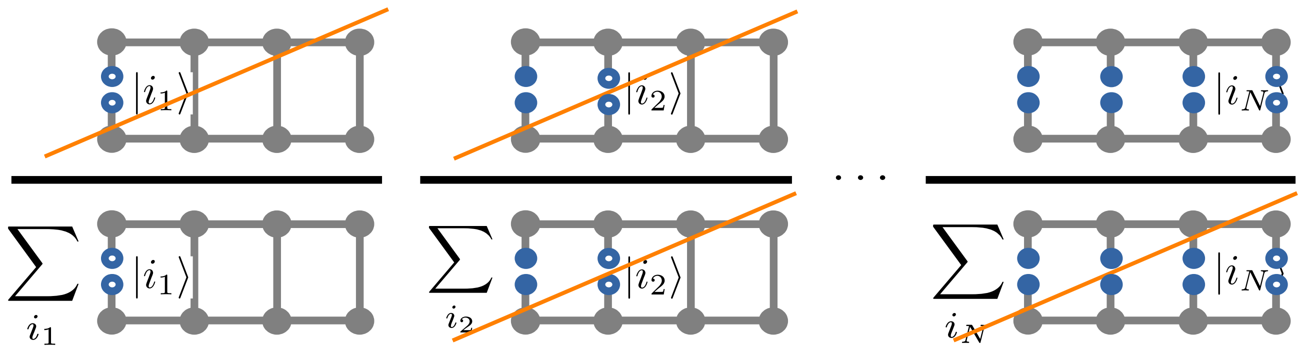
...

$$q_{i'\to i} = q_{i_1} q_{i_2} \cdots q_{i_N}; \quad |i\rangle = |i_1 i_2 \cdots i_N\rangle$$

[Stoudenmire, New J. Phys. (2010), White, PRL. (2009)]

Collapsing probability

$$q_{i' \to i} =$$



$$= \frac{\left|\langle i|\phi_{i'}\rangle\right|^2}{\langle\phi_{i'}|\phi_{i'}\rangle}$$

Comparison between purification and METTS

Required bond dimensions

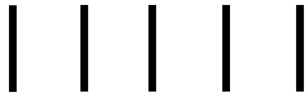
- T → ∞

  purification: 1
  METTS: 1 × lot of samplings

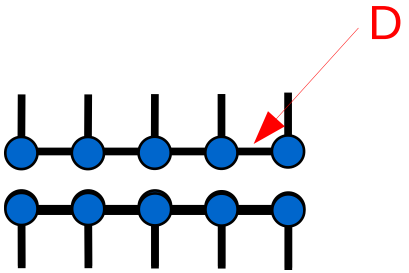
- T → 0

  purification: D^2
  METTS: D (1 sampling)

$\rho_\infty =$



$\rho_0 =$

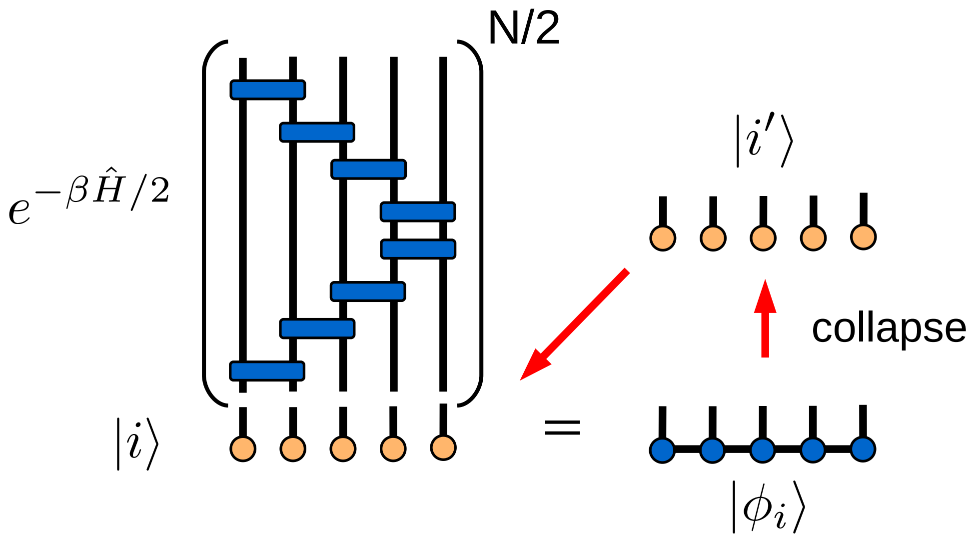


Purification is more efficient at **high** and **intermediate** temperature,

while **METTS** is more efficient at **low** temperature.

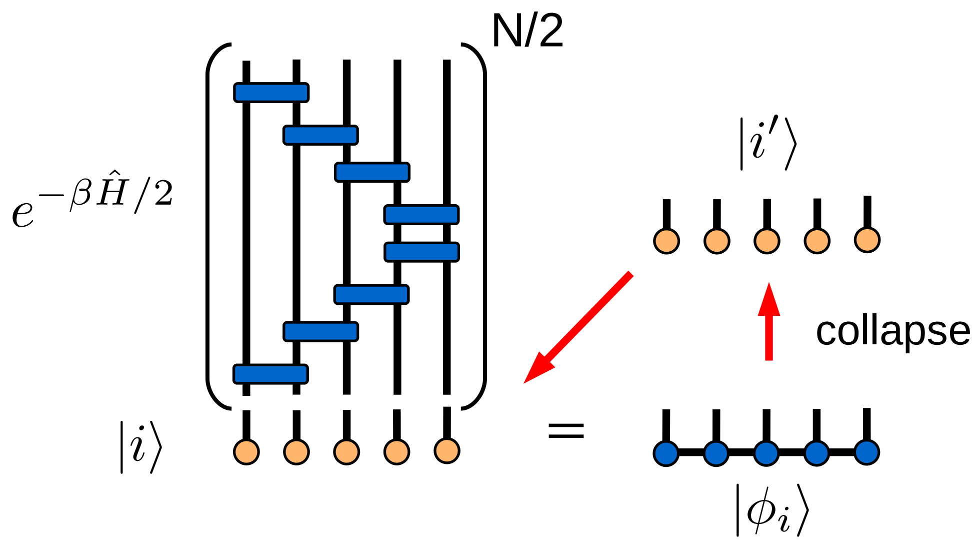
Quantum number and autocorrelation in METTS

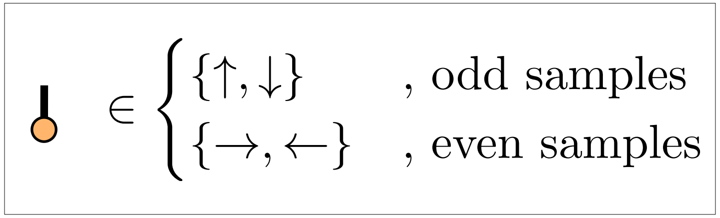
- If $|i\rangle$ and $\hat{H}$ conserve quantum number, the simulation will be stuck in the corresponding quantum number sector.
- For high T or small off-diagonal Hamiltonian, METTS algorithm will be stuck.



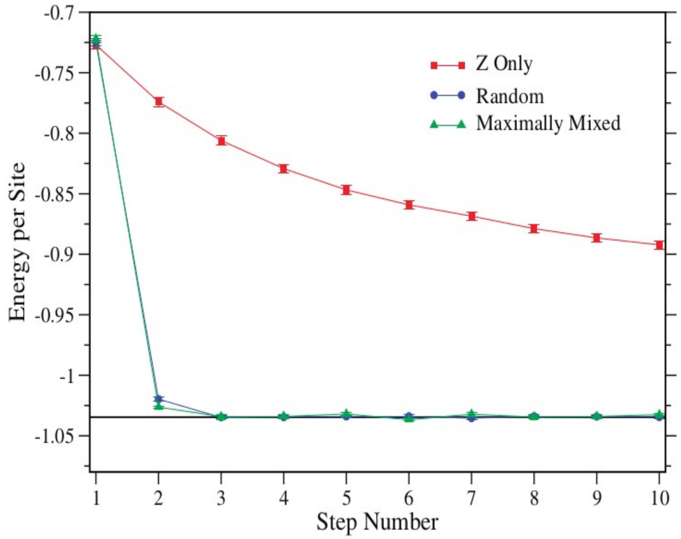
Collapse to orthogonal bases

[Stoudenmire, New J. Phys (2010)]





[Stoudenmire, New J. Phys (2010)]



Good:

- Reduce autocorrelation time.
- Grand canonical ensemble.

Bad:

- Require MPS with no quantum number

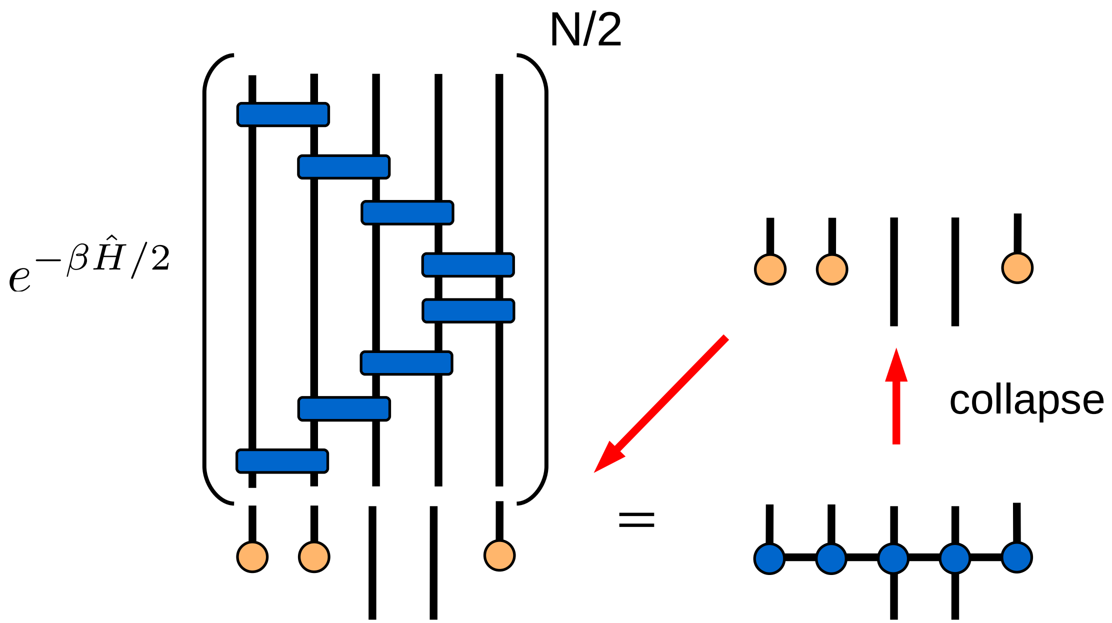
New algorithm [arXiv:1910.03329], see also [Jing Chen, arXiv:1910.09142]

We want:

- Use quantum number conserving MPS
- Reduce the autocorrelation

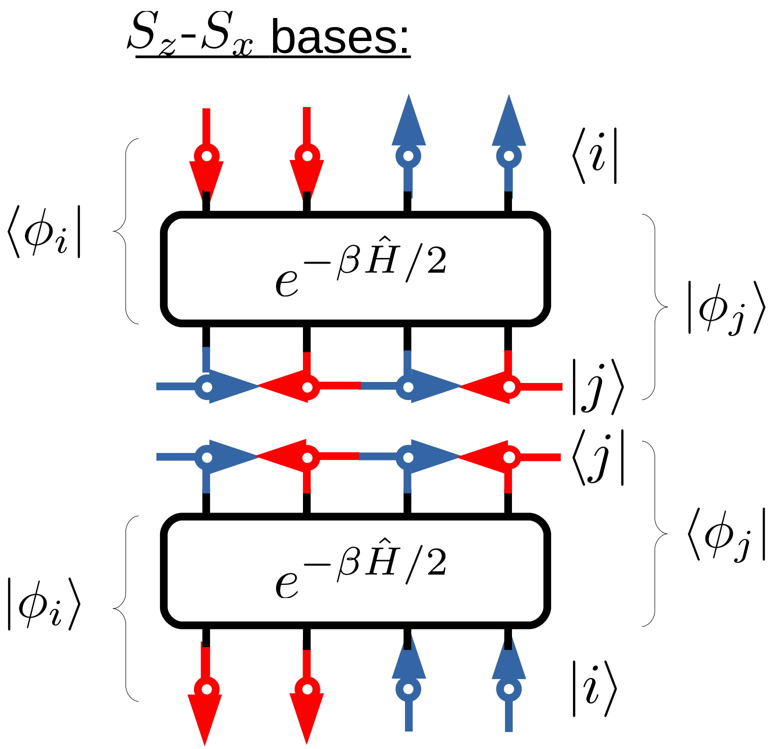
Key idea:

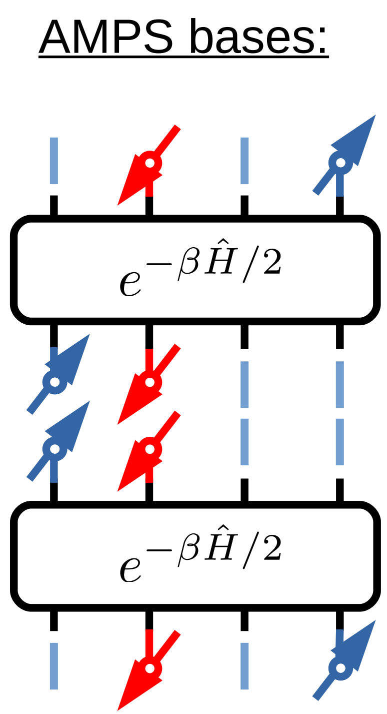
- Remain some sites **uncollapsed**



MPS with auxiliary indices
(auxiliary MPS, or AMPS)

METTS – “diagram” representation





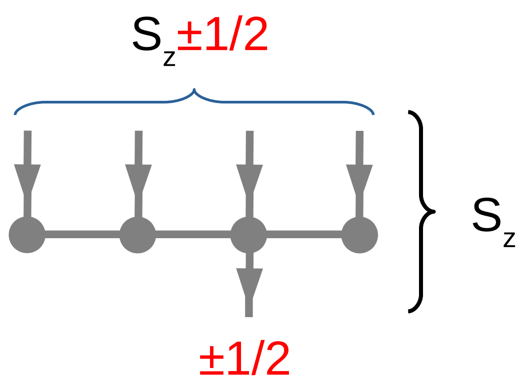
The uncollapsed sites play roles as “presuming” the partition function

New algorithm

[arXiv:1910.03329], see also [Jing Chen, arXiv:1910.09142]

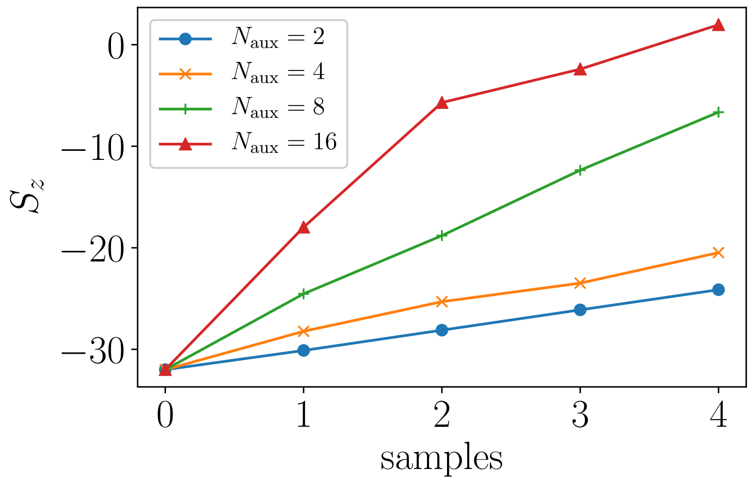
Auxiliary sites induce the quantum number fluctuation

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

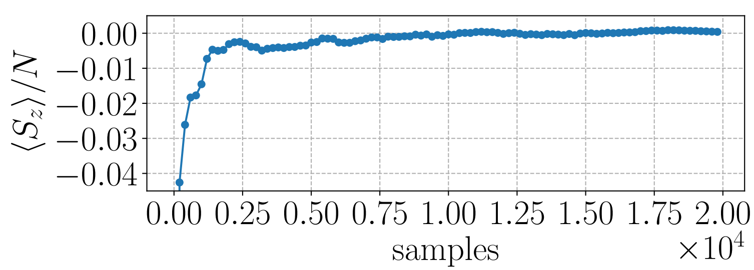


$\Delta Q = 1$

L=64 Heisenberg chain at β=2
Starting from all down spins

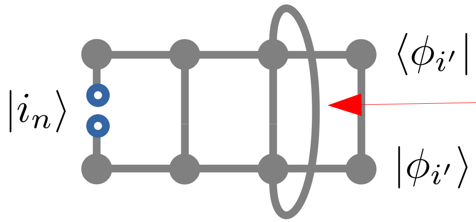


$N_{\mathrm{aux}} = 2$



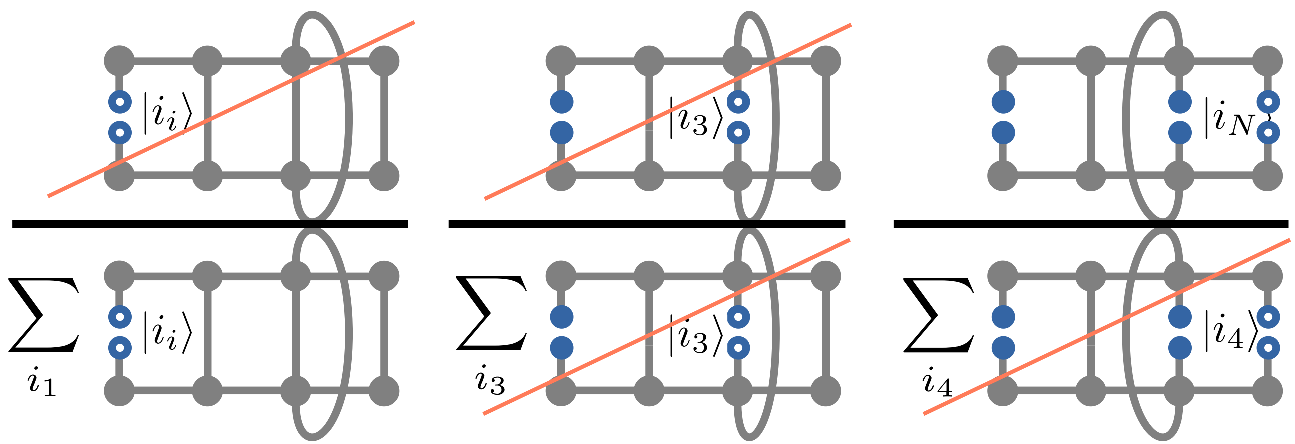
- Collapsing algorithm

$q_{i_n} \propto$



contract both the physical
and auxiliary indices

$q_{i' \to i} =$

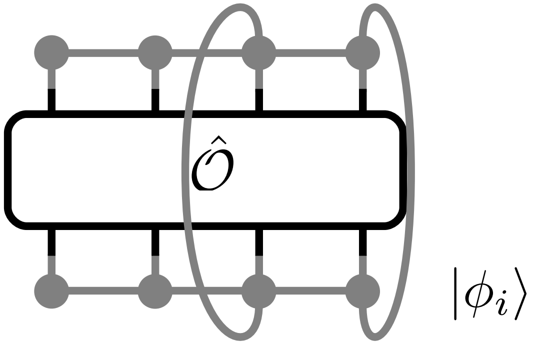


$$= \frac{|\langle i|\phi_{i'}\rangle|^2}{\langle\phi_{i'}|\phi_{i'}\rangle}$$

Grand canonical METTS

- Measure:

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



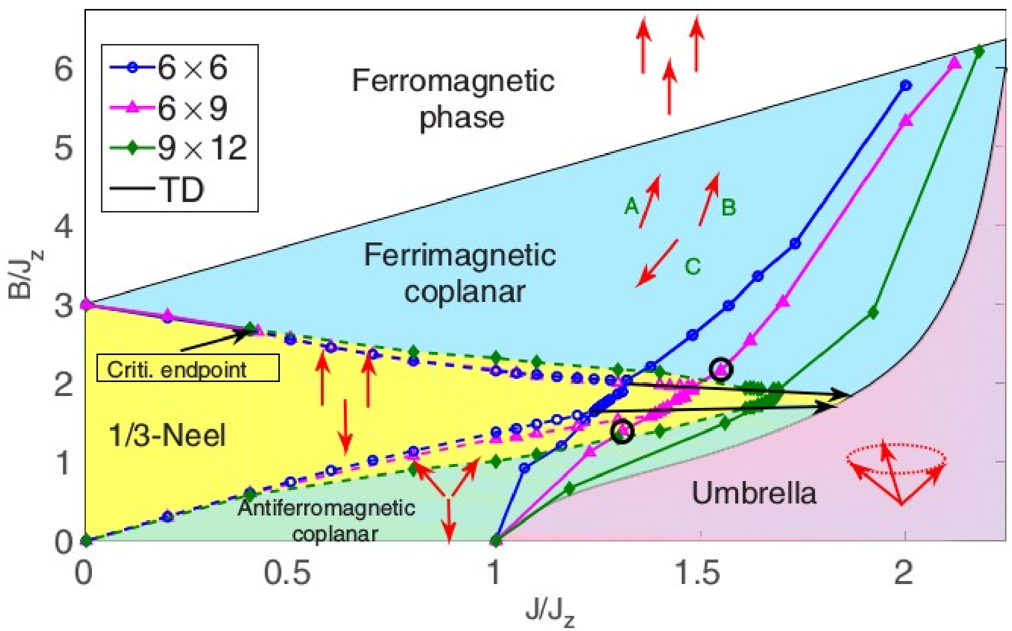
contract both the physical the auxiliary sites

Benchmark on trianglular lattice, XXZ model, Jz=0.8

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

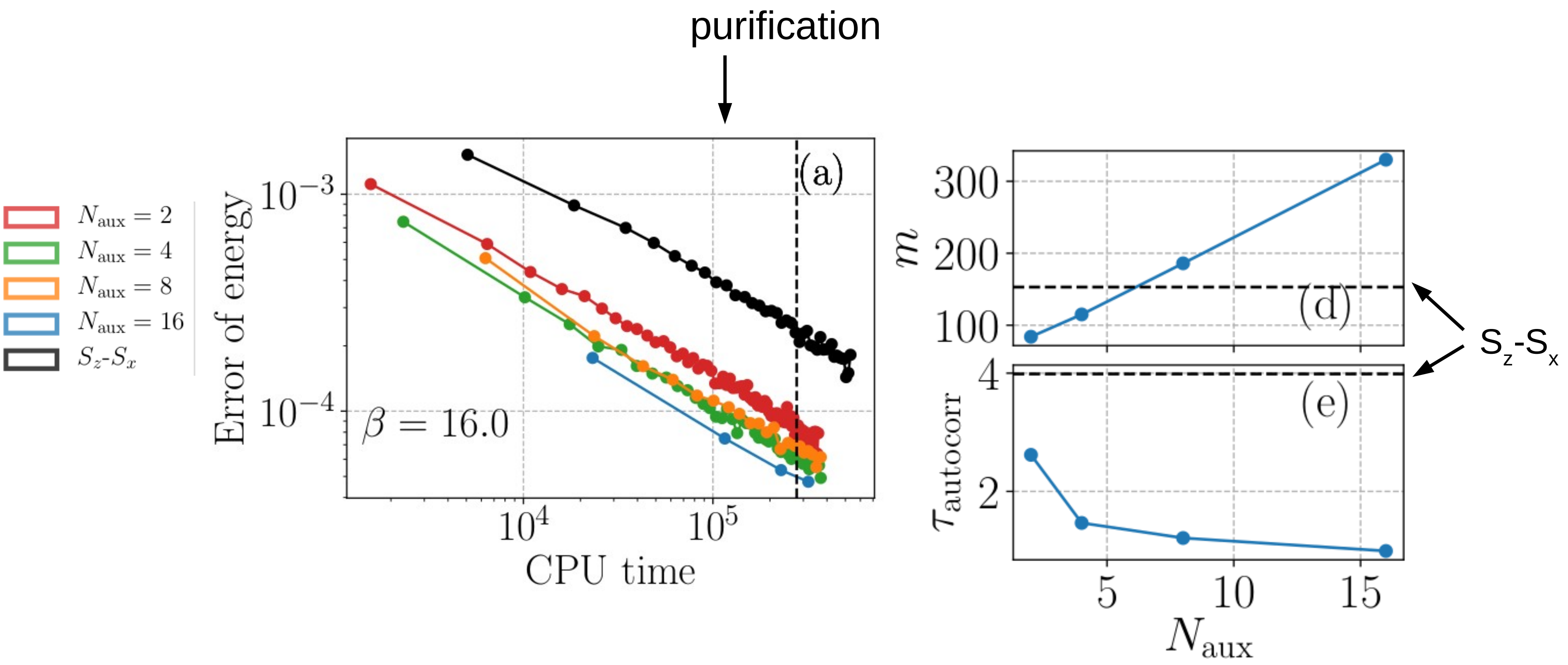
- Sign problem in the quantum Monte Carlo
- We consider B=0, J_z=0.8

[Sellmann, PRB 91, 081104(R) (2015)]



Benchmark: 12x3 trianglular lattice, XXZ model, Jz=0.8

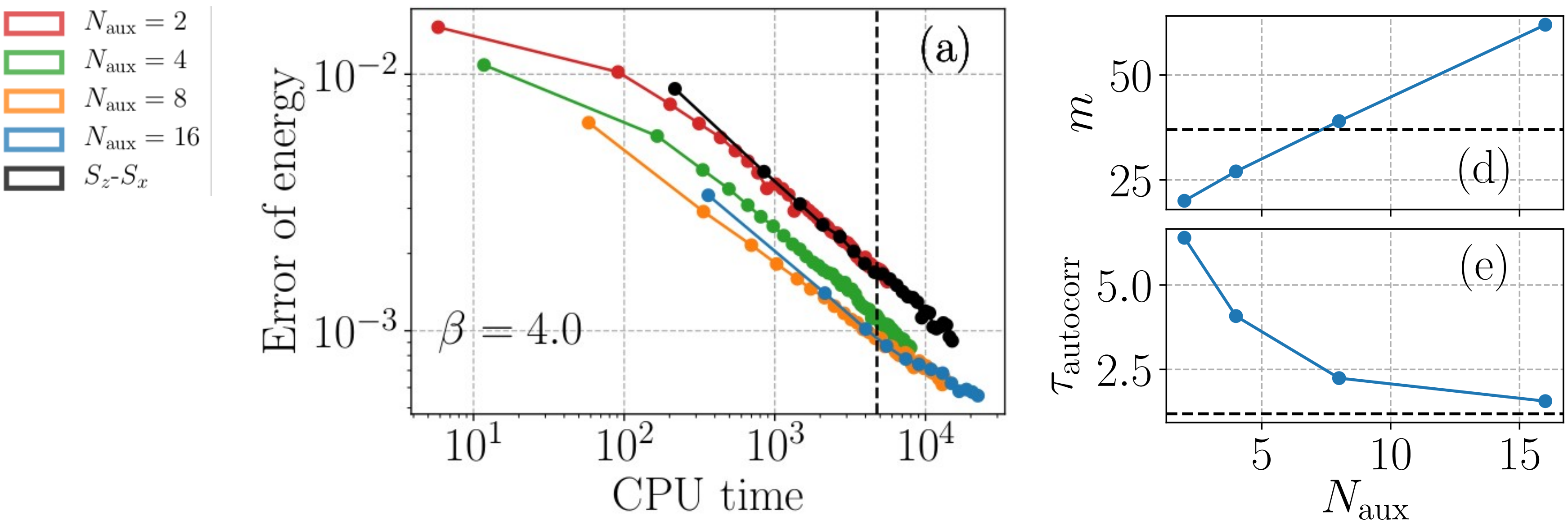
β=16



AMPS-METTS outperforms Sz-Sx METTS and purification at low temperature

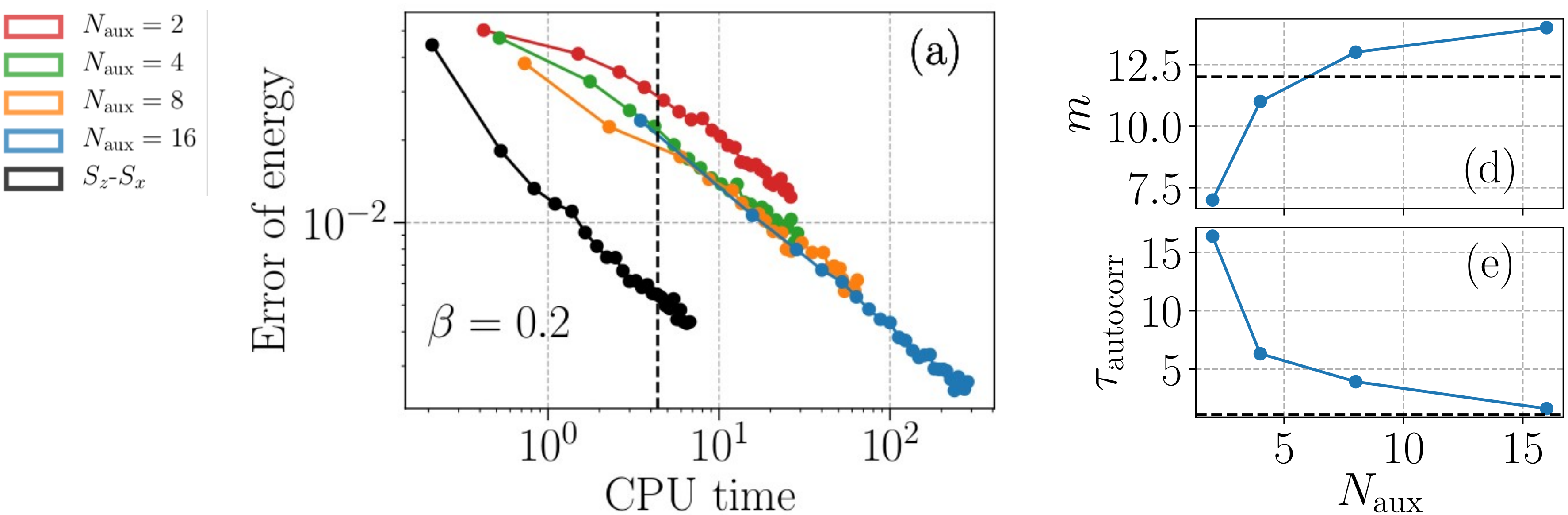
Benchmark: 12x3 trianglular lattice, XXZ model, Jz=0.8

β=4



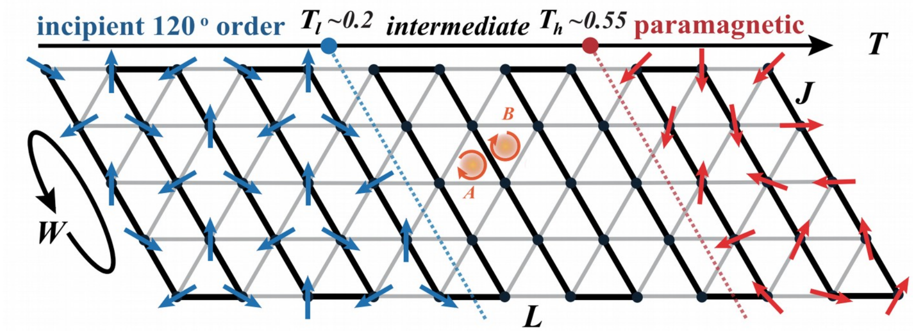
Benchmark: 12x3 trianglular lattice, XXZ model, Jz=0.8

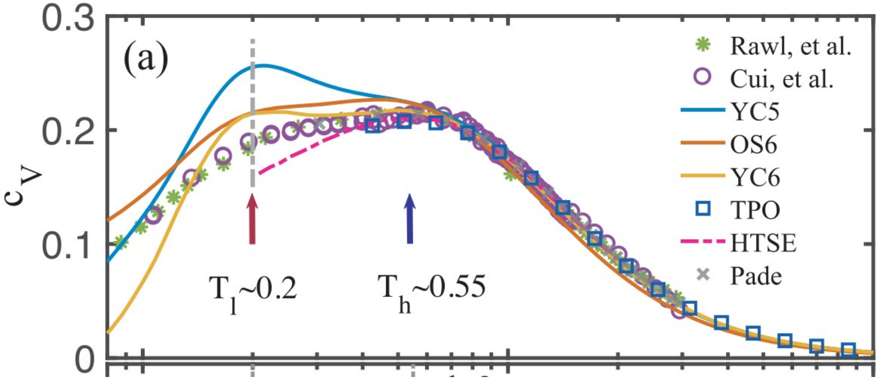
β=0.2



Heisenberg model on triangular lattice

Lei Chen, PRB 99, 140404(R) (2019)





Benchmark: 12x3 trianglular lattice, XXZ model, Jz=0.8

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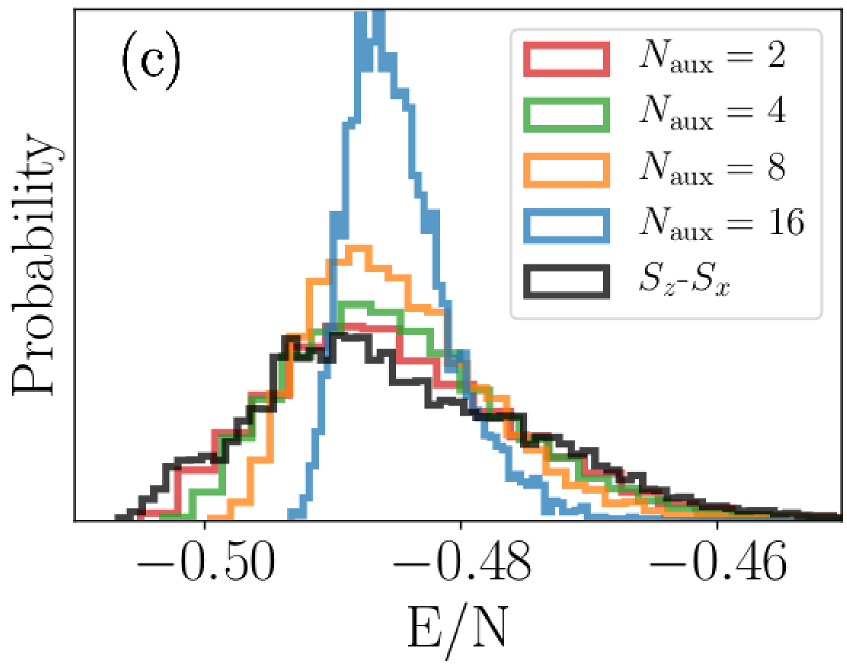
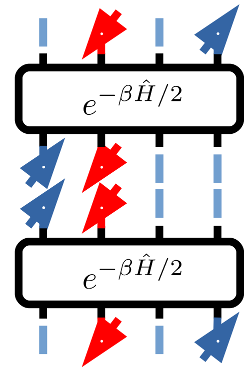




The identities = “presum” of the partition function

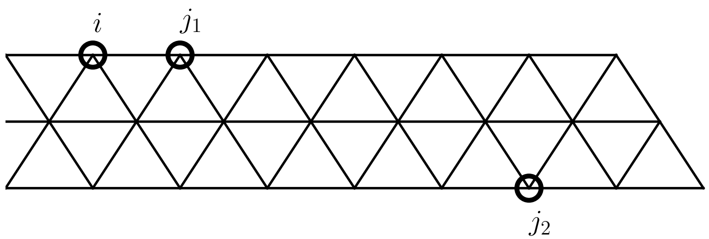
Effects of auxiliary indices:

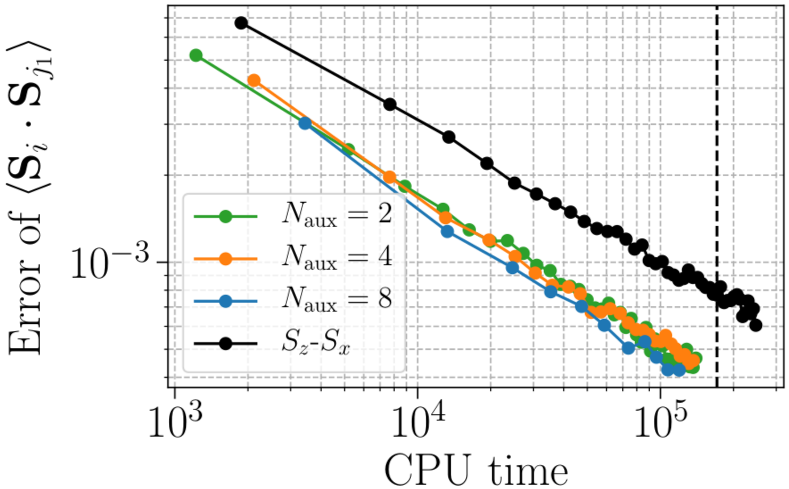
- Induce quantum number fluctuation
- Reduce autocorrelation time
- Narrow the probability distribution

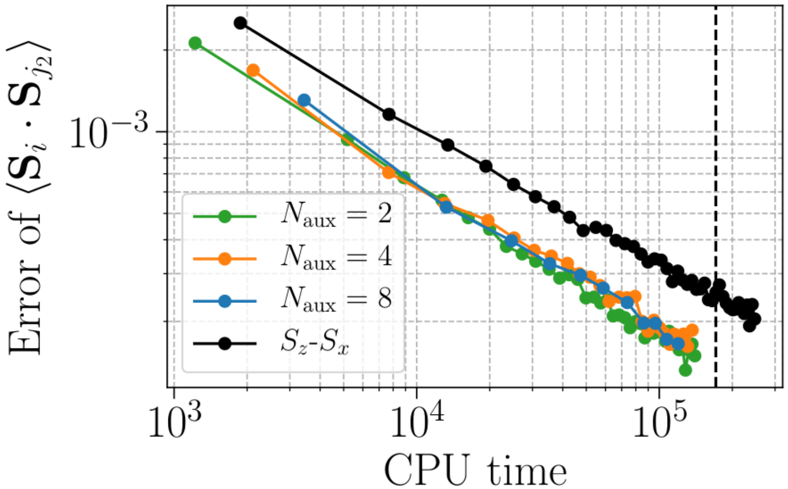
Benchmark: 12x3 trianglular lattice, XXZ model, Jz=0.8

β=16

$\langle S_i \cdot S_j \rangle$







Conclusion

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)

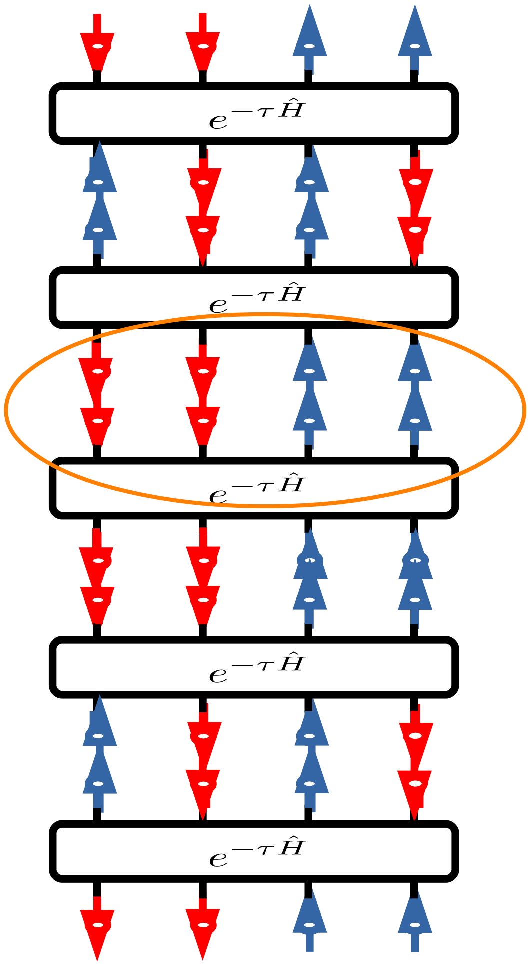
Discussion

Approach the path-integral Monte Carlo

$$\mathrm{Tr} e^{-\beta \hat{H}} = \mathrm{Tr}(e^{-\tau \hat{H}} \cdots\cdots e^{-\beta \hat{H}})$$

$$\hat{1} = \sum_i |i\rangle\langle i|$$

Can update the configuration by collapsing



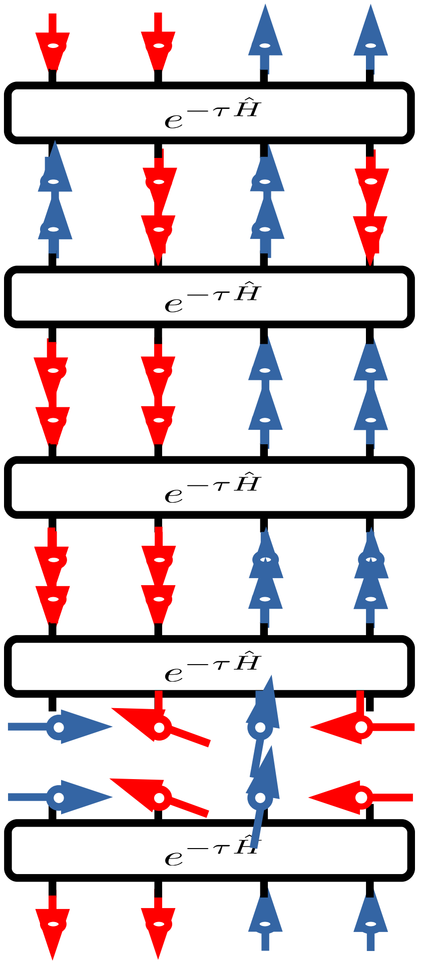
- Sign problem will come back
- Completely flexible in choosing bases

→ New hope?

Discussion

Example of possible bases:

- Local rotation
  [D. Hangleiter, arXiv:1906.02309 (2019)]

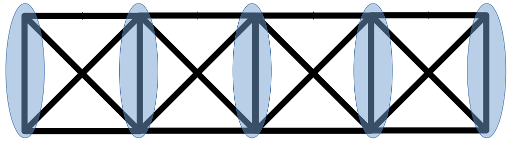


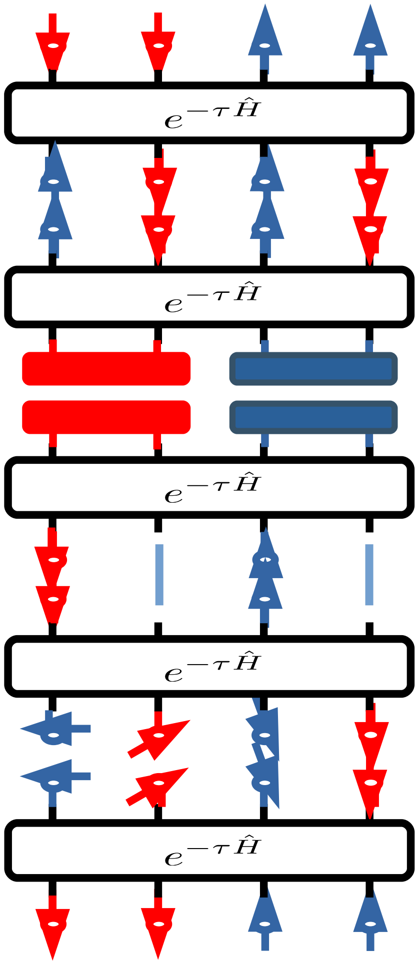
Discussion

Example of possible bases:

- Local rotation
  [D. Hangleiter, arXiv:1906.02309 (2019)]
- 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).

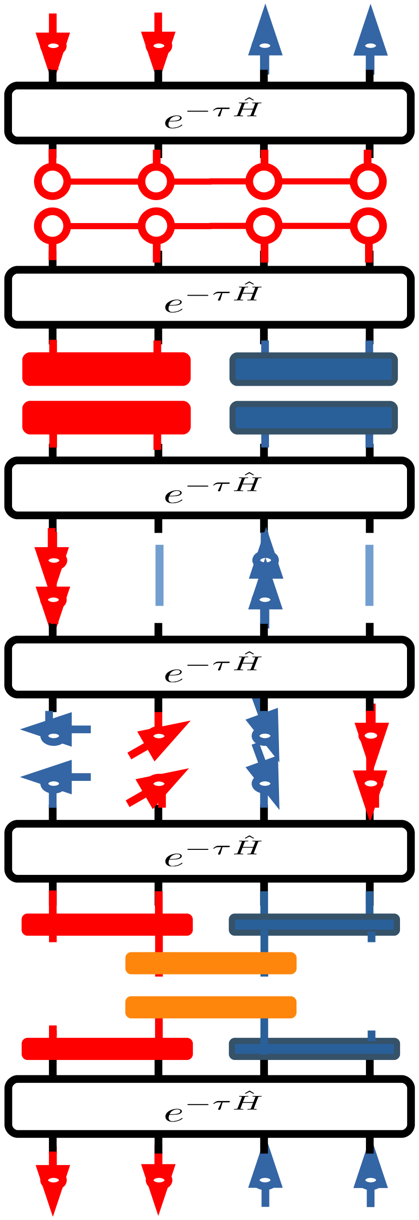




Discussion

Example of possible bases:

- Local rotation
  [D. Hangleiter, arXiv:1906.02309 (2019)]
- Multiple-site bases
  [Alet, et. al. PRL 117, 197203 (2016)]
- MPS bases
- MERA-like bases



Discussion

Example of possible bases:

- Local rotation
  [D. Hangleiter, arXiv:1906.02309 (2019)]
- Multiple-site bases
  [Alet, et. al. PRL 117, 197203 (2016)]
- MPS bases
- MERA-like bases
- Rotation of single particle basis
  [R. Levy, arXiv:1907.02076(2019)]

$\longrightarrow$ New hope???