

# A Subpolynomial-Time Algorithm for the Free Energy of One-Dimensional Quantum Systems in the Thermodynamic Limit

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## Abstract

We introduce a classical algorithm to approximate the free energy of local, translation-invariant, one-dimensional quantum systems in the thermodynamic limit of infinite chain size. While the ground state problem (i.e., the free energy at temperature  $T = 0$ ) for these systems is expected to be computationally hard even for quantum computers, our algorithm runs for any fixed temperature  $T > 0$  in subpolynomial time, i.e., in time  $O((\frac{1}{\varepsilon})^c)$  for any constant  $c > 0$  where  $\varepsilon$  is the additive approximation error. Previously, the best known algorithm had a runtime that is polynomial in  $\frac{1}{\varepsilon}$  where the degree of the polynomial is exponential in the inverse temperature  $1/T$ . Our algorithm is also particularly simple as it reduces to the computation of the spectral radius of a linear map. This linear map has an interpretation as a noncommutative transfer matrix and has been studied previously to prove results on the analyticity of the free energy and the decay of correlations. We also show that the corresponding eigenvector of this map gives an approximation of the marginal of the Gibbs state and thereby allows for the computation of various thermodynamic properties of the quantum system.

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## 1 Introduction and Main Result

Multipartite quantum systems are described by a Hilbert space, which is a tensor product of the single-particle  $d$ -dimensional spaces. The behaviour of a quantum-many body system is described by a Hamiltonian which models the interaction between the different particles. Of particular interest are  $k$ -local Hamiltonians that can be written as a sum of terms acting nontrivially on at most  $k$  particles, with  $k$  being a constant. At thermal equilibrium, the system is described by the Gibbs state



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$$\rho = e^{-\beta H} / Z_\beta(H) \quad (1)$$

where  $\beta = 1/T$  is the inverse temperature, and  $Z_\beta(H) = \text{tr} [e^{-\beta H}]$  is the partition function. The free energy of the system at inverse temperature  $\beta$  is defined as

$$F_\beta(H) = -\frac{1}{\beta} \log Z_\beta(H). \quad (2)$$

At zero temperature, i.e.,  $\beta = +\infty$ ,  $F_\beta(H)$  becomes  $\lambda_{\min}(H)$ , the ground energy of  $H$ . The problem of computing the ground energy for a given local Hamiltonian is known to be QMA-complete [14], and is the central problem in the area of Hamiltonian complexity [10]. This problem remains QMA-complete even if we restrict ourselves to 2-local Hamiltonians that are translation-invariant on a chain [11, 4], i.e.,  $H = \sum_i h_{i,i+1}$  where the operators  $h_{i,i+1}$  are given by some Hermitian operator  $h$  (the same one for every  $i$ ) acting on particles  $i$  and  $i + 1$ .<sup>1</sup>

In order to understand the physical properties of the system at nonzero temperature, it is crucial to understand not only the ground energy, but also the free energy function  $F_\beta(H)$  as a function of  $\beta > 0$  [2]. Indeed, computing  $F_\beta(H)$  and its derivatives with respect to  $\beta$  and parameters of the Hamiltonian determines phase transitions and gives access to fundamental physical properties of the system in thermal equilibrium such as the internal energy, specific heat, or magnetic susceptibility [19].

## 1.1 Main result

In this paper, we focus on 2-local translation-invariant quantum systems on an infinite chain. As the free energy scales with the system size, in the thermodynamic limit of infinite systems we consider the free energy per particle  $f_\beta(h)$ . Note that  $f_\beta(h)$  only depends on the finite matrix  $h$  of size  $d^2 \times d^2$ . Our objective is to design an algorithm to approximate  $f_\beta(h)$  with a good scaling in terms of the target error  $\varepsilon$  and the local dimension  $d$ . As argued in recent works on Hamiltonian complexity in the thermodynamic limit [25, 1], understanding the dependence of the complexity in terms of the desired precision for infinite systems is often closer to capturing the fundamental problems in many-body physics than understanding the dependence in the system size. Our main result is an algorithm that given as input  $h$  and a target error  $\varepsilon$  outputs an approximation of  $f_\beta(h)$  and of the  $k$ -particle marginals of the Gibbs state.

► **Theorem 1.** *There is a deterministic algorithm that takes as input a Hermitian operator  $h$  acting on  $\mathbb{C}^d \otimes \mathbb{C}^d$  satisfying  $\|h\| \leq 1$  and  $\varepsilon \in (0, 1/e)$  and outputs an approximation  $\tilde{f}_\beta$  satisfying  $|\tilde{f}_\beta - f_\beta(h)| \leq \varepsilon$ , where  $f_\beta(h)$  is the free energy per particle of the infinite translation-invariant Hamiltonian on a chain defined by  $h$ . For any fixed  $\beta > 0$ , the running time of the algorithm is  $\exp\left(O\left(\log d \frac{\log(1/\varepsilon)}{\log \log(1/\varepsilon)}\right)\right)$ . Moreover, this algorithm can also compute an  $\varepsilon$ -approximation of the marginal of the Gibbs state on an interval of size  $k$  with the same running time for any fixed  $k$ .*

Before describing the algorithm and proof method, we make some remarks and discuss related works.

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<sup>1</sup> Technically, because of the choice of specification of input in [11], the problem is complete for a scaled version of QMA called  $\text{QMA}_{\text{EXP}}$ .

## Remarks

We note that the temperature dependence of the running time is hidden in the  $O(\cdot)$  notation as we are interested in the algorithm for fixed temperature. If we want to make the dependence on the inverse temperature  $\beta$  explicit, the running time takes the form  $\exp\left(O\left(\log d \frac{\log(1/\varepsilon)}{\log \log(1/\varepsilon)}\right) \exp(O(\beta))\right)$ , where  $O(\cdot)$  only hides universal constants.<sup>2</sup> An improvement to an exponential dependence in  $\beta$  should not be expected due to the  $\text{QMA}_{\text{EXP}}$ -hardness of the ground energy problem [11]. The ground energy can be approximated by the free energy for a large value of  $\beta$ . In particular, by reduction of the ground state problem to the free energy problem, we establish  $\text{QMA}_{\text{EXP}}$ -hardness of the infinite translation-invariant free energy problem with the temperature as an additional problem input. This shows that, unless  $\text{QMA}_{\text{EXP}} = \text{EXP}$ , no algorithm can have a running time of the form  $\exp(\text{polylog}(\beta, 1/\varepsilon))$ .

To appreciate the algorithm we use to prove Theorem 1, it is instructive to consider first a naive algorithm for this problem sometimes called exact diagonalization. The idea of this algorithm is to consider the Hamiltonian  $H_{[1,n]} = \sum_{i=1}^{n-1} h_{i,i+1}$  restricted to only  $n$  particles. Computing the free energy per particle  $f_{\beta,n}$  of  $H_{[1,n]}$  (for any value of  $\beta$ ) can be done in time polynomial in  $d^n$  by explicitly writing the  $d^n \times d^n$  matrix  $H_{[1,n]}$ . The sequence  $f_{\beta,n}$  does converge to  $f_\beta$  as  $n \rightarrow \infty$ , but the convergence is in general slow with an error decaying as  $\frac{1}{n}$  due to the missing interaction term at the boundary. As a result, for a desired precision  $\varepsilon$ , we obtain a runtime which is exponential in  $1/\varepsilon$ . In order to obtain the subpolynomial dependence on  $1/\varepsilon$  in Theorem 1, we need to develop a more refined algorithm.

## 1.2 Related work

In recent years, there have been multiple works about computing the free energy (or equivalently the partition function) at finite inverse temperature for a given Hamiltonian. In particular, for local Hamiltonians on an arbitrary bounded-degree graph, algorithms have been developed in [15, 12, 18] with performance guarantees when the inverse temperature  $\beta$  is below some critical inverse temperature. The runtime of these algorithms is polynomial or quasi-polynomial in the number of particles and in  $1/\varepsilon$ . These works rely on the so called cluster expansion, which, at its core, is a Taylor expansion of the partition function at  $\beta = 0$ . Truncating this expansion at a certain order and bounding the remainder terms allows for the approximation of the free energy for  $\beta$  small enough. Indeed, the sum of remainder terms no longer converges if  $\beta$  is too large which introduces a critical inverse temperature above which such algorithms do not have convergence guarantees.

However, a different method was used in [16] to obtain an algorithm for all temperatures for one-dimensional finite quantum systems. This algorithm combines several results from the analysis of 1D-systems: quantum belief propagation [13], together with a locality result about Gibbs states which was only recently proven in general [6]. For a system of  $n$  particles in 1D, the running time of the algorithm is  $n(\frac{1}{\varepsilon})^{O(1)}$ , where  $O(1)$  is a constant that depends exponentially on  $\beta$ . This algorithm can readily be applied to the infinite translation-invariant chain by setting  $n = 1/\varepsilon$  and this leads to an algorithm that is polynomial in  $1/\varepsilon$ . For its implementation, the algorithm involves several choices of length scales to ensure convergence and numerical integrations to obtain the operators from the belief propagation.

<sup>2</sup> The dependence is worse when computing marginals of the Gibbs state, see full version [8].

In a different regime, classical algorithms have been designed in [7] to compute the free energy of dense Hamiltonians based on convex relaxations. These algorithms have a runtime that is exponential in  $1/\varepsilon$ .

Besides this line of work on provably convergent algorithms to which our work shall also contribute, there are numerous algorithms that effectively address the problem despite having no convergence results or only in special cases. For the free energy problem this includes most notably Quantum Monte Carlo methods [24, 23]. These probabilistic algorithms lack rigorous results on their runtime except for few special cases and are known to fail for Hamiltonians that have the so-called sign problem. Another example of effective algorithms for the ground state energy problem ( $\beta = +\infty$ ) in one dimension are tensor networks and the DMRG algorithm [26, 20]. The convergence of a related algorithm to the ground state energy has been proven under the additional assumption that the Hamiltonian is gapped [17].

### 1.3 Proof technique

Before giving an overview of the algorithm establishing Theorem 1, it is worth mentioning that the analogous classical problem has a very simple solution. In fact, using the technique of transfer matrices (see e.g. [9]), for any  $\beta$  the free energy per particle can be obtained from the eigenvalue of a simple  $d \times d$  matrix and thus the problem reduces to standard numerical algorithms applied to some fixed matrix. This implies very efficient algorithms for any  $\beta$  including  $\beta = +\infty$ .

However, the quantum case is significantly more complicated. This is illustrated for example by the fact that, when  $\beta = +\infty$ , the problem is QMA-hard, and also that the simple Markov property for classical Gibbs states in one-dimension does not hold in the quantum setting. In his seminal work, Araki [3] proposed a quantum analogue of the transfer matrix, but it is a linear map between infinite-dimensional spaces. In our algorithm, we use a finite-dimensional approximation to this map. Our main technical result is to prove that the spectral radii of these finite-dimensional approximations converge superexponentially fast to  $e^{-\beta f_\beta(h)}$ . The algorithm (see Algorithm 2) is then simply to choose the finite-dimensional approximation parameter  $L$  for the transfer matrix as a function of the desired precision  $\varepsilon$  and then compute the spectral radius of the corresponding linear map.

■ **Algorithm 2** Algorithm for computing the free energy per particle. The constant  $C$  is a number that can be obtained from our proofs.

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**Parameters:** Inverse temperature  $\beta$ , universal constant  $C$   
**Input:**  $d$  local dimension, Hamiltonian term  $h \in \mathbb{C}^{d^2 \times d^2}$  such that  $\|h\| \leq 1$ , error  $\varepsilon$   
**Output:**  $\tilde{f}_\beta$  approximation to the free energy  $f_\beta(h)$

- 1  $L \leftarrow \log(1/\varepsilon) \exp(C(\beta + 1)) / \log(\log(1/\varepsilon));$  /\* parameter for approximation \*/  
/\* matrix representation of linear map from  $\mathbb{C}^{d^{L-1} \times d^{L-1}}$  to itself: \*/
- 2  $\mathcal{L}_L^*(\cdot) \leftarrow \text{tr}_L (e^{-\beta H_{[1,L]}/2} e^{\beta H_{[2,L]}/2} (\mathbf{1} \otimes \cdot) e^{\beta H_{[2,L]}/2} e^{-\beta H_{[1,L]}/2});$
- 3  $r_L \leftarrow$  spectral radius of  $\mathcal{L}_L^*$ ;
- 4  $\tilde{f}_\beta \leftarrow -(\log r_L) / \beta$ ;

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To analyse the algorithm we make extensive use of Araki's expansions [3] to show that the marginal  $\rho_L$  on the first  $L-1$  sites of the infinite Gibbs state, is an *approximate eigenvector* of the finite-dimensional map  $\mathcal{L}_L^*$ , i.e., that  $\|\mathcal{L}_L^*(\rho_L) - e^{-\beta f_\beta(h)} \rho_L\|_1$  decays superexponentially fast in  $L$ . By using variational expressions of the spectral radius of positive maps (so called Collatz-Wielandt formula), this allows us to show that the spectral radius of  $\mathcal{L}_L^*$

is superexponentially close to  $e^{-\beta f_\beta(h)}$ . We note that standard perturbation bounds for eigenvalues of non-normal operators have a very bad dependence on dimension, and are thus not usable here, see e.g., [5, Chapter VIII]. To prove that the corresponding eigenvector of  $\mathcal{L}_L^*$  is close to  $\rho_L$ , we establish a quantitative *primitivity* condition for  $\mathcal{L}_L^*$ , i.e., we prove that a sufficiently high power of  $\mathcal{L}_L^*$  maps nonzero positive semidefinite operators to positive *definite* ones. Using tools from the Perron-Frobenius theory of positive operators – more precisely the Hilbert projective metric –, this allows us to show that  $\rho_L$  is superexponentially close to the eigenvector of  $\mathcal{L}_L^*$  associated to its spectral radius.

Let us also mention that the above techniques based on [3] are specific to one dimension. In particular, the results in there are related to the absence of thermal phase transitions, which do occur in higher dimensions so an extension of this approach to higher dimension is not possible, see also [21, 22] for hardness results of the classical partition function on bounded degree graphs.

## 1.4 Numerical implementation

We also implement our algorithm and run it on a Hamiltonian for which the free energy function is known exactly. We observe very small errors (machine precision) already for moderate choices of  $L$ . We also observe that for this example the scaling of the error with inverse temperature is better than the worst-case estimates derived theoretically.

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