Thermal States as Convex Combinations of Matrix Product States

Mario Berta – arXiv:1709.07423

with Fernando Brandão, Jutho Haegeman, Volkher B. Scholz, and Frank Verstraete

Strongly Interacting Spin Chains: Ground States

- Matrix product states (MPS) form a sub-manifold $M_{MPS}^D \subset \mathbb{C}^{d^n}$ of the state space of n distinguishable spin-d particles. They are represented as

$$|\psi[A]\rangle := \sum_{i_1,\ldots,i_n} \text{Tr}[A_{i_1} \cdots A_{i_n}] |i_1\rangle \cdots |i_n\rangle,$$

where for $j = 1, \ldots, n$ the A_{i_j} are $D \times D$ dimensional complex matrices. The parameter D is called the bond dimension.
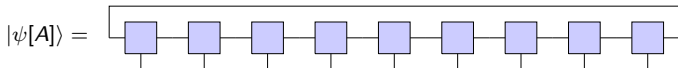
$$|\psi[A]\rangle =$$

Figure from [Bridgeman & Chubb '17]

- MPS with low bond dimension D capture the ground state physics of one-dimensional local gapped Hamiltonians [Hastings '07].
- Various algorithms that (efficiently) find the best approximate state within the sub-manifold M_{MPS}^D for the ground state, e.g., variationally using the density matrix renormalization group (DMRG).

Strongly Interacting Spin Chains: Thermal States

- We are interested in thermal states of one-dimensional local Hamiltonians H at non-zero temperature $T > 0$:

$$\rho(H, T) := \frac{\exp\left(H/T\right)}{\text{Tr}\left[\exp\left(H/T\right)\right]}.$$

- Matrix product operators (MPO) provide a faithful approximation [Hastings '06] and (efficient) algorithms for finding them are known [Verstraete *et al.* '04].

Major conceptual drawback

No distinction made between classical and quantum correlations $\Rightarrow$ classical correlations should be dealt with by using Monte Carlo sampling techniques and one should not waste a large bond dimension to those fluctuations.

- MPO based algorithms have some further practical drawbacks, such as positivity issues as well as blow up of bond dimension for purification based methods

Imperial College London

Main Result

- Let $H = \sum_{i \in I} h_i$ be a one-dimensional local Hamiltonian with uniform bound on the interaction strength $\|h_i\|_\infty \leq 1 \ \forall i \in I$.
- Can we approximate the thermal state

$$\rho(H, T) = \frac{\exp(H/T)}{\mathrm{Tr}\left[\exp(H/T)\right]} \text{ for fixed temperature } T > 0$$

as a convex combination of MPS with low bond dimension?

Thermal states as convex combinations of MPS

For any $\varepsilon \in (0, 1]$ there exists a bond dimension $D \in \mathbb{N}$ and a probability measure $\mathrm{d}\mu_\varepsilon$ on the manifold M_{MPS}^D such that

$$\left\| \rho(H, T) - \underbrace{\int \mathrm{d}\mu_\varepsilon\left([A]\right) |\psi[A]\rangle\langle\psi[A]|}_{=: \ \rho[\mu_\varepsilon]} \right\|_1 \leq \varepsilon \,,$$

where $\|X\|_1 := \mathrm{Tr}\left[|X|\right]$. The bond dimension D scales quasi-polynomially in ε^{-1} and system size, and doubly exponential in T^{-1}.
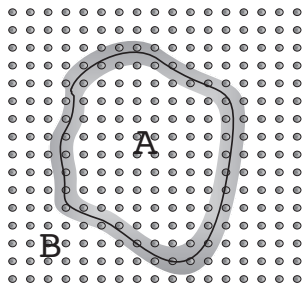
Proof Ideas I

Figure from [Wolf *et al.*, 08].

- Thermal states with finite correlation length have an area law for the quantum mutual information (QMI) [Wolf *et al.* '08]

$$I(A : B)_\rho := H(A)_\rho + H(B)_\rho - H(AB)_\rho$$

for $H(A)_\rho := -\text{Tr}\left[\rho_A \log \rho_A\right]$. That is,

$$I(A : B)_\rho \lesssim |\delta A|.$$

- QMI measures (quantum and classical) correlations ⇒ can area law be extended to other entanglement measures?

Proof Ideas II

- For our purposes we are interested in an area law for entanglement of formation

$$E_F(A:B)_\rho := \inf \sum_i p_i H(A)_{\rho^i}, \quad \text{with decompositions } \rho_{AB} = \sum_i p_i |\rho^i\rangle\langle\rho^i|_{AB}.$$

$\Rightarrow$ this would imply exactly what we want — up to $H(A)_\rho \approx H_{\max}(A)_\rho$.

- One might think that

$$E_F(A:B)_\rho \overset{?}{\leq} I(A:B)_\rho.$$

- However, using concentration of measure phenomena [Hayden et al. '06] show that maybe somewhat surprisingly

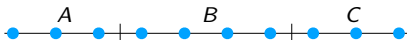$$E_F(A:B)_\rho \gg I(A:B)_\rho \text{ is possible.}$$

- Another entanglement measure (tripartite) is the conditional quantum mutual information (CQMI)

$$I(A:C|B)_\rho := H(AB)_\rho + H(BC)_\rho - H(B)_\rho - H(ABC)_\rho \geq 0.$$

Proof Ideas III

- Exponential decay of $I(A:C|B)_\rho$ in the system size of B connecting A and C?

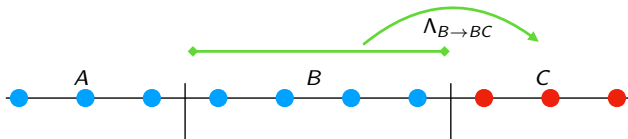
  [Brandão & Kastoryano '16] and [Swingle & McGreevy '16]

- Connection to Markov chain structure [Fawzi & Renner '15] and [many more]

  $$I(A:C|B)_\rho \geq \frac{1}{4} \left\| \rho_{ABC} - (\mathcal{I}_A \otimes \Lambda_{B\to BC})(\rho_{AB}) \right\|_1^2 ,$$

  where $\Lambda_{B\to BC}$ denotes quantum channel only acting on the region B.

- However, statement about CQMI not known for general systems of interest.

Proof Ideas IV

Local Markov chain structure [Kato & Brandão '16]

Let $H = \sum_{i \in I} h_i$ be a one-dimensional local Hamiltonian with $\|h_i\|_\infty \leq 1 \; \forall i \in I$. Then, for any tripartite split of the lattice $\alpha\beta\gamma$, there exists a local quantum channel $\Lambda_{\beta \to \beta\gamma}$ only acting on the region β such that

$$\left\| \rho_{\alpha\beta\gamma}(H, T) - \left(\mathcal{I}_\alpha \otimes \Lambda_{\beta \to \beta\gamma}\right)\left(\rho_{\alpha\beta}(H, T)\right) \right\|_1 \leq \exp\left(-q(T)\sqrt{d(\alpha, \gamma)}\right),$$

where $d(\alpha, \gamma) \geq \ell_0$ denotes the minimal distance in system size between α and γ, and $q(T) := C \exp(-c/T)$ for some universal constants $0 < \ell_0, C, c < 100$.
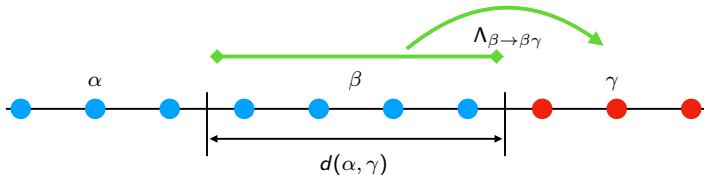
Proof Sketch

- For fixed $T > 0$ and $\varepsilon \in (0, 1]$ use [Kato & Brandão '16] in parallel to:
  1. Construct global MPS $|\Psi(D, \varepsilon)\rangle$ with quasi-polynomial scaling in n and $1/\varepsilon$
  2. Show that $|\Psi(D, \varepsilon)\rangle$ is purification of convex combination of MPS — denoted by $\rho[\mu_\varepsilon]$
  3. Show that $\rho[\mu_\varepsilon]$ is close to thermal state $\rho(H, T)$
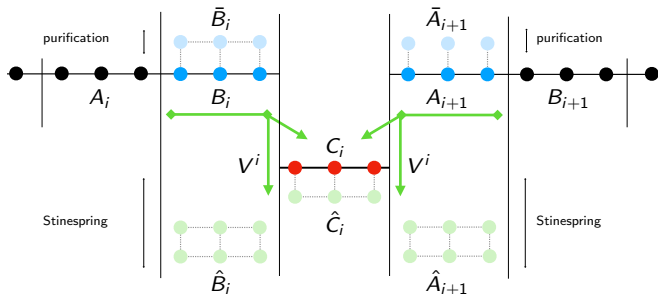
$L = A_1 B_1 C_1 \, A_2 B_2 C_2 \cdots A_l B_l C_l$ with $|A_i| = |B_i| = 2^{\log^2(n/\varepsilon)}$, $|C_i| = 2^{5\xi \cdot \log^2(n/\varepsilon)}$ and ξ corr. length
$\Rightarrow$ choose $\alpha_i = L/(\beta_i \gamma_i)$, $\beta_i = B_i A_{i+1}$, $\gamma_i = C_i$

Application: Numerics

- MPO numerical methods to approximate thermal state [Verstraete *et al.* '04]
- Alternatively minimally entangled typical thermal states (METTS) [White '09]:

  1 Randomly choose product state $|\vec{i}\rangle := |i_1\rangle \cdots |i_n\rangle$

  2 Approximate the imaginary time evolved

  $$|\phi(T, \vec{i})\rangle := p(\vec{i})^{-1/2} \exp\left(-\beta H/2\right) |\vec{i}\rangle, \quad \text{with } p(\vec{i}) := \langle\vec{i}| \exp\left(-\beta H\right) |\vec{i}\rangle$$

  by an MPS with low bond dimension

  3 Collapse a new product state $|\vec{i'}\rangle$ from $|\phi(T, \vec{i})\rangle$ with probability $p(\vec{i} \to \vec{j}) := |\langle\vec{i'}|\phi(T, \vec{i})\rangle|^2$ and return to step 2

  $\Rightarrow$ approximately creates convex combination of MPS with low bond dimension

  $$\frac{1}{Z} \sum_{\vec{i}} p(\vec{i}) |\phi(T, \vec{i})\rangle\langle\phi(T, \vec{i})|$$

- Mathematical justification for (heuristic) METTS algorithm
- Similar mathematical justification for extension to algorithms time evolving quantum systems — hydrodynamics [Leviatan *et al.* '17]

Conclusion

Main result

The thermal state of every one-dimensional local Hamiltonian with uniform bound on the interaction strength is approximated as a convex combination of MPS with bond dimension scaling quasi-polynomially in ε^{-1} and system size:

$$\rho(H, T) \approx_\varepsilon \int d\mu_\varepsilon \left([A]\right) |\psi[A]\rangle\langle\psi[A]| .$$

- Can the parameter in our main result be improved? ⇒ quasi-polynomial versus polynomial scaling of bond dimension in terms of system size [Kim '17].
- For our proof strategy, this boils down to improving [Kato & Brandão '16]

$$\left\| \rho_{\alpha\beta\gamma}(H, T) - \left(\mathcal{I}_\alpha \otimes \Lambda_{\beta\to\beta\gamma}\right)\left(\rho_{\alpha\beta}(H, T)\right) \right\|_1 \leq \exp\left(-q(T)\sqrt{d(\alpha,\gamma)}\right)$$

  to $\exp\left(-q(T)d(\alpha,\gamma)\right)$ dependence. Examples in [Swingle & McGreevy '16].
- Alternatively we could start from known MPO methods [Hastings '06].
- Physics: say more about numerics for METTS algorithm and hydrodynamics?

Thanks. Check out arXiv:1709.07423.