Spectral Gap Amplification

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Many problems in quantum information reduce to preparing a specific eigenstate of some Hamiltonian H. The generic cost of quantum algorithms for these problems is determined by the inverse spectral gap of H for that eigenstate and the cost of evolving with H for some fixed time. The goal of spectral gap amplification is therefore to construct a Hamiltonian H' with the same eigenstate as that of H but a bigger spectral gap, requiring that constant-time evolutions with H' and H can be implemented with nearly the same cost. We show that a quadratic spectral gap amplification is possible when H satisfies a frustration-free property and give H' for this case. This results in quantum speedups for some adiabatic evolutions. Defining a suitable oracle model, we establish that the quadratic amplification is optimal for frustration-free Hamiltonians and that no spectral gap amplification is possible if the frustration-free property is removed. A corollary is that finding a similarity transformation between a stoquastic Hamiltonian and the corresponding stochastic matrix is hard in the oracle model, setting strong limits in the power of some classical methods that simulate quantum adiabatic evolutions. Implications of spectral gap amplification for quantum speedups of optimization problems and the preparation of projected entangled pair states (PEPS) are discussed.

I. INTRODUCTION

It is well known that many problems in physics and optimization, such as describing quantum phases of matter or solving satisfiability, can be reduced to the computation of low-energy states of Hamiltonians (see, e.g.[1, 2]). Methods to compute such states exist, with adiabatic state transformation (AST) being one of the most acknowledged and powerful heuristics for that goal [2–7]. Typically, the problem in AST involves transforming a pure quantum state $|\psi_0\rangle$ into $|\psi_1\rangle$; these being the endpoints of a state path $|\psi_s\rangle$, $0 \leq s \leq 1$. Each $|\psi_s\rangle$ is an eigenstate of a Hamiltonian $H(s)$. One strategy to solve the AST problem is given by the quantum adiabatic theorem and requires smoothly changing the interaction parameter s in time [8, 9], but more efficient strategies exist [10–12].

Methods to solve the AST problem typically require evolving with the Hamiltonians for some time $T > 0$, which determines the cost of the method and depends on properties of the path. Let L be the angular length determined by $\{|\psi_s\rangle\}_{0\leq s\leq 1}$ and $\Delta_s \geq \Delta$ the spectral gap to the other nearest eigenvalue of $H(s)$. Recently, we provided fast quantum methods for eigenpath traversal that do not exploit the structure of the Hamiltonians and prepare $|\psi_1\rangle$ from $|\psi_0\rangle$ in optimal time $T \in \Omega(L/\Delta)$ [12, 13]. If required, such evolutions can be simulated in the standard circuit model of quantum computing using Trotter-Suzuki-like formulas available in the literature [14, 15]. The resulting circuit size increases with T, usually as $T^{1+\gamma}$, and $\gamma > 0$ an arbitrary constant. Ref. [13] does not forbid, however, the existence of faster methods for solving the AST problem if additional knowledge of the structure of $H(s)$ is available. Our paper focuses on this observation and introduces the spectral gap amplification problem or GAP, which roughly answers: For which $H(s)$ can we construct $H'(s)$ that also has $|\psi_s\rangle$ as eigenstate, but spectral gap $\Delta'_s \gg \Delta_s$?

When spectral gap amplification is possible, it can be used as a technique to find new quantum speedups. In [16, 17], for example, we constructed the so-called quantum simulated annealing algorithm that provided speedups of the well-known simulated annealing method implemented using Monte-Carlo. The reason for such speedups is a gap amplification step: if Δ is the spectral gap of the stochastic matrix S used in Monte-Carlo, there is a Hamiltonian H' with spectral gap $\Delta' \geq \sqrt{\Delta}$ and eigenstate that allows to sample from the fixed point of S. To build H' we used previously-developed tools for quantum walks [18, 19].

Motivated by the results in [16, 17] we study the GAP in different scenarios. We first show that, for Hamiltonians that satisfy a frustration-free property [20–23], a quadratic spectral gap amplification is possible and *optimal* in some suitable oracle model. Quadratic spectral gap amplification was previously known only for Hamiltonians that result from a similarity transformation of stochastic matrices [16–18]. These Hamiltonians, which are the so-called discriminants of stochastic matrices, are also stoquastic, i.e. the off-diagonal entries are non-positive. A direct

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consequence of our new construction is that spectral gap amplification can now be achieved for frustration-free Hamiltonians used in quantum adiabatic simulations of quantum circuits, improving upon the results in [24–26]. The eigenstate in our construction is not the lowest-energy state of the Hamiltonian induced by the quantum circuit (which was the case in [24–26]). Nevertheless, techniques for AST work for any eigenstate and still apply to our case, giving more efficient quantum adiabatic simulations to prepare the circuit's output state. In addition, some low-energy eigenstates of general frustration-free Hamiltonians (termed PEPS) were shown to play an important role in physics, renormalization, and optimization [20, 23, 27]. Fast methods to prepare PEPS are desired. Our method for spectral gap amplification can be used to speedup the preparation of PEPS on a quantum computer, with an expected improvement of other methods for this goal (e.g., [28]).

Interestingly, it seems hard to achieve spectral gap amplification for Hamiltonians that do not satisfy the frustration-free property. We support this claim by showing that, in an oracle model in which Hamiltonians are given as matrix oracles, no gap amplification is possible. It would otherwise imply quantum methods to solve, for example, the search problem in time less than than $\sqrt{N}$. This would contradict known complexity bounds [29]. Moreover, our technique for quadratic gap amplification of a frustration-free H outputs a Hamiltonian H' that approximates $\sqrt{H}$, and hence the amplification. (The approximation is not direct from our construction but can be made precise). However, even deciding whether a general Hamiltonian H has a Hermitian square root or not (or, equivalently, whether H is semidefinite positive or not) with some polynomially-small error bound is hard, as a solution to this problem could be used to estimate the lowest eigenvalue of H, a problem in the class QMA [30].

Our previous result on no general gap amplification has additional consequences. For example, it is known that stoquastic Hamiltonians are related to stochastic matrices through a similarity transformation [21, 31, 32]. The fixed point of the stochastic matrix is given by the probability distribution obtained after a simple measurement is made in the ground state of the Hamiltonian. Finding such stochastic matrix would allow us to build a Monte Carlo method to sample from the fixed point and classically solve the AST problem in this case. Further, it would allow us to specify the stoquastic Hamiltonian as a frustration-free one. Because no gap amplification is possible in general, finding the stochastic matrix is hard (in the oracle model), or otherwise we could use the results in [16] to amplify the gap.

A. Theorems and overview of proofs

To state our results we first formulate the GAP in more detail:

Definition 1. *Let $H \in \mathbb{C}^N \times \mathbb{C}^N$ be a finite-dimensional Hamiltonian, $|\psi\rangle$ a (unique) eigenstate of H with eigenvalue λ, and Δ the gap to the other nearest eigenvalue of λ; i.e. Δ is the spectral gap. The goal of the GAP is to find a new Hamiltonian H' that has $|\psi\rangle \otimes |\mathsf{o}\rangle$ as (unique) eigenstate and eigenvalue gap $\Delta' \in \Omega(\Delta^{1-\epsilon})$, for $\epsilon > 0$. $|\mathsf{o}\rangle$ is any subsystem's state for which an efficient quantum circuit is known. The implementation cost of $\exp\{-iH't\}$ in the circuit model must be of the same order as the implementation cost of $\exp\{-iHt\}$.*

The last requirement forbids naive constructions such as $H' = cH$ for $c \gg 1$. If both H and H' have a bounded number of (efficiently computable) non-zero entries per row (i.e., they are sparse) the last requirement can be satisfied [14, 33–35].

Definition 2. *A Hamiltonian $H \in \mathbb{C}^N \times \mathbb{C}^N$ is frustration free if it is efficiently specified as $H = \sum_{k=1}^{L} \alpha_k \Pi_k$, with $0 \le \alpha_k \le 1$, $(\Pi_k)^2 = \Pi_k$ projectors, and $L \in \mathcal{O}[polylog(N)]$. Further, if $|\psi\rangle$ is a ground state (i.e., a lowest-eigenvalue eigenstate) of H, then $\Pi_k|\psi\rangle = 0 \;\forall\; k$.*

$|\psi\rangle$ is then a ground state of every term in the decomposition of H. Frustration-free Hamiltonians naturally appear as the "parent" Hamiltonians of projected entangled pair states (PEPS) that are useful variational states reproducing the local physics with high accuracy [27, 36] and for optimization problems [31]. With no loss of generality we assume that $\alpha_k = 1 \;\forall k$. (Note that the gap of H cannot decrease by making all the α_ks equal to 1.) Then $H = \sum_k \Pi_k$ is still frustration free, it has $|\psi\rangle$ as ground state, and $\|H\| \le L$. While the Π_k's often correspond to local operators, we do not make that assumption here.

Our first result on the GAP is:

Theorem 1. *Let $H = \sum_{k=1}^{L} \Pi_k$ be a frustration-free Hamiltonian, $|\psi\rangle$ a ground state, and Δ the lowest nonzero eigenvalue or spectral gap. Then, there exists a Hamiltonian H' satisfying $H'|\psi\rangle|\mathsf{o}\rangle = 0$, $\|H'\| \le 1$, and the corresponding spectral gap of H' is $\Delta' \in \Omega(\sqrt{\Delta/L})$. There are no other eigenstates of H' with eigenvalue 0.*

Proof. (Sketched.) The proof is constructive and is based on geometry arguments. It reduces to finding a unitary operator acting on a bigger Hilbert space that satisfies

$$PUP = (\mathbb{1} - (2/L)H) \otimes P \;, \tag{1}$$

where $P = |\mathfrak{o}\rangle\langle\mathfrak{o}|$ is a projector into a simple state. This means that a block of the matrix U contains $\mathbb{1} - (2/L)H$. If $|j\rangle$ is an eigenstate of H with eigenvalue λ_j, the quantity $1 - (2/L)\lambda_j$ is the inner product or overlap between $|j\rangle|\mathfrak{o}\rangle$ and $U|j\rangle|\mathfrak{o}\rangle$. Then, these two unit states have an angular distance of order $\sqrt{\lambda_j}$. The Hamiltonian H' is designed so that its eigenvalues are such distances, providing a quadratic amplification of the gap. In our construction we choose $H' = i(PU - UP)/2$, which clearly satisfies $\|H'\| \leq 1$. □

Interestingly, it is possible to find a unitary U so that H' is sparse if H is. But more importantly, a constant-time evolution with H' for time t, i.e. $\exp\{-iH't\}$, can be simulated in the circuit model with nearly the same cost than that required for simulating $\exp\{-iHt\}$:

Lemma 1. *A discrete simulation of* $\exp\{-iH't\}$ *with precision* ϵ *uses a number of "black-box" calls to unitaries* $\exp\{-i\Pi_k\tau\}$, $|\tau| \leq \pi$, *and other standard quantum gates, that is of order* $e^{1/\gamma}\left(\frac{Lt}{\epsilon}\right)^{1+\gamma}$. $\gamma > 0$ *is an arbitrary constant.*

It is because of Lemma 1 that quantum speedups can be obtained: the AST problem can be solved *quadratically faster* in this case if we use the H's instead. While we often assume that circuit decompositions of constant size to simulate each black-box $\exp\{-i\Pi_k\tau\}$ exist, our construction of U does not exploit the structure of each Π_k. Restricted to this black box model, our construction is optimal:

Theorem 2. *Let* Δ *be the spectral gap or nearest-to-0 eigenvalue of* $H = \sum_{k=1}^{L}\Pi_k$ *and* $|\psi\rangle$ *a ground state. Consider the GAP problem of finding* H' *such that implementing* $\exp\{-iH't\}$ *requires* $\mathcal{O}(|t|)$ *uses of the black boxes. Then,* $\Delta' \in \Theta(\sqrt{\Delta})$ *in the black-box model.*

Proof. (Sketched) To prove optimality we reduce instances of the search problem [37] to instances of the GAP. A call to the black box $\exp\{-i\Pi_k\tau\}$ will be related to a call of the black box or oracle of the search problem. We construct a Hamiltonian H of spectral gap $1/N$ and show that, using H' of gap Δ', search can be solved with $1/\Delta'$ oracles. If a bigger-than-quadratic gap amplification were possible, search could be solved with less than $\sqrt{N}$ oracles, contradicting known complexity bounds [29]. □

To prove limits on the power of quantum computing it is useful to work in other oracle models as well. For Hamiltonian simulations, it is often assumed that a Hamiltonian H is given as a matrix oracle for which, on input $i \in \{1, \ldots, N\}$, the oracle outputs the list of nonzero matrix elements of the Hamiltonian corresponding to the i th row as well as their positions (i.e., H is row-computable). In quantum computation we assume a reversible version of such an oracle. If H is sparse, for example, the evolution $\exp\{-iHt\}$ can be implemented using $\mathcal{O}(\text{polylog}(N))$ oracles [14, 33–35]. Unfortunately, working in this oracle model it is possible to show that no spectral gap amplification for general Hamiltonians exist. More specifically, we have:

Theorem 3. *There are families of sparse Hamiltonians for which gap amplification is not possible in the oracle model.*

Proof. (Sketched) As before, the idea is to construct a family of sparse Hamiltonians such that their unique ground states encode the solution to the search problem. The Hamiltonians in this case are stoquastic and already have spectral gap $1/\sqrt{N}$; Search can be solved using order of $\sqrt{N}$ calls to the Hamiltonian oracle. A call to a Hamiltonian oracle is equivalent to a call to the oracle for the search problem, which can be solved in complexity $\sqrt{N}$ (the inverse gap) in this case. If gap amplification were possible, this would also contradict the known complexity bounds [29]. □

The previous theorem has additional consequences in the classical simulation of quantum adiabatic evolutions. One is that, while stoquastic Hamiltonians are in one-to-one relationship with stochastic matrices [21, 31, 32], finding such matrices from the Hamiltonians could be computationally hard. Otherwise one would be able to amplify the gap and, moreover, solve search with a classical probabilistic algorithm that uses $\sqrt{N}$ calls to the oracle, which is impossible. This sets limits in the power of classical methods like quantum Monte Carlo that could be used to solve the AST problem classically [5, 38].

Some of the proofs are highly technical and were left in the long version of the paper, which also contains additional results. The longer version is attached.

[1] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, UK, 2001).
[2] E. Farhi, J. Goldstone, S. Gutmann, J. Lapan, A. Lundgren, and D. Preda, Science **292**, 472 (2001).
[3] P. Amara, D. Hsu, and J. E. Straub, The J. of Phys. Chem. **97**, 6715 (1993).
[4] A. B. Finnila, M. A. Gomez, C. Sebenik, C. Stenson, and J. D. Doll, Chem. Phys. Lett. **219**, 343 (1994).

[5] T. Kadowaki and H. Nishimori, Phys. Rev. E **58**, 5355 (1998).
[6] E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser, quant-ph/0001106 (2000).
[7] E. Farhi, J. Goldstone, and S. Gutmann, quant-ph/0201031 (2002).
[8] A. Messiah, *Quantum Mechanics* (Dover Publications, 1999).
[9] S. Jansen, M. Ruskai, and R. Seiler, J. of Math. Phys. **48**, 102111 (2007).
[10] S. Boixo, E. Knill, and R. D. Somma, Quantum Inf. and Comp. **9**, 833 (2009).
[11] P. Wocjan and A. Abeyesinghe, Phys. Rev. A p. 042336 (2008).
[12] S. Boixo, E. Knill, and R. D. Somma (2010), arXiv:1005.3034.
[13] S. Boixo and R. D. Somma, Phys. Rev. A **81**, 032308 (2010).
[14] D. Berry, G. Ahokas, R. Cleve, and B. Sanders, Comm. Math. Phys. **270**, 359 (2007).
[15] N. Wiebe, D. Berry, P. Hoyer, and B. C. Sanders, J. Phys. A: Math. Theor. **43**, 065203 (2010).
[16] R. D. Somma, S. Boixo, H. Barnum, and E. Knill, Phys. Rev. Lett. **101**, 130504 (2008).
[17] R. Somma and G. Ortiz, Lect. Notes Phys. **802**, 1 (2010).
[18] M. Szegedy, Proceedings of the 45th Annual IEEE Symposium on Foundations of Computer Science pp. 32–41 (2004).
[19] A. Ambainis, Proceedings of the 45th Annual IEEE Symposium on Foundations of Computer Science pp. 22–31 (2004).
[20] D. Perez-Garcia, F. Verstraete, J. I. Cirac, and M. Wolf, Quant. Inf. Comp. **8**, 0650 (2008).
[21] S. Bravyi and B. Terhal, SIAM J. Comput. **39**, 1462 (2009).
[22] N. de Beaudrap, M. Ohliger, T. Osborne, and J. Eisert, Phys. Rev. Lett. **105**, 060504 (2010).
[23] M. M. Wolf, G. Ortiz, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **97**, 110403 (2006).
[24] D. Aharonov, W. van Dam, J. Kempe, Z. Landau, S. Lloyd, and O. Regev, SIAM J. Comp. **37**, 166 (2007).
[25] A. Mizel, D. A. Lidar, and M. Mitchell, Phys. Rev. Lett. **99**, 070502 (2007).
[26] D. Aharonov, D. Gottesman, S. Irani, and J. Kempe, Comm. Math. Phys. **287**, 41 (2009).
[27] F. Verstraete, M. Wolf, D. Perez-Garcia, and J. Cirac, Phys. Rev. Lett. **96**, 220601 (2006).
[28] M. Schwarz, K. Temme, and F. Verstraete, arXiv:1104.1410 (2011).
[29] C. Bennett, E. Bernstein, G. Brassard, and U. Vazirani, SIAM J. Comput. **26**, 1510 (1997).
[30] A. Y. Kitaev, A. Shen, and M. Vyalyi, *Classical and Quantum Computation* (American Mathematical Society, 2002).
[31] R. Somma, C. Batista, and G. Ortiz, Phys. Rev. Lett. **99**, 030603 (2007).
[32] S. Bravyi, D. P. DiVicenzo, R. Oliveira, and B. M. Terhal, Quant. Inf. and Comp. **8**, 0361 (2008).
[33] R. Somma, G. Ortiz, J. Gubernatis, E. Knill, and R. Laflamme, Phys. Rev. A **65**, 042323 (2002).
[34] D. Aharonov and A. Ta-Shma, Proceedings of the 35th ACM Symposium on Theory of Computing pp. 20–29 (2003).
[35] A. Childs and R. Kothari (2010), arXiv:1003.3683.
[36] F. Verstraete and J. Cirac, Phys. Rev. A **70**, 060302(R) (2004).
[37] L. K. Grover, Proceedings of the 28th Annual ACM Symposium on the Theory of Computing pp. 212–219 (1996).
[38] A. Das and B. K. Chakrabarti, *Quantum Annealing And Related Optimization Methods* (Springer, 2005).