A quantum algorithm for Gibbs state preparation

Based on arXiv:1603.02940 [Chowdhury & Somma 2017] [CS 17]

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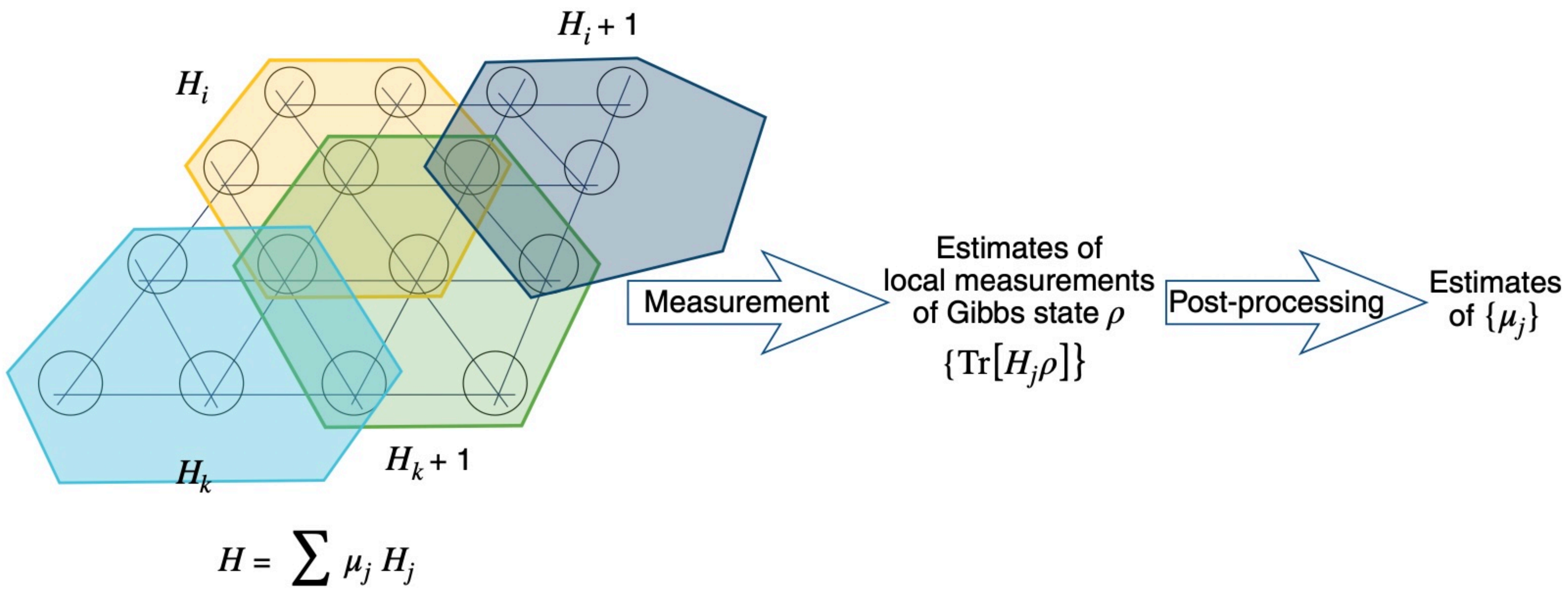
Motivation

- The Gibbs State of a many-qubit system encodes information about its underlying Hamiltonian
- Helps better understand Statistical Mechanics
- Sampling the gibbs state can be used to “learn” an approximate underlying Hamiltonian [AAKS 21, arXiv:2004.07266, Nature]



Nature viewpoint “Inside quantum black boxes” by Vedran Dunjko, 2021

Problem Statement

- Given: An n-qubit Hamiltonian $H = H^\dagger \in \mathbb{C}^{N\times N}$ ($N = 2^n$) as a "frustration-free" projector decomposition
$$H = \sum_{k=1}^{K} \alpha_k \Pi_k$$
- Where $K = poly(n)$ and each Π_k is a projector $\Rightarrow \Pi_k^2 = \Pi_k \quad \forall k$
- Also given: A quantum computer in the state $|0^n\rangle$ with access to poly(n) ancillas
- A Hamiltonian is "frustration-free" if the ground state of H is also the ground state of Π_k $\forall k$
- Aside: Not all local Hamiltonians with commuting terms are frustration-free

Problem Statement

- Task (Informal): Prepare $$\rho_G = \frac{e^{-\beta H}}{tr(e^{-\beta H})} = \frac{e^{-\beta H}}{Z} = \sum_{j=0}^{N-1} \frac{e^{-\beta E_j}}{Z} |\psi_j\rangle\langle\psi_j|$$ $$\left(H = \sum_{j=0}^{N-1} E_j |\psi_j\rangle\langle\psi_j|\right)$$

- More formally: Give a description of a unitary V such that

$$\text{tr}_\text{a}\left(V\left(|0^n\rangle\langle 0^n| \otimes |0\rangle\langle 0|_\text{a}\right)V^\dagger\right) = \hat{\rho}$$

$$\text{so that } \frac{1}{2}||\hat{\rho} - \rho_G||_1 \leq \epsilon$$

- Subscript "a" represents the full set of ancillary qubits. We would like $|\text{a}| \leq \text{poly}(n)$ qubits

- All the ancillaries are traced out at the end of the computation. What remains must be ϵ-close to the Gibbs State in trace norm

Improvement over previous work

- [PW 09, arXiv:0905.2199] use QPE to find effective gate complexity of V as

$$O\left(\frac{\beta^6}{\epsilon^3}\sqrt{\frac{N}{Z}}\ \text{polylog}(\epsilon^{-1})\right)$$

- [CS 17, present work] use several tools (but excluding QPE) to find gate complexity of V as

$$O\left(\sqrt{\frac{N\beta}{Z}}\text{polylog}\left(\frac{1}{\epsilon}\sqrt{\frac{N\beta}{Z}}\right)\right)$$

- Polynomial improvement in β, exponential improvement in $1/\epsilon$

Algorithm: Step 1: Spectral Gap Amplification

- Construct $\widetilde{H}$ acting on a larger Hilbert space [$(n + \log K)$ qubits] as

$$\left(H = \sum_{k=1}^{K} \alpha_k \Pi_k \right) \qquad \widetilde{H} = \sum_{k=1}^{K} \sqrt{\alpha_k} \Pi_k \otimes (|k\rangle\langle 0| + |0\rangle\langle k|)_{a_1}$$

- In a rough sense, $\widetilde{H} \sim \sqrt{H}$ in this larger Hilbert space

$$(\widetilde{H})^2 |\phi\rangle \otimes |0\rangle_{a_1} = \left(H|\phi\rangle\right) \otimes |0\rangle_{a_1} \quad \text{for all states} \quad |\phi\rangle \in \mathbb{C}^{2^n}$$

- This is called "Spectral Gap Amplification". If $\text{gap}(H) = \Delta$ and $\text{gap}(\widetilde{H}) = \Delta'$, then $\Delta' \geq \Omega\left(\sqrt{\Delta}\right)$ if H is frustration-free.
- [Somma Boixo 11, arXiv:1110.2494]

Algorithm: Step 2: LCU in larger Hilbert space

- Denote $M_k = \big(|k\rangle\langle 0| + |0\rangle\langle k| \big)_{a_1}$

  Now note by Euler's formula that $M_k = \frac{i}{2}\left(e^{-i\pi M_k/2} - e^{i\pi M_k/2}\right)$

  Also, for any projector Π_k , there exists a unitary U_k s.t. $\Pi_k = \frac{1}{2}\left(I + U_k\right)$

$$\Rightarrow \widetilde{H} = \sum_{k=1}^{K} \sqrt{\alpha_k}\Pi_k \otimes M_k = \sum_{k=1}^{\widetilde{K}} \widetilde{\alpha}_k \widetilde{U}_k$$

- Here $\widetilde{K} = 4K,$ and $\widetilde{\alpha}_k$ & $\widetilde{U}_k$ can be directly expressed using α_k and U_k, M_k respectively.

- Takeaway from Step 1+Step2: Given a projector decomposition of H, we can explicitly construct $\widetilde{H}$ as a Linear Combination of Unitaries (LCU) in the larger Hilbert space

Algorithm: Step 3: “Hubbard-Stratonovich Transformation” (HST)

- We painstakingly constructed $\widetilde{H}$ from H. What benefit do we gain out of this?
- Express $e^{-\beta H/2}$ (~gibbs state) purely in terms of $e^{-\sqrt{\beta H}}$, and hence $e^{-\sqrt{\beta}\widetilde{H}}$

$$e^{-\beta H/2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy\ e^{-y^2/2} \exp(-iy\sqrt{\beta H}) \qquad [HST]$$

- Integral needs $\sqrt{H}$, we instead use $\widetilde{H}$!
- However y is a continuous variable. Hence we have to discretize the HST integral into a finite sum, which has the LCU form. Continued next slide

Algorithm: Step 3 continued: Discretize HST

- Lemma (informal):

$$X_\beta = \frac{1}{\sqrt{2\pi}} \sum_{j=-J}^{+J} c_j \exp\left(-i y_j \sqrt{\beta}\ \widetilde{H}\right) \qquad c_j := \delta y\ e^{-y_j^2/2}$$

is ϵ-close (in L_2 norm) to $e^{-\beta H/2}$ over its action on **any** state $|\phi\rangle|0\rangle_{a_1} \in \mathbb{C}^N \otimes \mathbb{C}^K$

if

$$J = \Theta\left(\sqrt{\frac{||H||}{\beta}} \log(\epsilon^{-1})\right)$$

$$\Rightarrow ||(X_\beta - e^{-\beta H/2})|\phi\rangle|0\rangle_{a_1}|| \leq \Theta(\epsilon)$$

Algorithm: Step 4: Hamiltonian Simulation

- Use cutting-edge Hamiltonian Simulation, like [BCCKS 14, arXiv:1412.4687]

  to approximate $\exp(-iy_j\sqrt{\beta}\widetilde{H})$ for each $j \in \{-J, \ldots\ J\}$ by an

  ϵ-close (in spectral norm) unitary construction W_j so that

$$X_\beta \approx \sum_{j=-J}^{J} c_j W_j$$

- Example of how such a W_j is constructed? Continued next slide

Algorithm: Step 4: Construct W_j (example)

- To get W ϵ-close to $e^{-i\widetilde{H}t}$ given $\widetilde{H} = \sum_{k=1}^{\widetilde{K}} \widetilde{\alpha}_k \widetilde{U}_k$

  i) Assume query access to with $|a_2| = O(\log K)$ ancillas $\widetilde{Q} = \sum_{k=1}^{\widetilde{K}} \widetilde{U}_k \otimes |k\rangle\langle k|_{a_2}$

  ii) Use [BCCKS 14] to construct W with optimal query complexity

- Total gate complexity of W is equal to

$$O\left((K + C_U \log K)\tau \frac{\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\right) \quad \text{with} \quad \tau = |t| \sum_k \widetilde{\alpha}_k$$

Algorithm: Step 5: Implement $X_\beta|\phi\rangle$ for maximally entangled $|\phi\rangle$

- At this point, we know $\{c_j\}$ as well as gate constructions of $\{W_j\}$ such that $X_\beta = \sum c_j W_j$ is ϵ-close to $e^{-\beta H/2}$.

- Now implement $X_\beta|\phi\rangle$ for $|\phi\rangle = \frac{1}{\sqrt{N}}\sum_{\sigma=0}^{N-1}|\sigma\rangle|\sigma\rangle_{a_4}$ with two more new sets of ancillas: $|a_3| = \log(2J+1)$ & $|a_4| = n$ qubits, where the $|a_3|$ ancillas act as controls for an LCU protocol

- Result: $X_\beta|\phi\rangle = \epsilon$-close to $e^{-\beta H/2}|\phi\rangle$ and we know that $e^{-\beta H/2}|\phi\rangle \equiv$ Gibbs state @ temp $\frac{2}{\beta}$

- Note: $|a| = (|a_1| + |a_2| + |a_3| + |a_4|) = n + \log(K^2(2J+1))$ ancillas used in total

Algorithm: Step 6: Measure and Stop

$$\hat{\rho} = \mathrm{tr}_{a_1 a_2 a_3 a_4}\left(\frac{X_\beta|\phi\rangle\langle\phi|X_\beta^\dagger}{||X_\beta|\phi\rangle||^2}\right)$$

satisfies $||\hat{\rho} - \rho_G|| \leq \Theta(\epsilon)$

Summary

- A quantum algorithm for Gibbs state preparation was constructed using several tricks including SGA, LCU, AA and fourier analysis.
- Relative to [Poulin Wocjan 09], authors prove improvements in gate complexity

Thank you for listening!