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, which is a modification of the original Metropolis-Hastings algorithm that eliminates random walk behavior. 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. As the probability of accepting new samples scales like the exponential of the energy difference, and since Hamiltonian evolution naturally preserves energy, every sample is theoretically accepted ignoring numerical integration errors. By implementing a quantum version of HMC, which does not have a rejection filter, we are able to avoid the dealbreakers of Marriot-Watrous rewinding [1] or other weak measurement schemes [2] present when trying to adapt standard Metropolis-Hastings algorithms to quantum computers.

The quantum algorithm we developed can be summarized as follows. First, prepare the system in a state diagonal in the Hamiltonian basis, the maximally mixed state or a Haar random pure state are sufficient, and a single ancilla qubit in a thermal state $\frac{e^{-\beta H_E}}{1+e^{-\beta\gamma}}$, with an energy gap γ that can be chosen uniformly at random from the interval $[0, 4\,||H_S||]$. Then, choose an interaction term with Haar random eigenvectors and I.I.D Gaussian eigenvalues and add it to the system and environment Hamiltonians with a coupling constant α. Finally, simulate the system-environment Hamiltonian wth interaction for a time t and then trace out the ancilla qubit. This yields our overall channel

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

	Harmonic Oscillator	Zero Knowledge	Perfect Knowledge
Env. Gap	$\gamma = \Delta$	$\gamma \in [0, 4\|\|H_S\|\|]$	$\Pr\left[\gamma = \|\Delta_S(i,j)|\right] = 1/\binom{\dim_S}{2}$
$\|\rho(\beta) - \Phi(\rho(\beta))\|_1$	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.

which is then repeated L times.

To analyze this algorithm we perform a weak-coupling expansion of the combined system-environment output of Φ as given in Eq. (1). The technical tools used for this involve only applications of Duhamel's formula and second moment Haar integrals. The computation of this weak-coupling expansion is completely generic and could be used in future work to study problems such as thermometry and spectroscopy. For Gibbs sampling, we use this expansion to reduce the quantum dynamics of Φ to a classical Markov chain over the system eigenbasis. Once this is obtained we can compute the fixed points of the channel, compute spectral gaps, and show ergodicity. 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 four theorems (Theorems 10 - 13) in the complete manuscript and are summarized in Figure 1, we leave out the single qubit scenario due to space constraints. A further result that is left out is that the fixed point of the Zero Knowledge case may appear to diverge in the $\beta \to \infty$ limit, as we show that it is a controllably approximate fixed point, but in this same limit we show that the ground state is the exact fixed point with no approximation, indicating our approximation bounds are rather loose.

Our manuscript also provides extensive numerics that explore various behaviors of the channel Φ, a few of which we replicate here. For small harmonic oscillator instances we are able to study the β and ϵ dependence of the channel. The β dependence of the total simulation time exhibits unexpected behavior even for $\dim_S = 4$ truncations, where it appears that the spectral gap of the Markov chain *increases* with β, meaning ground states can be prepared faster than intermediate temperatures when starting from the maximally mixed state. When probing the ϵ scaling of the algorithm we push the algorithm in regimes beyond prescribed values of α and t as given by our weak-coupling expansion. We find that at $\epsilon = 0.005$ the total simulation time can be reduced by over 4 orders of magnitude. This suggests that the upper bounds on our runtime are very loose and could be improved with strong coupling analysis.

Lastly, we explore the behavior of the algorithm for small benchmark systems of Hydrogen chains. In Figure [] we show the error scaling with respect to the number of interactions for a pair of hydrogen atoms for various α and t settings and again observe that strong coupling cools much faster but has a higher error floor. In practice, one would want to start with large values of α that decrease over time. In Figure [] we quantify the effects of noise on our Perfect Knowledge results for a chain of 3 Hydrogen atoms. This plot is generated by

sampling values of γ from the exact eigenvalue spectrum and then adding Gaussian noise to the sample. The total simulation time needed to thermalize is plotted as a function of the width of this added noise, demonstrating an even interpolation from the scenario with a priori eigenvalue knowledge to no uniform sampling across the eigenvalue spectrum.

To compare these results with existing quantum algorithms is a difficult task as there is now a plethora of techniques, each with their own drawbacks and advantages. Previous quantum algorithms can be roughly grouped into three approaches: the earliest algorithms proposed tend to be inspired more by computational approaches than physical models, the bulk of the more recent algorithms proposed are based on Linbladian schemes from open quantum systems literature, and the last approach is to model dissipation with an explicit bath. We will briefly discuss these categories in order before moving on to our results. The earliest batch of algorithms for preparing arbitrary thermal states either utilize phase estimation to work explicitly in the Hamiltonian eigenbasis [3] or attempt to adopt the original Metropolis-Hastings algorithm to a quantum setting [1]. These two approaches suffer from serious drawbacks: phase estimation is a rather oblivious algorithm that offers no scenarios for special case analysis to eliminate dimensionful factors, and [1] involves delicate Marriot-Watrous rewinding techniques [4] and offers a tenuous proof of correctness.

The second and largest group of algorithms are those based on Linbladian approaches [5, 6, 7, 8]. These approaches design a Linbladian, typically based on physical models such as the Davies generator [9], and rely on conditions such as the Kubo-Martin-Schwinger (KMS) or the Gelfand–Naimark–Segal (GNS) [10] to show that the thermal state is a fixed point. Proofs of ergodicity are further necessary typically provided separately; for example, ergodicity of the sampler in [5] was not provided until a year later in [6]. These approaches offer many strengths over the previous results: they work for very generic systems, low temperatures, have rigorous proofs of correctness, and have logarithmic error scaling. Some of the downside of these approaches is that they are relatively complex and compiling these routines into concrete circuits is highly nontrivial and sometimes involve intermediate steps of Stochastic Differential Equation (SDE) solvers or operator square roots. Further, many of the runtimes are parametrized by a "mixing time", which is still unbounded for arbitrary non-commuting Hamiltonians at the ground state limit.

The final category of Gibbs samplers involve simulating dissipation with explicit baths. More computational inspired approaches are given by [11, 2] and involve using weak measurement. The algorithm given in [2] relies on phase estimation and [11] relies on careful tuning of measurement probabilities and is modeled via a stopped process, meaning the runtime is stochastic. The closest algorithm to ours is given in [12], in which they propose two algorithms. The first involves time evolution of the system coupled to many ancilla bath qubits with random interactions. This routine is only provably correct for Eigenstate Thermalization Hypothesis (ETH) satisfying Hamiltonians and does not extend to low temperatures. The second algorithm works for arbitrary Hamiltonians but has a prohibitively high failure probability, involves a rejection step similar to [1], and does not extend to low temperatures.

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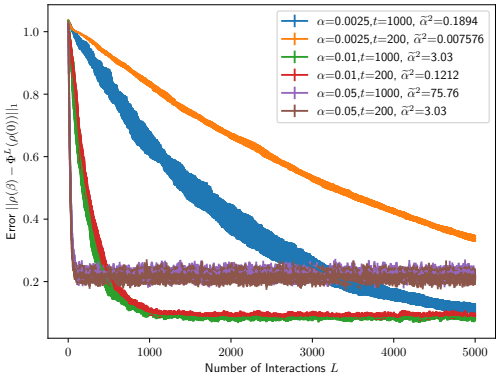
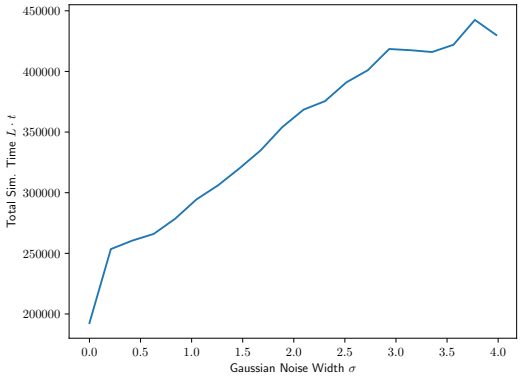


(a) Hydrogen-2 Chain Error



(b) Hydrogen-3 Chain Simulation Time

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