Does Adiabatic Quantum Optimization Fail for NP-Complete Problems?

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It has been recently argued that adiabatic quantum optimization would fail in solving NP-complete problems because of the occurrence of exponentially small gaps due to crossing of local minima of the final Hamiltonian with its global minimum near the end of the adiabatic evolution. Using perturbation expansion, we analytically show that for the NP-hard problem known as maximum independent set, there always exist adiabatic paths along which no such crossings occur. Therefore, in order to prove that adiabatic quantum optimization fails for any NP-complete problem, one must prove that it is impossible to find any such path in polynomial time.

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Adiabatic quantum optimization (AQO) was originally proposed [1] as a possible means for solving NP-complete problems faster than classical computation. In AQO, the Hamiltonian of the system is evolved from an initial form, H_B, whose ground state defines the initial state of the system, to a final Hamiltonian H_P, whose ground state is the optimal solution to an optimization problem. To ensure a large amplitude of the ground state at the end of the evolution, the computation time t_f should increase as $t_f \sim g_{\min}^{-2}$, where $g_{\min}$ is the minimum energy gap between the ground and first excited states during the evolution. The complexity of AQO is therefore determined by the scaling of $g_{\min}$ with the problem size.

Since its proposal, the complexity of AQO for solving NP-complete problems has been a subject of controversy. Early works suggested the possibility of polynomial scaling with the size of the problem [1], but soon counterexamples were found [2,3]. Later it was shown that the size of the gap in those counterexamples can be increased significantly by changing the adiabatic path [4] or the initial Hamiltonian [5]. However, until recently, little insight existed on the physical process that can lead to exponentially small gaps.

Using perturbation expansion, it was shown that a local minimum of H_P crossing with the global minimum near the end of the evolution, sometimes called a first order quantum phase transition, can result in an extremely small $g_{\min}$, exponential in the Hamming distance between the two minima [6]. Using the same perturbation argument, Altshuler *et al.* [7] showed that for random exact cover instances, the probability of having such crossings increases with the system size and the crossing point moves toward the end of the evolution leading to an exponentially small gap. They, therefore, concluded that AQO would *fail* in solving random exact cover problems and possibly all NP-complete problems. Others also came to similar conclusions in different ways [8,9]. Later, Knysh *et al.* [10] questioned the result of [7] based on neglecting degeneracies of the minima and correlations between them. Moreover, the possibility of avoiding small gaps by changing adiabatic path was again pointed out by Farhi *et al.* [11], and the fact that one problem can be mapped into many different Hamiltonians with different gap behavior was mentioned by Choi [12]. Those arguments, however, were based on numerical calculations for small problems, therefore inconclusive for large scales.

In this Letter, we study the NP-hard [13] maximum independent set (MIS) problem, into which the exact cover problem can be mapped in polynomial steps [12]. Using perturbation expansion, we analytically show that (i) for problems with nondegenerate local minima, or degenerate local minima distant from each other by more than 2 bit flips, it is trivial to choose an H_P so that no crossing occurs between any local minimum (minima) and the global minimum, and (ii) if H_P has degenerate local minima, some exactly 2 bit flips apart, it is still always possible (although not as trivial) to avoid such crossings by changing H_B. Since there are infinite possibilities of choosing the total Hamiltonian, a valid proof of AQO failure must show that it is impossible to find an adiabatic path with no level crossing in polynomial time. Moreover, remaining in the ground state is not a necessary condition for solving NP-complete problems. As shown in Ref. [14], approximate solutions can also be used to solve NP-complete problems exactly in polynomial time. A proof of failure, therefore, must also show that no such approximate solutions can be obtained by AQO.

The MIS problem is that of finding a largest set M of nodes in a given graph G, such that there are no edges of G between any nodes in M. If n is the total number of nodes in G, the problem of finding an MIS M can be expressed as minimizing a cost function (energy) on n binary variables x_i using [15]

$$x_i = \begin{cases} 1 & \text{if } i \in M, \\ 0 & \text{if } i \notin M' \end{cases}$$

$$E_P = -\sum_{i \in \text{nodes}} x_i + \sum_{(i,j) \in \text{edges}} c x_i x_j, \qquad (1)$$

with $c > 1$. The last term in (1) is zero for every independent set of nodes, because there is no edge between nodes for which $x_i = 1$. Every dependent set, on the other hand, gets a positive contribution from the sum for every pair of adjacent nodes within it, thus resulting in a larger cost or energy. Therefore, without the linear term, (1) would have a hugely degenerate global minimum consisting of all independent sets. Such a cost function (without the linear term) has no local minima, because from every state it is always possible to remove nodes (i.e., switch x_i from 1 to 0) one by one to make all nonzero bilinear terms vanish. Therefore, it is always possible to get from any state to the ground state without ever increasing the energy. The role of the linear term in (1) is to assign costs (energies) to different independent sets based on their sizes so that the global minimum (or minima) of (1) becomes an MIS. There can also be many local minima, which are maximal independent sets of G, i.e., independent sets that cannot be made larger by adding nodes.

Our goal is to solve the MIS problem using AQO. We first represent every node with a qubit by substituting $x_i \rightarrow \frac{1}{2}(\sigma_i^z + 1)$, where σ_i^z is a Pauli matrix. Equation (1), therefore, turns into a 2-local Hamiltonian

$$H_P = \sum_i h_i \sigma_i^z + \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z, \tag{2}$$

with $h_i = n_i c/4 - 1/2$, where n_i is the number of edges connected to node i (degree of i), and $J_{ij} = c/4$ ($= 0$) whenever there is an (no) edge between i and j. We introduce time evolution Hamiltonian

$$H = H_P + \lambda H_B, \qquad H_B = -\sum_i \Delta_i \sigma_i^x, \tag{3}$$

where λ changes from ∞ to 0.

Near the end of the evolution, where $\lambda \ll 1$, we can use perturbation expansion in λ, taking H_P as the unperturbed Hamiltonian, to calculate eigenstates of H. Let S be any maximal independent set (which could also be an MIS) of size s and $|S^{(0)}\rangle$ be its corresponding state representing a local (or global) minimum of (2). From (1) we immediately find $E_S^{(0)} = -s$. Upon perturbation, the energy eigenvalue becomes $E_S(\lambda) = E_S^{(0)} + \lambda E_S^{(1)} + \lambda^2 E_S^{(2)} + \ldots$. The first order correction $E_S^{(1)} = \langle S^{(0)}|H_B|S^{(0)}\rangle = 0$, because the operators σ_i^x in H_B each flip only one qubit. The lowest order nonzero term is therefore second order, which as we shall see is the dominant one.

Now suppose that $|M^{(0)}\rangle$ is the global minimum and $|M'^{(0)}\rangle$ is a local minimum of (2), each representing a maximal independent set (M and M') of size m and m' ($< m$), respectively. Let $\delta E(\lambda) \equiv E_{M'}(\lambda) - E_M(\lambda) = \delta E^{(0)} + \lambda^2 \delta E^{(2)} + O(\lambda^4)$ denote the energy separation between the two states. To zeroth order, $\delta E^{(0)} = m - m' > 0$, as expected since M is the MIS. If at some λ within the convergence radius of the perturbation, $\delta E(\lambda) < 0$ for a finite order of perturbation [16], this means that at some point $\lambda = \lambda^*$ the two levels should cross. This can lead to an extremely small minimum gap at the (anti)crossing point, which is exponentially dependent on the Hamming distance between the two minima [6].

We first consider the simplest case with no degeneracy and a uniform transverse field, $\Delta_i = 1$. The second order correction to the energy is (with $S = M, M'$)

$$E_S^{(2)} = \sum_{k \neq S} \frac{\langle S^{(0)}|H_B|k^{(0)}\rangle\langle k^{(0)}|H_B|S^{(0)}\rangle}{E_S^{(0)} - E_k^{(0)}}. \tag{4}$$

Since H_B involves only 1 bit flip operators σ_i^x, the sum is nonzero only for states $|k^{(0)}\rangle$ that are 1 bit flip from $|M^{(0)}\rangle$:

$$E_S^{(2)} = -\sum_i \frac{1}{B_i}, \qquad B_i = \begin{cases} 1 & \text{if } i \in S, \\ cd_i - 1 & \text{if } i \notin S, \end{cases} \tag{5}$$

where B_i is the energy cost of flipping qubit i from state $|S^{(0)}\rangle$, and d_i is the number of edges between i and nodes in S. Notice that $d_i \geq 2$, since $d_i = 0$ implies that node i is not connected to any nodes in S, i.e., S is not maximal, and $d_i = 1$ implies that there is a degenerate state 2 bit flips away. Up to second order in λ, we find

$$E_S(\lambda) = -(1 + \lambda^2)s - \lambda^2 \sum_{i \notin S} \frac{1}{cd_i - 1}. \tag{6}$$

Since s is largest for the MIS, the first term in (6) is minimum for the global minimum as desired. The sum, however, depends on d_i and could be larger for a local minimum than the global minimum. As a result, at large enough λ, it can cause the two energy levels to cross. However, since c can be chosen to be arbitrarily large, it is possible to reduce the effect of the sum and therefore eliminate the anticrossing by increasing c. Physically, increasing c will push low lying excited states (specifically dependent sets) adjacent to the global and local minima upward while keeping the minima energies fixed. This would reduce the relative magnitude of $E_S^{(2)}$ in (4), as it inversely depends on the excited state energies. For example, by choosing $c = n$, we get

$$\delta E(\lambda) > (1 + \lambda^2)(m - m') - \lambda^2 \frac{n - m'}{2n - 1} > 1 + \frac{\lambda^2}{2}, \tag{7}$$

because $m - m' \geq 1$, $m' \geq 1$, $d_i' \geq 2$, and the number of nodes not in M' is $n - m'$. This is strictly positive; therefore, no anticrossing occurs between those minima.

The above argument holds beyond second order perturbation. Assuming $c = n$ and that a minimum S is sufficiently isolated from other minima so that up to q bit flips the energy of the state always increases, the qth order perturbation correction to the energy is

$$E_S^{(q)} = \frac{(-1)^{q/2}(q-2)!}{(q/2-1)!(q/2)!} s + O(1). \tag{8}$$

The radius of convergence deduced from (8) is $\lambda_c = \frac{1}{2}$, and the contribution from each successive term

monotonically decreases within λ_c, so the second order term remains dominant. Moreover, neglecting the $O(1)$ part of (8) compared to the first $\Theta(s)$ term, we find that up to the qth order perturbation, where validity of (8) stands, we can write $E_{M'}(\lambda) = (m'/m)E_M(\lambda)$, therefore $\delta E(\lambda) = [(m' - m)/m]E_M(\lambda) > 0$, which follows from $m > m'$ and $E_M(\lambda) < 0$. This means that up to the qth order perturbation, the levels do not cross.

The price to pay for eliminating the level crossings is to increase the coupling constant c linearly with the size of the problem. Alternatively, one can keep c constant, but divide the linear terms in (1) by n to achieve the same goal, as was done in [12] (although the local minima in [12] are degenerate). This leads to smaller energy steps in the spectrum of H_P and therefore higher required precision. In both cases, the scaling of the coupling constant or precision with n is polynomial (linear), whereas the gain in eliminating the crossings could be exponential.

One may argue that by increasing c with n, or equivalently dividing the linear terms in (1) by n, we reach a regime in which the bilinear terms in (1) become dominant and determine the dynamics of the system. Thus, although there is no level crossing for $\lambda \ll 1$ considered above, there could be one for $1 \ll \lambda \ll n$. In this region, one can neglect the linear terms in (1) and repeat the above perturbative argument keeping only the bilinear terms. However, as mentioned earlier, the Hamiltonian without the linear terms has no local minima, but only a hugely degenerate global minimum consisting of all independent sets. Such a Hamiltonian, therefore, cannot produce a crossing in the way discussed above.

So far, we have only considered nondegenerate states, which is indeed the level of discussion in Refs. [7,11]. We now take a step further and discuss cases with degenerate minima. We first have to generalize (4) to include degeneracies. Suppose there are K maximal (or maximum) independent sets S_k of size s, with $k = 1, \ldots, K$. States $|S_k^{(0)}\rangle$ and also every superposition of them are therefore degenerate eigenstates of H_P. Perturbation in λ removes this degeneracy. Let $|S^{(0)}\rangle = \sum_k C_k |S_k^{(0)}\rangle$ represent the lowest energy superposition after the degeneracy is lifted. With the positive sign of Δ_i, C_k will all be positive real numbers with the constraint: $\sum_k C_k^2 = 1$. The first order correction is zero because all S_k are the same size (s) and therefore one cannot get from one minimum to another by a single bit flip (adding or removing a single node). The second order correction is

$$E_S^{(2)} = -\sum_{(k,k'),(i,j)}{}' \frac{\Delta_i \Delta_j C_k C_{k'}}{B_{k,i}}, \tag{9}$$

where $B_{k,i}$ is the cost of flipping qubit i from state $|S_k^{(0)}\rangle$, and the prime sign on the sum means that the sum is over all the paths from $|S_k^{(0)}\rangle$ to $|S_{k'}^{(0)}\rangle$ with 2 bit flips by first flipping qubit i and then qubit j.

If there are no two minima $|S_k^{(0)}\rangle$ and $|S_{k'}^{(0)}\rangle$ that are exactly 2 bit flips distant from each other, (9) becomes similar to the nondegenerate Eq. (4). In that case, the argument deduced from (4) holds, i.e., level crossings can be eliminated by increasing c linearly with n. The exceptions, therefore, are cases with minima 2 bit flips apart from each other. The worst cases would have only one global minimum but numerous local minima 2 bit flips apart. The negative contribution to $E_{M'}^{(2)}$ can then become large enough to bring down the total energy of the local minima below that of the global minimum at a $\lambda < \lambda_c$. This is the case we shall consider now.

To eliminate the above crossing, we need to make the energy difference $\delta E(\lambda) = m - m' + \lambda^2 \delta E^{(2)}$ strictly positive. This is achieved if

$$\delta E^{(2)} = \sum_i \frac{\Delta_i^2}{B_i} - \sum_{(k,k'),(i,j)}{}' \frac{\Delta_i \Delta_j C_k C_{k'}}{B'_{k,i}} > 0. \tag{10}$$

Here, B_i ($B'_{k,i}$) is the cost of flipping qubit i in the global minimum M (local minimum M'_k). A sufficient condition, which is independent of C_k, is

$$\sum_i \frac{\Delta_i^2}{B_i} - \max_k \sum_{k',(i,j)}{}' \frac{\Delta_i \Delta_j}{B'_{k,i}} > 0. \tag{11}$$

This can be proved using the fact that for every nonnegative, symmetric matrix A operating on unit vectors v, we have $\max_v v^T A v \le \max_k \sum_{k'} A_{kk'}$. For simplicity, here we focus on the large c regime (e.g., $c = n$) for which the states that violate edges can be neglected. All calculations can be generalized to the small c regime, but the equations become more complicated. Condition (11) becomes $\mathcal{F}(\{\Delta_i\}) > 0$, where

$$\mathcal{F}(\{\Delta_i\}) \equiv \sum_{i \in M} \Delta_i^2 - \max_k \sum_{i \in M'_k} \left[\Delta_i^2 + \sum_{k',j}{}' \Delta_i \Delta_j \right]. \tag{12}$$

Since there is freedom in choosing values of Δ_i, one can choose them such that $\mathcal{F}(\{\Delta_i\}) > 0$. A successful assignment makes the first term in (12) large and/or the second term small so that the result becomes positive. A trivial choice is $\Delta_{i \in M} = \alpha$ and $\Delta_{i \notin M} = 1$. Let $p_k = |M \cap M'_k|$. Since M'_k is a local minimum, we have $p_k \le m - 2$. Also, there are at most $n - m'$ local minima all 2 bit flips away from M'_k. Therefore,

$$\begin{aligned} \mathcal{F} &\ge \alpha^2 m - \max_k (\alpha^2 p_k + m' - p_k + \alpha(n - m')) \\ &\ge 2\alpha^2 - \alpha(n - m') - m' + 1, \end{aligned} \tag{13}$$

which is positive if

$$\alpha > \frac{n - m' + \sqrt{(n - m')^2 + 8(m' - 1)}}{4} \approx \frac{n - m'}{2}. \tag{14}$$

Such an assignment, however, is not very useful, since it assumes knowing the solution to the problem.

Nevertheless, it proves the existence of at least one assignment of Δ_i for which no crossing occurs.

We now consider another assignment which does not assume the solution. Let $M' = \cup_k M'_k$ and $p = |M \cap M'|$. We assign $\Delta_{i\in M'} = \beta$ and $\Delta_{i\notin M'} = 1$. The last term in (12) is multiplied by β^2 and the first term becomes $m - p + \beta^2 p$. We find $\mathcal{F} \geq m - p + \beta^2 p - \beta^2[m' + n - m']$. In order for $\mathcal{F} > 0$, it is sufficient to have $\beta < \sqrt{(m-p)/(n-p)}$. Therefore, as long as $m > p$, that is as long as there is at least one node in the global minimum that is not in any of the local minima, there exists an assignment of Δ_i for which no crossing happens during the adiabatic evolution. As before, the scaling of β with the size of the system is only polynomial.

This assignment does not require knowledge of the global minimum (solution), but only knowledge of the local minima, which can be obtained by running the evolution multiple times with $\Delta_i = 1$. If there is a crossing between the global minimum and the state comprising the local minima, every time the system does not reach the global minimum, it falls into one of the local minima. Moreover, other degenerate local minima in the neighborhood of the one reached can be obtained in polynomial time using local search. The more information is obtained from such suboptimal evolutions, the more one can adjust Δ_i to avoid the crossing.

The above assignment may not eliminate all such crossings if $m = p$. However, there are an infinite number of ways to define the input parameters. For example, one can choose nonuniform Δ_i within M' or nonuniform J_{ij}. Combining these and other ideas may also give a Hamiltonian that satisfies (11). There are therefore infinitely many possibilities to define a Hamiltonian for solving an NP-hard problem instance, many of which may not have level crossings. An iterative numerical method that follows from the above ideas has proven to be successful in eliminating crossings in extremely difficult instances with highly degenerate local minima, even where $m = p$ [17]. Other methods have also been proposed for finding an optimal path [18].

It is important to note that we are not trying to prove that all level crossings between a global minimum and local minima can be eliminated in polynomial time. Neither are we claiming that if they are eliminated, the MIS problem can be solved in polynomial time. Even if all level crossings are eliminated, the scaling of the minimum gap in the rest of the spectrum is still unknown. What we are stating here is that there always exist paths along which no crossing occurs, at least up to second order perturbation. Since MIS is NP hard, any NP problem can be polynomially mapped onto it. Therefore, a valid proof that any NP-complete problem cannot be solved using AQO because of level crossings must prove that for the problem mapped onto MIS, it is impossible to find an assignment of parameters for which there is no level crossing. Further, due to the NP hardness of approximating solutions to MIS [14], even if there are multiple crossings, AQO may produce sufficient solutions to solve NP-complete problems.

In conclusion, using perturbation expansion, we have shown that for the NP-hard problem of MIS, it is always possible to write down a Hamiltonian for which during the adiabatic evolution no crossing occurs between a global minimum and any local minima. If there is no degeneracy in the local minima, or if there are degenerate local minima but no pair of them is exactly 2 bit flips apart, such a Hamiltonian can be trivially obtained by increasing the coupling coefficient between the qubits linearly with the size of the problem. In cases with local minima exactly 2 bit flips away from each other, one can use the freedom of choosing the initial Hamiltonian to avoid level crossings. In the latter case, finding an assignment for tunneling amplitudes Δ_i could be nontrivial. However, we have shown that such an assignment always exists. In general, there are infinite ways of defining the Hamiltonian, including those where many approximate solutions suffice; therefore, it seems infeasible to prove that no successful Hamiltonian can be obtained in polynomial time.

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