LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

ARNOLD SOMMERFELD CENTER FOR THEORETICAL PHYSICS

CeNS Center for NanoScience | LMU

# Energy scales and exponential speed up in thermal tensor network simulations

arXiv:1801.00142 [cond-mat.str-el]

Andreas Weichselbaum

Brookhaven National Lab, Upton, New York
Ludwig Maximilians University, Munich

Collaboration Bin-Bin Chen, Lei Chen, Ziyu Chen, Wei Li (Beihang University, Beijing)

Supported by DFG (TR12, WE4819/1-1, WE4819/2-1 Heisenberg, WE4819/3-1)
Cluster of Excellence NanoSystems Initiative, Munich (NIM)

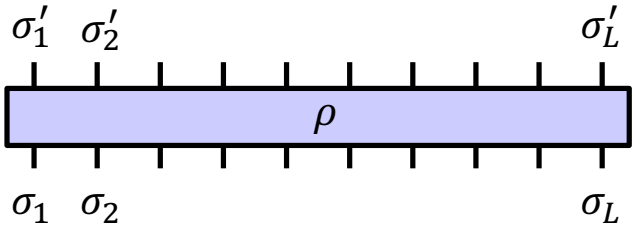
# Outline

- Representation of thermal states
- Recent insights into entanglement scaling in thermal states (1D)
- Exponential energy scales
  - benefits of logarithmic $\beta$ grid
  - compare to coarse graining renormalization group approaches
- Results
  - benchmark: performance (numerical cost and accuracy)
  - 1D Heisenberg chain
    - entanglement scaling at large and small $\beta$
    - specific heat and scaling exponents
    - entanglement flow diagram vs. energy scales
  - 2D square Heisenberg model: specific heat and entanglement
- Summary & outlook

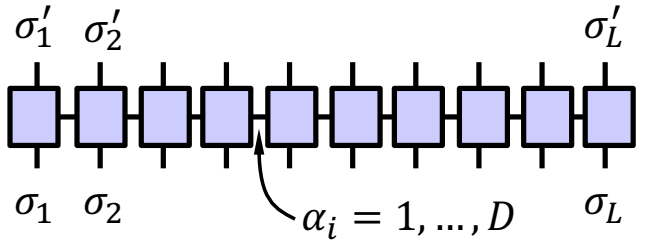
# Representation of thermal density matrix

$$\hat{\rho}(\beta) \equiv e^{-\beta \hat{H}} = \sum_s e^{-\beta E_s} |s\rangle\langle s| = \sum_s \rho_{(\sigma_1 \sigma_2 \ldots \sigma_L),\,(\sigma_1' \sigma_2' \ldots \sigma_L')} |\sigma_1 \sigma_2 \ldots \sigma_L\rangle\langle \sigma_1' \sigma_2' \ldots \sigma_L'| \qquad (\sigma_i = 1, \ldots, d)$$

$\equiv$

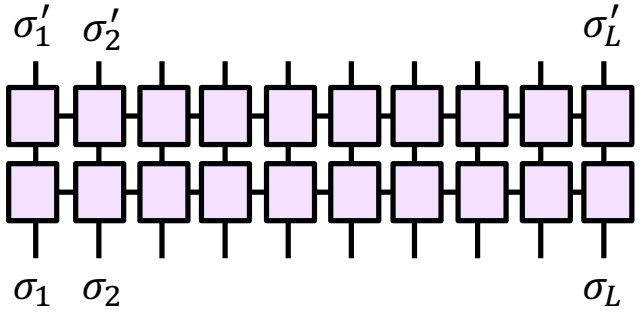



$\equiv$




matrix product operator (MPO)

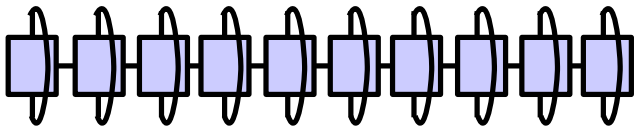
$$\hat{\rho}(\beta) = \left[e^{-\frac{\beta}{2}\hat{H}}\right]^2 = \rho\left(\frac{\beta}{2}\right) * \rho\left(\frac{\beta}{2}\right) =$$



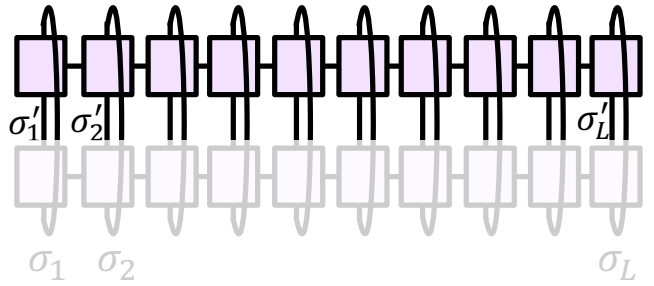

$\equiv \hat{\Psi}^\dagger \hat{\Psi}$

always positive

$$Z = \mathrm{tr}[\hat{\rho}(\beta)] =$$



$=$




$\equiv \langle\Psi|\Psi\rangle$

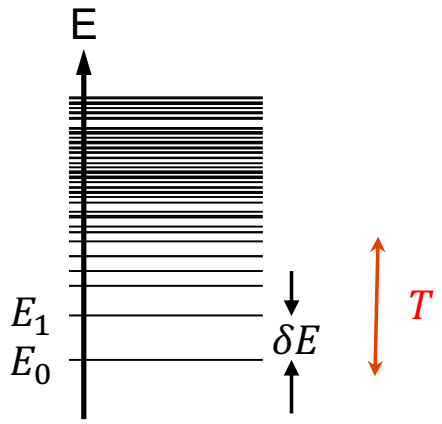
purification

$$\langle \hat{A} \rangle \equiv \frac{1}{Z}\mathrm{tr}\left[\hat{\rho}\hat{A}\right] \equiv \frac{1}{Z}\mathrm{tr}\left[\hat{\Psi}\hat{A}\hat{\Psi}^\dagger\right] \equiv \frac{1}{Z}\langle\Psi|\hat{A}|\Psi\rangle$$

Verstraete (2004)
Schollwoeck (review DMRG; 2010)
Thermofield approach (de Vega, Banuls; 2015)

# Entanglement scaling in thermal states in 1D

- Many-body finite size spectrum (critical systems, or $\delta E \gg$ gap $\Delta$)



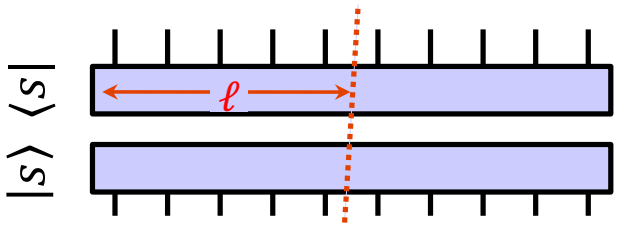

$$\rho(T) = \sum_s e^{-\beta E_s} |s\rangle\langle s|$$

finite size level-spacing $\delta E \sim 1/L$

$$\Rightarrow T \gtrsim \delta E \Rightarrow \beta \lesssim L$$

minimal requirement for thermal simulations

$$L \sim \beta$$




$$S(\ell) \sim 2 \times \frac{c}{6} \log(\ell)$$

Calabrese (2004)

entropy of thermal state

$$\Rightarrow S(\ell) \sim \frac{c}{3} \log(\ell)$$

$$\Downarrow \quad \ell \to \beta$$

$$\boxed{S(\beta) \sim \frac{c}{3} \log(\beta)}$$

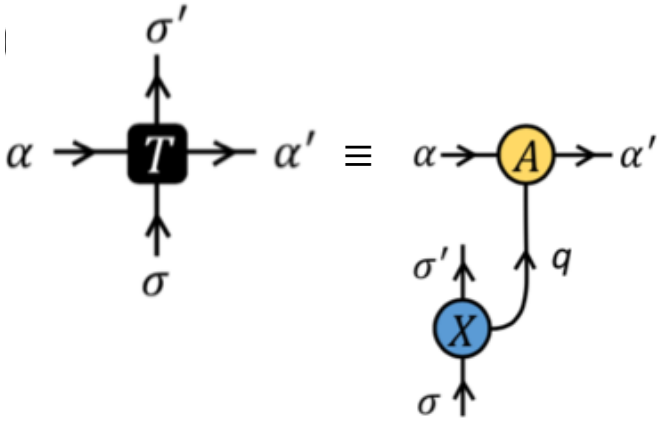
More rigorous arguments based on conformal field theory (CFT)

- J. Dubail [J. Phys. A: Math. Theor. **50** (2017) 234001]
- T. Barthel [arXiv:1708.09349 [quant-ph], 2017]

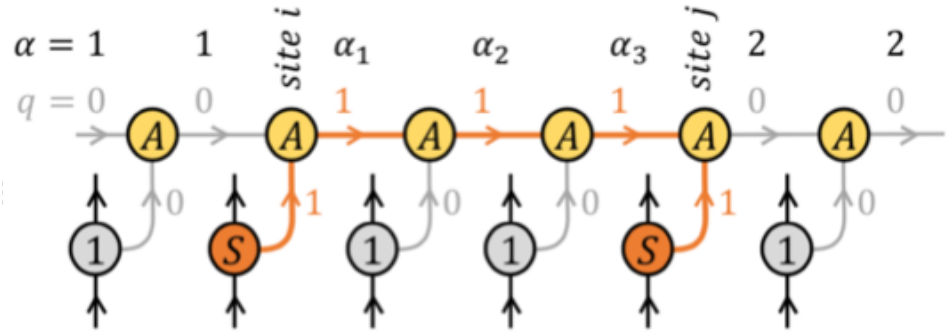
allows for efficient simulations of thermal states (entanglement entropy comparable to pure states with periodic BC)

# Thermal correlation length and symmetries

- $S(\beta) \lesssim \frac{c}{3}\log(\beta)$ independent of $L$ for $L \to \infty$
  - finite correlation length $\xi \sim \beta$ in thermal state
- Can use finite systems to simulate thermodynamic limit
  - can use finite size MPS in $|\Psi\rangle$
  - can exploit all symmetries (abelian and non-abelian) in an optimal way




$\boldsymbol{S}_i^\dagger \cdot \boldsymbol{S}_j =$




*e.g. spin-half site:* $X \in \{1, \boldsymbol{S}\}$

# Exponential energy scales

- Weak growth of block entropy of thermal state $S(\beta) \sim \frac{c}{3}\log(\beta)$
  - good for numerical efficiency
  - however: ill-suited for *linear* imaginary time evolution schemes
    e.g. Trotter: $\beta \to \beta + \tau$ with $\tau \ll \beta$

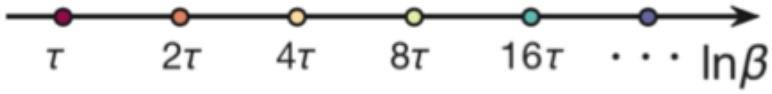
$$e^{-H\tau} \simeq e^{-H_{even}\tau} e^{-H_{odd}\tau}$$

small Trotter error enforces small constant $\tau$ for any $\beta$


- rather need to make bold steps in $\beta$ with increasing $\beta$
  to see a significant change in physical properties within a critical regime

  natural choice: $\beta \to \Lambda\beta \quad (\Lambda > 1) \quad \Rightarrow \quad \delta S \sim \text{const.}$
  simple choice: $\Lambda = 2$

$$\hat{\rho}(\tau_0) \to \hat{\rho}(\tau_0) * \hat{\rho}(\tau_0) = \hat{\rho}(2\tau_0) \to \hat{\rho}(2\tau_0) * \hat{\rho}(2\tau_0) = \hat{\rho}(4\tau_0) \to \cdots$$

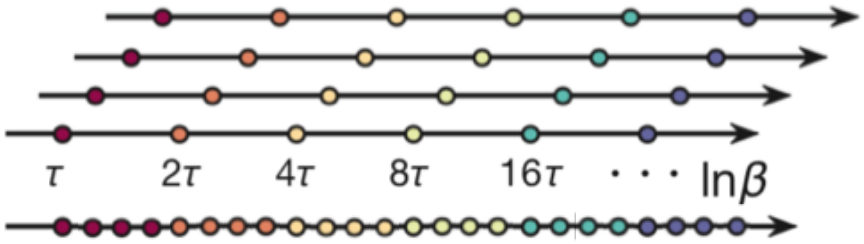



$$\beta_n = \tau_0 2^n$$

exponential tensor renormalization group (XTRG)

# Benefits of logarithmic temperature grid

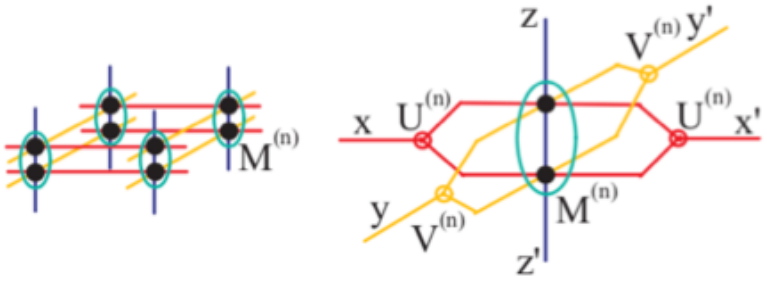
- Simple initialization of $\rho(\tau_0)$
  - can start with *exponentially* small $\tau_0$ such that $\rho(\tau_0) = 1 - \tau_0 H$
  - simply use the MPO of $H$ $\Rightarrow$ up to minor tweak, *same* MPO for $\rho(\tau_0)$
- No requirement for bipartite setup etc. as required for Trotter
  - simply applicable to longer range Hamiltonians
  - including (quasi-) 2D systems
  - no swap gates to deal with Trotter steps
- Maximal speed to reach large $\beta$ with minimal number of truncation steps
- Fine grained temperature resolution!
  - using $z$-shifted temperature grids $\beta_n = \tau_0 2^{n+z}$



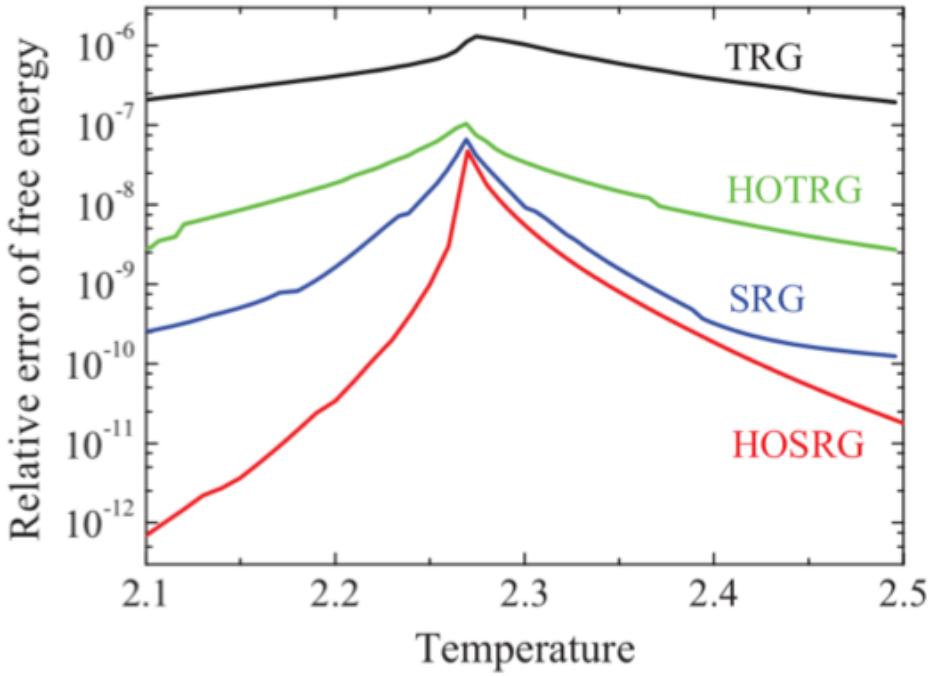

  - equivalent to using $\tau_0 \to \tau_0 2^z$ with $z \in [0,1[$
  - easy to parallelize: independent runs for logarithmically interleaved data sets

# Brief comparison to coarse graining renormalization

- Xie et al. (PRB 2012)
  Coarse-graining renormalization by higher-order singular value decomposition




2D Ising model (D=24)



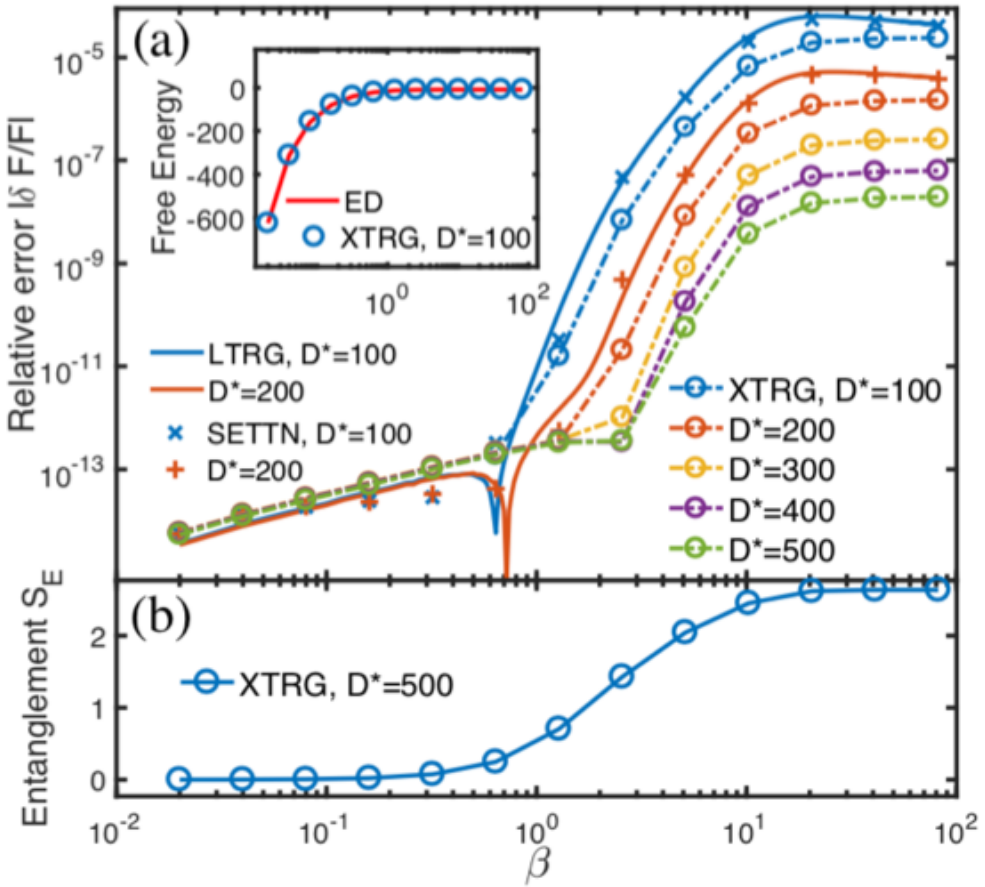

- starting point: Trotter gates
- infinite tensor network
  - no clean orthogonal vector spaces
  - no symmetries used
- no interleaved temperatures
  - „However, the number of temperature points that can be studied with this approach is quite limited […], since the temperature is reduced by a factor of 2 at each contraction along the Trotter direction."
  - therefore largely favors linearized imaginary time evolution

Similarly for Czarnik et al. (PRB 2015)

# Benchmark: performance

Free energy $F = -\frac{1}{\beta}\log Z$

L=18 spin-1/2 Heisenberg chain (PBC)




XTRG = exponential tensor renormalization group
LTRG = linearized tensor renormalization group
SETTN = series expansion thermal tensor network

- XTRG is most accurate
- XTRG is clearly fastest

speed gain (for D*=100,200)

LTRG $\xrightarrow{\times 10}$ SETTN $\xrightarrow{\times 10}$ XTRG

starting from the same $\rho = \rho(\tau_0)$, proceed

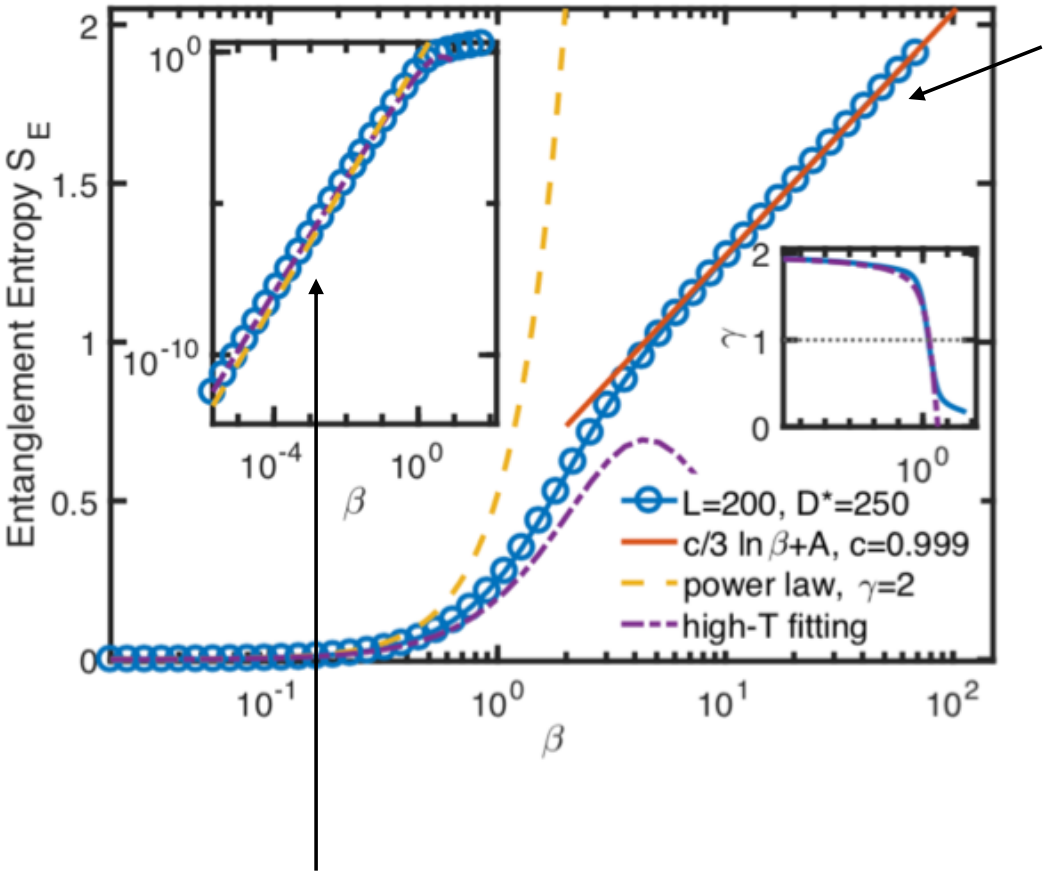
$\rho \to \rho * \rho$

$\rho \to \rho * \rho(\tau_0)$

$\rho \to \rho(\beta) * e^{-\beta H/2}$

# Block entanglement entropy

L=200 spin-1/2 Heisenberg chain (OBC)




log. growth $S \sim \frac{c}{3} \log \beta$
with $c = 0.999$

This offers an alternative to obtain central charge via finite-T calculations!

In comparison to Calabrese (2004) for obtaining $c$ from ground states with periodic BC

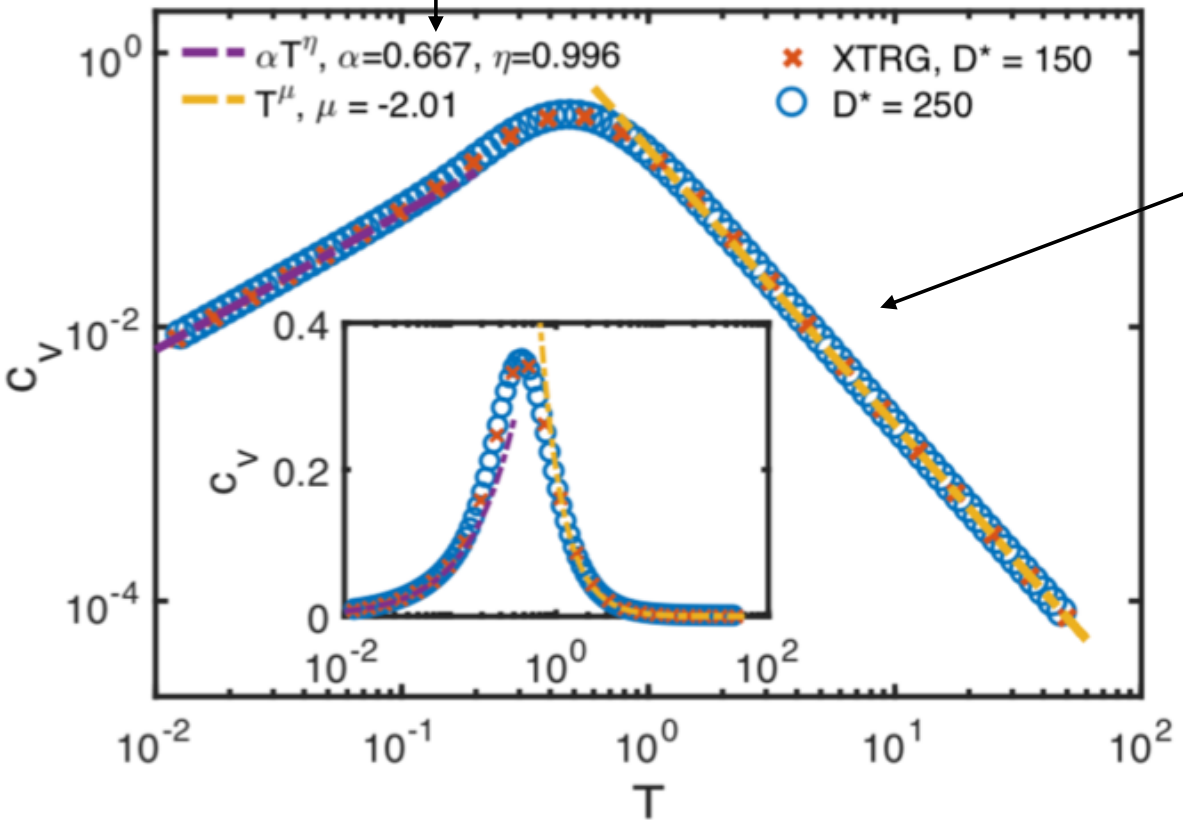
- comparable block entropy scaling
- no system size dependence as long as $L \gtrsim \xi$

universal $S \sim \beta^2$ behavior for extremly large temperatures where $S \ll 1$
(irrespective of the physics or dimensionality of the model!)

# Specific heat and critical exponents

L=300 spin-1/2 Heisenberg chain D*=250

*Specific heat at low temperatures* $c_V = \frac{\pi c}{3v} T$ with $v = \frac{\pi}{2} \Rightarrow c = 0.996$

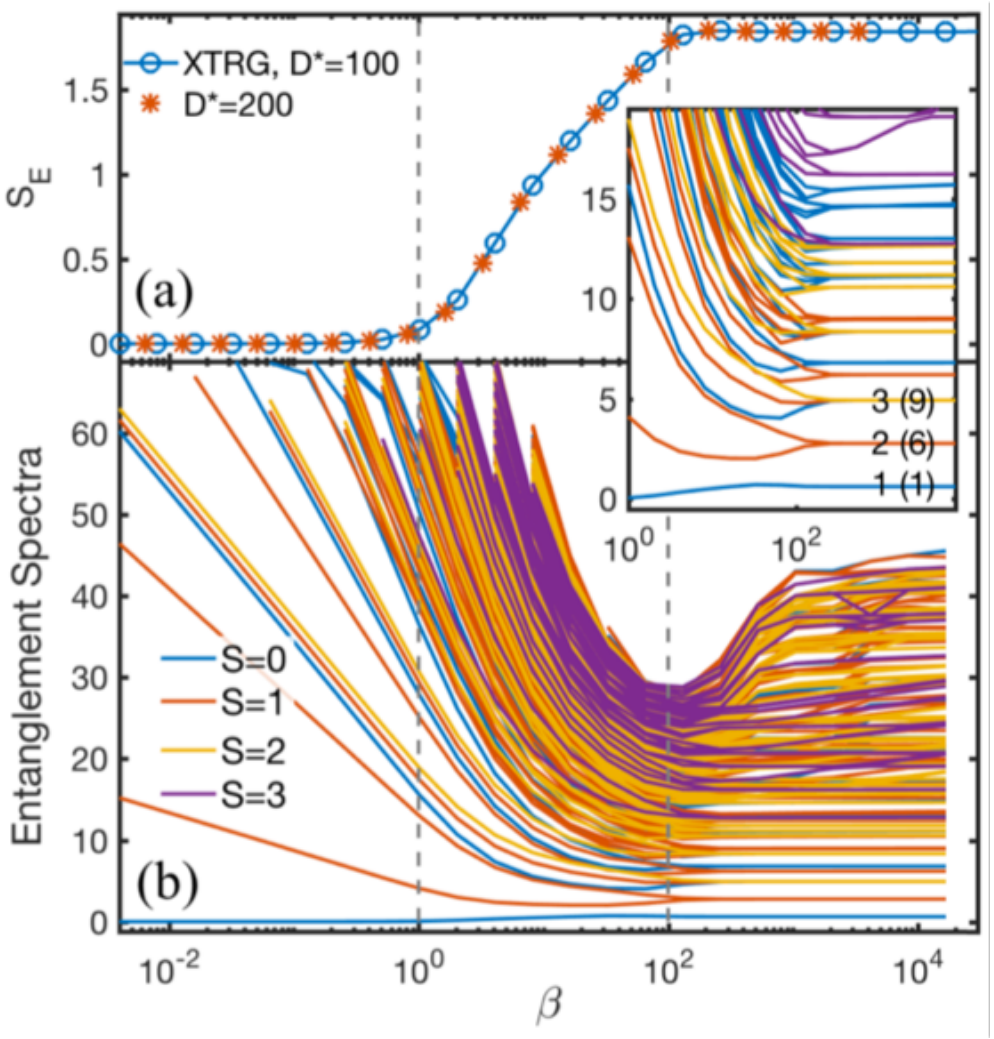



*at large temperatures: universal* $1/T^2$ *behavior*

*(*irrespective of the physics or dimensionality of the model!)

# Entanglement flow diagram

L=100 spin-1/2 Heisenberg chain (OBC)

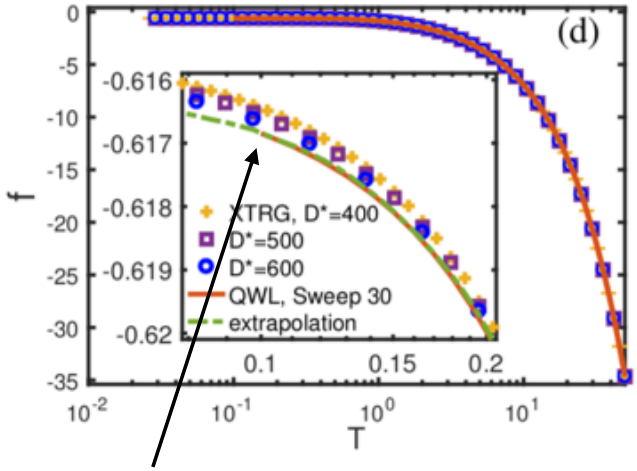



- spectra flow towards low-energy regime
- can identify qualitative changes for finite-T phase transitions
- here: transition to (artificial) gapped phase due to finite size

# 2D lattice models: benchmark

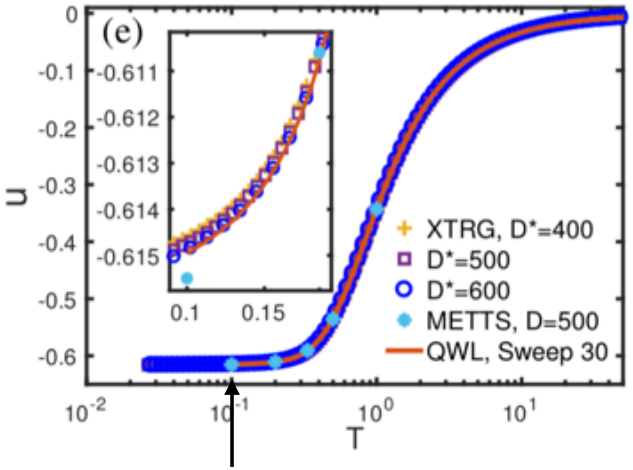
16×5 spin-1/2 Heisenberg square lattice

free energy /site ($f \sim \frac{1}{\beta}\log Z$)



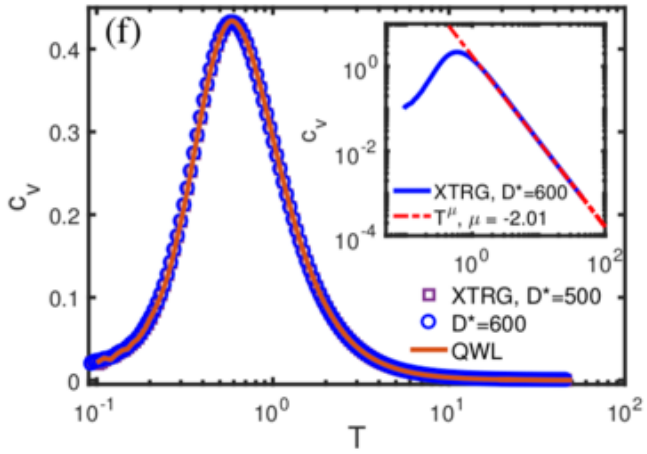

*excellent agreement after extrapolation* $D^* \to \infty$

internal energy / site ($u \sim \mathrm{tr}(\rho H)$)




*lowest temperatures reachable by METTS and QWL at comparable numerical* cost

specific heat / site ($c_V \sim \frac{\partial u}{\partial T}$)

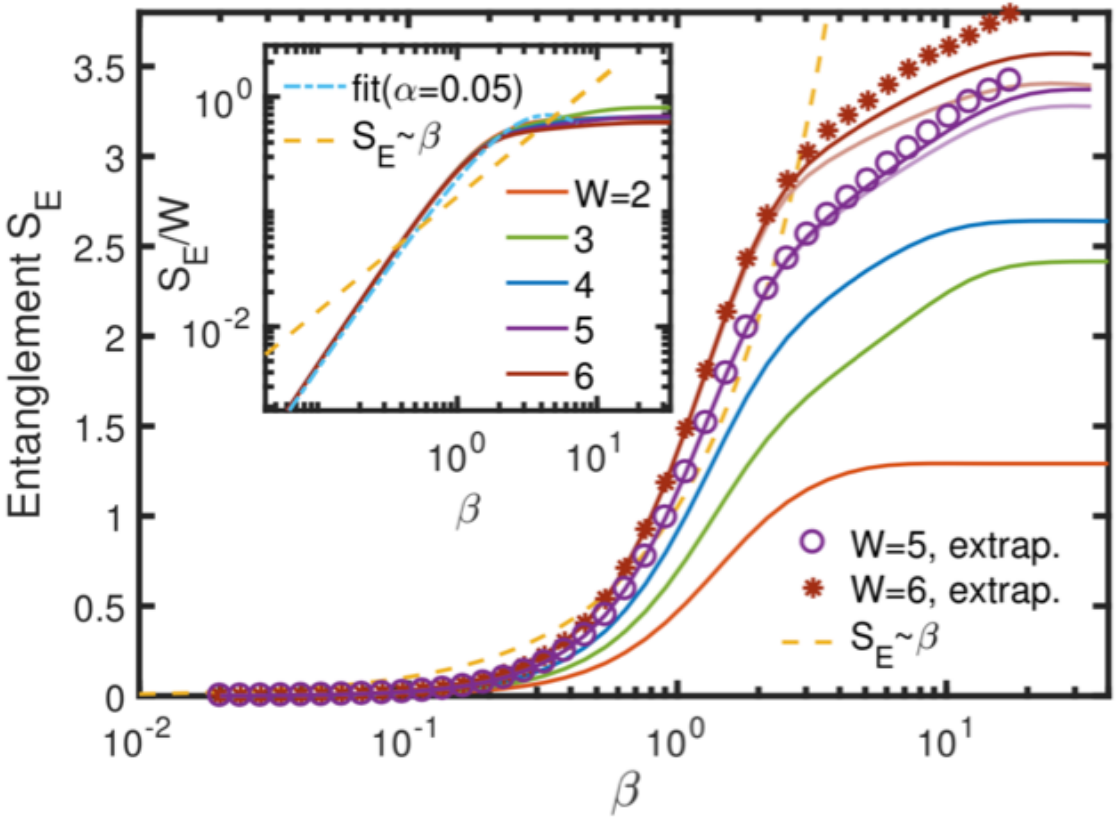



QWL = quantum Wang-Landau (Monte Carlo; ALPS 2011)

METTS = minimally entangled typical thermal states (S. R. White, 2009; data by B. Bruognolo)

# Entanglement scaling in 2D system

$L = 10$ spin-1/2 Heisenberg square lattice (OBC)




- also log. corrections at low temperatures (large $\beta$)
- due to spontaneously broken symmetries, leading to the presence of Goldstone modes *)
- effectively: a systematic efficient generalization to cluster expansion to 2D systems

*) also confirmed by Melitski et al. (arXiv:1112.5166 [cond-mat.str-el], 2011)
or Monte Carlo simulations: A. Kallin et. al. (Phys. Rev. B 84, 165134 (2011))

## Summary

[arXiv:1801.00142]

- XTRG is an extremely simple, yet efficient approach to thermal states in quasi-1D
  - $\rho \to \rho * \rho$ resulting in $\beta \to 2\beta$
  - easy to parallelize for fine temperature resolution
  - no Trotter setup required whatsoever,
    and therefore no Trotter error or error from swap gates
  - clean exploitation of all symmetries in the Hamiltonian
  - relates to energy scales [much like the Numerical Renormalization Group (NRG)]
- motivated by entanglement scaling $S \sim \frac{c}{3} \log \beta$
- Outlook: reducing thermal entanglement by disentangling
  e.g. via unitary transformations on auxiliary state space? $\hat{\rho} = \left(U\hat{\Psi}\right)^{\dagger}\left(U\hat{\Psi}\right)$

Supported by DFG (TR12, WE4819/1-1, WE4819/2-1 Heisenberg)
Cluster of Excellence NanoSystems Initiative, Munich (NIM)