

Thermal State Prep

Nathan Wiebe, Matthew Hagan

May 2022

1 Introduction

The computational task of preparing states of the form $\frac{e^{-\beta H}}{\mathcal{Z}}$ in a usable approximation on a quantum computer is both incredibly useful and difficult. The closely related problem of estimating the free energy, defined as $F = -(1/\beta) \log \mathcal{Z}$, up to additive error is known to be QMA-Hard for 2-local Hamiltonians [1]. Intuitively, finding the ground state of a k -local Hamiltonian is known to be QMA-Hard [2] and the thermal state $e^{-\beta H} \mathcal{Z}^{-1}$ can be constructed with arbitrarily high overlap with the ground state as $\beta \rightarrow \infty$ or the temperature approaches 0.

Preparing thermal states for arbitrary Hamiltonians for arbitrary temperatures is QMA-Hard, however thermal states are incredibly useful inputs whenever low energy states are needed, such as when training Boltzmann machines [3], preparing ground states for quantum error correcting codes [4], or starting states for chemistry simulations [5].

Want to include here the main methods for preparing thermal states that currently exist, mainly the Poulin and Wocjan paper and Quantum-Quantum Metropolis Hastings. Where should more niche/advanced methods go?

2 Preliminaries

We denote the Hilbert space of the system as \mathcal{H}_{sys} and the environment as \mathcal{H}_{env} . The algorithm we propose for preparing thermal states for a Hamiltonian $H_{sys} \in \text{Herm}(\mathcal{H}_{sys})$ involves direct time simulation of the system coupled to an environment governed by $H_{env} \in \text{Herm}(\mathcal{H}_{env})$. We denote the interaction $H_{int} \in \text{Herm}(\mathcal{H}_{sys} \otimes \mathcal{H}_{env})$. At a broad level, the algorithm starts from some initial state (what is the distribution over inputs?) we denote as ρ , undergoes time evolution with $H = H_{sys} + H_{env} + H_{int}$ for some time t , after which we trace out the environment leaving

$$\mathcal{P}(\rho) = \text{Tr}_{Env} [e^{iHt} \rho e^{-iHt}]. \quad (1)$$

The goal of this paper is to provide subsets of possible systems, environments, and interactions that can lead to efficient thermalization.

Can thermal state preparation be written as a SDP? Brandao and Svore showed that thermal states can be used as a resource for a quantum Aurora-Kale SDP solver, but what about the inverse problem? We know that the thermal state satisfies the following:

$$\rho_G = \arg \max_{\rho} \text{Tr} [-\rho \log \rho] \quad \text{such that} \quad (2)$$

$$\text{Tr} [\rho H] = E? \quad (3)$$

References

- [1] Sergey Bravyi, Anirban Chowdhury, David Gosset, and Pawel Wocjan. On the complexity of quantum partition functions, October 2021. Number: arXiv:2110.15466 arXiv:2110.15466 [quant-ph].