The Thermodynamic Cost of Ignorance: Thermal State Preparation with One Ancilla Qubit

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Extended Abstract

Thermal states are fundamental primitives for many quantum algorithms, ranging from quantum chemistry and materials simulations to Semi-Definite Program (SDP) solvers. They are also of utmost importance in physics, as systems tend to generically equilibrate to the temperature of their surrounding environments. Understanding the problem of thermalization, or how systems approach thermal states, is therefore a critical task for both the physics of open quantum systems and quantum computer science. In our paper we propose a quantum algorithm that is capable of preparing thermal states for arbitrary systems at arbitrary temperatures and is composed of simple Hamiltonian evolution circuits, thereby providing both new methods for thermal state preparation on quantum computers and an extension of the open quantum systems model of Repeated Interactions to arbitrary systems.

Our algorithm is inspired by the classical Hamiltonian Monte Carlo (HMC) algorithm, a modification of Metropolis-Hastings. HMC works by extending the state space of the system of interest to include momentum variables and then utilizes time-evolution of the extended Hamiltonian to transition to new states. Our algorithm is described as follows. We first prepare a single ancilla qubit in a thermal state for a chosen energy gap γ. This gap can be chosen according to eigenvalue differences known to the user or sampled uniformly at random from an interval containing all eigenvalue differences, we outline both techniques in our paper. Then, choose an interaction term $G \sim U_{\text{haar}} \Lambda U_{\text{haar}}^\dagger$, whre U_{haar} can be sampled from a 2-design and Λ is a diagonal matrix with I.I.D Gaussian entries. Simulating the total Hamiltonian with the randomized interaction then yields the channel

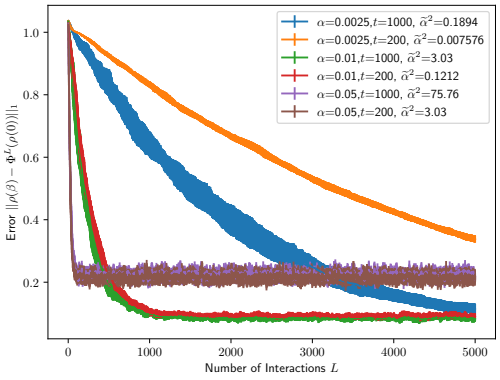
$$\Phi(\rho) = \mathbb{E}_G \operatorname{Tr}_{\text{env}} \left[e^{-i(H_S + H_E + \alpha G)t} \left(\rho \otimes \frac{e^{-\beta H_E}}{\mathcal{Z}_E(\beta)} \right) e^{+i(H_S + H_E + \alpha G)t} \right], \tag{1}$$

which is then repeated L times.

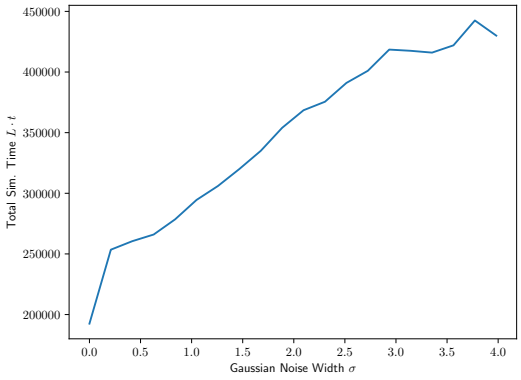
In our paper we provide a detailed analysis of this algorithm using a weak-coupling expansion. We are able to prove fixed point properties and convergence rates in terms of the spectral gap of an underlying Markov chain. One remarkable property of our algorithm is that the spectral gap of this system is *exactly* computable in the ground state limit, as $\beta \to \infty$. We perform this analysis in four settings: first for a single qubit system, second for a truncated harmonic oscillator, third for a generic system with no a priori eigenvalue knowledge, and fourth for a generic system with exact eigenvalue knowledge. These results are presented in

	Harmonic Oscillator	Zero Knowledge	Perfect Knowledge
Env. Gap	$\gamma = \Delta$	$\gamma \in [0, 4\|\|H_S\|\|]$	$\Pr[\gamma = \|\Delta_S(i,j)|] = 1/\binom{\dim_S}{2}$
$\|\|\rho(\beta) - \Phi(\rho(\beta))\|\|_1$	0	$O\left(\alpha^2 t e^{\beta\delta_{\min}}\right)$	0
t	$\frac{\dim_S^2}{\Delta\sqrt{\epsilon\lambda_\star(\beta)}}$	$\frac{\dim_S^2 \|\|H_S\|\|}{\delta_{\min}^2\lambda_\star(\beta)\epsilon}$	$\frac{\dim_S^2}{\delta_{\min}\sqrt{\epsilon\lambda_\star(\beta)}}$
# of Interactions L	$\widetilde{O}\left(\frac{\dim_S^8}{\lambda_\star(\beta)^2\epsilon^2}\right)$	$\widetilde{O}\left(\frac{\dim_S^{14}\|\|H_S\|\|^6}{\epsilon^5\delta_{\min}^6\lambda_\star(\beta)^6}\right)$	$\widetilde{O}\left(\frac{\dim_S^{14}}{\epsilon^2\lambda_\star(\beta)^3}\right)$
$\lim_{\beta\to\infty}\lambda_\star(\beta)$	1	≥ 2.43	≥ 1

Figure 1: Worst-case bounds to guarantee thermalization of the form $\left|\left|\rho_S(\beta) - \Phi^L(\rho)\right|\right|_1 \in \widetilde{O}(\epsilon)$. $\lambda_\star(\beta)$ denotes the spectral gap of the underlying Markov chain.



(a) Hydrogen-2 Chain Error



(b) Hydrogen-3 Chain Simulation Time

four theorems (Theorems 10 - 13) in the complete manuscript and are summarized in Figure 1, although we leave out the single qubit scenario due to space constraints.

As previously mentioned, our algorithm can be straightforwardly compiled to time-independent Hamiltonian simulation circuits. We were able to simulate these dynamics exactly for a few small systems on classical devices to benchmark the algorithm. Here we include two indicative plots of the performance of our algorithm as applied to hydrogen chains of 2 and 3 atoms. Figure 2a demonstrates the error scaling as a function of the number of interactions L using the trace of the Hamiltonian as a heuristic for tuning the environment gap *gamma*. This plot showcases the relatively rapid speed of strong coupling, indicating that our weak-coupling expansion may be leaving improvements on the table. Figure 2b showcases the number of interactions needed to thermalize to a set β and ϵ for noisy samples of *gamma*. We plot the number of interactions needed as a function of the noise added to a sample of *gamma* taken from the exact eigenvalue spectrum, and we see that although perfect samples do indeed have the fastest thermalization it is still possible to prepare accurate thermal states with no knowledge of the spectrum whatsoever, even for standard chemistry benchmark systems.