Energy scales and exponential speed up in thermal tensor network simulations

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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
\[ \hat{\rho}(\beta) \equiv e^{-\beta \hat{H}} = \sum_s e^{-\beta E_s} |s\rangle \langle s| = \sum_s \rho(\sigma_1 \sigma_2 ... \sigma_L), (\sigma_1' \sigma_2' ... \sigma_L') |\sigma_1 \sigma_2 ... \sigma_L\rangle \langle \sigma_1' \sigma_2' ... \sigma_L'| \quad (\sigma_i = 1, ..., d) \]

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

\[ \langle \hat{A} \rangle \equiv \frac{1}{Z} \text{tr}[\hat{\rho} \hat{A}] \equiv \frac{1}{Z} \text{tr}[\Psi \hat{A} \Psi^\dagger] \equiv \frac{1}{Z} \langle \Psi | \hat{A} | \Psi \rangle \]

\[\]

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 $\delta E \gg \text{gap } \Delta$)

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

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

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

minimal requirement for thermal simulations

$$L \sim \beta$$

entropy of thermal state

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

Calabrese (2004)

More rigorous arguments based on conformal field theory (CFT)


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

\[ S_i^\dagger \cdot S_j = \]

\[ e.g. \text{spin-half site: } X \in \{1, S\} \]
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: $\beta \rightarrow \beta + \tau$ with $\tau \ll \beta$
    
    $e^{-H\tau} \approx e^{-H_{\text{even}}} e^{-H_{\text{odd}}\tau}$

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

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

  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 $\beta_n = \tau_0 2^{n+z}$

  $\tau$, $2\tau$, $4\tau$, $8\tau$, $16\tau$, $\cdots$ $\ln \beta$

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

- 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 is most accurate
- XTRG is clearly fastest

speed gain (for $D^*=100,200$)

LTRG $\rightarrow$ SETTN $\rightarrow$ XTRG

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

$\rho \rightarrow \rho \ast \rho$

$\rho \rightarrow \rho \ast \rho(\tau_0)$

$\rho \rightarrow \rho(\beta) \ast e^{-\beta H/2}$

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

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

\[ \log \text{growth } S \sim \frac{c}{3} \log \beta \]
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 extremely 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 $c_V = \frac{\pi c}{3\nu} T$ with $\nu = \frac{\pi}{2} \Rightarrow c = 0.996$

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 \( (f \sim \frac{1}{\beta} \log Z) \)

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

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

**excellent agreement after extrapolation** \( D^* \to \infty \)

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

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))
XTRG is an extremely simple, yet efficient approach to thermal states in quasi-1D

- $\rho \rightarrow \rho \ast \rho$ resulting in $\beta \rightarrow 2\beta$
- 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? $\hat{\rho} = (U\Psi)^\dagger (U\Psi)$