# Rapid Mixing of Quantum Gibbs Samplers for Weakly-Interacting Quantum Systems

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**Thermalisation** – The theoretical study of thermalisation of quantum many-body systems weakly coupled to a heat bath at a fixed temperature dates back to the work of Davies [1] in the seventies.[1] Since then, the quantum Markov semigroups $e^{t\mathcal{L}}{}_{t\geq 0}$ generated by Lindbladians $\mathcal{L}$ of Davies type have been extensively studied in the mathematical physics literature. It has been shown that, for various relevant quantum systems, these Lindbladians exhibit *fast* thermalisation, occurring within polynomial time in the system size, see, e.g., [4–6] and references therein. The most direct approach to bounding the *mixing time* is to analyse the Lindbladian spectrum and establish a constant lower bound on its gap. There are also techniques which can — in some cases — avoid the need of estimating the spectral gap of the full generator by treating the coherent and dissipative part separately [7]. Nonetheless, a polynomial growth of the mixing time can actually be a severe overestimate, and some Lindbladians can even thermalise *rapidly*, that is, in polylogarithmic time. Such bounds are not obtainable from the spectrum of the Lindbladian, but rather require a finer understanding of the structure of the dynamics.

**Algorithmic aspects** – Davies generators, however, are not directly suitable for algorithmic applications, as their non-local transitions do not directly allow efficient simulation protocols. Recent seminal works on quantum algorithms for Gibbs state preparation have succeeded in combining algorithmic efficiency with an exact notion of *quantum detailed balance* relative to the target Gibbs state [8–10]. These algorithmic Lindbladians mimic the thermalisation of Davies generators while retaining efficient simulability by enforcing locality of the induced jumps. Implementing their dynamics thus constitutes the fully quantum analogue of the highly successful classical *Markov chain Monte Carlo* methods. The central challenge in analysing the complexity of thermal state preparation then lies in bounding the relevant, model-dependent mixing times. In our work, we address this question for a wide range of physically relevant systems. Building on previous rapid mixing results for high-temperature regimes [11, 12] and ground states [13], we establish efficient mixing of quantum Gibbs samplers *at any temperature* for broad classes of weakly interacting quantum systems with varying particle statistics. Specifically, we consider qudit spin, fermionic, and bosonic systems, and prove the following results on their mixing times and consequences:

**Main findings**

- Rapid mixing for weakly-interacting (non-commuting) qudits, governed by Hamiltonians of the form $H = \sum_i h_i + \lambda \cdot V$, where each $h_i$ is supported strictly at qudit $i$, and $\lambda$ is smaller than some explicitly evaluable constant $\lambda_{\max}$.
- Rapid mixing of free fermions, governed by Hamiltonians of the form $H = \sum_{i,j} c_i^\dagger M_{ij} c_j$, as well as weakly-interacting (non-commuting) perturbations of non-hopping fermions with $H = \sum_i \varepsilon_i c_i^\dagger c_i + \lambda \cdot V$, again up to some maximal explicitly evaluable strength $\lambda_{\max}$.
- Adapting techniques from separable qudits to the fermionic case, we also prove rapid mixing for the strongly-interacting regime of the Fermi-Hubbard model, given by $H = -t \sum_{\langle i,j\rangle,\sigma} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \right) + U \sum_{i=1}^n N_{i,\uparrow} N_{i,\downarrow}$. In this setting, the system mixes rapidly up to some maximal explicitly evaluable hopping strength $t_{\max}$ (which depends on $U$ and $\beta$).
- Rapid mixing of free bosons, governed by Hamiltonians of the form $H = \sum_{i,j} a_i^\dagger h_{ij} a_j$, when initiating the evolution in the vacuum state $\rho_0 = |\mathbf{0}\rangle\langle\mathbf{0}|$.
- Consequently, we obtain $\widetilde{\mathcal{O}}(n^2)$ algorithmic complexity for Gibbs state preparation, as well as $\widetilde{\mathcal{O}}(n^4)$ complexity for partition function estimation — using $\widetilde{\mathcal{O}}(n)$ many qubits.
- Our results hold in any fixed dimension and for any constant temperature, and do not require the underlying Hamiltonian to be gapped.

[1] We refer to [2, 3] for modern discussions originating in quantum information.

**Comments** – Rapid mixing times $t_{\text{mix}} = \mathcal{O}(\log(n/\varepsilon))$ have immediate consequences for the corresponding quantum algorithms. As sketched above and following the construction of [9], a logarithmic mixing time brings down the algorithmic complexity to $\widetilde{\mathcal{O}}(n^2 \log(1/\varepsilon))$ query complexity with $\widetilde{\mathcal{O}}(n)$ qubits for Gibbs state preparation. Efficient thermal state preparation can then readily be applied to the calculation of the *partition function* for the corresponding systems, as explained in [12, 14], yielding $\widetilde{\mathcal{O}}(n^4/\varepsilon^2)$ query complexity for the estimation of free energy. Faster mixing times also lead to shallower quantum circuits, making them more suitable for near term quantum devices. On top of that, it has been shown that the dynamics of rapidly mixing Lindbladians is stable under perturbation [15], further improving their potential resilience to noise. Last but not least, the study of rapid mixing is of general interest for several other reasons, like implications on exponential decay of correlations in the steady states [16], and applications to self-correcting quantum memories [17].

**Approach: Non-interacting systems** – Our approach starts from understanding the mixing times of non-interacting systems, which is summarised in the following proposition.

**Proposition 1** (Rapid mixing of non-interacting systems)**.** *For non-interacting quantum systems, including separable qudit spin Hamiltonians $H_s = \sum_{i=1}^n h_i$ with each $h_i$ supported strictly at the qudit $i$, free fermionic Hamiltonians $H_f = \sum_{i,j=1}^n c_i^\dagger M_{ij} c_j$ with $c_i$'s obeying $\{c_i, c_j^\dagger\} = \delta_{ij}$, and free bosonic Hamiltonians $H_b = \sum_{i,j=1}^n a_i^\dagger h_{ij} a_j$ with $a_i$'s obeying $[a_i, a_j^\dagger] = \delta_{ij}$, after making appropriate design choices for the transition operators $\{A_\nu^{(\text{type})}\}_{\nu=1}^{\mathcal{O}(n)}$ as specified in the main text, the algorithmic Lindbladian $\mathcal{L}$ from [9] for Gibbs state preparation mixes rapidly in logarithmic time,*

$$t_{\text{mix}}^{(\text{type})}(\varepsilon) \leq c_1^{(\text{type})} \cdot \log\left(c_2^{(\text{type})} \cdot \frac{n}{\varepsilon}\right), \tag{1}$$

*with $c_1$ and $c_2$ being size-independent constants specified in the main text, where $c_1 \sim \frac{1}{\text{gap}(\mathcal{L})}$, and $\varepsilon$ specifying the accuracy in trace distance.*

**Approach: Perturbation theory** – Subsequently, we wish to understand the behaviour of the mixing times as we perturb the Hamiltonians $H \to H + \lambda \cdot V$. To do so, we firstly need to understand locality of the Lindbladian and strength of the perturbation as in the following lemma.

**Lemma 2.** *Consider a system with $n$ sites. Let $\mathcal{L}^0$ be the algorithmic Lindbladian associated to the non-interacting Hamiltonian $H^0$ and $\mathcal{L}$ that associated to $H = H^0 + \lambda V$. Assume that*

1. *$V = \sum_{r \geq 1} \sum_{C \in C(r)} W_C$, where $C(r)$ is the set of balls of radius $r$ and $\max_{C \in C(r)} \|W_C\| \leq K e^{-\nu r}$*
2. *the jump operators for $\mathcal{L}, \mathcal{L}^0$ are $\{A_\nu^{(\text{type})}\}_{\nu=1}^{\mathcal{O}(n)}$ as previously (and specified for each case in the main text).*

*Denote by $\mathcal{L}_i$ the Lindbladian part associated with all the jump operators at site $i$ and by $\mathcal{L}_i^{(r)}$ its truncation to a ball of radius $r$ around $i$. Then there are constants $C, \chi, C' \geq 0$ such that*

$$\|\mathcal{L}_i^{(r)} - \mathcal{L}_i^{(r-1)}\|_{\infty\to\infty} \leq C e^{-\chi r} \equiv \zeta(r), \quad \|\mathcal{L}_i - \mathcal{L}_i^0\|_{\infty\to\infty} \leq C'|\lambda| \equiv \xi(\lambda). \tag{2}$$

Finally, for suitable systems, we are able to use these properties to argue for the stability of the rapid mixing time, up to some maximal interaction strength $\lambda_{\max}$.

**Theorem 3** (Rapid mixing of perturbed systems)**.** *For separable qudits under (quasi-local) perturbation, given by $H_s(\lambda) = \sum_{i=1}^n h_i + \lambda \cdot V$, and for non-hopping free fermions under (quasi-local) perturbation, given by $H_f(\lambda) = \sum_{i=1}^n \varepsilon_i c_i^\dagger c_i + \lambda \cdot V$, there exist corresponding maximal interaction strengths $\lambda_{\max}$ such that for $|\lambda| \leq \lambda_{\max}$, the Lindbladian $\mathcal{L}$ remains rapidly mixing. Further, the constant $\lambda_{\max}$ can be explicitly evaluated for any given system.*

**Proposition 4** (Rapid mixing of strongly-interacting Fermi-Hubbard model)**.** *For the Fermi-Hubbard model given by* $H = -t\sum_{\langle i,j\rangle,\sigma}\left(c^\dagger_{i,\sigma}c_{j,\sigma} + c^\dagger_{j,\sigma}c_{i,\sigma}\right) + U\sum_{i=1}^{n} N_{i,\uparrow}N_{i,\downarrow}$*, where* $\langle i,j\rangle$ *represents nearest neighbours on the lattice,* $\sigma \in \{\uparrow,\downarrow\}$ *represents the spin of the fermions, and* $N_{i,\sigma} = c^\dagger_{i,\sigma}c_{i,\sigma}$*, there exists a maximal hopping strength* $t_{\max}$ *(which depends on the fixed interaction strength* $U$ *and temperature* $\beta$*) such that for* $|t| \leq t_{\max}$*, the corresponding Lindbladian* $\mathcal{L}$ *mixes rapidly. Further, the constant* $t_{\max}$ *can be explicitly evaluated.*

**Novel techniques** – To prove rapid mixing, which is not accessible by studying the spectrum of the generator on its own, our techniques rely primarily on the study of the *oscillator norm*, which was originally proposed in [18, 19], and more recently employed in [5, 12, 13]. The main technical novelty of our work for rapid mixing proofs lies in the generalisation and adaptation of the oscillator norm to each particular Lindbladian we consider, i.e. making it problem-specific, and hence greatly extending its original applicability. We expect these ideas to pave the way for extensive follow-up work in the quantum information community on understanding rapid mixing of many Lindbladians of interest. This technique further allows for an explicit evaluation of the maximal covered interaction strengths, which is not attainable from the stability of the spectral gap.

**Applications** – Understanding the efficient preparation of thermal states has extensive applications throughout science, from molecular dynamics and material design to quantum optimisation and quantum machine learning. Fermionic systems like the Fermi-Hubbard model are used as a central benchmark in computational physics, as well as for modelling high-temperature superconductors and phase transitions between metals and insulators. Perturbed qudit systems cover for example spin Hamiltonians like the Heisenberg model in a strong external magnetic field. Having at hand the demonstrated end-to-end polynomial time quantum algorithms for resolving the phase diagram of such systems, promises strong quantum advantages in quantum simulation compared to state-of-the-art classical methods (although larger scale numerics for classically hard regimes would reveal more on that point). We emphasise that in contrast to popular quantum phase estimation based methods around ground state energy estimation — which suffer from the Ansatz state bottleneck — the presented complexities here are truly end-to-end.

**Conclusion** – Our work provides the first rapid mixing results of dissipative quantum algorithms for preparing thermal states of weakly-interacting qudit and fermionic systems *at any temperature*. As far as we are aware, we also provide the first rapid mixing result for any bosonic Lindbladian. The improved mixing times scaling logarithmically further imply several desirable qualities, such as, e.g., increased resilience towards noise. We believe this work constitutes a paradigm shift in quantum simulation: It significantly advances the state of the art by showing that recent digital schemes based on Lindbladian dynamics can be made efficient for a wide class of physically relevant and classically hard models, offering pathways towards practical quantum advantage.

*We note that after our paper has been published, a new work [20] has proven an efficient classical algorithm for calculating local expectation values in the thermal states of weakly-interacting fermions, as well as evaluating their partition functions. This lowers the expectations of a strong quantum advantage in these weakly-interacting regimes, however, we remark that not all cases covered by our work currently have an efficient classical counterpart. Moreover, while this classical algorithm is designed specifically for the weakly-interacting regime, dissipative quantum Gibbs sampling has the potential to be efficient beyond this regime, only our analysis is restricted to weak perturbations.*

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