The Importance of the Spectral Gap in Estimating Ground-State Energies

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Abstract

The field of quantum Hamiltonian complexity lies at the intersection of quantum many-body physics and computational complexity theory, with deep implications to both fields. The main object of study is the Local Hamiltonian problem, which is concerned with estimating the ground-state energy of a local Hamiltonian and is complete for the class QMA, a quantum generalization of the class NP. A major challenge in the field is to understand the complexity of the Local Hamiltonian problem in more physically natural parameter regimes. One crucial parameter in understanding the ground space of any Hamiltonian in many-body physics is the spectral gap, which is the difference between the smallest two eigenvalues. Despite its importance in quantum many-body physics, the role played by the spectral gap in the complexity of the Local Hamiltonian problem is less well-understood. In this work, we make progress on this question by considering the precise regime, in which one estimates the ground-state energy to within inverse exponential precision. Computing ground-state energies precisely is a task that is important for quantum chemistry and quantum many-body physics.

In the setting of inverse-exponential precision (promise gap), there is a surprising result that the complexity of Local Hamiltonian is magnified from QMA to PSPACE, the class of problems solvable in polynomial space (but possibly exponential time). We clarify the reason behind this boost in complexity. Specifically, we show that the full complexity of the high precision case only comes about when the spectral gap is exponentially small. As a consequence of the proof techniques developed to show our results, we uncover important implications for the representability and circuit complexity of ground states of local Hamiltonians, the theory of uniqueness of quantum witnesses, and techniques for the amplification of quantum witnesses in the presence of postselection.

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1 Introduction and Main Results

The local Hamiltonian problem is a central object in the field of Hamiltonian complexity, a field of study at the intersection of quantum information, many-body physics, and complexity theory. This problem concerns finding the ground-state energy of a Hamiltonian defined on n qubits to an additive error, or the "promise gap", that scales as an inverse polynomial in n. Kitaev's famous result establishing the QMA-completeness of this problem gives strong evidence that it is intractable for general k-local Hamiltonians [20]. Since then, there has been a concerted effort to understand the complexity of this problem in more physically natural settings. First, we have seen this from the perspective of strengthened hardness results, where the problem has been studied with additional physically motivated constraints on the Hamiltonian [25, 4, 6, 15]. From the other side, heuristic quantum algorithms such as the variational quantum eigensolver (VQE) have been proposed to compute ground-state energies of certain specific classes of Hamiltonians [26]. Understanding more rigorously the conditions under which heuristic algorithms can hope to be successful in spite of hardness results has become a major open question for the field.

To understand this better, we need to identify certain structural properties of Hamiltonians that could help us classify their complexity. In this work, we focus on two often-identified properties of Hamiltonians that may make the local Hamiltonian problem easier, neither of which has been completely characterized from the perspective of complexity theory.

The first of these is the spectral gap, defined to be the difference between the ground-state energy and the energy of the first excited state. The spectral gap is an important quantity in the study of any physical Hamiltonian, and is known to make the study of ground-state physics significantly more tractable in certain specific senses, such as in one dimension [16, 21]. From the perspective of hardness results, however, it has been noted [8, 14] that current techniques (namely the clock construction) will not suffice to argue for the hardness of Hamiltonians with a constant spectral gap. Indeed, it is currently unknown whether the local Hamiltonian problem stays QMA-hard even with an inverse-polynomial lower bound on the spectral gap, despite efforts in this direction [3, 17].

Another possible structural property that could potentially make estimating ground-state energies easier is the existence of a polynomial-size description of the ground state, such as a tensor-network description (see, e.g. [7]) or a circuit to prepare the ground state. In the language of complexity theory, the question of whether such classical descriptions (or "witnesses") can simplify the local Hamiltonian problem is the subject of the QMA vs. QCMA question [2, 10].

In this work, we make progress on both of these questions in a potentially less natural context: the precise regime, where we estimate the ground-state energy to inverse-exponential precision. Despite this, we will be able to use the additional flexibility afforded by this setting to prove very general complexity separations which seem beyond the capabilities of present techniques in the setting of inverse-polynomial precision. In the regime of inverse-exponential precision, it is known from prior results [11, 12] that the local Hamiltonian problem is PreciseQMA$(=$ PSPACE$)$-complete in general.

Table 1 Complexity of variants of the local Hamiltonian problem in the setting of inverse-exponential promise gap. The column "Low circuit-complexity promise" corresponds to problems where one is promised the existence of a polynomial-sized circuit to prepare a low-energy state, which corresponds to a classical witness. The problems in the third column have no such promise and correspond to a quantum witness. The row with $\Delta = 0$ corresponds to the usual setting of there being no promise on the spectral gap. The row with $\Delta = 1/\mathsf{poly}(n)$ denotes the modified problem in which there is an inverse-polynomial lower bound on the spectral gap.

Spectral gap (Δ)	Low circuit-complexity promise	No promise on circuit complexity
$1/\mathsf{poly}(n)$	PP-complete	PP-complete
0	$\mathsf{NP}^{\mathsf{PP}}$-complete	PSPACE-complete [12]

Result 1

The first main result of our work [9] is that in the setting of inverse-exponential precision, the existence of a spectral gap provably makes a difference in the complexity of the local Hamiltonian problem. Specifically, we show that under the promise of an inverse-polynomial lower bound on the spectral gap, denoted as $\Delta = \Omega(1/\mathsf{poly}(n))$, the analogous problem is PP-complete. Assuming the commonly-held belief that $\mathsf{PP} \neq \mathsf{PSPACE}$, we see that a lower bound on the spectral gap greatly reduces the complexity from PSPACE to PP.

Result 2

Secondly, in the same setting of inverse-exponential precision and inverse-polynomial spectral gap, we show that a quantum witness offers no advantage over a classical witness. Namely, in this specific setting, QMA equals QCMA. Moreover, both these classes collapse to PP.

It is important to note that the result above is truly a consequence of the spectral gap, not the increased precision alone. This is because when there is no lower bound on the spectral gap, the precise versions of QMA and QCMA are $\mathsf{PreciseQMA} = \mathsf{PSPACE}$ and $\mathsf{PreciseQCMA} = \mathsf{NP}^{\mathsf{PP}}$ [23, 13], respectively, which are believed to be distinct. The results in the previous two paragraphs are summarized in Table 1.

Discussion

Therefore, to summarize, we have given a rigorous setting in which a). The spectral gap strictly reduces the complexity of the local Hamiltonian problem (assuming $\mathsf{PP} \neq \mathsf{PSPACE}$), and b). When there is a lower bound on the spectral gap, the promise of there being an efficient description of the ground state makes no difference to the complexity of the local Hamiltonian problem.

This brings up the tantalizing possibility that an inverse-polynomial spectral gap already implies the existence of a polynomial-size circuit to prepare a low-energy state of the Hamiltonian. This conjecture, if true, would explain why allowing the witness to be quantum does not help. Further, in the non-precise regime, this conjecture would imply that many important Hamiltonians (in particular, those with inverse-polynomial spectral gaps) have ground states with polynomial circuit complexity. This implication might yield cases where heuristic algorithms could potentially succeed in finding ground-state energies. Our study is also of interest to the high-energy and gravitational physics communities [18, 28], since preparing a low-energy state of an interacting quantum field theory is the first step in simulating it on a quantum computer.

In the regime of inverse-exponential precision, our work explains a seemingly puzzling fact, namely the PSPACE-completeness of the local Hamiltonian problem [12]. This fact is counterintuitive because in the regular setting of inverse-polynomial precision, QMA is in the class PP [22]; and moreover, the classical class "PreciseP", is, by definition, PP. Therefore, there is an unexplained boost in complexity from PP to PSPACE when the precision is changed from inverse-polynomial to inverse-exponential. Our work shows that this boost is in fact a consequence of tiny spectral gaps, specifically those scaling inverse-exponentially in the system size.

Moreover, we note that our results in the precise regime serve to rule out techniques in the non-precise regime, much in the same way as how oracle results rule out techniques that relativize with respect to the oracle. As an example, our results imply that any proof attempt to show QMA-hardness of the local Hamiltonian problem with a spectral gap in the regular setting must not carry over to the precise regime (unless PP = PSPACE). Similarly, as a result of our proof techniques, we rule out a sufficiently strong "in-place amplification" [22, 24] for a class called postQMA [23].

Techniques

In order to prove our results in the setting of inverse-exponential promise gaps, we introduce a few techniques that might be more broadly applicable in Hamiltonian complexity.

The first of these is a technique to obtain local Hamiltonians with nontrivial lower bounds on the spectral gap. The technique is a modification of the clock construction [20, 19], where we allow for the penalty term at the end of the verifier's circuit to be of small strength, say $\Theta(1/\mathsf{poly}(n))$ or $\Theta(1/\exp(n))$. We call this the small-penalty clock construction. This construction enables us to apply formal tools like the Schrieffer-Wolff transformation [27, 5]. This, in turn, enables us to analytically track the entire low-energy spectrum of the Hamiltonian resulting from the clock construction, instead of only keeping track of the ground-state energy. We also anticipate this technique to be more widely applicable in other situations in the precise regime, such as for modified clock constructions based on perturbation theory and clock constructions dealing with constraints such as spatial locality and translation-invariance.

In order to show a PP upper bound on the complexity of the local Hamiltonian problem with a lower bound on the spectral gap in the precise regime, we use a technique commonly known as the power method. This method relies on the idea that by taking powers of a matrix with a spectral gap, the limiting behavior converges to that of the eigenstate with extremal eigenvalue. This method also has a physical interpretation. The idea is that time-evolving the maximally mixed state under the Hamiltonian H for "imaginary time" $-i\beta$ produces the state $\rho \propto \exp[-2\beta H]$. This state, in the limit of large β, has a large enough overlap with the ground state if the spectral gap is lower bounded. The map produced by imaginary-time evolution $\exp[-\beta H]$, while not unitary, is nevertheless linear, and a PP(= postBQP) algorithm can simulate linear maps of this form [1]. We show that in PP, it is possible to simulate the action of the operation $\exp[-\beta H]$ to inverse-exponential precision. This allows us to give a PP upper bound on the complexity of precisely computing ground-state energies of Hamiltonians with an inverse-polynomial spectral gap.

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