Finite-temperature simulations with stoMPS

May, 2024

Journal Club - Third Season

Franco Lisandrini (AG Kollath)

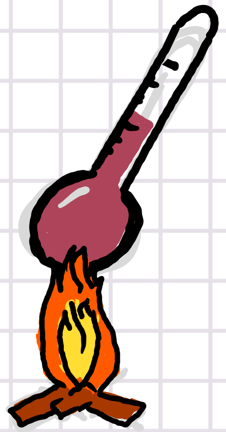
Presenting results from: arXiv:2312.04420

Jianxin Gao, Yuan Gao, Qiaoyi Li, and Wei Li

We focus on...

Finite temperature

- Necessary to compare with experiments



Many methods in general

- QMC, FTLM (ED), Series expansion, etc...

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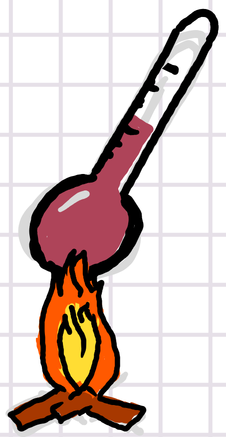
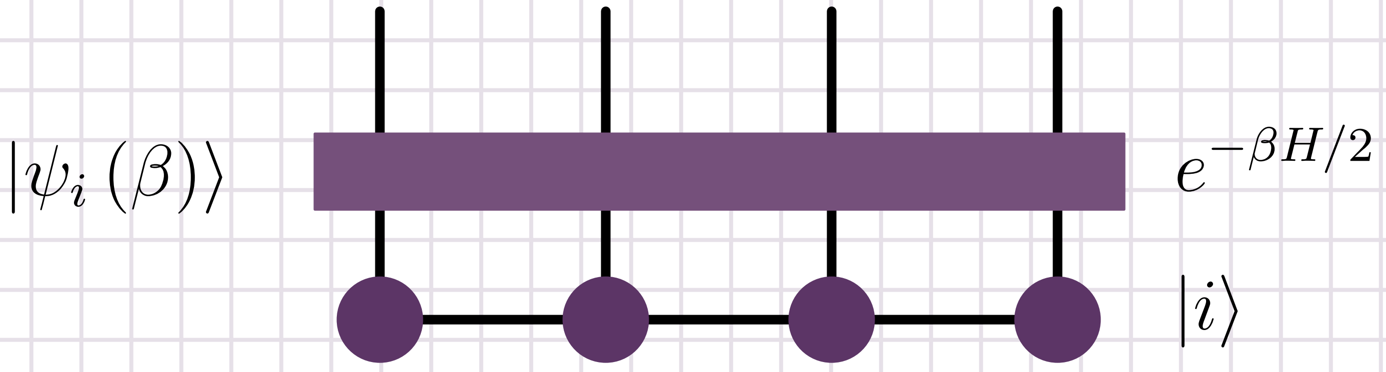


Many methods in general

- QMC, FTLM (ED), Series expansion, etc...

Tensor networks?

- MPS + imaginary time evolution



Purification and Sampling (METTS and stoMPS)

Methods in this talk

Purification

- Density matrix as an MPS

METTS (Minimally Entangled Typical Thermal States)

- Well stablished sampling method

Stocasthic MPS (stoMPS)

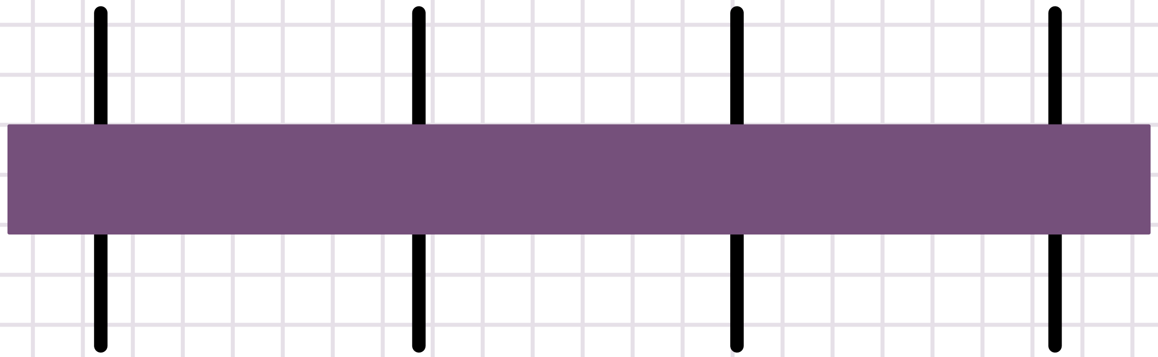
- New sampling method

Verstraete et al., PRL **93**, 207204 (2004)
Barthel et al., PRB **79**, 245101 (2009)

Purification

$$\langle A \rangle_\beta = \frac{1}{Z_\beta} \mathrm{Tr}\left(e^{-\beta H} A\right)$$

Operator
$e^{-\beta H}$



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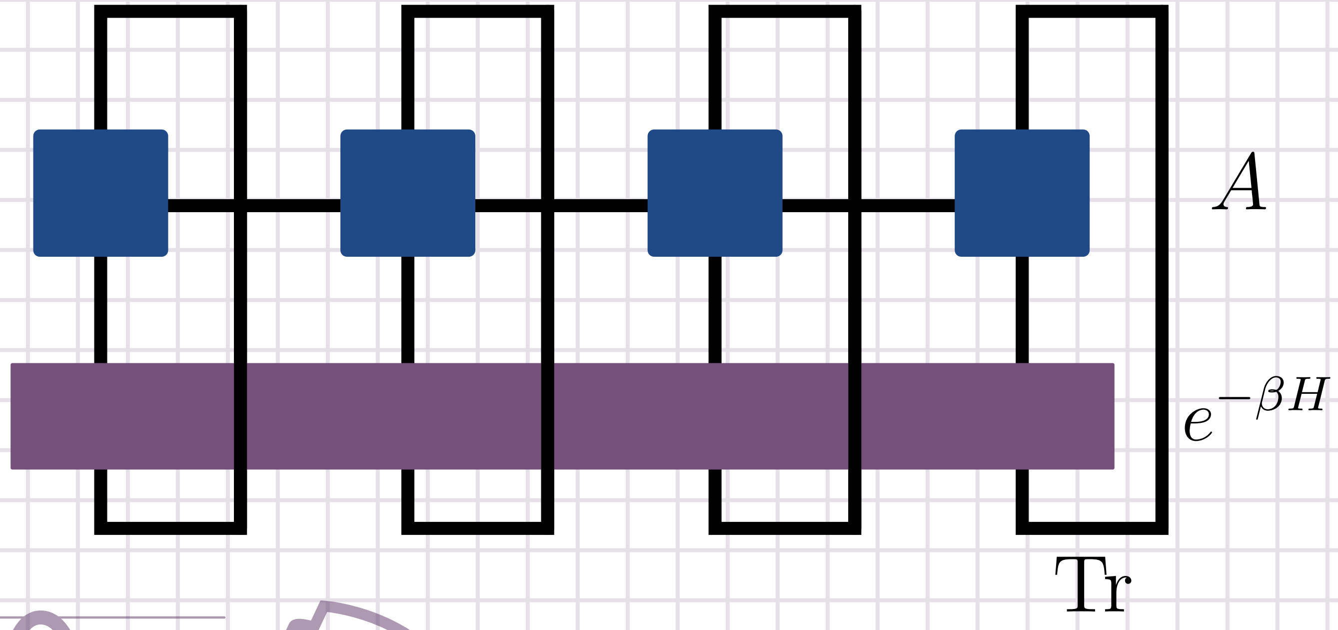

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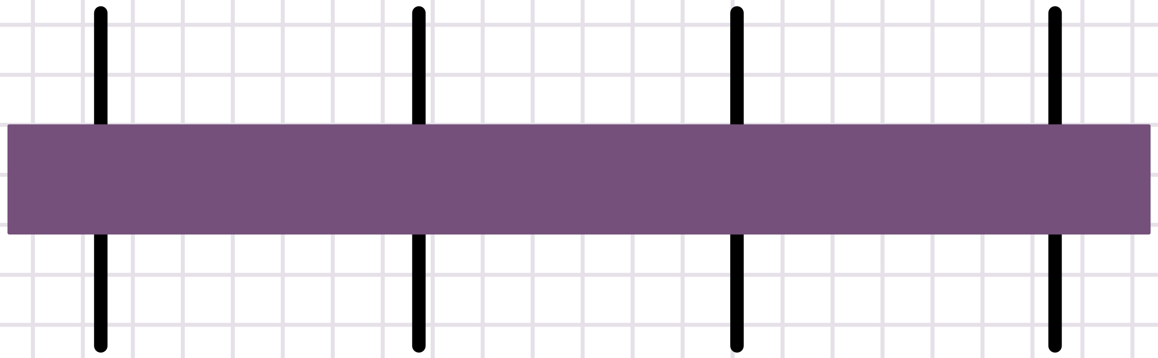

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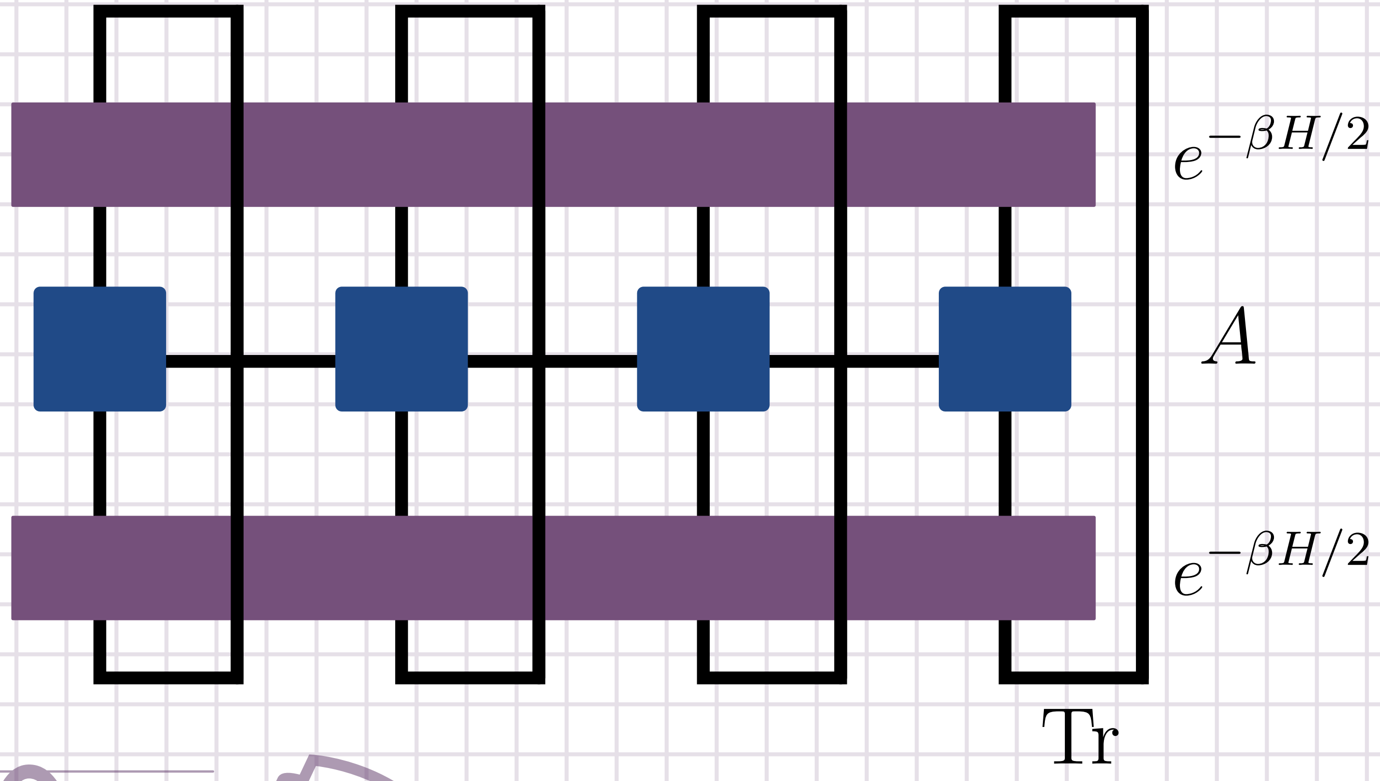

Verstraete et al., PRL **93**, 207204 (2004)
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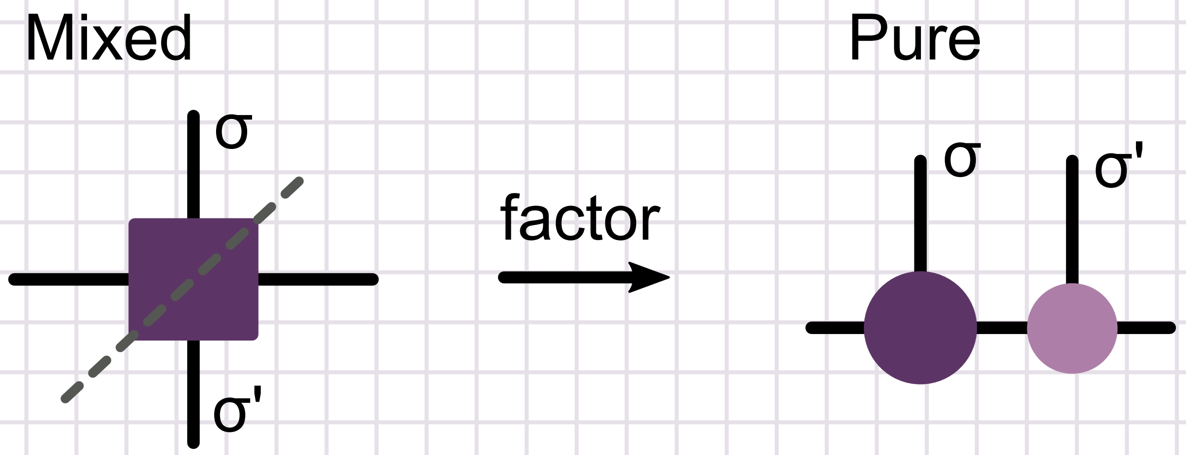

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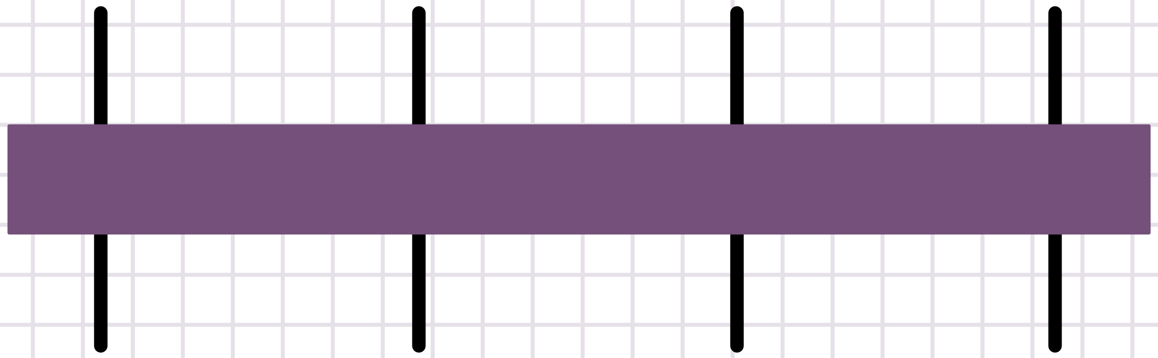

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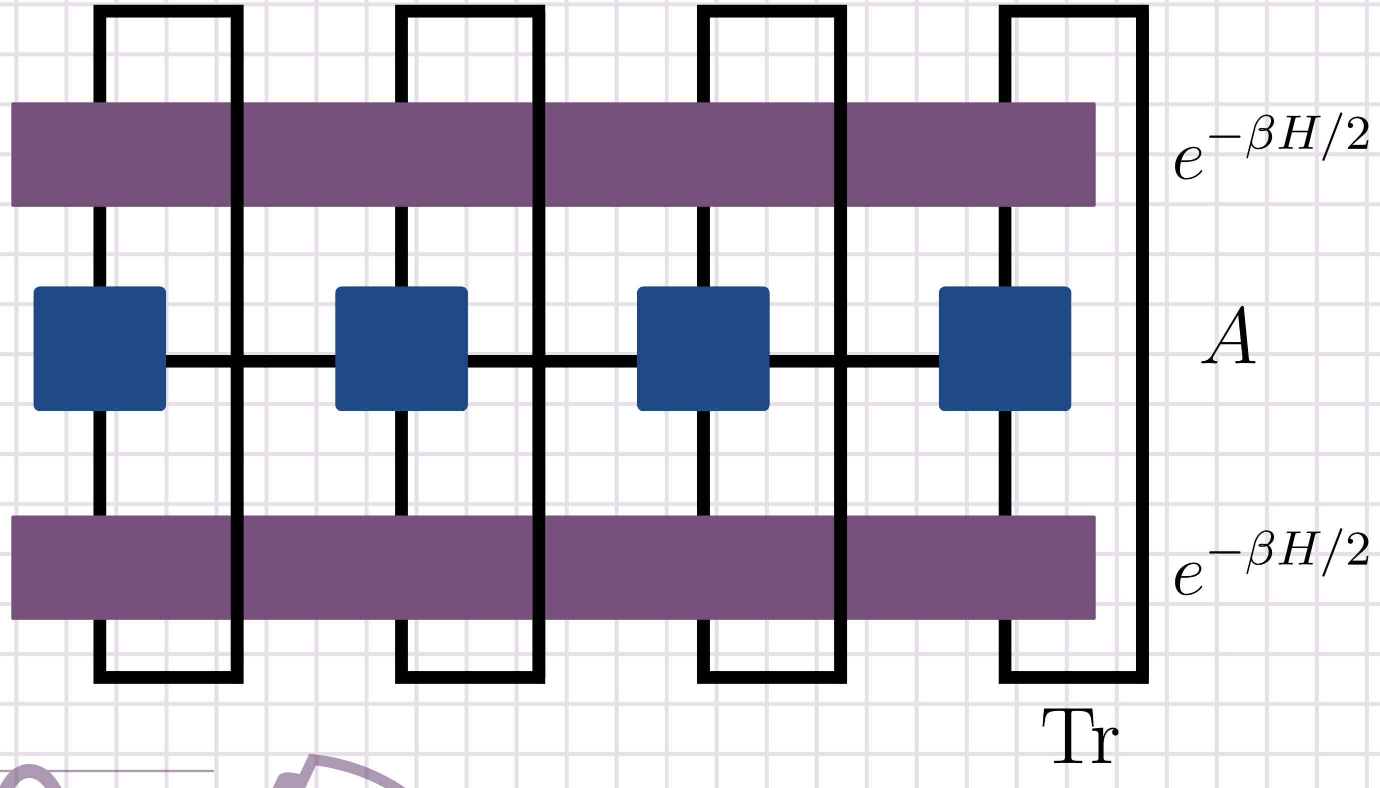

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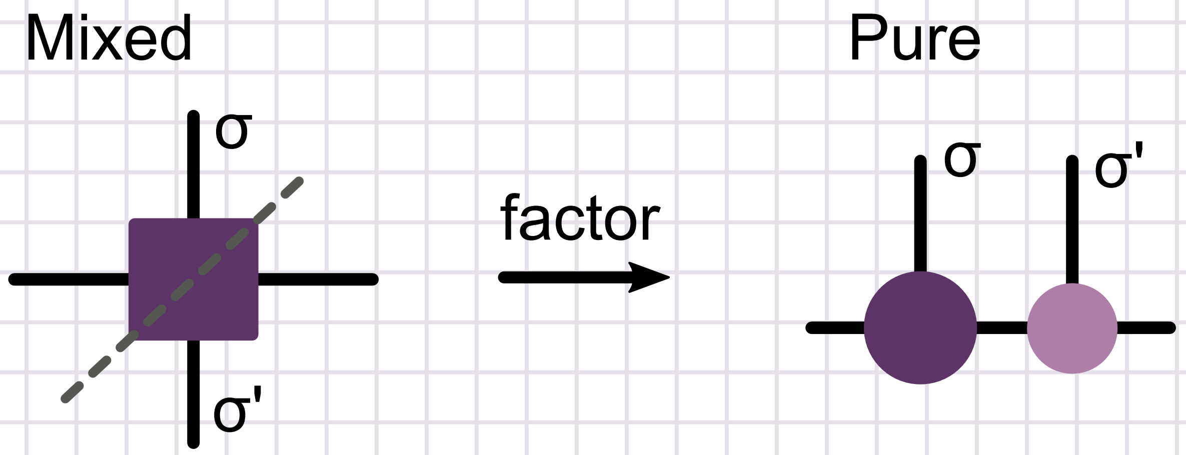

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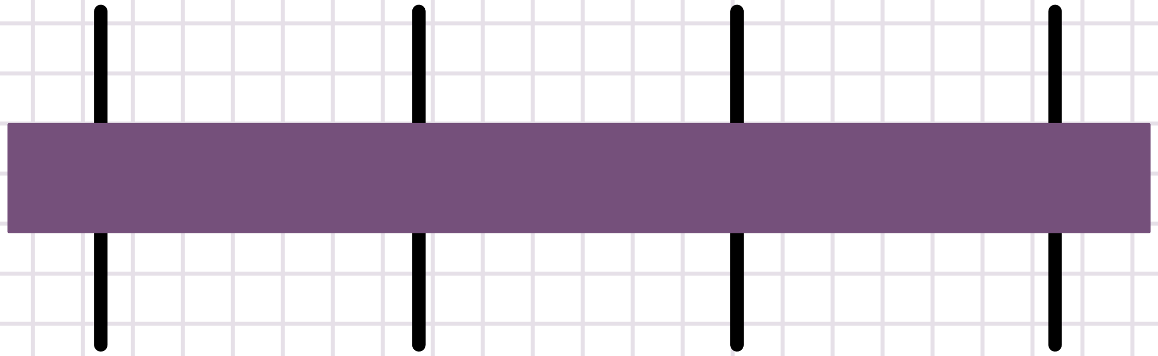
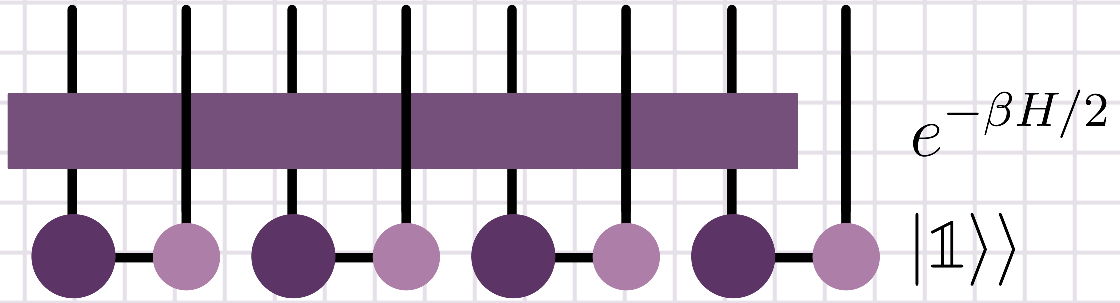


MPS

$|\psi(\beta)\rangle\rangle =$



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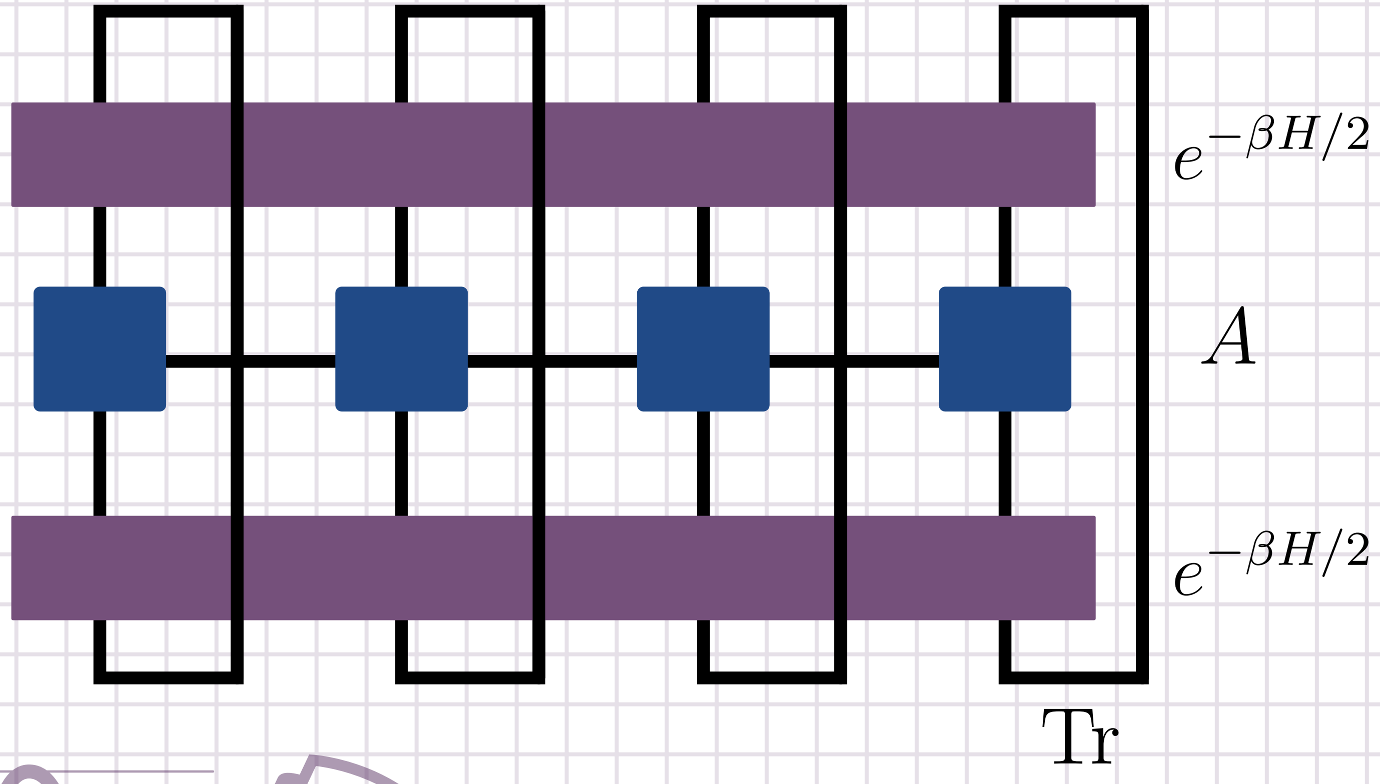

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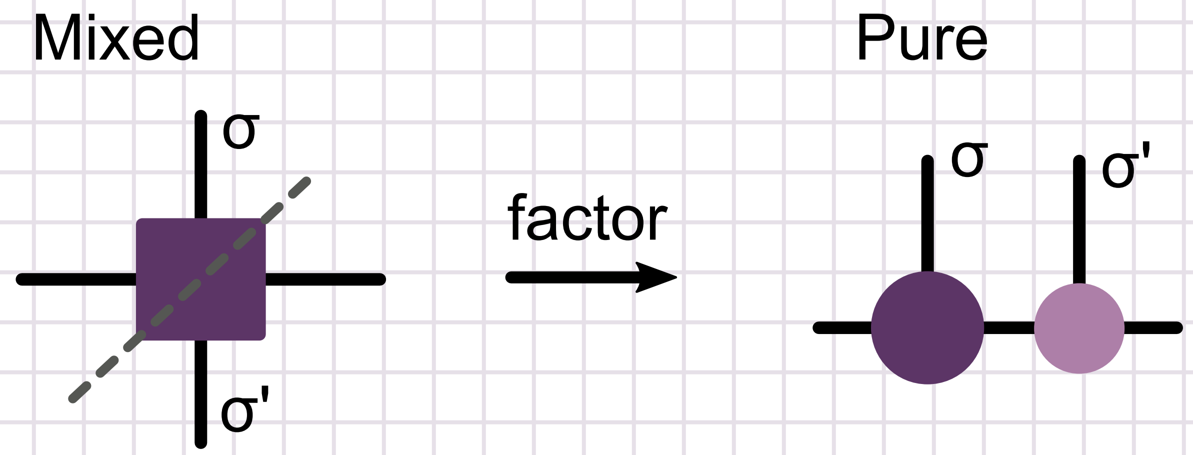

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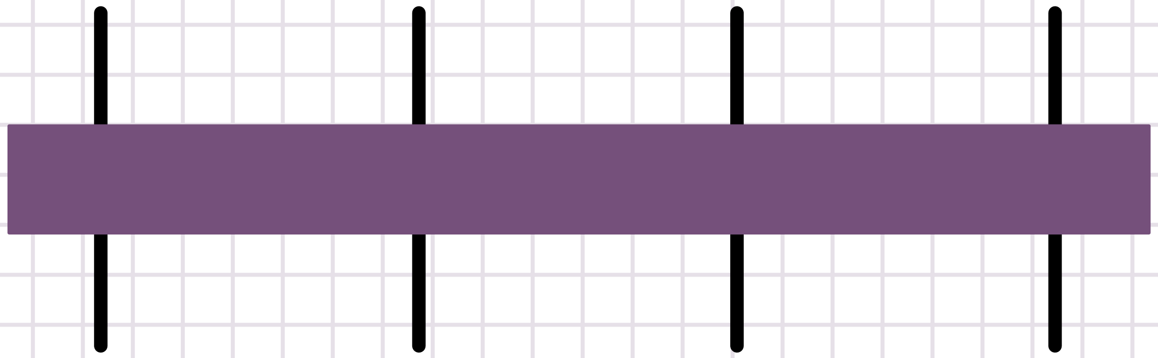

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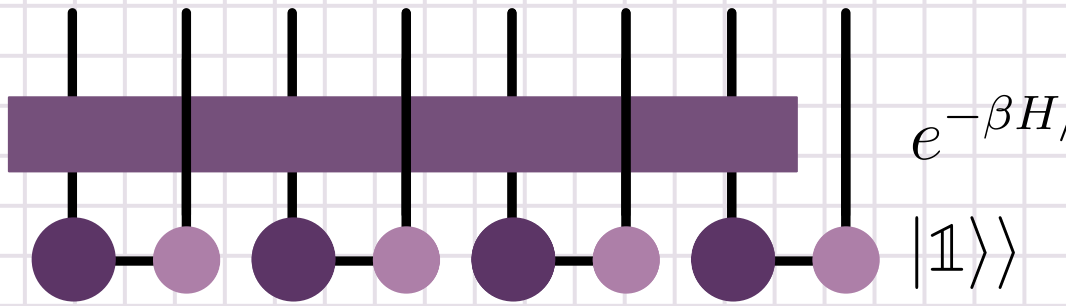

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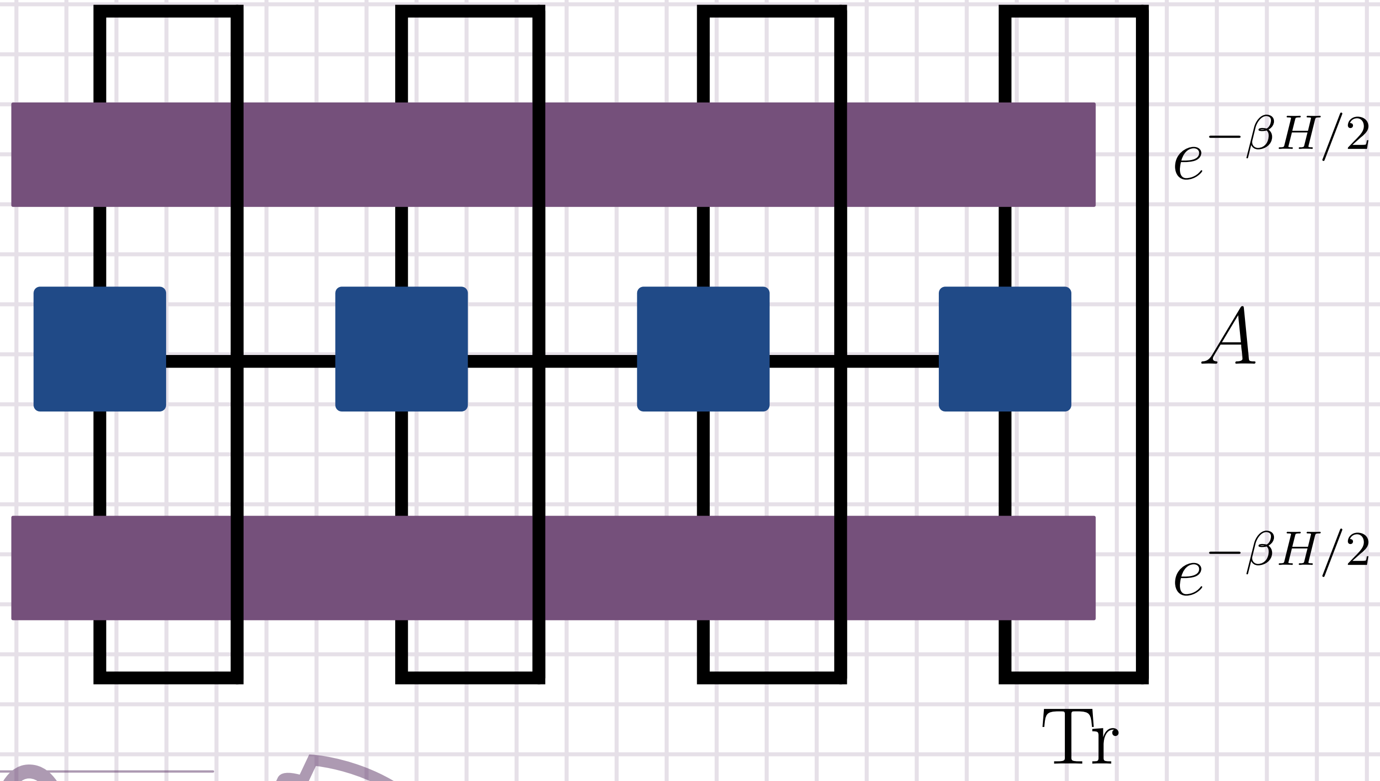

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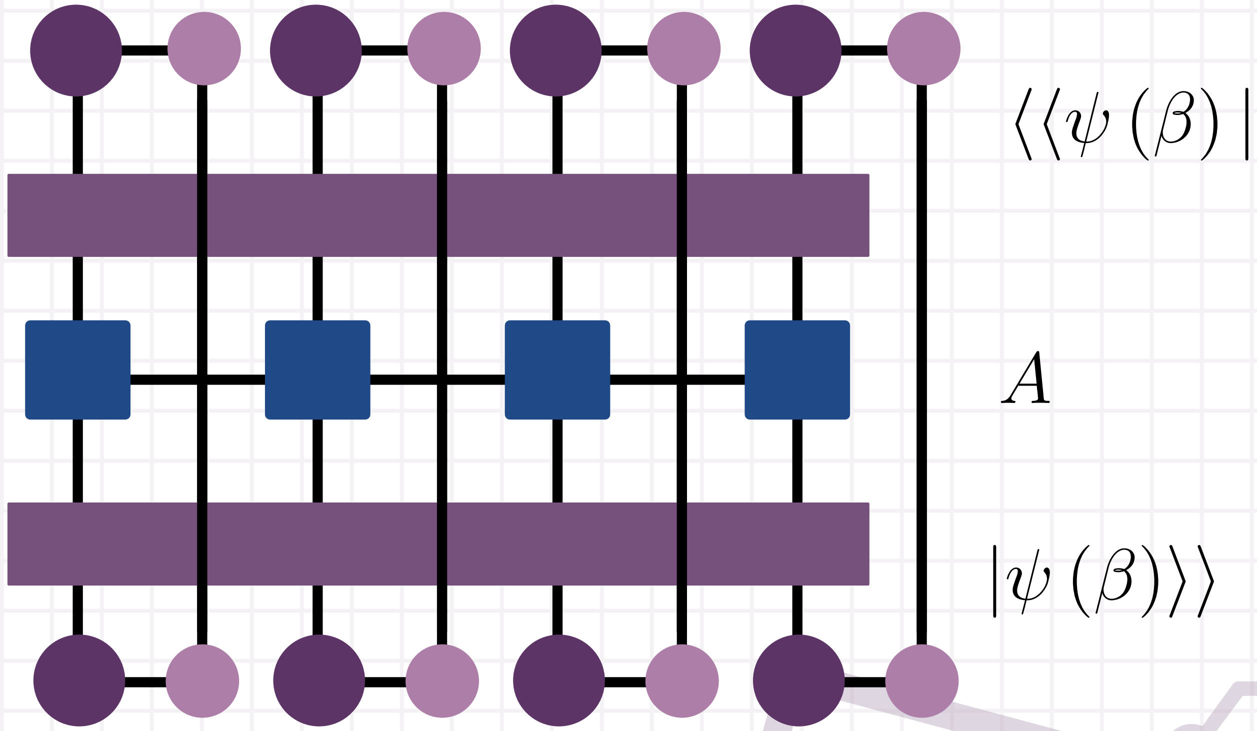
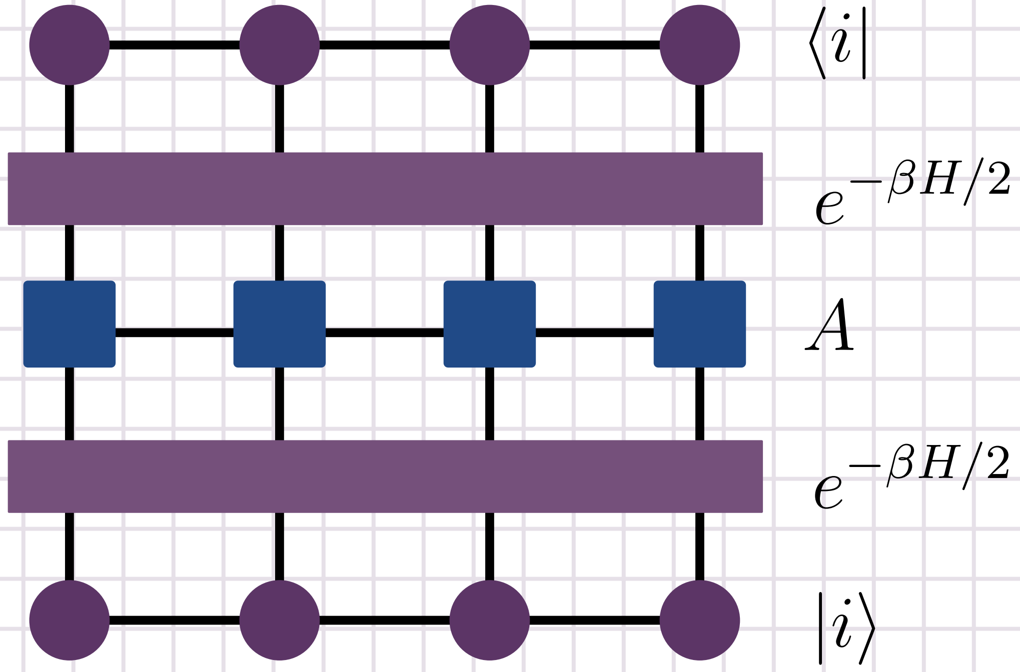


Sampling methods

$$\langle A\rangle_\beta = \frac{1}{Z_\beta}\sum_i \langle i|e^{-\beta H/2} A e^{-\beta H/2}|i\rangle$$

$$\langle A\rangle_\beta = \frac{1}{N_s}\sum_i$$

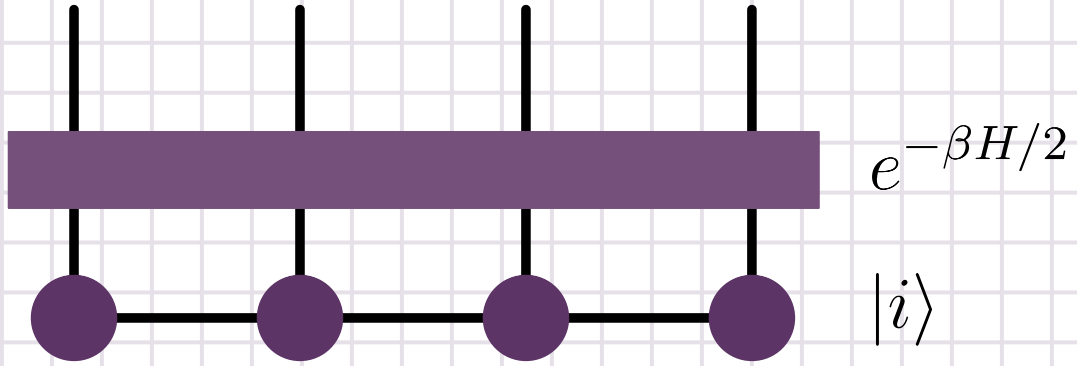


Pure state sampling

$$\langle A\rangle_\beta = \sum_i \frac{P_i(\beta)}{Z_\beta}\langle \psi_i(\beta)|A|\psi_i(\beta)\rangle$$

$$|\psi_i(\beta)\rangle = \frac{1}{P_i(\beta)^{1/2}} e^{-\beta H/2}|i\rangle$$

$|\psi_i(\beta)\rangle$



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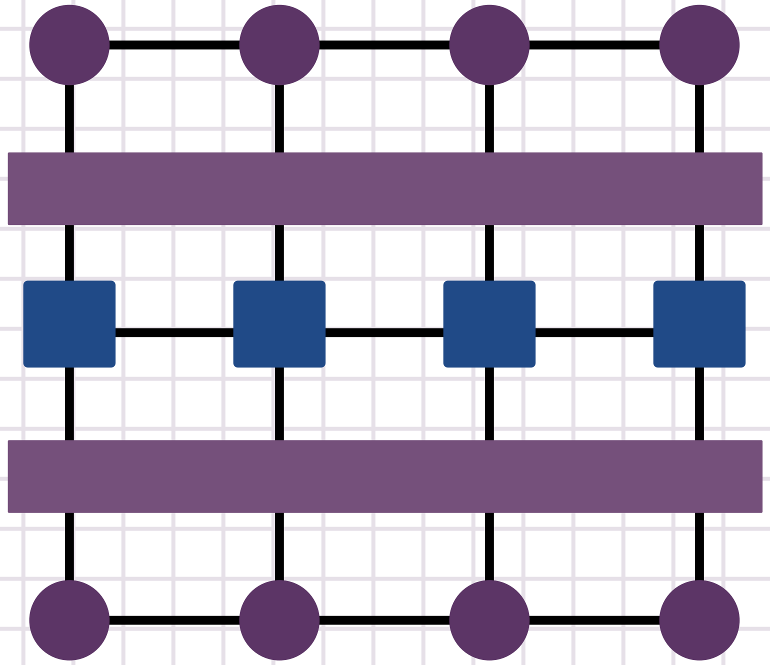

β → 0: $\langle A\rangle_{\beta=0} = \frac{1}{N_s}\sum_i \langle i|A|i\rangle$

β → ∞: $\langle A\rangle_{\beta=\infty} = \frac{1}{N_s}\sum_i \langle GS|A|GS\rangle$

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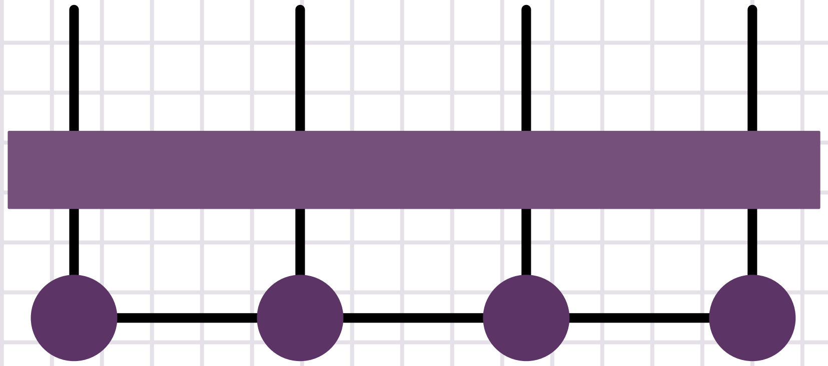
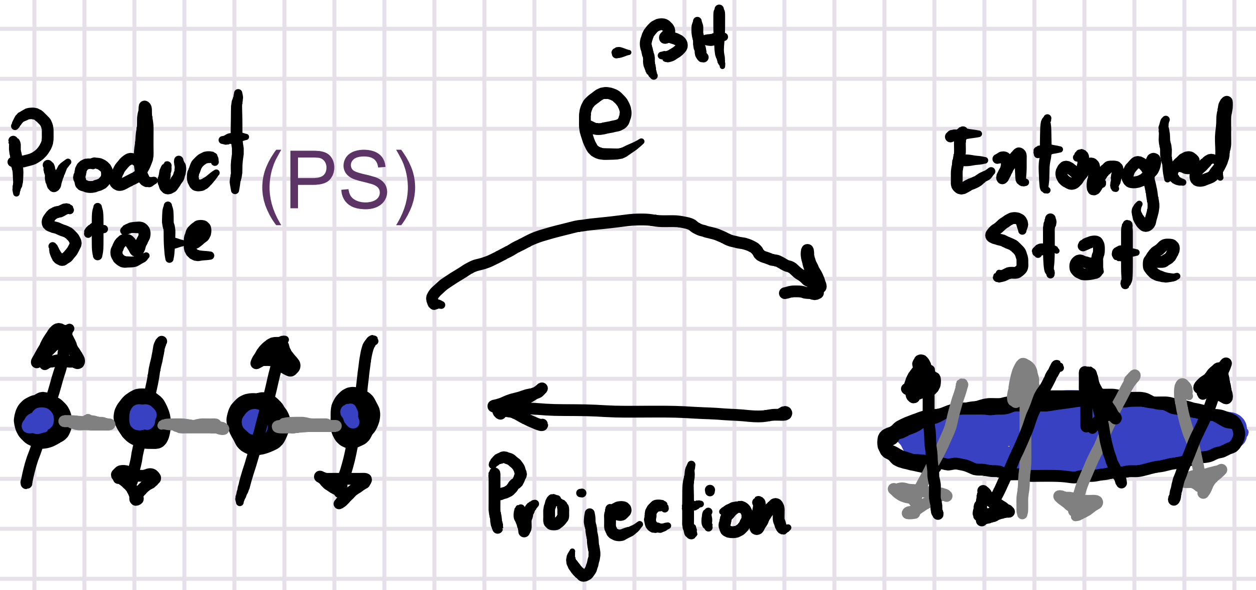


How to sample?

White, PRL **102**, 190601 (2009)
Stoudenmire et al., New J. Phys. **12** 055026 (2010)

METTS, a Markovian random walk

$$\langle A\rangle_\beta = \sum_i \frac{P_i(\beta)}{Z_\beta}\langle\psi_i(\beta)|A|\psi_i(\beta)\rangle \qquad |\psi_i(\beta)\rangle = \frac{1}{P_i(\beta)^{1/2}} e^{-\beta H/2}|i\rangle$$



1) init random PS
2) time evolve until β
3) collapse to PS'(β) go to (2)

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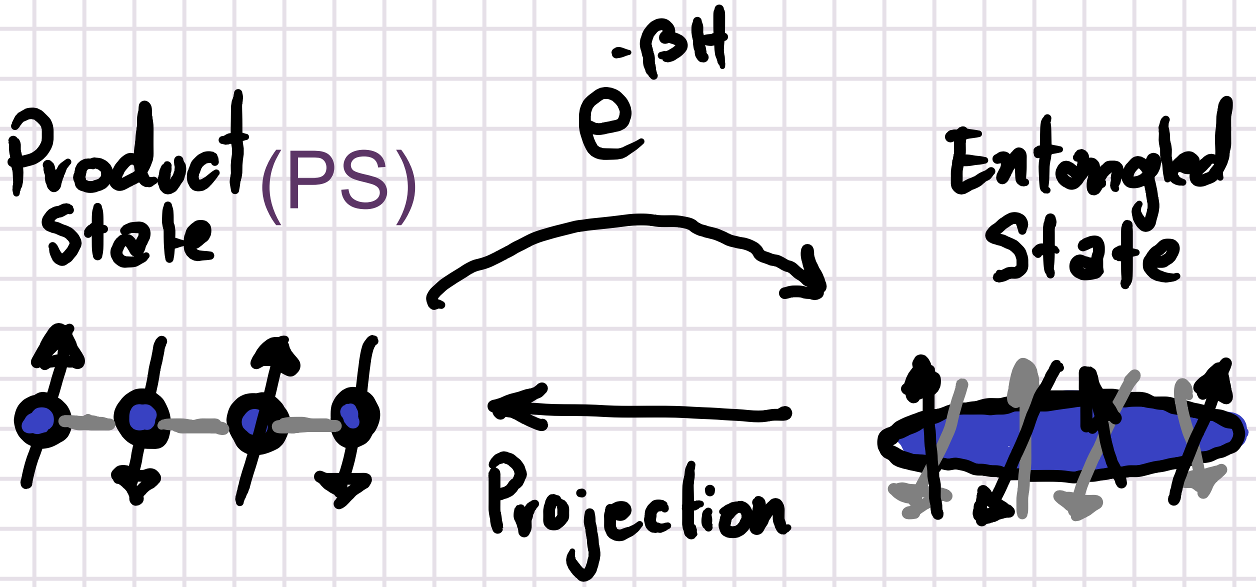

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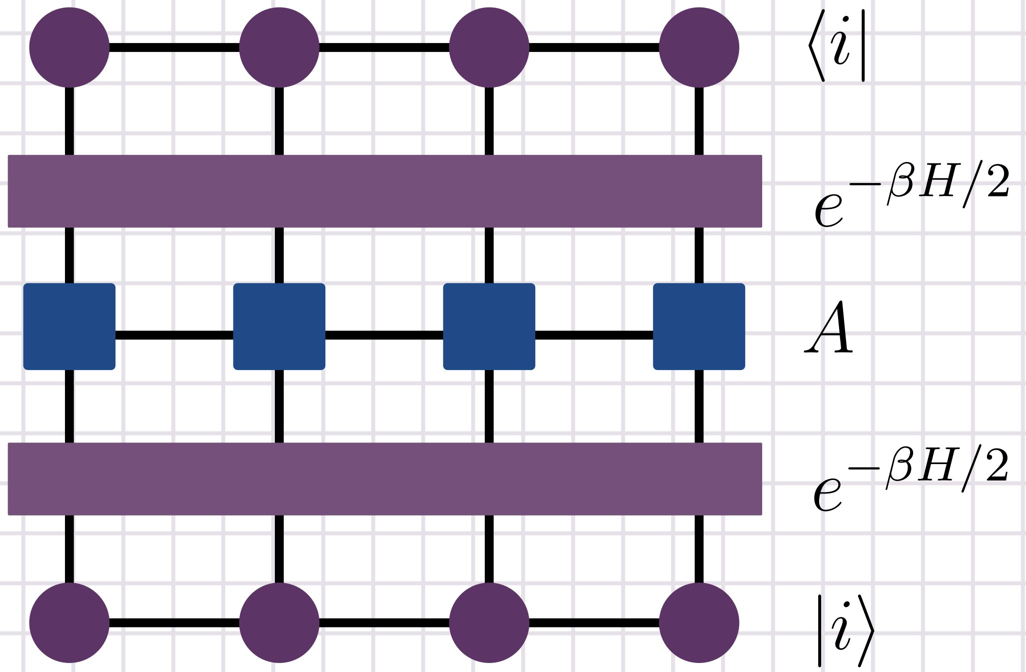
- Ensures the correct sampling distribution
- PS → Minimally entangled states
- Good results at low temperatures and ladders (Wietek et al., PRX 11, 031007 (2021))

J. Gao et al., arXiv:2312.04420

stoMPS is not a Markov chain

$$\langle A \rangle_\beta = \frac{1}{N_s} \sum_i \langle \psi_i(\beta) | A | \psi_i(\beta) \rangle$$

$$\langle A \rangle_\beta = \frac{1}{N_s} \sum_i$$



Sampling an MPS with bond dim D

Product state (D=1)

- $|s_i\rangle = |\uparrow\rangle$ or $|\downarrow\rangle$ (Z_2)
- $|s_i\rangle = \cos\theta\,|\uparrow\rangle + \sin\theta\,|\downarrow\rangle$

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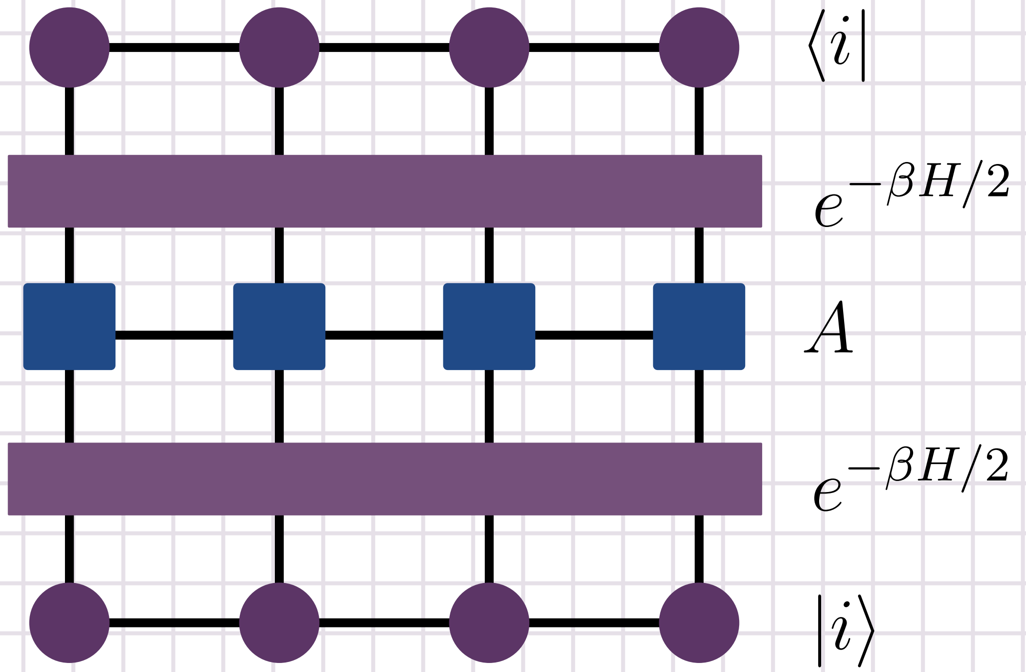

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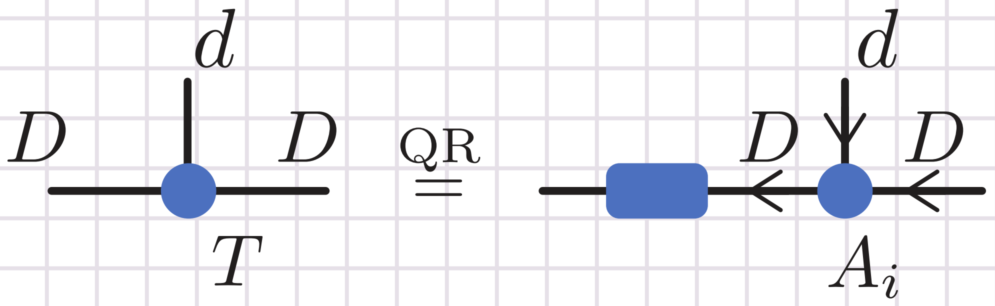
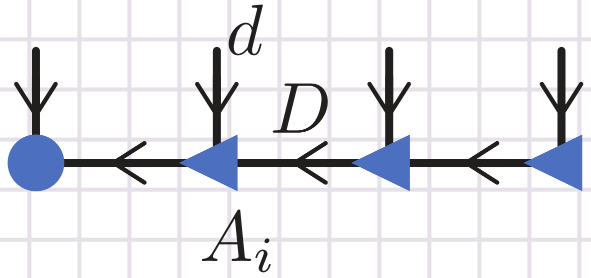
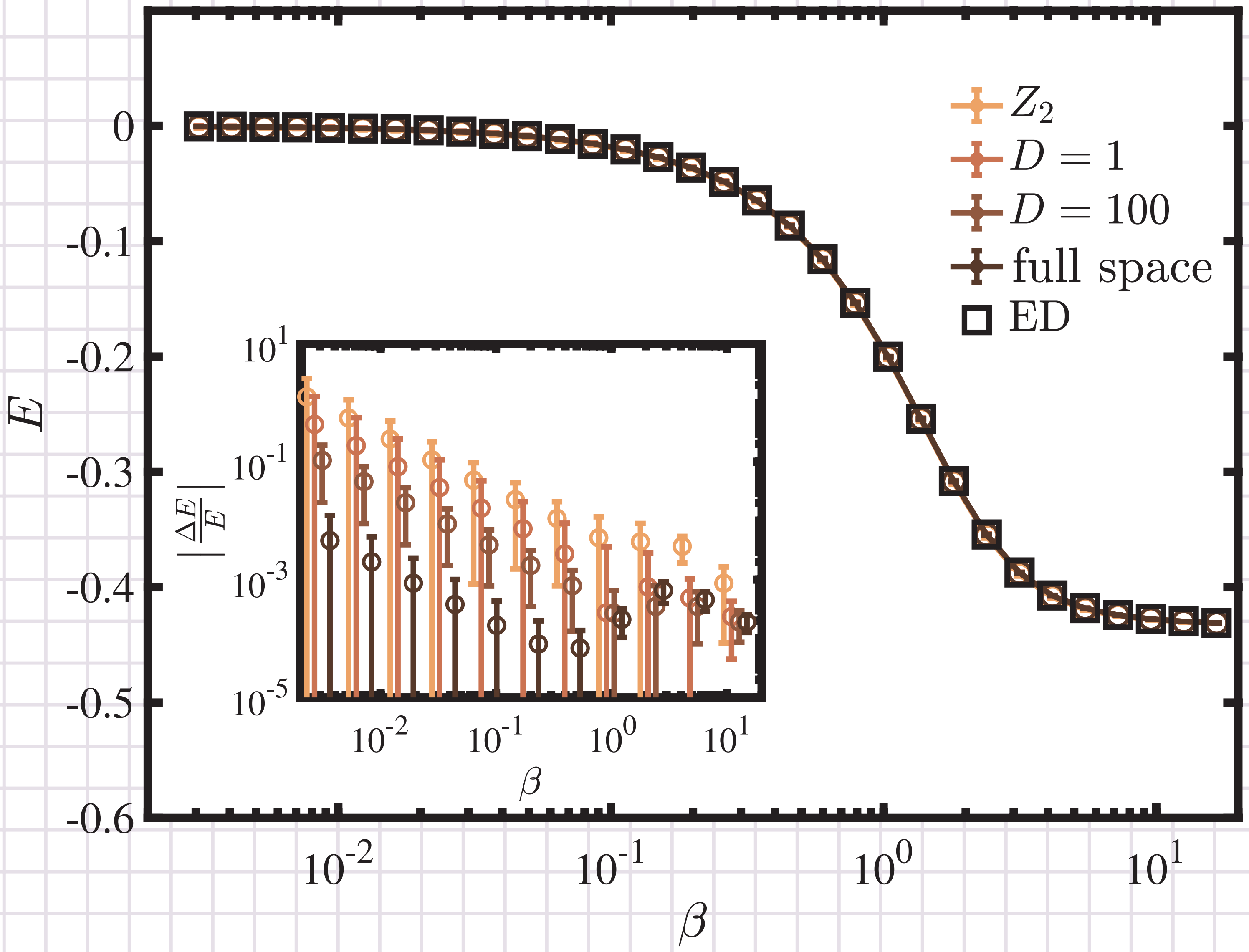
MPS (D>1)

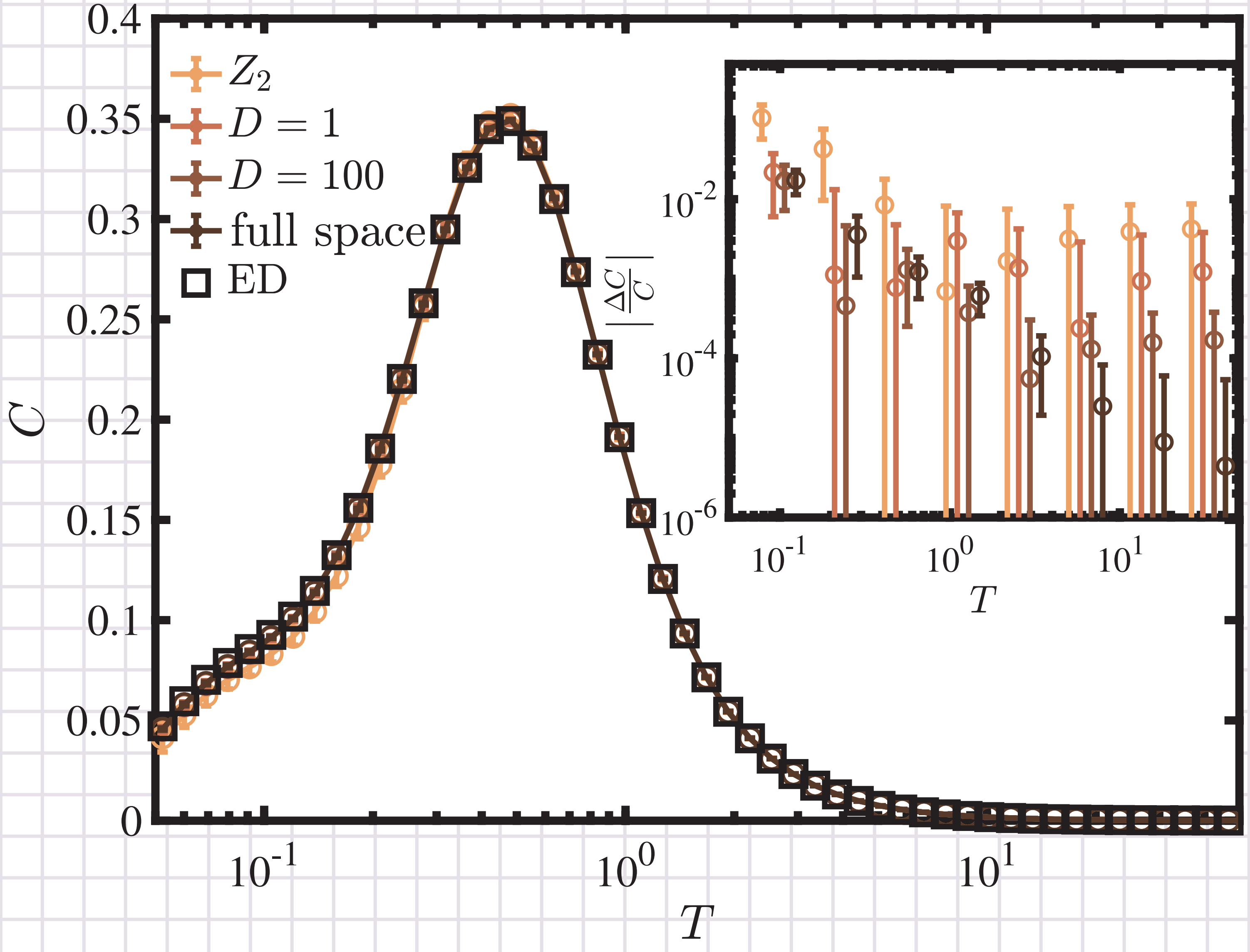


$$T^m_{\alpha,\beta} \sim \mathcal{N}(0,1)$$



stoMPS coincides with ED





J. Gao et al., arXiv:2312.04420

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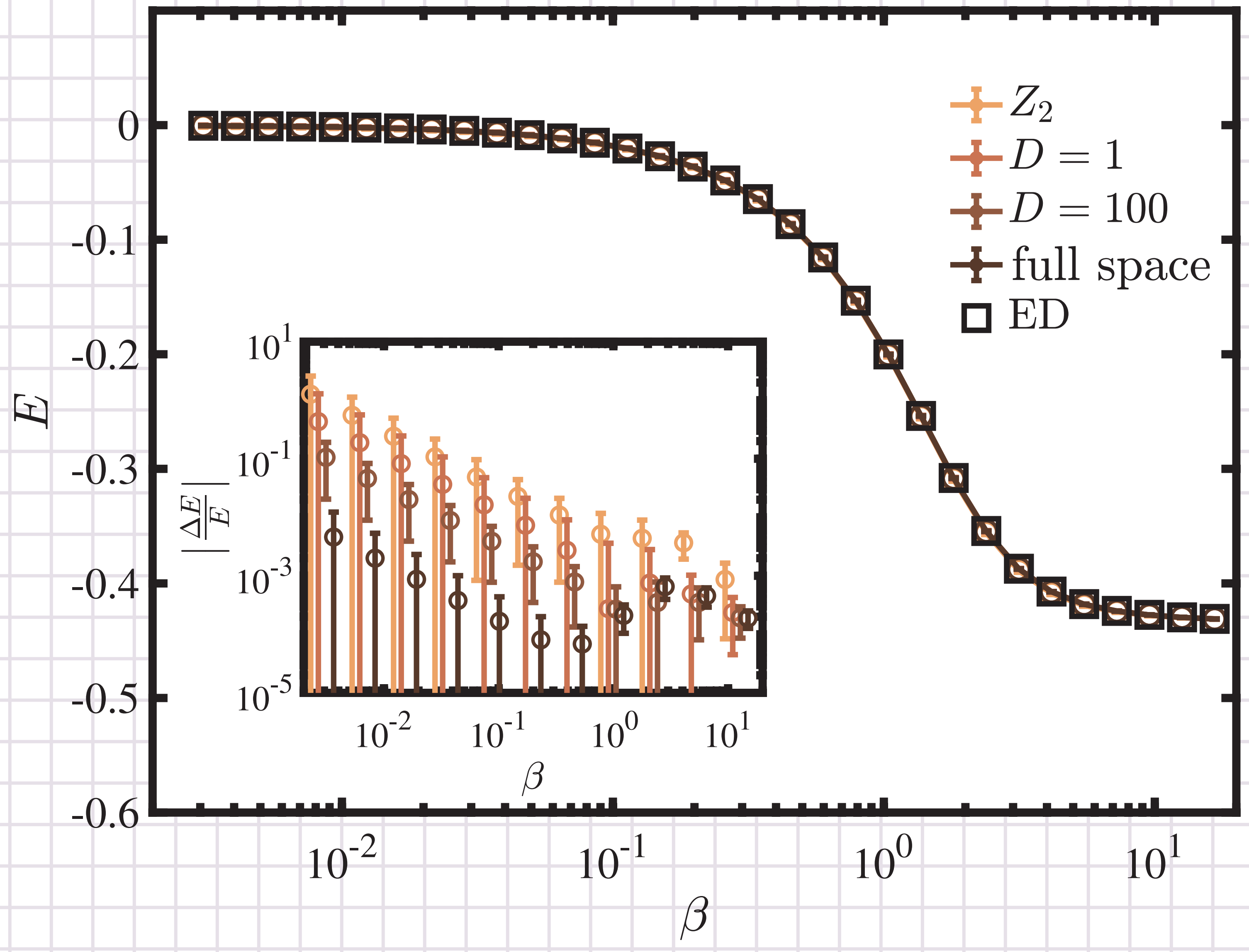
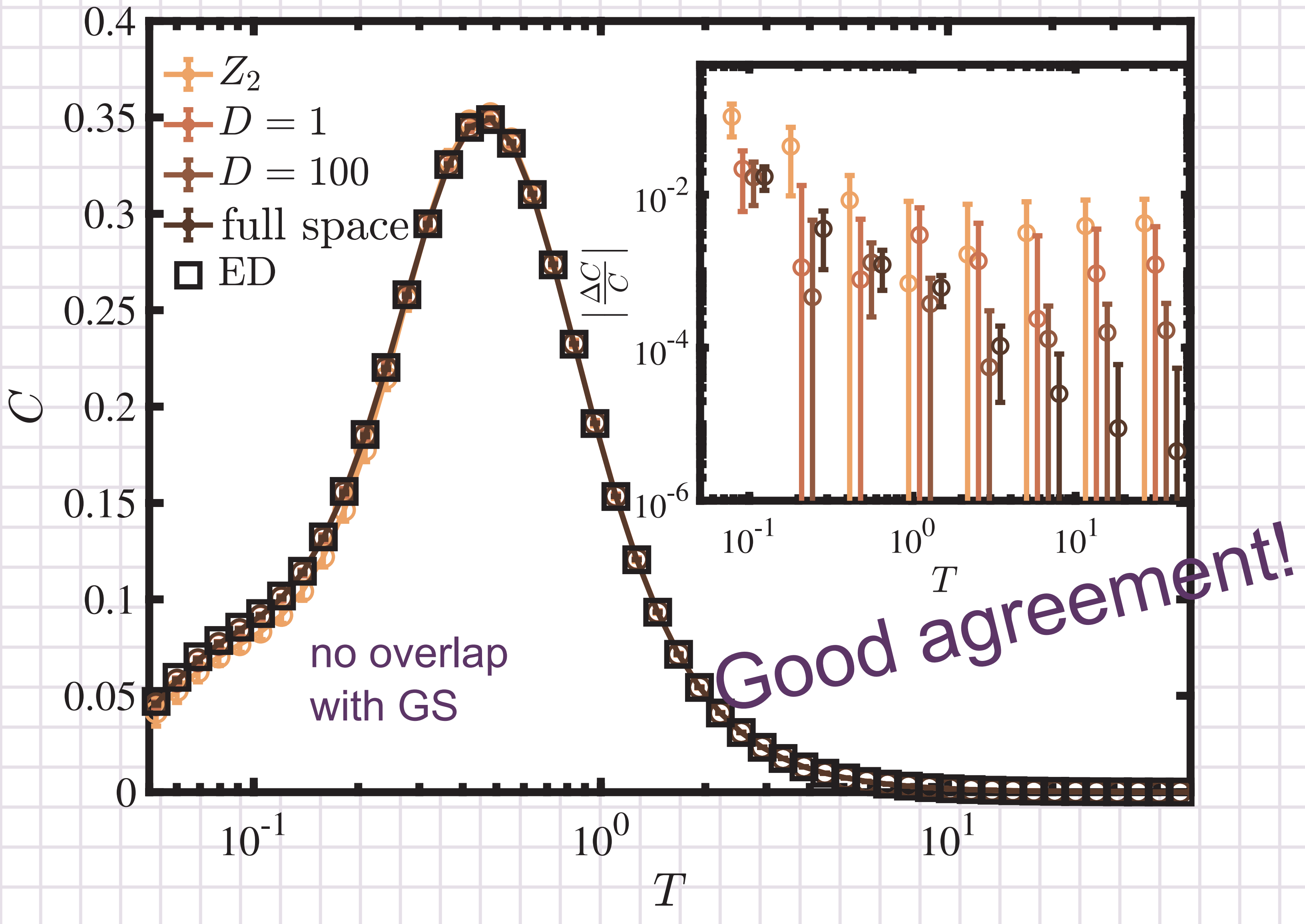
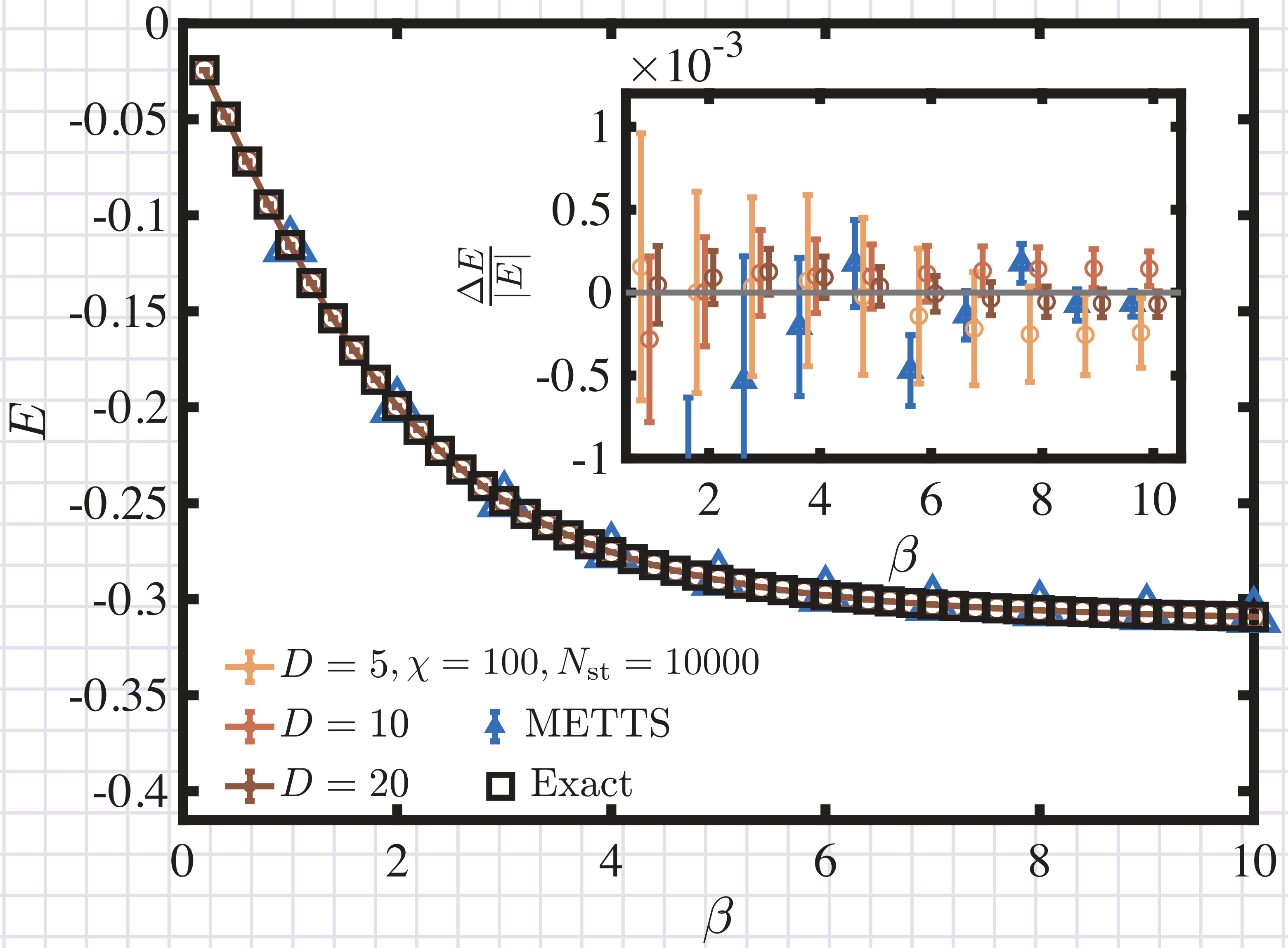
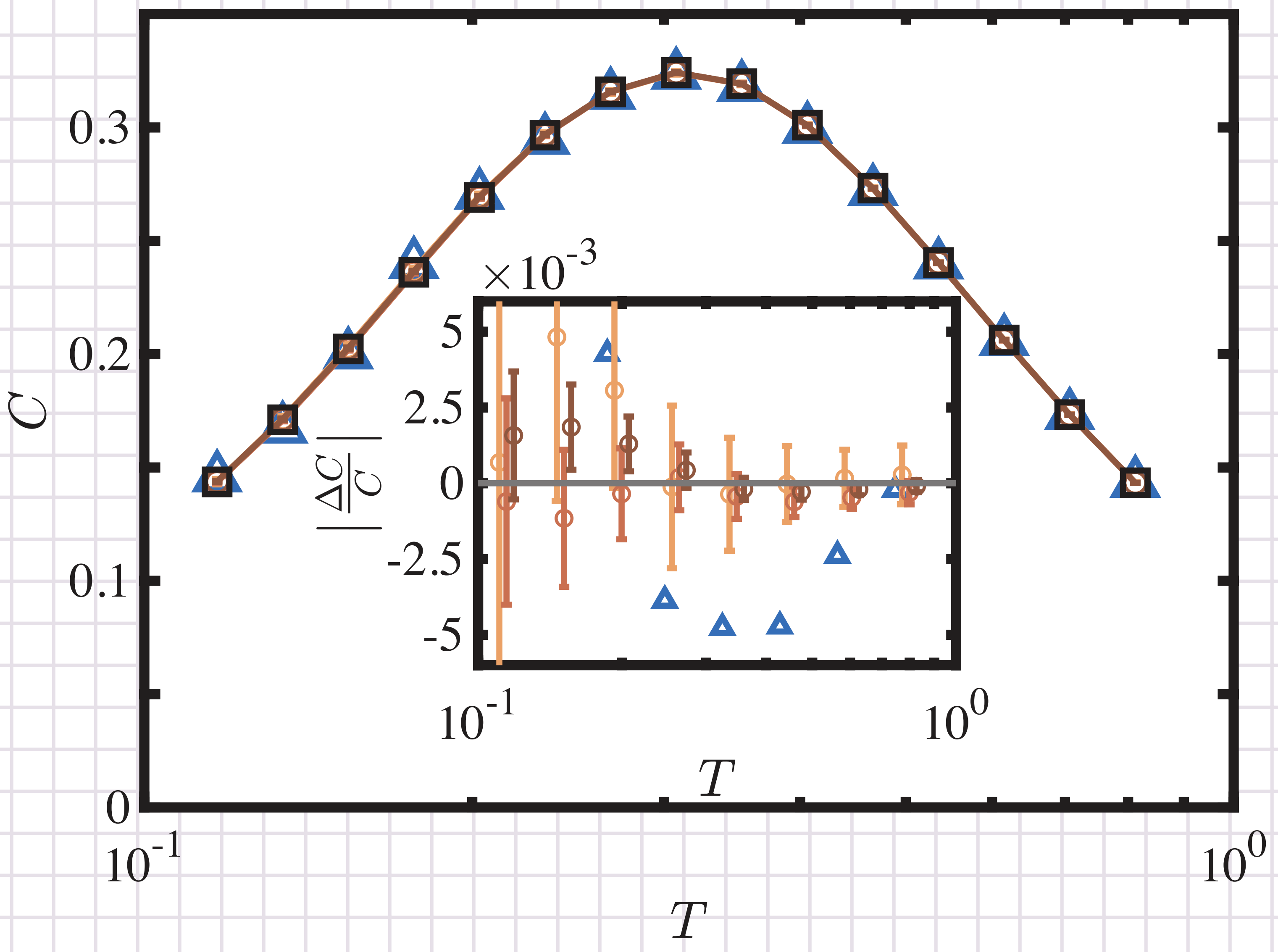




J. Gao et al., arXiv:2312.04420

stoMPS outperforms METTS





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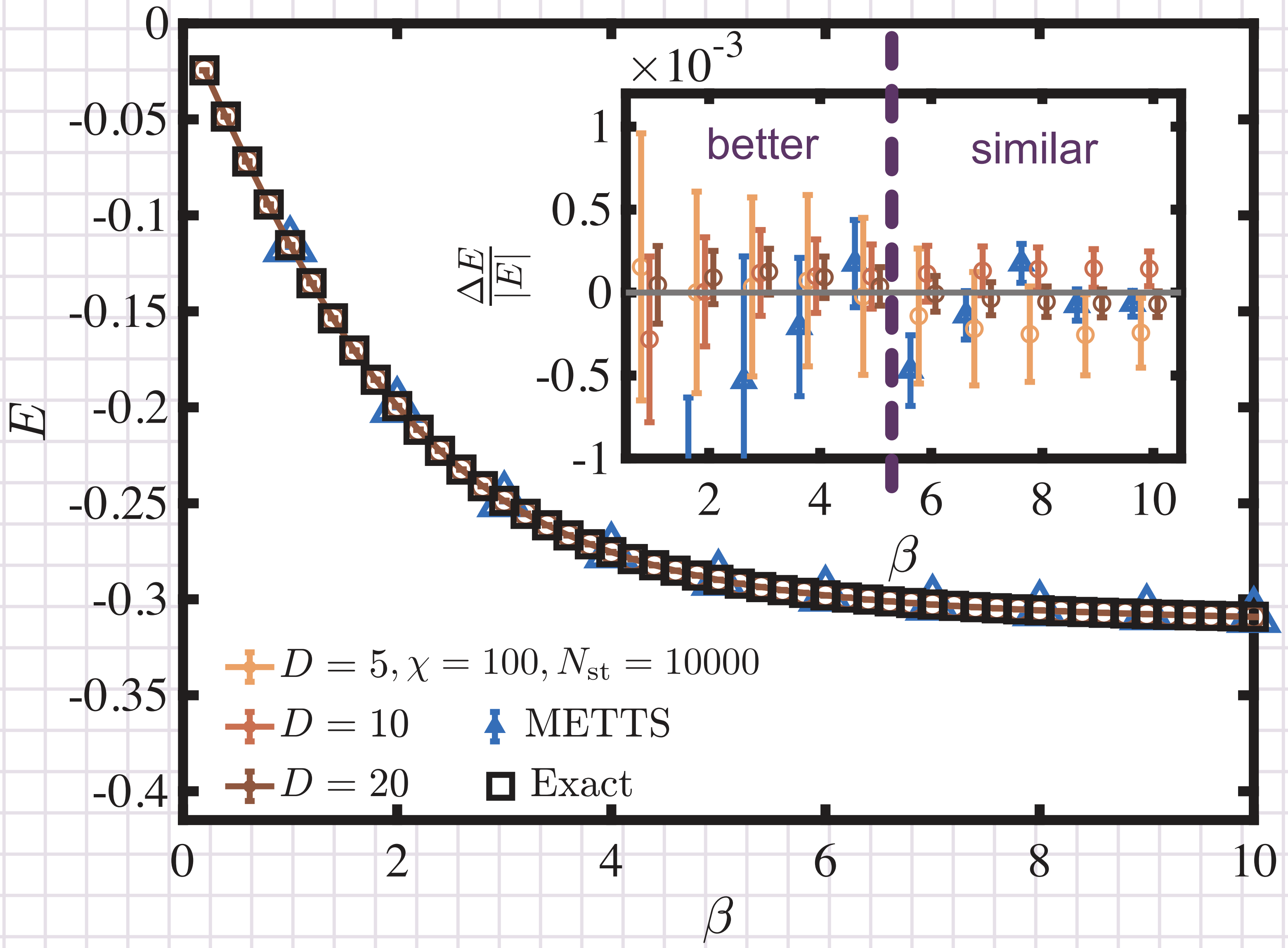

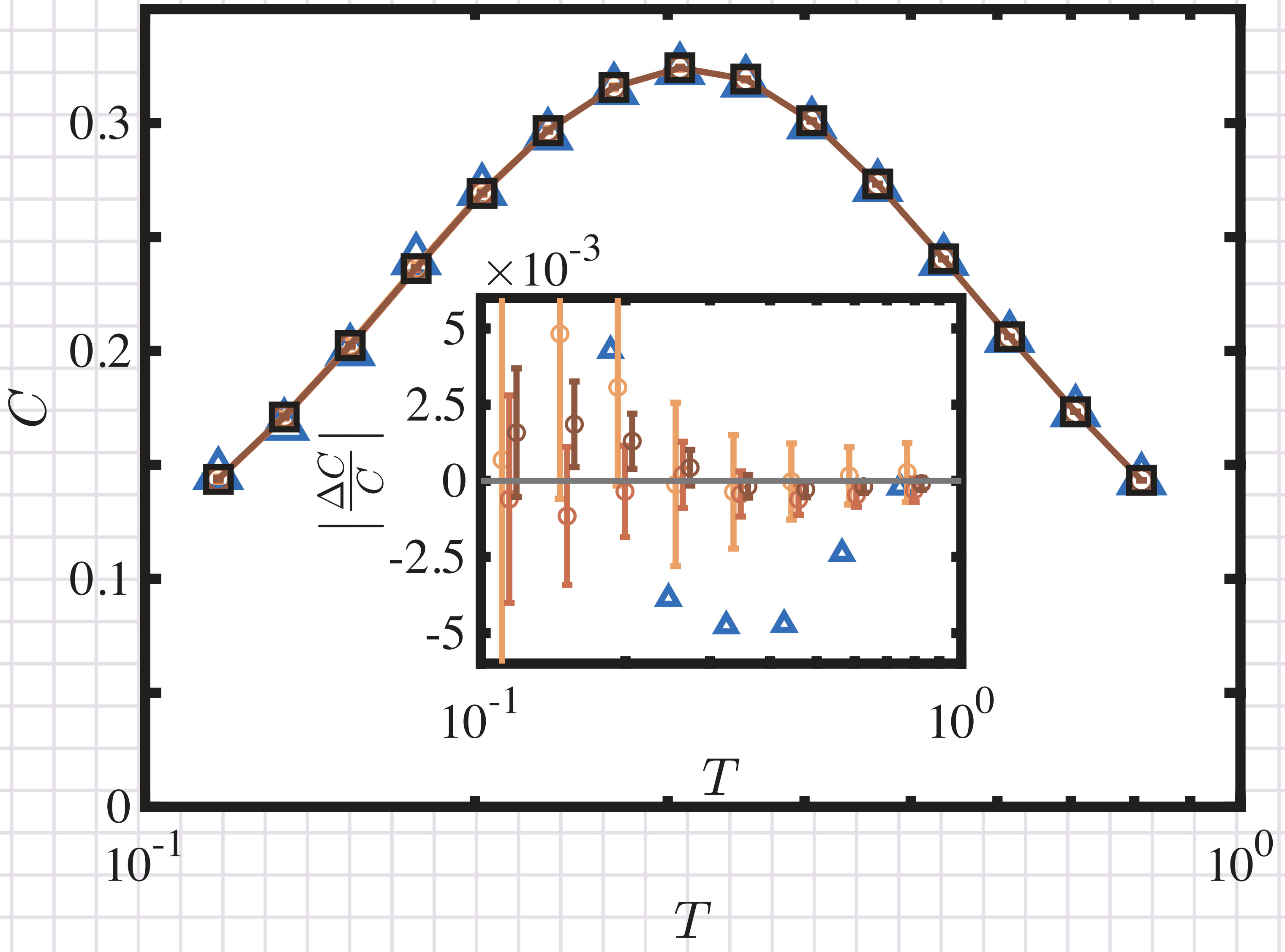

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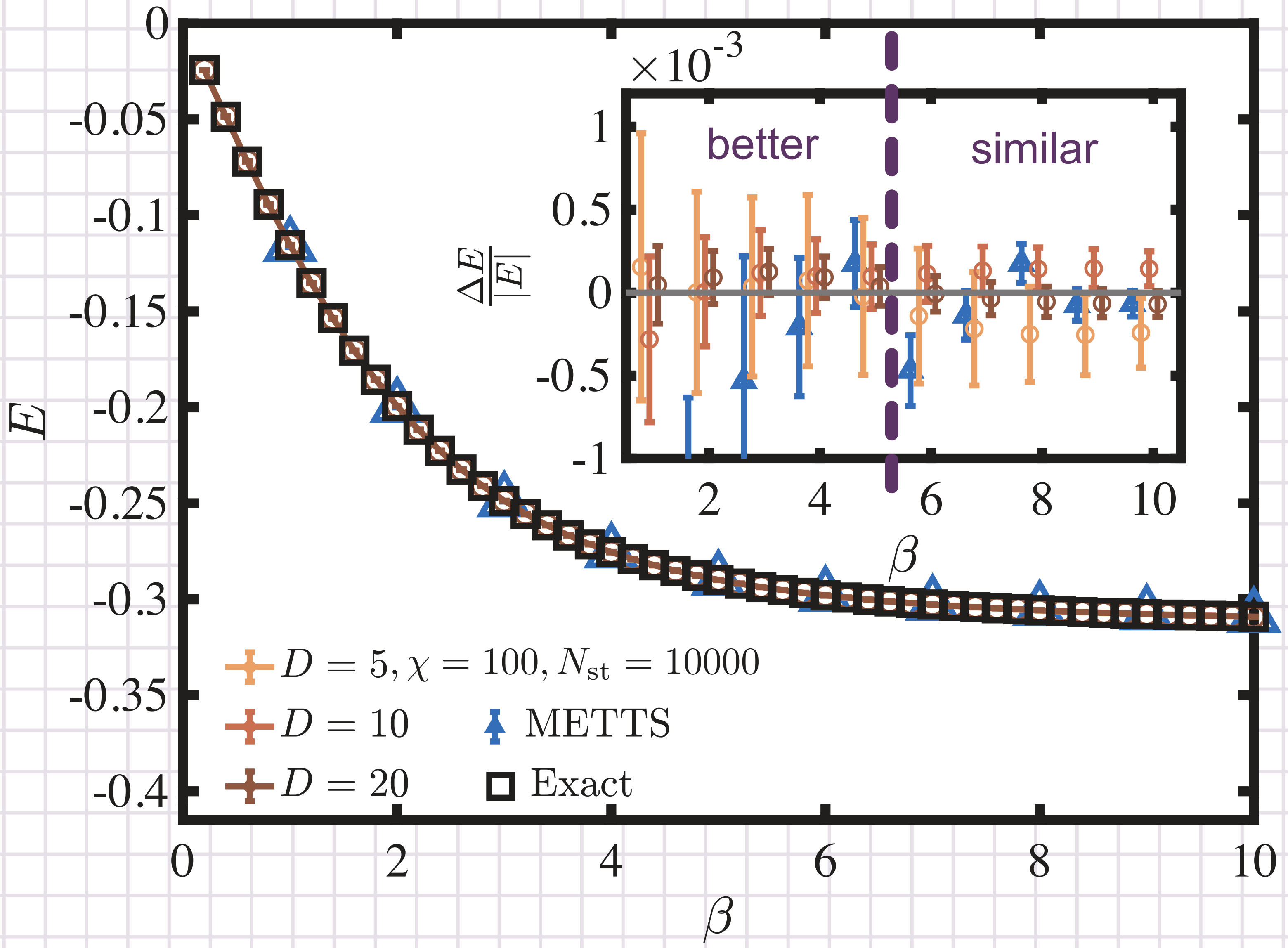
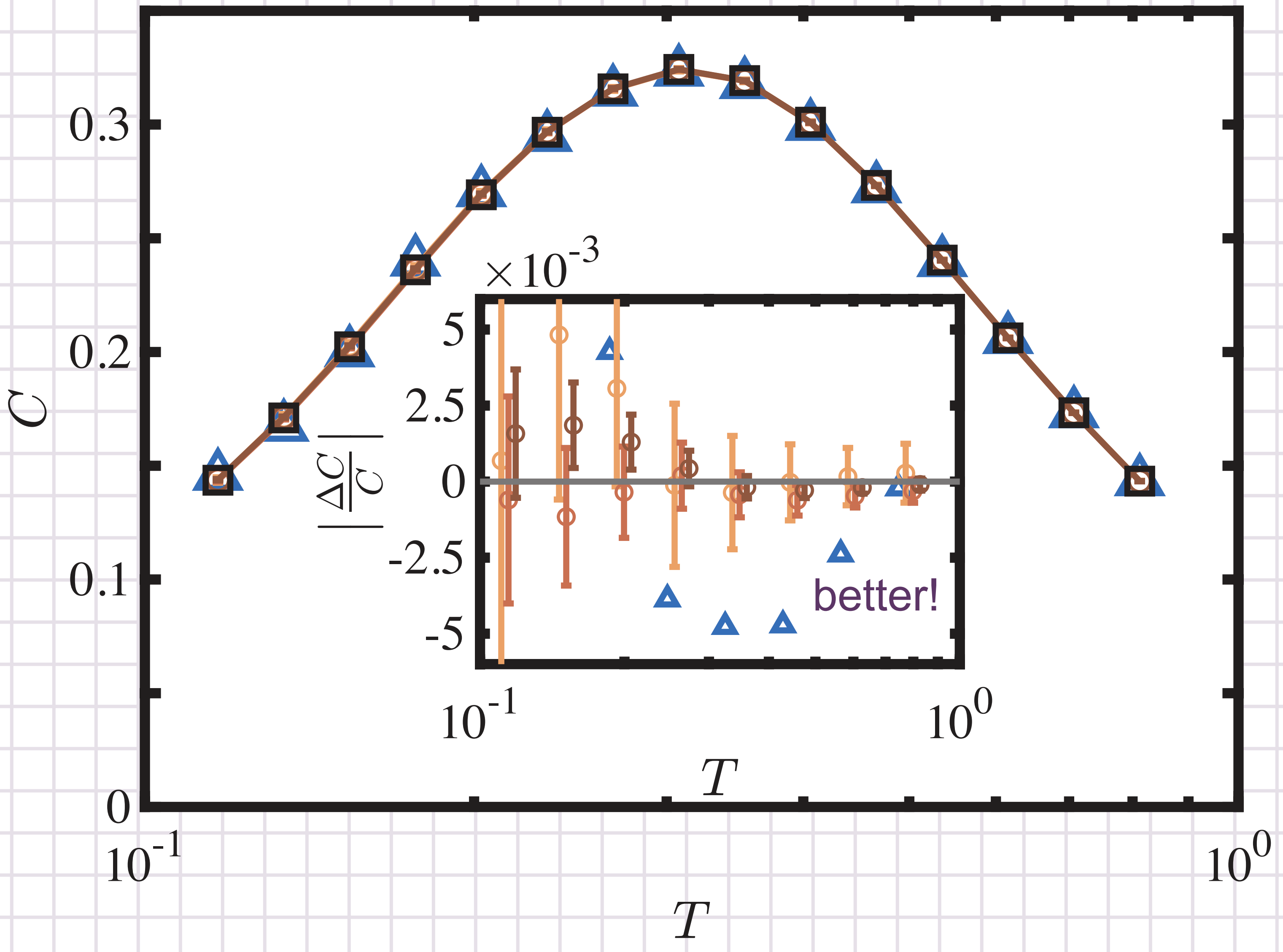
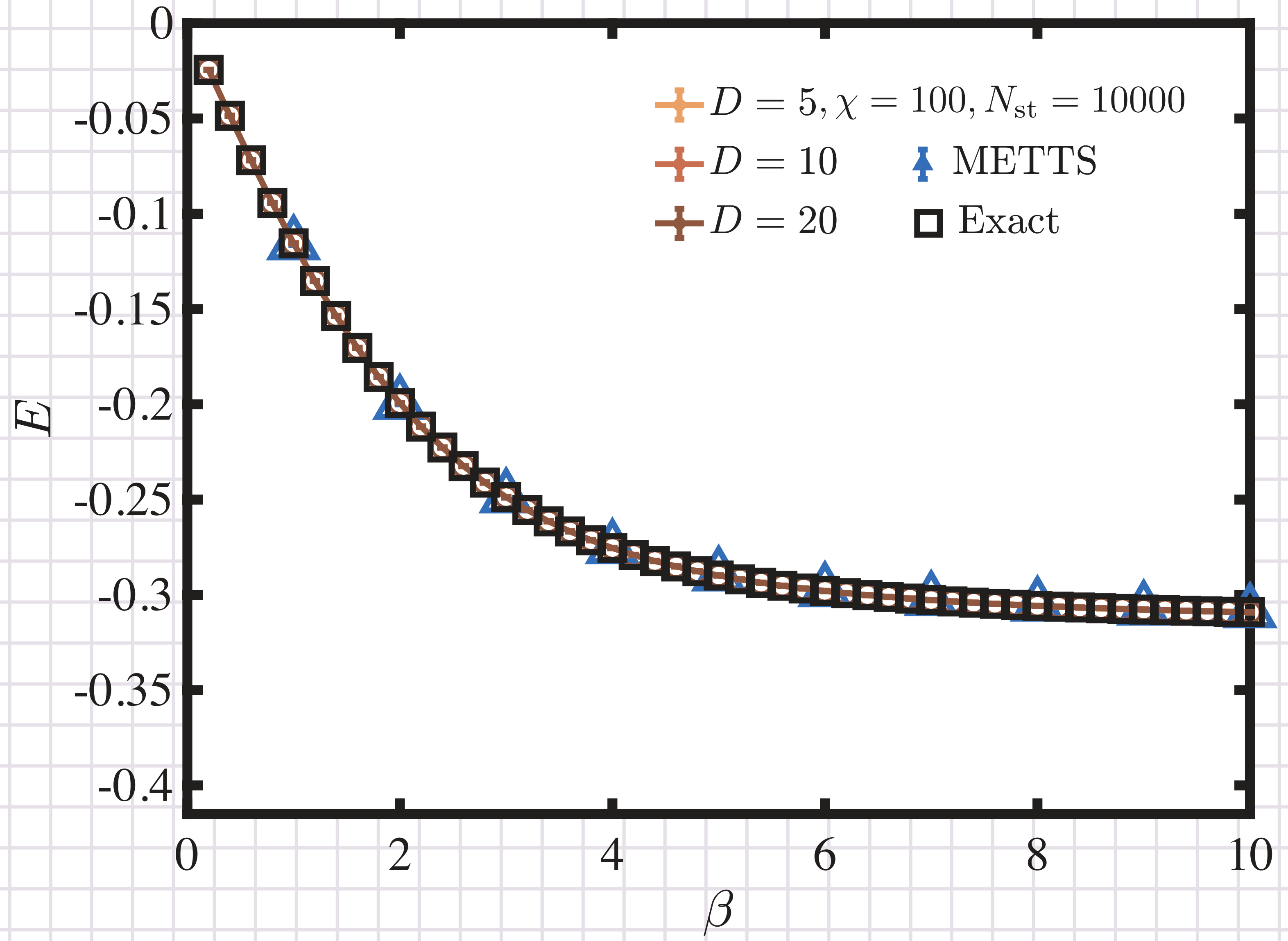
J. Gao et al., arXiv:2312.04420





J. Gao et al., arXiv:2312.04420

stoMPS takes independent trajectories



stoMPS

- One run for all βs!

METTS

- One run for each β!

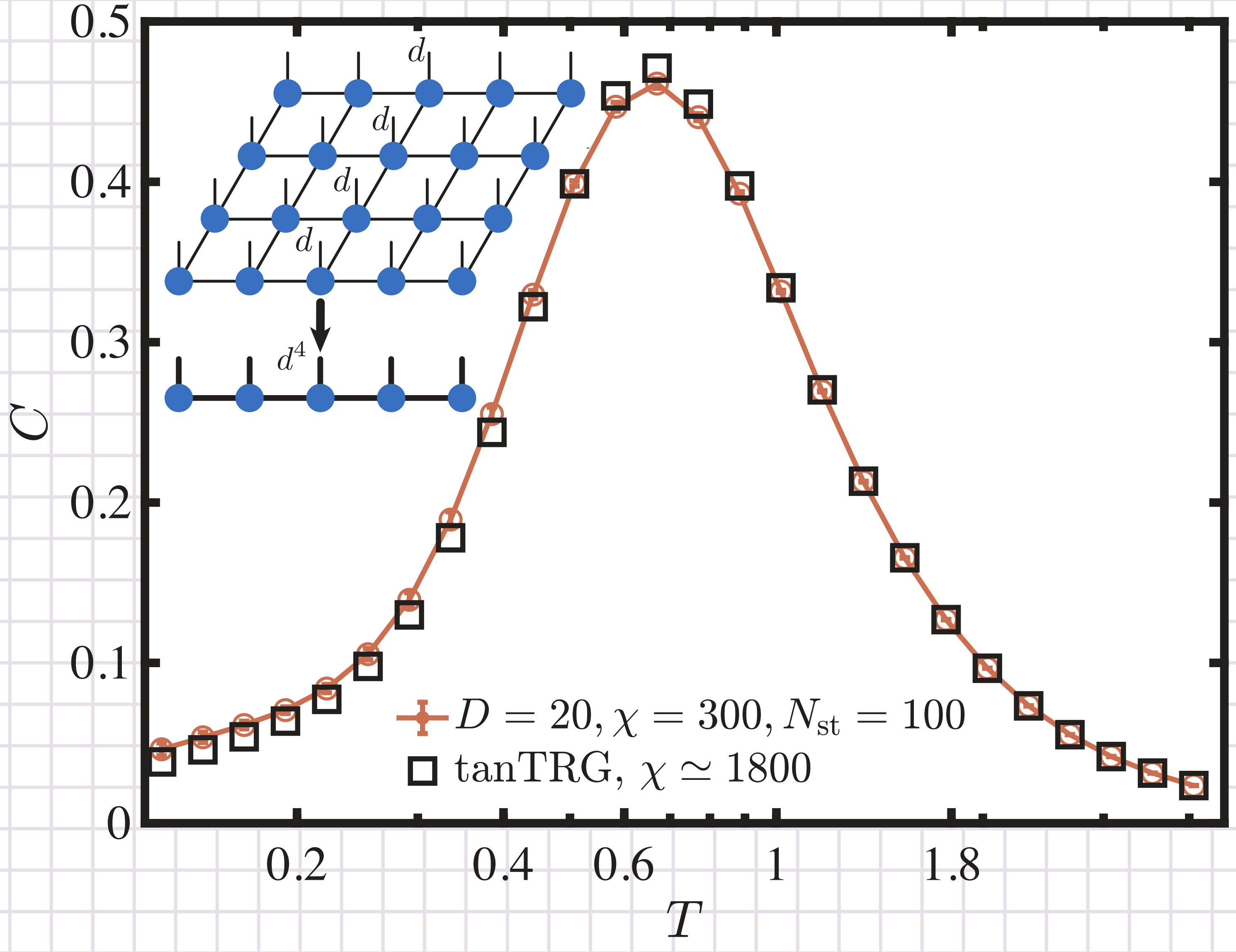
2) time evolve until β

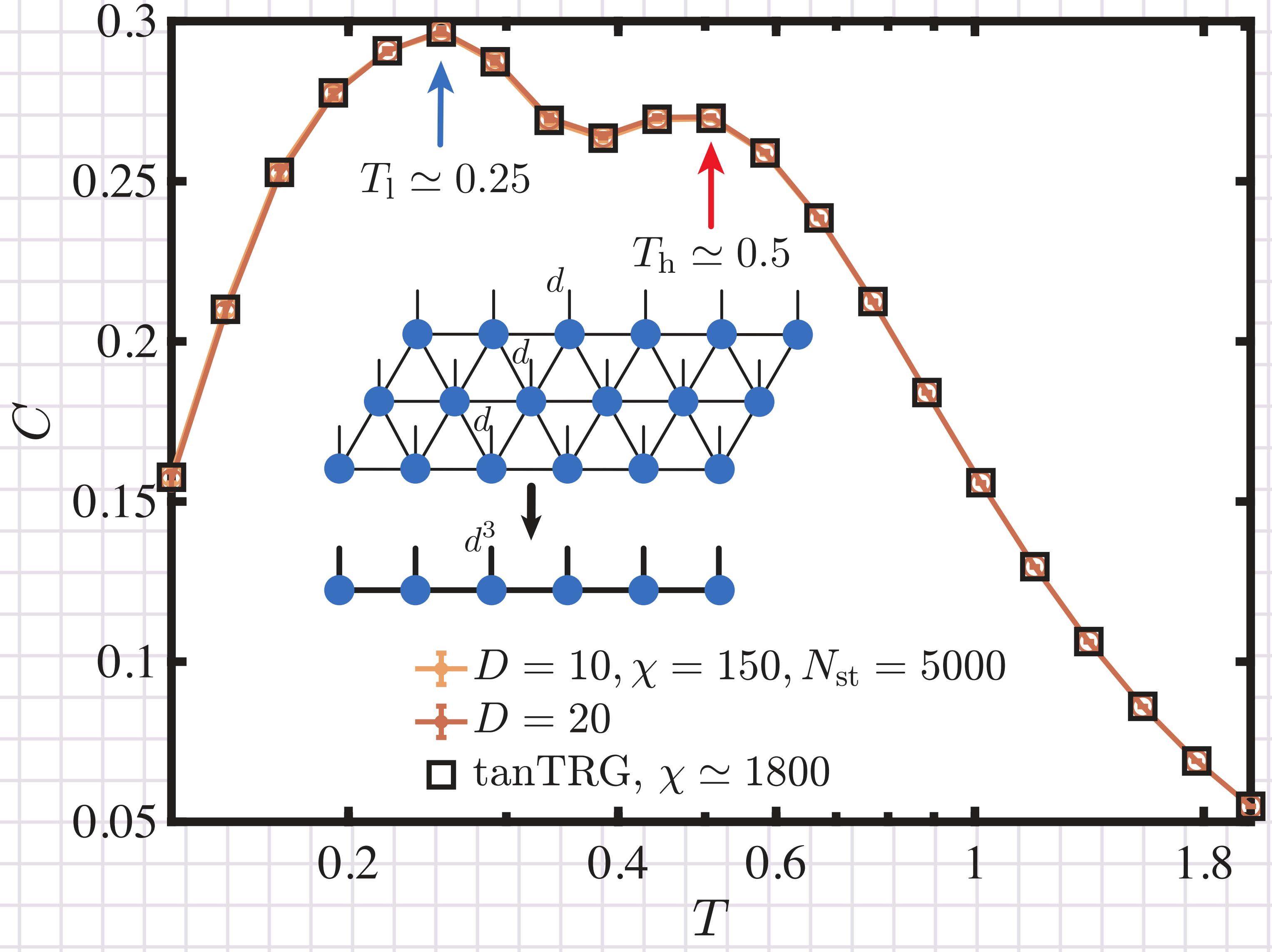
3) collapse to PS'(β) go to (2)

Example:
large-β ferromagnetic case → sample around ferro
No information about small β!
Cannot reuse small β data, one calculation per β!

J. Gao et al., arXiv:2312.04420

stoMPS works for ladders





Conclusions

Interesting new sampling method

Comparable with METTS

- Better in some situations?

Independent trajectories

- Good for thermodynamic integration

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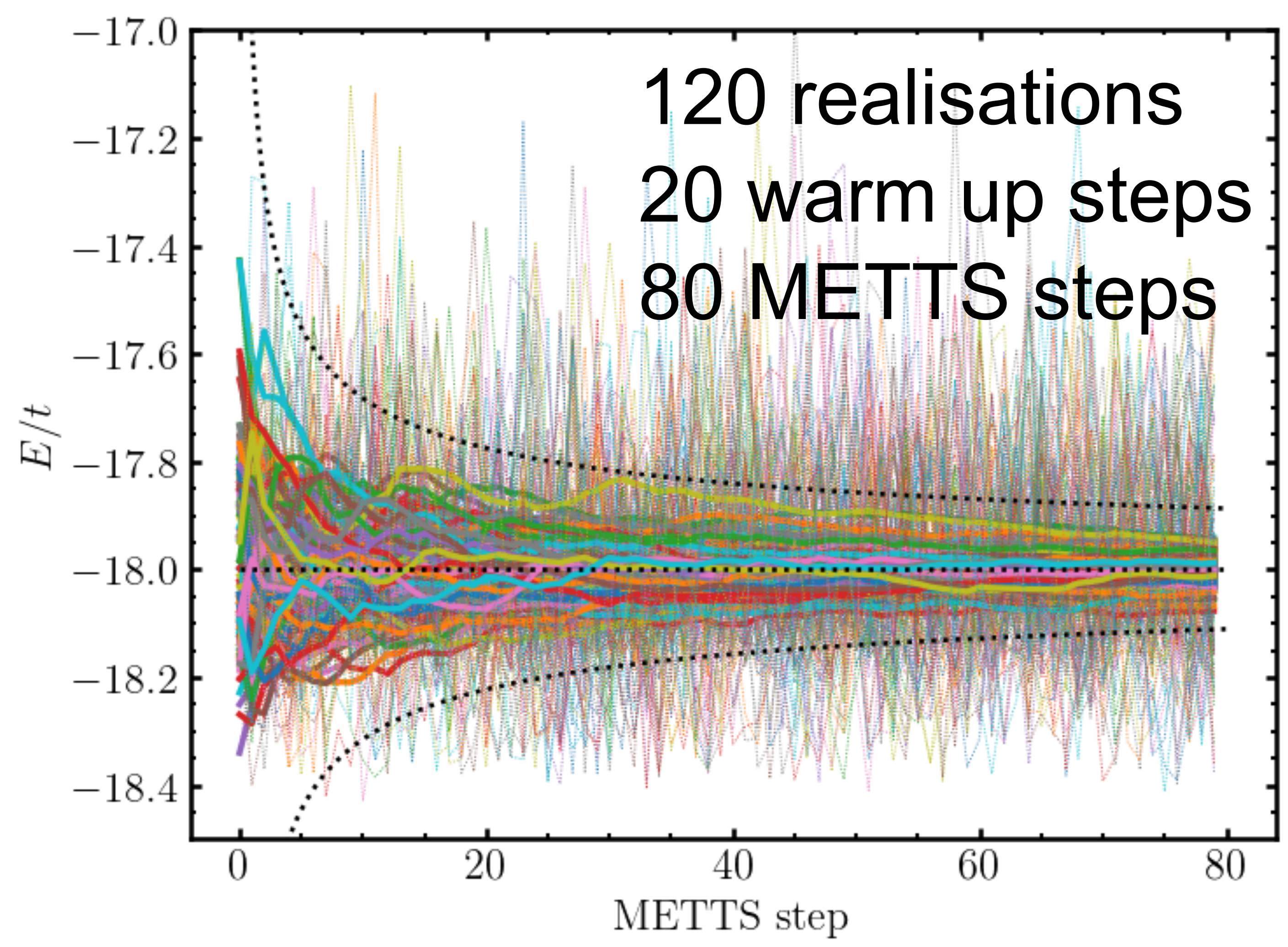
Performance?

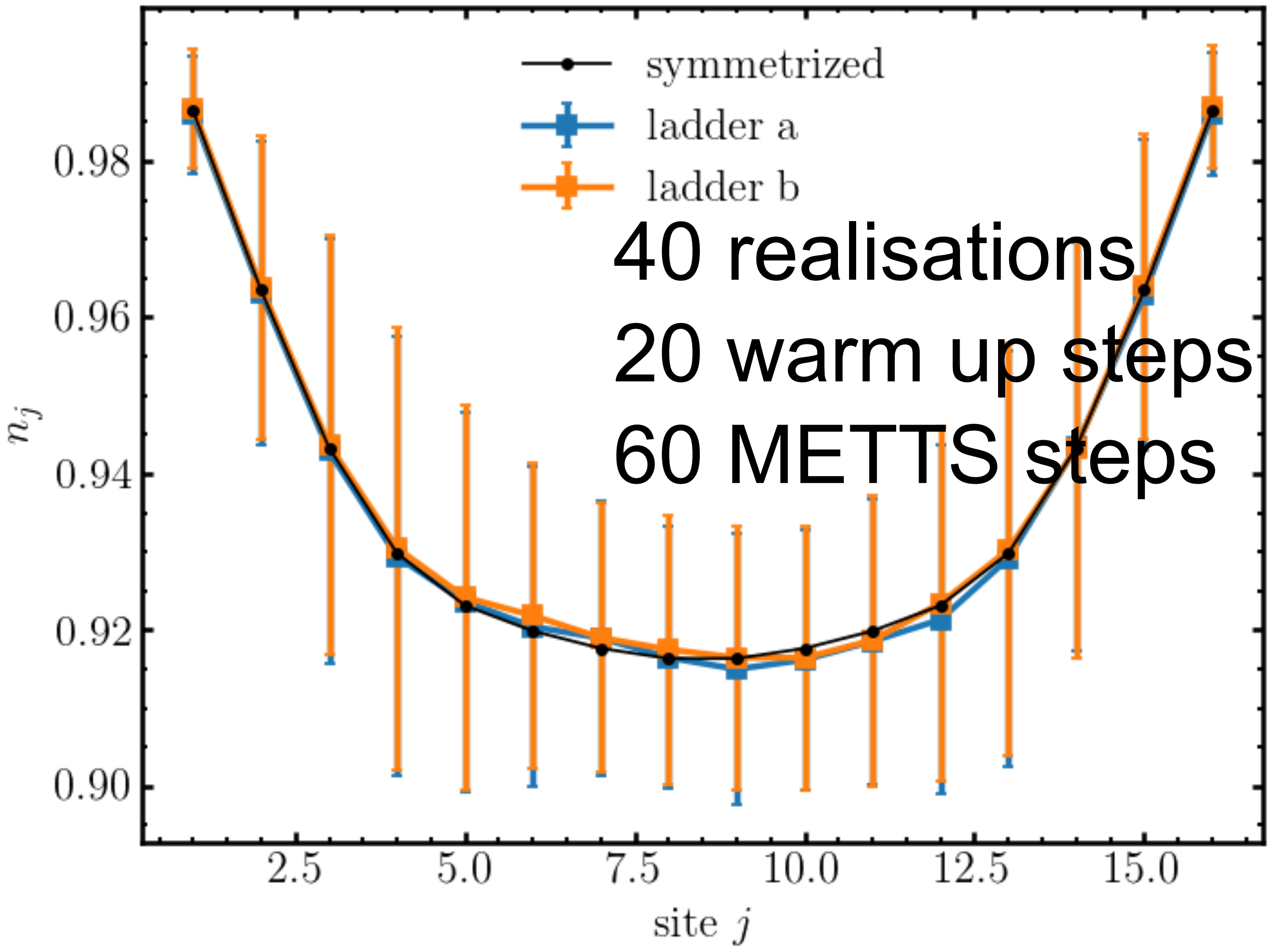
- 5 times faster?

Improvements

EXTRA: METTS observables



L=16
U=8t
ty=1.2t
n=0.9375
$k_B T$=0.13t



L=16
U=8t
ty=1.4t
n=0.94
$k_B T$=0.08t