Extended abstract of arXiv:1409.3435

Quantum Gibbs Sampling: the commuting case

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(Dated: September 12, 2014)

Physical systems in nature very often are in thermal equilibrium. Statistical mechanics provides a microscopic theory justifying the relevance of thermal states of matter. However, fully understanding the ubiquity of this class of states from the laws of quantum theory remains an important topic in theoretical physics. The problem can be broken up into two sets of questions: (i) under what conditions does a system thermalize in the long time limit, and (ii) assuming a system does eventually thermalize, how much time does one have to wait before this is so? Our work is concerned with the latter question in the setting of quantum lattice spin systems.

The problem of the speed of thermalization is also of practical relevance in the context of quantum simulators, where one wants to analyze the properties of a real physical system by simulating a controllable idealization of it on a classical or quantum computer. Given that many of the systems which one would want to simulate are thermal, it is an important task to develop simulation and sampling algorithms that can prepare large classes of thermal states of local Hamiltonians. A large body of work has already been done on the classical problem, starting with the development and analysis of Gibbs sampling algorithms of lattice systems called Glauber dynamics, which include the Metropolis and Heat-bath algorithms as spacial cases. A peculiar feature of many of these algorithms is that they often provide reliable results in practice, but a systematic certification of their accuracy and efficiency is often elusive. Although a very hard problem in general, estimation of the convergence time of classical Gibbs samplers has seen a number of breakthroughs in the past few decades. The centerpiece of this theory is a structural theorem which says that the Gibbs state of a local Hamiltonian on a lattice has exponentially decaying correlations *if, and only if,* the Glauber dynamics are rapidly mixing. *In this submission, we extend this main structural theorem to the quantum setting.*

In this submission we will restrict ourselves to commuting Hamiltonians. It is worth noting that the case of commuting Hamiltonians does not effectively reduce to classical systems, as these allow for intrinsic quantum phenomena, such as topological quantum order. In particular, this setting encompasses all stabilizer Hamiltonians, which have been a useful playground for exploring unique quantum features of many-body systems.

The physical relevance of our results is twofold. First, we consider a class of Gibbs samplers (called Davies generators [2]) which can be derived from the weak coupling of a finite quantum system to a large thermal bath. Hence our analysis pertains to the time it takes to reach thermal equilibrium in naturally occurring systems. Secondly, all Gibbs samplers which we consider are local and bounded maps, and therefore can be prepared by dissipative engineering or digital simulation on quantum computers, or quantum simulators [**?**].

Summary of results

In order to present our main results, we need to evoke the theory of non-commutative $\mathbb{L}_p$ spaces. This typically involves an $\mathbb{L}_p$ inner product $\langle f, g\rangle_\rho := \mathrm{tr}\left[\sqrt{\rho} f^\dagger \sqrt{\rho} g\right]$, and a family of $\mathbb{L}_p$ norms $||f||_{p,\rho}^p := \mathrm{tr}\left[\ |\ \rho^{\frac{1}{2p}} f \rho^{\frac{1}{2p}}\ |^p\ \right]$, where f, g are observables, and both objects are defined with respect to some faithful state $\rho > 0$. In our case, ρ is the Gibbs state of a local commuting Hamiltonian of a finite lattice system (see Ref. [1] for a proper definition, and a discussion of the extension of DLR theory to the quantum setting). What we mean by Gibbs sampler is a quantum dynamical semigroup (whose generator $\mathcal{L}$ can be conveniently written in Lindblad form), and with the Gibbs state as its unique stationary state.

We introduce a class of maps called conditional expectations $\mathbb{E}$ which serve as local quasi-projectors onto the Gibbs state of the system. These maps play a central role in our analysis. We identify two special classes of conditional expectations: the first is purely dynamical and inherits many of the properties of the underlying dissipative generator $\mathcal{L}$, the second is purely static, and only depends on the reference (Gibbs) state of the system ρ. We prove that both are local maps when the underlying Hamiltonian is commuting.

We similarly construct two classes of Gibbs samplers: *Davies Generators* and *Heat-Bath Generators*. The Davies generators are obtained from a canonical weak-coupling between a system and a large thermal bath [11], whereas the heat-bath generators are constructed in a manner reminiscent of the classical heat-bath Monte-Carlo algorithm [12]. Generators of Gibbs samplers are characterized by being: (i) generators of completely positive and trace preserving maps, (ii) local, meaning that each individual Lindblad term $\mathcal{L} = \sum_k \mathcal{L}_k$ acts non-trivially only on a constant neighborhood of constant size around k, (iii) locally primitive and locally reversible with respect to the global Gibbs state ρ, (iv) frustration free.

Reversibility means that that the generator $\mathcal{L}$ is similar to a Hermitian (super)-operator, and frustration freedom means that the global stationary state is in the stationary subspace of locally restricted generators. Local primitivity is roughly the property that extending the support of the generator $\mathcal{L}$ decreases the size of the stationary subspace, and the stationary subspace converges to a single point when $\mathcal{L}$ acts on the whole system (see Ref. [1] for proper definitions).

The main purpose of the paper is to show an equivalence between the convergence time of the Gibbs sampler and the correlation behaviour of the Gibbs state. The analogous classical equivalence builds heavily on the DLR theory of boundary conditions [3, 4]. As a naive extension of the DLR theory does not hold for quantum systems, we are lead to define a different notion of clustering (which we call *strong clustering*), that somehow incorporates the *strong mixing* (or complete analyticity) condition for classical systems: for all observables f, and overlapping subsets $A, B \subset \Lambda$, where $A \cap B \neq \emptyset$, and Λ is the full lattice, we get

$$\mathrm{Cov}_{A\cup B}(\mathbb{E}_A(f), \mathbb{E}_B(f)) \leq ||f||^2_{\rho,2}\, e^{-d(A^c,B^c)/\xi}, \tag{1}$$

where A^c (B^c) is the complement of A (B). This condition relies on a conditional covariance, which is identical to the usual covariance ($\langle f - \mathrm{tr}\,[f\rho]\,, g - \mathrm{tr}\,[g\rho]\rangle_\rho$) except that the full expectation ($\mathrm{tr}\,[f\rho]$) is replace by a condition expectation ($\mathbb{E}_A(f)$) with respect to some lattice restriction ($A \subset \Lambda$). We show that Eqn. (1) implies the standard clustering of correlation (which we call *weak clustering*) condition that is more commonly considered in quantum lattice systems. We also flesh out the connection between our notions of clustering and the local indistinguishability of Gibbs states that differ only by a distant perturbation; i.e. a Gibbs state version of the LTQO condition [13].

Having introduced the framework of Gibbs samplers, and defined what we mean by clustering of correlations, the main theorem of our paper can be stated:

Theorem 1 (informal) *Both the Davies Gibbs sampler and Heat-Bath Gibbs sampler of commuting local Hamiltonians have a gap which is independent of the system size if, and only if, the Gibbs state satisfies strong clustering.*

The gap of a Gibbs sampler is defined as the largest non-zero eigenvalue of $\mathcal{L}$ and is related to the rate of convergence of the Gibbs sampler to equilibrium.

We prove the necessity and sufficiency parts of the theorem separately, as they require quite distinct proof techniques. The *only if* statement is proved via methods reminiscent of the analogous classical result [7]. The main idea of the proof is to consider the variational characterization of the spectral gap, and show, by a clever manipulation of conditional variances, that the gap of the Gibbs sampler restricted to a subsystem of minimum side length L is roughly the same as the gap restricted to a subsystem of side length $2L$, whenever strong clustering holds. Then using the same argument iteratively shows that the gap of the dynamics is asymptotically scale invariant. The *if* part of the statement, on the other hand, exploits methods from quantum information theory and quantum many-body theory. In particular, we find a mapping of our problem to properties of frustration-free gapped local Hamiltonians, and leverage the machinery of the so-called detectability lemma of [6].

Our main theorem becomes especially compelling for one dimensional lattice systems, where it was shown by Araki [8] that Gibbs states always satisfy weak clustering. We prove that weak clustering and strong clustering are equivalent for one dimensional systems, getting that all Gibbs samplers in this case are gapped. Exploring our mapping between Gibbs samplers and local Hamiltonians, we also prove that at high enough temperature (independent of the size of the system) the Gibbs samplers are gapped. We then obtain:

Theorem 2 (informal) *Both the Davies or Heat-Bath Gibbs samplers give polynomial-time quantum algorithms for preparing the Gibbs state of every 1D commuting Hamiltonian at any constant temperature. Above a given universal critical temperature T_c, the result this holds true in any dimension.*

We note that since Gibbs states of 1D commuting Hamiltonians are matrix-product operators, one can prepare them efficiently on a quantum computer using e.g. [9] (in fact this is also true for general non-commuting 1D Gibbs states [10]); here we only show another way of preparing them, which might be more resilient to noise in some circumstances.

Finally, we discuss extensions and further implications of our results, including the prospect of rigorous no-go results for self-correcting quantum memories based on stabilizer codes. Indeed, as all stabilizer hamiltonians satisfy LTQO (in the ground state), it is plausible that the under certain circumstances the Gibbs state also satisfies some form of local indistinguishability. This is very close in spirit to the notion of strong clustering which we introduce. Hence if one were able to establish slightly stronger connections between the notions of clustering introduced in Ref. [1], then we could prove rigorous no-go theorems for self-correction based on stabilizer codes, as well as better understand the notion of topological order at non-zero temperature.

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