Avoid First Order Quantum Phase Transition by Changing Problem Hamiltonians

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October 7, 2010

Abstract

The problem Hamiltonian of the adiabatic quantum algorithm for the maximum-weight independent set problem (MIS) that is based on the reduction to the Ising problem (as described in [6]) has flexible parameters. We show that by choosing the parameters appropriately in the problem Hamiltonian (without changing the problem to be solved) for MIS on CK graphs [8], we can prevent the first order quantum phase transition [4] and significantly change the minimum spectral gap. Furthermore, the result also serves to concretely clarify that it is not sufficient to consider one specific problem Hamiltonian for proving the failure of adiabatic quantum optimization for a problem as in [25, 2]. We also raise the basic question about what the appropriate formulation of adiabatic running time should be.

1 Introduction

Adiabatic quantum computation (AQC) was proposed by Farhi et al. [11] in 2000 as an alternative quantum paradigm to solve NP-hard optimization problems, which are believed to be classically intractable. Later, it was shown that AQC is not just limited to optimization problems, and is polynomially equivalent to conventional quantum computation (quantum circuit model) [1, 19]. A quantum computer promises extraordinary power over a classical computer, as demonstrated by Shor [23] in 1994 with the polynomial quantum algorithm for solving the factoring problem, for which the best known classical algorithms are exponential. Just how much more powerful are quantum computers? In particular, we are interested in whether an adiabatic quantum computer can solve NP-complete problems *more* efficiently than a classical computer.

Unlike classical computation or conventional quantum model in which an algorithm is specified by a finite sequence of *discrete* operations via classical/quantum gates, the adiabatic quantum algorithm is *continuous*. It has been assumed (see Section 2 for more discussion) that, according to the adiabatic theorem, the dominant factor of the adiabatic running time (ART) of the algorithm scales polynomially with the inverse of the *minimum spectral gap* $g_{\min}$ of the system Hamiltonian (that describes the algorithm). Therefore, in order to analyze the running time of an adiabatic algorithm, it is necessary to be able to bound $g_{\min}$ analytically. However, $g_{\min}$ is in general difficult to compute (it is as hard as solving the original problem if computed directly). Rigorous analytical analysis of adiabatic algorithms remains challenging. Most of studies have to resort to numerical calculations. These include numerical integration of Schrödinger equation [11, 5], eigenvalue computation (or exact diagonization)[28, 22],

and quantum Monte Carlo (QMC) technique [26, 27]. However, not only are these methods limited to small sizes (as the simulations of quantum systems grow exponentially with the system size), but also little insight can be gained from these numbers to design and analyze the time complexity of the algorithm.

Perhaps, from the algorithmic design point of view, it is more important to unveil the quantum evolution black-box and thus enable us to obtain insight for designing efficient adiabatic quantum algorithms. For this purpose, we devise a visualization tool, called Decomposed State Evolution Visualization (DESEV). Through the aid of this tool, we constructed a family of instances of MIS, called CK graphs [8]. The numerical results of an adiabatic algorithm for MIS on these graphs suggested that g_{min} is exponentially small and thus the algorithm requires exponential time. These results were then explained by the first order quantum phase transition (FQPT) in [4]. Since then, there have been some other papers (Altshuler et al., [2] ; Farhi et al., [13]; Young et al., [27]; Jorg et al., [17, 18]) investigating the same phenomenon, i.e., first order quantum phase transition. In particular, Farhi et al. in [13] suggested that the exponential small gap caused by the FQPT could be overcome (for the set of instances they consider) by randomizing the choice of initial Hamiltonian. In this paper, we show that by changing the parameters in the problem Hamiltonian (without changing the problem to be solved) of the adiabatic algorithm for MIS on CK graphs, we prevent the FQPT from occurring and significantly increase g_{min}. To the best of our knowledge, this is the first time that such a result has been shown. We do so by scaling the vertex-weight of the graph, namely, multiplying the weights of vertices by a scaling factor. In order to determine the best scaling factor, we raise the basic question about what the appropriate formulation of adiabatic running time should be. Furthermore, our result serves to further clarify (see [7] for explanation) that it is not sufficient to consider one specific problem Hamiltonian for proving the the failure of adiabatic quantum optimization for a problem as in [25, 2].

This paper is organized as follows. In Section 2, we review the adiabatic quantum algorithm, and the adiabatic running time(ART). In Section 3, we recall the adiabatic quantum algorithm for MIS based on the reduction to the Ising problem. In Section 4, we describe the visualization tool DESEV and the CK graphs. We show examples of DESEV on the MIS adiabatic algorithm for CK graphs. In Section 5, we describe how changing the parameters affects g_{min}, and raise the question about ART. We conclude with the discussion in Section 6.

2 Adiabatic Quantum Algorithm

An adiabatic quantum algorithm is described by a time-dependent system Hamiltonian

$$\mathcal{H}(t) = (1 - s(t))\mathcal{H}_{\mathsf{init}} + s(t)\mathcal{H}_{\mathsf{problem}}$$

for $t \in [0, T]$, $s(0) = 0$, $s(T) = 1$. There are three components of $\mathcal{H}(.)$: (1) initial Hamiltonian: $\mathcal{H}(0) = \mathcal{H}_{\mathsf{init}}$; (2) problem Hamiltonian: $\mathcal{H}(T) = \mathcal{H}_{\mathsf{problem}}$; and (3) evolution path: $s : [0, T] \longrightarrow [0, 1]$, e.g., $s(t) = \frac{t}{T}$. $\mathcal{H}(t)$ is an adiabatic algorithm for an optimization problem if we encode the problem into the problem Hamiltonian $\mathcal{H}_{\mathsf{problem}}$ such that the ground state of $\mathcal{H}_{\mathsf{problem}}$ corresponds to the answer to the problem. The initial Hamiltonian $\mathcal{H}_{\mathsf{init}}$ is chosen to be non-commutative with $\mathcal{H}_{\mathsf{problem}}$ and its ground state must be known and experimentally constructable, e.g., $\mathcal{H}_{\mathsf{init}} = -\sum_{i \in \mathsf{V}(G)} \Delta_i \sigma_i^x$. Here T is the running time of the algorithm. According to the adiabatic theorem, if $\mathcal{H}(t)$ evolves "slowly" enough, or equivalently, if T is "large" enough (see Adiabatic Running Time below) the system remains in the ground state of $\mathcal{H}(t)$, and consequently, ground state of $\mathcal{H}(T) = \mathcal{H}_{\mathsf{problem}}$ gives the solution to the problem.

Notice that given a problem, there are three components (initial Hamiltonian, problem Hamiltonian, and evolution path) that specify an adiabatic algorithm for the problem. A change in one component (e.g. initial Hamiltonian) will result in a different adiabatic algorithm for the same problem.

In this paper, we fix the evolution path by the linear interpolation function $s(t) = \frac{t}{T}$. Hereafter, we describe an adiabatic algorithm by the re-parametrized Hamiltonian

$$\mathcal{H}(s) = (1-s)\mathcal{H}_{\mathsf{init}} + s\mathcal{H}_{\mathsf{problem}}$$

where $s \in [0,1]$, with understanding that $s(t) = t/T$. For a more general interpolation path see [21]. Furthermore, throughout this paper, we fix the initial Hamiltonian to be $\mathcal{H}_{\mathsf{init}} = -\sum_{i \in \mathsf{V}(G)} \sigma_i^x$. When it is clear from context, we also refer to the problem Hamiltonian as the adiabatic algorithm for the problem.

Adiabatic Running Time. In their original work [10], the running time of the adiabatic algorithm is defined to be the same as the adiabatic evolution time T, which is given by the adiabatic condition of the adiabatic theorem. However, this definition is under the assumption of some physical limit of the maximum energy of the system (see e.g., [16]), and is not well-defined from the computational point of view, as observed by Aharonov et al. [1]. They re-define $\mathsf{ART}(\mathcal{H})$ as $T \cdot \max_s ||\mathcal{H}(s)||$, taking into the account of the time-energy trade-off in the Schrödinger's equation[1].

On the other hand, given the extensive work on the rigorous proofs of the adiabatic theorem, it is interesting (if not confusing) that many different versions of the adiabatic conditions have been recently proposed. These include [29, 30, 31, 32, 34, 33, 37, 39, 35, 36, 38] in the quantum physics community, and [20, 1, 3] in the computer science community. Most of these studies suggest that ART scales polynomially with the inverse of the spectral gap of the system Hamiltonian, which is sufficient when one is interested in the coarse computational complexity of algorithms, namely, the distinction between polynomial and exponential running time.

However, from both the practical and algorithmic point of view, it is important to have a more precise formulation of ART. First, this is because the specification of the adiabatic evolution time T is required in an adiabatic algorithm, and therefore a tight and simple upper bound is desired. Second, we are interested in the actual time complexity of the algorithm, and not just the polynomial vs. exponential distinction. It is necessary to have a more precise formulation of ART such that basic algorithmic analysis can be carried out. Third, at this stage of research, it is particularly important to have such a formulation because the spectral gap, which plays the dominating role in the formulation of ART, is difficult to analyze. All current efforts on the spectral gap analysis resort to numerical studies, and that means the studies are restricted to small problem sizes only. Therefore, to gain insight into the time complexity of algorithms from these small instances, it is important that the formulation of ART applies to small sizes. So what is the appropriate formulation of ART? What should the adiabatic condition(s) be? This is in contrast to the study in [21] where the exact form of adiabatic condition is not essential. In Section 5.2, we compare three closely related versions and raise the question about what the appropriate adiabatic running time should be.

3 An Adiabatic Algorithm for MIS

In this section, we recall the adiabatic algorithm for MIS that is based on the reduction to the Ising problem, as described in [6]. First, we formally define the Maximum-Weight Independent Set (MIS) problem (optimization version):

Input: An undirected graph $G(= (\mathsf{V}(G), \mathsf{E}(G)))$, where each vertex $i \in \mathsf{V}(G) = \{1, \ldots, n\}$ is weighted by a positive rational number c_i

Output: A subset $S \subseteq \mathsf{V}(G)$ such that S is independent (i.e., for each $i, j \in \mathsf{V}(G)$, $i \neq j$, $ij \notin \mathsf{E}(G)$) and the total *weight* of S $(= \sum_{i \in S} c_i)$ is maximized. Denote the optimal set by $\mathsf{mis}(G)$.

[1] Namely, $i\frac{d|\psi(s)\rangle}{ds} = T \cdot \mathcal{H}(s)|\psi(s)\rangle = \frac{T}{K} \cdot K\mathcal{H}(s)|\psi(s)\rangle$ where $K > 0$ is a constant.

There is a one-one correspondence between the MIS problem and the Ising problem, which is the problem directly solved by the quantum processor that implements 1/2-spin Ising Hamiltonian. We recall the quadratic binary optimization formulation of the problem. More details can be found in [6].

Theorem 3.1 (Theorem 5.1 in [6]). *If $J_{ij} \geq \min\{c_i, c_j\}$ for all $ij \in \mathsf{E}(G)$, then the maximum value of*

$$\mathcal{Y}(x_1, \ldots, x_n) = \sum_{i \in \mathsf{V}(G)} c_i x_i - \sum_{ij \in \mathsf{E}(G)} J_{ij} x_i x_j \tag{1}$$

is the total weight of the MIS. In particular if $J_{ij} > \min\{c_i, c_j\}$ for all $ij \in \mathsf{E}(G)$, then $\mathsf{mis}(G) = \{i \in \mathsf{V}(G) : x_i^* = 1\}$, where $(x_1^*, \ldots, x_n^*) = \arg\max_{(x_1,\ldots,x_n)\in\{0,1\}^n} \mathcal{Y}(x_1, \ldots, x_n)$.

Here the function $\mathcal{Y}$ is called the pseudo-boolean function for MIS. Notice that in this formulation, we only require $J_{ij} > \min\{c_i, c_j\}$, and thus there is freedom in choosing this parameter. In this paper we will show how to take advantage of this.

By changing the variables ($x_i = \frac{1+s_i}{2}$), it is easy to show that MIS is equivalent to minimizing the following function, known as the *Ising energy function*:

$$\mathcal{E}(s_1, \ldots, s_n) \quad = \quad \sum_{i \in \mathsf{V}(G)} h_i s_i + \sum_{ij \in \mathsf{E}(G)} J_{ij} s_i s_j, \tag{2}$$

which is the eigenfunction of the following *Ising Hamiltonian*:

$$\mathcal{H}_{\mathsf{Ising}} = \sum_{i \in \mathsf{V}(G)} h_i \sigma_i^z + \sum_{ij \in \mathsf{E}(G)} J_{ij} \sigma_i^z \sigma_j^z \tag{3}$$

where $h_i = \sum_{j \in \mathsf{nbr}(i)} J_{ij} - 2c_i$, $\mathsf{nbr}(i) = \{j : ij \in \mathsf{E}(G)\}$, for $i \in \mathsf{V}(G)$.

That is, an adiabatic algorithm for MIS in which the problem Hamiltonian is $\mathcal{H}_{\mathsf{Ising}}$ is described by the following system Hamiltonian:

$$\mathcal{H}(s) = (1 - s)\mathcal{H}_{\mathsf{init}} + s\mathcal{H}_{\mathsf{Ising}}$$

where $s \in [0, 1]$ with the assumption that $s(t) = t/T$. If T is sufficiently large according to the adiabatic theorem, then the ground state of $\mathcal{H}(1)$, say $|x_1^* x_2^* \ldots x_n^*\rangle$, corresponds to the maximum-weight independent set, namely $\mathsf{mis}(G) = \{i : x_i^* = 0\}$[2].

4 DESEV and CK Graphs

In this section, we describe a visualization tool, called Decomposed State Evolution Visualization (DESEV), which aims to "open up" the quantum evolution black-box from a computational point of view. Consider the above adiabatic algorithm for MIS. Recall that according to the adiabatic theorem, if the evolution is slow enough, the system remains in the instantaneous ground state. Let $|\psi(s)\rangle$ be the ground state of $\mathcal{H}(s)$, for $s \in [0, 1]$. For a system of n-qubits, $|\psi(s)\rangle$ is a superposition of 2^n possible computational states, namely,

$$|\psi(s)\rangle = \sum_{x \in \{0,1\}^n} \alpha_x(s)|x\rangle, \qquad \text{where} \sum_{x \in \{0,1\}^n} |\alpha_x(s)|^2 = 1.$$

[2]Notice we use $x_i = \frac{1+s_i}{2}$ instead of $x_i = \frac{1-s_i}{2}$.

For example, we have the initial ground state $|\psi(0)\rangle = \frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} |x\rangle$, which is uniform superposition of all 2^n states, while the final ground state $|\psi(1)\rangle = |x_1^* x_2^* \dots x_n^*\rangle$, corresponding to the solution state. A natural question is: what are the instantaneous ground states $|\psi(s)\rangle$, for $0 < s < 1$, like? In particular, we would like to "see" how the instantaneous ground state evolves? A naïve solution would be to trace the 2^n amplitudes α_x. The task becomes unmanageable even for $n = 10$, which has 1024 amplitudes, even though many may be negligible (close to zero).

To make the "visualization" feasible, we introduce a new measure Γ_k. Suppose that $\mathcal{H}(1)$, has $(m+1) \leq 2^n$ distinct energy levels: $E_0 < E_1 < \ldots < E_m$. For $0 \leq k \leq m$, let $D_k = \{x \in \{0,1\}^n : \mathcal{H}(1)|x\rangle = E_k|x\rangle\}$ be the set of (degenerate) computational states that have the same energy level E_k (with respect to the problem Hamiltonian $\mathcal{H}(1)$), and define

$$\Gamma_k(s) = \sum_{x\in D_k} |\alpha_x(s)|^2.$$

In other words, $\Gamma_k(s)$ is the total percentage of (computational) states of the same energy level E_k participating in $|\psi(s)\rangle$. The idea is now to trace Γ_k instead of α_x. Here we remark that Γ_k are defined for any eigenstate $|\psi\rangle$ and not just for the ground state.

For our purpose, we constructed a special family of vertex-weighted graphs for the MIS problem, called CK graphs [8]. We designed the problem instances such that the global minimum is "hidden" in the sense that there are many local minima to mislead local search based algorithms. Note that the size of the smallest instances needs to be necessarily smaller than 20 as we are relying on the eigenvalue computation (or exact diagonization) to compute Γ_k.

CK Graph Construction. Let r, g be integers, and w_A, w_B be positive rational numbers. Our graphs are specified by these four parameters. There are two types of vertices in the graph: vertices of a $2g$-independent set, denoted by V_A, and vertices of g r-cliques (which form r^g maximal independent sets), denoted by V_B. The weight of vertex in V_A (V_B resp.) is w_A (w_B resp.). The graph is connected as follows. Partition the vertices in V_A into g groups of 2 (independent) vertices. There are also g groups of r-cliques in V_B. We label both groups accordingly such that each group in V_A is adjacent to all but one (the same label) r-cliques in V_B. Note if $w_B < 2w_A$, then we have V_A forming the (global) maximum independent sets of weight $2gw_A$, while there are r^g (local) maximal independent set of weight gw_B. See Figure 1 for an example of a graph for $r = 3$ and $g = 3$.

4.1 DESEV for the MIS Adiabatic Algorithm on a 15-vertex CK Graph

In the section, we fix the CK graph with $r = 3$, $g = 3$ as illustrated in Figure 1. We set $w_A = 1$, and consider $1 \leq w_B < 2$. The graph G consists of 15 vertices: $V_A = \{1, \ldots, 6\}$ forms the maximum-weight independent set of weight 6; while V_B, consisting of 3 groups of 3 triangles: $\{7, 8, 9\}$, $\{10, 11, 12\}$, and $\{13, 14, 15\}$, forms 3^3 maximal independent sets of weight $3w_B < 6$.

According to Eq.(3), the problem Hamiltonian (and thus the adiabatic algorithm) for MIS on G is

$$\mathcal{H}_1 = \sum_{i\in V_A} (6J - 2)\sigma_i^z + \sum_{i\in V_B} (6J - 2w_B)\sigma_i^z + J \sum_{ij\in \mathsf{E}(G)} \sigma_i^z \sigma_j^z \tag{4}$$

Here we fix $J_{ij} = J = 2 > w_B$ for all $ij \in \mathsf{E}(G)$.

Notation on representing the computational states. For a computational state $|x_1 x_2 \dots x_n\rangle$ where $x_i \in \{0, 1\}$, we adopt the zero position representation, namely, represent it by $|i_1 i_2 \dots i_k\rangle$ where $x_j = 0$ if and only if $j = i_t$ for some t. That is, we represent $|000000111111111\rangle$ (the solution state) by $|123456\rangle$. Further,

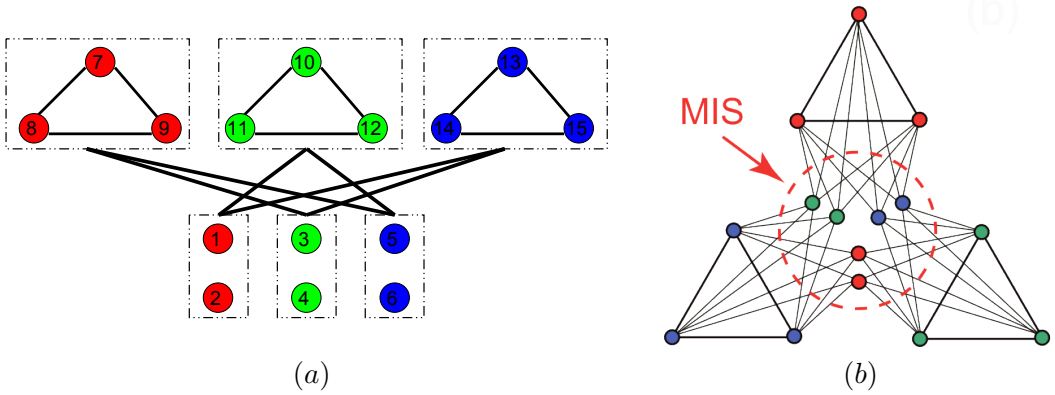

Figure 1: (a) A CK graph for $r = 3$ and $g = 3$. The graph consists of 15 vertices: $V_A = \{1, \ldots, 6\}$ forms an independent set of size 6, while V_B, consisting of $g(= 3)$ groups of $r(= 3)$ triangles: $\{7, 8, 9\}$, $\{10, 11, 12\}$, and $\{13, 14, 15\}$, forms 3^3 independent sets of size 3. The graph is connected as follows. The 6 vertices in V_A are divided into 3 groups: $\{1, 2\}$, $\{3, 4\}$, and $\{5, 6\}$. The vertices in each group are adjacent to vertices in two groups of three triangles in V_B (as illustrated by different colors). (b) The drawing of the graph with explicit connections. The weight of a vertex in V_A (V_B resp.) is w_A (w_B resp.). We set $w_A = 1$, and consider $1 \leq w_B < 2$. For explanation purpose, we represent a vertex in V_A by a $\bullet$, and a vertex in V_B by a $\triangle$. Therefore, $V_A = \{\bullet, \bullet, \bullet, \bullet, \bullet, \bullet, \}$, forms the MIS of weight 6; while $\{\triangle, \triangle, \triangle\}$ is a maximal independent set of weight $3w_B(< 6)$.

we use a $\bullet$ to denote a vertex in V_A, a $\triangle$ for a vertex in V_B. That is, the solution state is now represented by $|\bullet\bullet\bullet\bullet\bullet\bullet\rangle$, while $|\triangle\triangle\triangle\rangle$, corresponding to a local maximal independent set of weight $3w_B$ with one vertex from each triangle.

Maximum vs Minimum. The maximum of MIS corresponds to the minimum of the Ising energy. For explanation purpose, instead of referring to the energy values of the Ising Hamiltonian, we will refer to the values of MIS given by the pseudo-boolean function $\mathcal{Y}$ in Eq.(1) by "(-)energy", where "(-)" is to indicate the reverse ordering.

Example. The (-)energy of $|\bullet\bullet\bullet\bullet\bullet\bullet\rangle$ is 6; while $|\triangle\triangle\triangle\text{–}\triangle\rangle$ is $4w_B - J$, where $\triangle\text{–}\triangle$ represents two connected vertices from V_B, e.g. vertex 7 and 8 in Figure 1.

See Figure 2 for the DESEV of the the ground state of the adiabatic algorithm with $\mathcal{H}_1$ in Eq.(4) as the problem Hamiltonian for $w_B = 1.5$ and 1.8.

4.2 FQPT and Perturbation Estimation

To gain better understanding, we vary the weights of vertices: fix $w_A = 1$, while varying w_B from 1 to 1.9 with a step size of 0.1. That is, we fix the global maximum independent set, while increasing the weight of the local maximum. As the weight of w_B increases, the minimum spectral gaps get smaller and smaller (indeed, from 10^{-1} to 10^{-8} as w_B changes from 1 to 1.9 as shown in Table 1).

This was consequently explained by the FQPT in [4]. By FQPT, here we mean that there is a level anti-crossing between two states as illustrated in Figure 3. The minimum spectral gap (g_{min}) and the position (s^*) were then estimated based on the assumption of the level anti-crossing between the global minimum and the

w_B	s^*	$g_{\min}$
1.0	0.2368	5.23e-01
1.1	0.2517	4.12e-01
1.2	0.2708	2.90e-01
1.3	0.2964	1.68e-01
1.4	0.3323	7.14e-02
1.5	0.3805	2.04e-02
1.6	0.4422	3.63e-03
1.7	0.5217	3.39e-04
1.8	0.6276	1.04e-05
1.9	0.7758	4.14e-08

Table 1: The minimum spectral gap $g_{\min}$ (and position s^*) changes as w_B changes from 1 to 1.9, for the (unscaled) problem Hamiltonian $\mathcal{H}_1$ in Eq.(4).

local minima using perturbation method. In particular, $g_{\min}$ was estimated by the tunneling amplitude between the global minimum and the local minima. The formula so derived involves combinatorial enumeration of the all possible paths between local minima and the global minimum, and suggested $g_{\min}$ is exponentially (in terms of the problem size) small. See also [2, 4, 13, 27] for more explanation on the FQPT and the level anti-crossing.

5 Varying Parameters in the Problem Hamiltonian for MIS

In this section, we show that by changing the parameters in the problem Hamiltonian for MIS on CK graphs, the FQPT no longer occurs and we can significantly increase $g_{\min}$.

Recall that in the pseudo-boolean formulation of MIS as in Theorem 3.1, the requirement for J_{ij} is at least $\min\{c_i, c_j\}$, for each $ij \in \mathsf{E}(G)$. For simplicity, we consider the simplest case in which $J_{ij} = J$ for all $ij \in \mathsf{E}(G)$. In other words, we have the corresponding problem Hamiltonian:

$$\mathcal{H}_1 = \sum_{i \in \mathsf{V}(G)} (d_i J - 2c_i)\sigma_i^z + \sum_{ij \in \mathsf{E}(G)} J\sigma_i^z \sigma_j^z$$

where d_i is the degree of vertex $i \in \mathsf{V}(G)$.

The natural question is: how does the ART change when we vary J? Note that it is not sufficient to consider only the minimum spectral gap change (as almost all the other works on adiabatic quantum computation did) because by increasing J, the maximum energy of the system Hamiltonian also increases. Instead, in order to keep the maximum energy of the system Hamiltonian comparable, we keep J fixed and vary c_i instead, namely multiplying all weights c_i by a scaling factor, say $1/k$, for $k \geq 1$, which does not change the original problem to be solved. We remark that this is equivalent to multiplying J by k, and then multiply the problem Hamiltonian by $(1/k)$.

That is, we consider the following (scaled) problem Hamiltonian

$$\mathcal{H}_k = \sum_{i \in \mathsf{V}(G)} (Jd_i - 2c_i/k)\sigma_i^z + \sum_{ij \in \mathsf{E}(G)} J\sigma_i^z \sigma_j^z \tag{5}$$

where $k \geq 1$ is the scaling factor.

5.1 Minimum Spectral Gap g_{min} Without FQPT

The DESEVs of $\mathcal{H}_1$ and $\mathcal{H}_{10}$ are shown in Figure 4 and Figure 5. The anti-crossing between the global minimum and the local minima (for $k = 1$) no longer occurs for $k = 10$, and g_{min} increases from 1.04×10^{-5} to 0.145. A worthwhile observation is the change in the lowest few excited energy levels: for $k = 1$, the lowest few excited states (beyond the first excited state) of the problem Hamiltonian is mainly the superposition of states from V_B ($\triangle$) (which constitutes the local minima); while these states of the scaled ($k = 10$) problem Hamiltonian is mainly the superposition of states from V_A($\bullet$) (which constitutes the global minimum). That is, the minimum spectral gap can be increased drastically when the second or higher excited energy levels are changed (while the lowest and first excited energy level stay the same). The DESEVs of $\mathcal{H}_k$ for $k = 1, 2, 3, 5, 10, 50$ are shown in Figure 6.

In [4], based on the FQPT assumption, we estimate g_{min} (for $\mathcal{H}_1$) by the tunneling amplitude between the local minima and the global minimum, which suggests that g_{min} is exponentially small. However, for $k = 10$, from our numerical data and DESEV in Figure 4, we see that the FQPT (that causes g_{min} to be exponentially small) no longer occurs, and g_{min} increases significantly (from 10^{-5} to 0.145). This seems to suggest that g_{min} to be polynomially small instead. We are currently investigating how to analytically bound or estimate g_{min} of $\mathcal{H}_k$ for a general CK graph of size n. We remark here that the perturbation method is still valid (in fact, as we increase k, we also increase the minimum spectral gap position $s^* \rightsquigarrow 1$), however we can no longer assume that g_{min} can be approximated by the tunneling amplitude between the two (localized) states.

5.2 Scaling Factor and ART

In this section, we discuss what the good scaling factor should be, and how it affects the ART. To address this question, we need an appropriate formulation for ART. We point out that it is not sufficient to just consider g_{min}, but the matrix element of the time derivative of the Hamiltonian also matters. In particular, we adopt the following three formulations, which are related to the widely used traditional condition:

$$(*) \begin{cases} \mathsf{ART}_1(\mathcal{H}) = \frac{\max_{0\le s\le 1} \mathcal{M}(s)}{g_{\mathsf{min}}^2} \max_{0\le s\le 1} ||\mathcal{H}(s)|| \\ \mathsf{ART}_2(\mathcal{H}) = \frac{\mathcal{M}(s^*)}{g_{\mathsf{min}}^2} \max_{0\le s\le 1} ||\mathcal{H}(s)||, \text{ where } g_{\mathsf{min}} = E_1(s^*) - E_0(s^*) \\ \mathsf{ART}_3(\mathcal{H}) = \max_{0\le s\le 1} \frac{\mathcal{M}(s)}{(E_1(s)-E_0(s))^2} \max_{0\le s\le 1} ||\mathcal{H}(s)|| \end{cases}$$

where $\mathcal{M}(s) = |\langle E_1(s)|\frac{d\mathcal{H}}{ds}|E_0(s)\rangle|$ is the matrix element of the time derivative Hamiltonian at time s, and $\mathcal{H}(s)|E_i(s)\rangle = E_i(s)|E_i(s)\rangle$. See Table 2 for the numerical comparisons.

From Table2, we see that g_{min} increases as k increases from 1 to 10, however, decreases from 10 to 50 (even though it is still much larger than $k = 1$). The latter, perhaps, can be explained by the following: as k increases, the difference between the low energy levels decreases, and becomes dominate for $k > 10$. We remark that the optimal value for k seems to depend only on the vertex weights (for which J depends on), and independ of the problem size. By increasing the scaling factor, we also increase the precision (or dynamic range) requirement for representing the parameters (h_i & J_{ij}) in the problem Hamiltonian, which is one of the important physical resources.

Notice that $\mathsf{ART}_2 \le \mathsf{ART}_1 \le \mathsf{ART}_3$. The condition given in ART_3 is the formula that one would derive from the adiabatic approximation. The condition in ART_1 is the widely used traditional version. The condition in ART_2 was mentioned in [26]. The natural question is: when are they asymptotically equivalent? Indeed, the three versions of ART coincide for some Hamiltonians (e.g. for $k = 1$). However, they can be very different for the large k. The main reason is that the matrix element $\mathcal{M}(s)$ can be extremely small at the minimum spectral gap position s^*. For example, for $k = 50$, $s^* \rightsquigarrow 1$, $\mathcal{M}(s^*)$ is extremely small. Note one can

k	s^*	g_{min}	$\mathcal{M}(s^*)$	$\max_{0\le s\le 1}\mathcal{M}(s)$	$\max_{0\le s\le 1}\|\|\mathcal{H}\|\|$	ART_2	ART_1
1	0.62763727	1.04e-05	4.02e+00	4.02e+00	2.26e+02	8.34e+12	8.34e+12
2	0.54578285	6.37e-03	2.04e+00	2.04e+00	2.48e+02	1.24e+07	1.24e+07
3	0.54467568	3.30e-02	1.41e+00	1.41e+00	2.55e+02	3.32e+05	3.32e+05
4	0.55610853	6.83e-02	1.18e+00	1.18e+00	2.59e+02	6.57e+04	6.58e+04
5	0.57419149	9.67e-02	1.06e+00	1.07e+00	2.61e+02	2.96e+04	2.99e+04
10	0.66773072	1.45e-01	7.48e-01	7.92e-01	2.66e+02	9.45e+03	1.00e+04
20	0.80170240	1.30e-01	4.72e-01	5.68e-01	2.68e+02	7.48e+03	9.01e+03
30	0.99318624	7.97e-02	8.95e-09	4.26e-01	2.69e+02	3.78e-04	1.80e+04
40	0.99642154	5.99e-02	4.90e-10	4.35e-01	2.69e+02	3.67e-05	3.26e+04
50	0.99779592	4.79e-02	5.30e-11	4.41e-01	2.69e+02	6.20e-06	5.16e+04

k	s'	$g(s')$	$\mathcal{M}(s')$	$\frac{\mathcal{M}(s')}{g(s')^2}$	$\max_{0\le s\le 1}\|\|\mathcal{H}\|\|$	ART_3
1	0.62763727	1.04e-05	4.02e+00	3.70e+10	2.26e+02	8.34e+12
2	0.54578226	6.37e-03	2.04e+00	5.02e+04	2.48e+02	1.24e+07
3	0.54461081	3.30e-02	1.41e+00	1.30e+03	2.55e+02	3.32e+05
4	0.55545411	6.83e-02	1.18e+00	2.54e+02	2.59e+02	6.57e+04
5	0.57223394	9.68e-02	1.07e+00	1.14e+02	2.61e+02	2.97e+04
10	0.65682886	1.46e-01	7.75e-01	3.64e+01	2.66e+02	9.66e+03
20	0.77115481	1.33e-01	5.41e-01	3.08e+01	2.68e+02	8.24e+03
30	0.83962780	1.08e-01	4.43e-01	3.82e+01	2.69e+02	1.02e+04
40	0.88050519	8.82e-02	3.93e-01	5.05e+01	2.69e+02	1.36e+04
50	0.90581875	7.39e-02	3.63e-01	6.64e+01	2.69e+02	1.79e+04

where $g(s) = E_1(s) - E_0(s)$, and $s' = \arg\max_{0\le s\le 1}\frac{\mathcal{M}(s)}{g(s)^2}$.

Table 2: ART_1, ART_2, ART_3 for $\mathcal{H}_k$ in Eq.(5). Observations: (1) g_{min} increases as k increases from 1 to 10, but decreases from 10 to 50. (2) ART_1, ART_2, and ART_3 are close for $k < 5$. (3) The matrix element $\mathcal{M}(s^*)$ at the position of minimum spectral gap is extremely small for $k \ge 30$. (4) For $k > 10$, s^* (the position of the minimum spectral gap) is different from s', where $s' = \arg\max_{0\le s\le 1}\frac{\mathcal{M}(s)}{g(s)^2}$.

show that $\mathcal{M}(s) = |\langle E_1(s)|\mathcal{H}_{\mathsf{init}}|E_0(s)\rangle|/s$ for $s \in (0,1]$ because $\mathcal{M}(s) = |\langle E_1(s)|\mathcal{H}(1) - \mathcal{H}(0)|E_0(s)\rangle| = |\langle E_1(s)|\frac{\mathcal{H}(s)-\mathcal{H}(0)}{s}|E_0(s)\rangle| = |\langle E_1(s)|\mathcal{H}(0)|E_0(s)\rangle|/s$. Thus, for our initial Hamiltonian, $\mathcal{M}(s)$ measures the overlap of the states with one single bit flip, and in this case it is extremely small. Observe that the position of the minimum spectral gap s^* is not the same as the position s' where $\frac{\mathcal{M}(s)}{g(s)^2}$ is maximized. What should be the appropriate formulation of ART? Should it be ART_3? If so, under what condition, can ART_1 be a good approximation to ART_3? and under what condition, can we assume that g_{min} is the dominating factor (as have been assumed by all other works)?

6 Discussion

In this paper, we have shown that by changing the parameters in the problem Hamiltonian (without changing the problem to be solved) of the adiabatic algorithm for MIS on CK graphs, we prevent the FQPT, that causes the

exponential small g_{min}, from occurring and significantly increase g_{min}. We do so by scaling the vertex-weight of the graph, namely, multiplying the weights of vertices by a scaling factor. In order to determine the best scaling factor, we raise the basic question about what the appropriate formulation of adiabatic running time should be.

In [24, 25], van Dam et al. argued that adiabatic quantum optimization might be thought of as a kind of "quantum local search", and in [25], they constructed a special family of 3SAT instances for which the clause-violation cost function based adiabatic algorithm required exponential time. Farhi et al. [12] showed that the exponential small gap could be overcome by different initial Hamiltonians. In [7], we point out that the exponential small gap argument does not apply to a different adiabatic algorithm for 3SAT. Our CK graphs were designed to trap local search algorithms in the sense that there are many local minima to mislead the local search process. From DESEV on a 15-vertex CK graph, we see that indeed this is the case for $\mathcal{H}_1$ and the adiabatic algorithm would require exponential time due to the exponential small g_{min} caused by the FQPT or the level anti-crossing between the global minimum and the local minima. However, for $\mathcal{H}_k$ (say $k = 10$), the FQPT no longer occurs and g_{min} increases significantly, which might suggest the possibility of exponential speed-up over $\mathcal{H}_1$. It remains challenging on how to analytically bound g_{min} and/or ART of the adiabatic algorithm for $\mathcal{H}_k$ on general CK graphs. One worthwhile observation from this work is that the minimum spectral gap can be increased drastically when the second or higher excited energy states are overlapping with the ground state in spite of the large amount of first excited states (which constitutes the local minima). Recall that NP-complete problems can be polynomial reducible to each other. The reduction requires only the solution to be preserved, i.e. there is a polynomial time algorithm that maps the solution to the reduced problem to the solution to the original problem and vice versa (see e.g. [9]). In other words, the reduction might only preserves the solution (i.e. the ground state) and alter the energy levels of the problem Hamiltonian. Therefore, according to the observation, different reduction is possible to give rise to different problem Hamiltonians, and thus different adiabatic quantum algorithms, for the same problem. Indeed, we have shown in [7] that based on the NP-complete reductions, we describe different adiabatic quantum algorithms to which the arguments in [25, 2] for the failure of their adiabatic quantum algorithms do not apply.

In summary, although our result is only numerical and supported by visualization, this small example, nevertheless, serves to show that it is possible to avoid FQPT, and also to concretely clarify that it is not sufficient to consider one specific problem Hamiltonian (and thus one specific adiabatic quantum optimization algorithm) for proving the failure of adiabatic quantum optimization for a problem as in [25, 2].

7 Acknowledgments

I would like to thank my very enthusiastic students in my adiabatic quantum computing class: Ryan Blace, Russell Brasser, Mark Everline, Eric Franklin, Nabil Al Ramli, and Aiman Shabsigh, who also helped to name DESEV. I would like to thank Siyuan Han, Peter Young, Mohammad Amin, Neil Dickson, Robert Raussendorf, Tzu-Chieh Wei and Pradeep Kiran for their comments. Thanks also go to David Sankoff and David Kirkpatrick for the encouragement.

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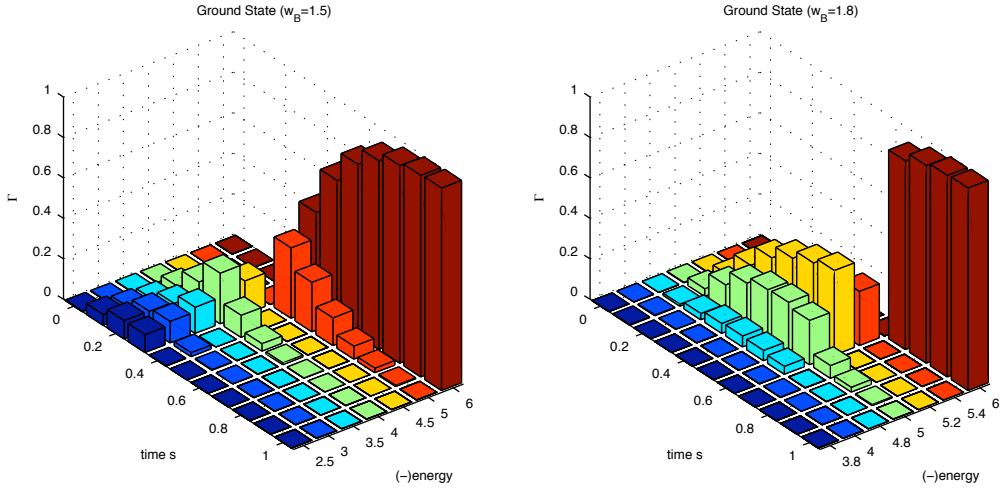


$s^* = 0.3805, g_{\min} = 2.04 \times 10^{-2}$

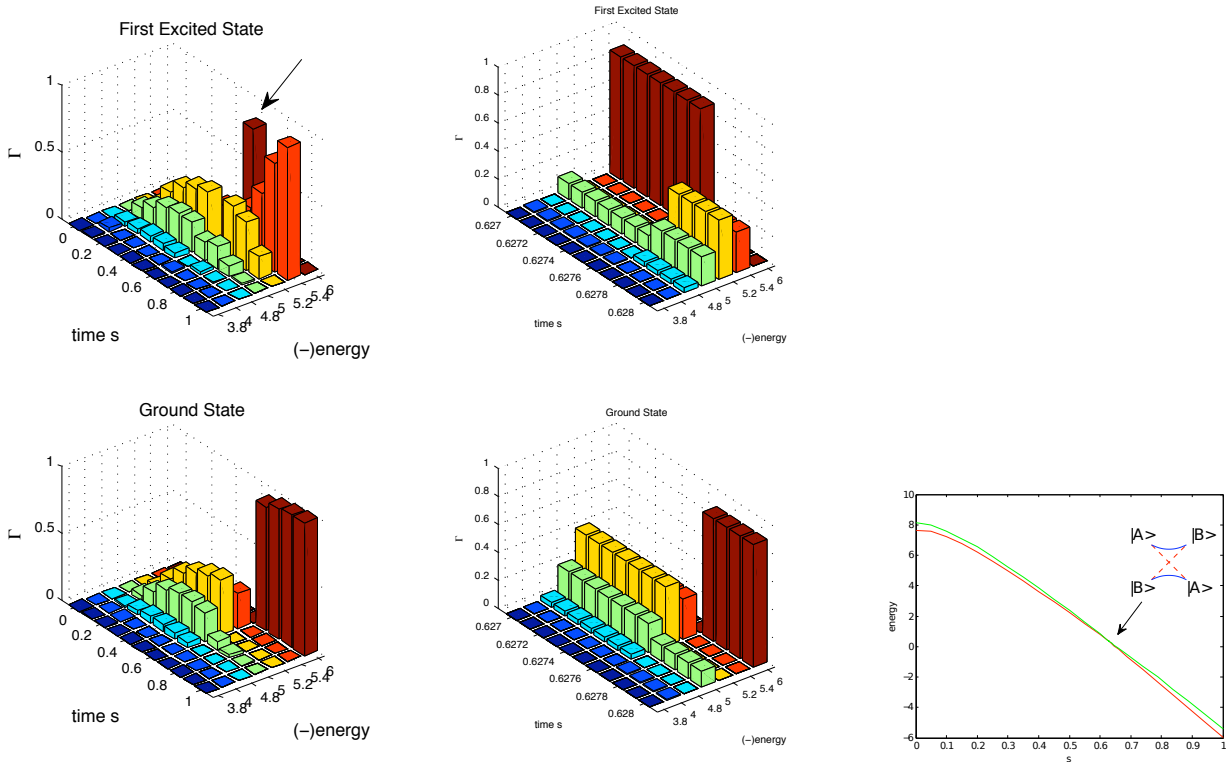
(-)energy	state
6	$\vert\bullet\bullet\bullet\bullet\bullet\bullet\rangle$
5	$\vert\bullet\bullet\bullet\bullet\bullet\rangle$
4.5	$\vert\triangle\triangle\triangle\rangle$
4	$\vert\bullet\bullet\bullet\bullet\rangle$
3.5	$\vert\bullet\bullet\triangle\rangle$
3	$\vert\bullet\bullet\bullet\rangle$
2.5	$\vert\bullet\triangle\rangle$

$s^* = 0.6276, g_{\min} = 1.04 \times 10^{-5}$

(-)energy	state
6	$\vert\bullet\bullet\bullet\bullet\bullet\bullet\rangle$
5.4	$\vert\triangle\triangle\triangle\rangle$
5.2	$\vert\triangle\triangle\triangle\text{–}\triangle\rangle$
5	$\vert\bullet\bullet\bullet\bullet\bullet\rangle + \vert\triangle\triangle\text{–}\triangle\triangle\text{–}\triangle\rangle$
4.8	$\vert\triangle\text{–}\triangle\triangle\text{–}\triangle\triangle\text{–}\triangle\rangle$
4	$\vert\bullet\bullet\bullet\bullet\rangle$
3.8	$\vert\bullet\bullet\triangle\rangle$

Figure 2: DESEV (only the 7 lowest energy levels shown) of the ground state of the MIS adiabatic algorithm with $\mathcal{H}_1$ in Eq.(4) as the problem Hamiltonian for $w_B = 1.5$ (left) and $w_B = 1.8$ (right). The x-axis is the time s. The y-axis is the (-)energy level. Each color corresponds to an energy level. The correspondence between (-)energy levels and the states are shown. The z-axis is Γ. As time s increases, one can see how Γ of each energy level evolves to get some sense of the evolution. For example, for $w_B = 1.5$ (left), for the (-)energy level 6 (which corresponds to the solution state), shown in brown, Γ changes from almost 0 at $s = 0.2$, to more than 0.4 at $s = 0.4$, to almost 1.0 at $s = 0.8$. For $w_B = 1.8$ (right), Γ of (-) energy level 6 changes from almost 0 before $s = 0.6$ to more than 0.9 at $s = 0.7$; while Γ of (-) energy level 5.4, which corresponds to the local minima, gradually increases from $s = 0$ to 0.6, but almost 0 after $s = 0.6$.

(Zoom:$s = 0.627 \ldots 0.628$)



$s^* = 0.6276, g_{\mathsf{min}} = 1.04 \times 10^{-5}$

(a) (b) (c)

3.8 $|\bullet\bullet\triangle\rangle$ 4 $|\bullet\bullet\bullet\bullet\rangle$ 4.8 $|\triangle\!\!-\!\!\triangle\!\!-\!\!\triangle\!\!-\!\!\triangle\!\!-\!\!\triangle\rangle$ 5 $|\bullet\bullet\bullet\bullet\bullet\rangle + |\triangle\!\!-\!\!\triangle\!\!-\!\!\triangle\!\!-\!\!\triangle\rangle$ 5.2 $|\triangle\triangle\!\!-\!\!\triangle\rangle$ 5.4 $|\triangle\triangle\triangle\rangle$ 6 $|\bullet\bullet\bullet\bullet\bullet\bullet\rangle$

Figure 3: DESEV of the ground state and the first excited state of the MIS adiabatic algorithm with $\mathcal{H}_1$ in (4) as the problem Hamiltonian for $w_B = 1.8$ (a) $s = 0 \ldots 1$; (b) Zoom in $s = 0.627 \ldots 0.628$; (c) The lowest two energy levels of $\mathcal{H}(s)$, $s = 0 \ldots 1$. The inset illustrates a level anti-crossing between two states $|B\rangle$ and $|A\rangle$, or the system has a FQPT from $|B\rangle$ to $|A\rangle$ at the anti-crossing s^*. In this example, $|A\rangle = |\bullet\bullet\bullet\bullet\bullet\bullet\rangle + |\bullet\bullet\bullet\bullet\bullet\bullet\rangle$ and $|B\rangle = |\triangle\!\!-\!\!\triangle\!\!-\!\!\triangle\!\!-\!\!\triangle\!\!-\!\!\triangle\rangle + |\triangle\triangle\!\!-\!\!\triangle\!\!-\!\!\triangle\rangle + |\triangle\triangle\triangle\rangle$.

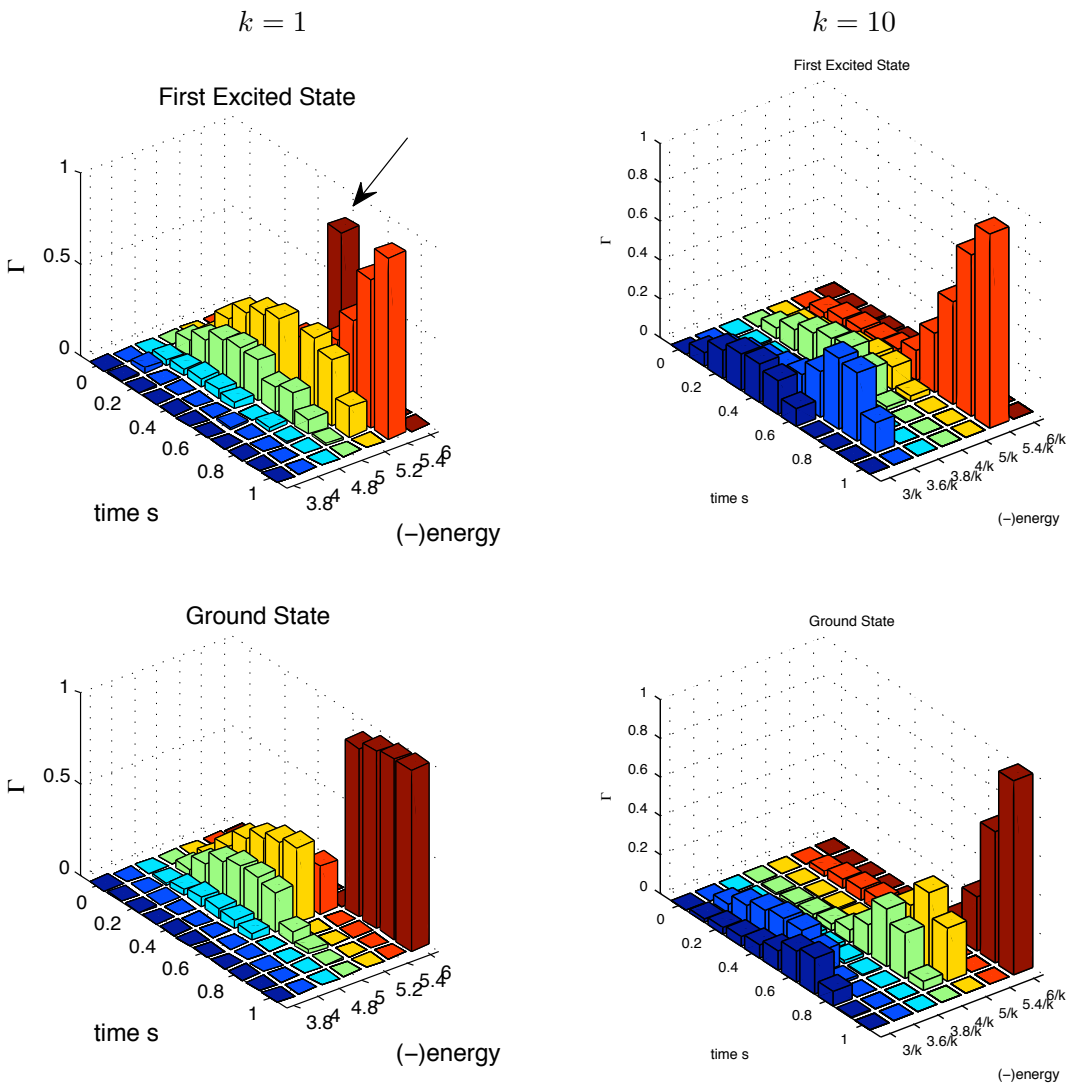
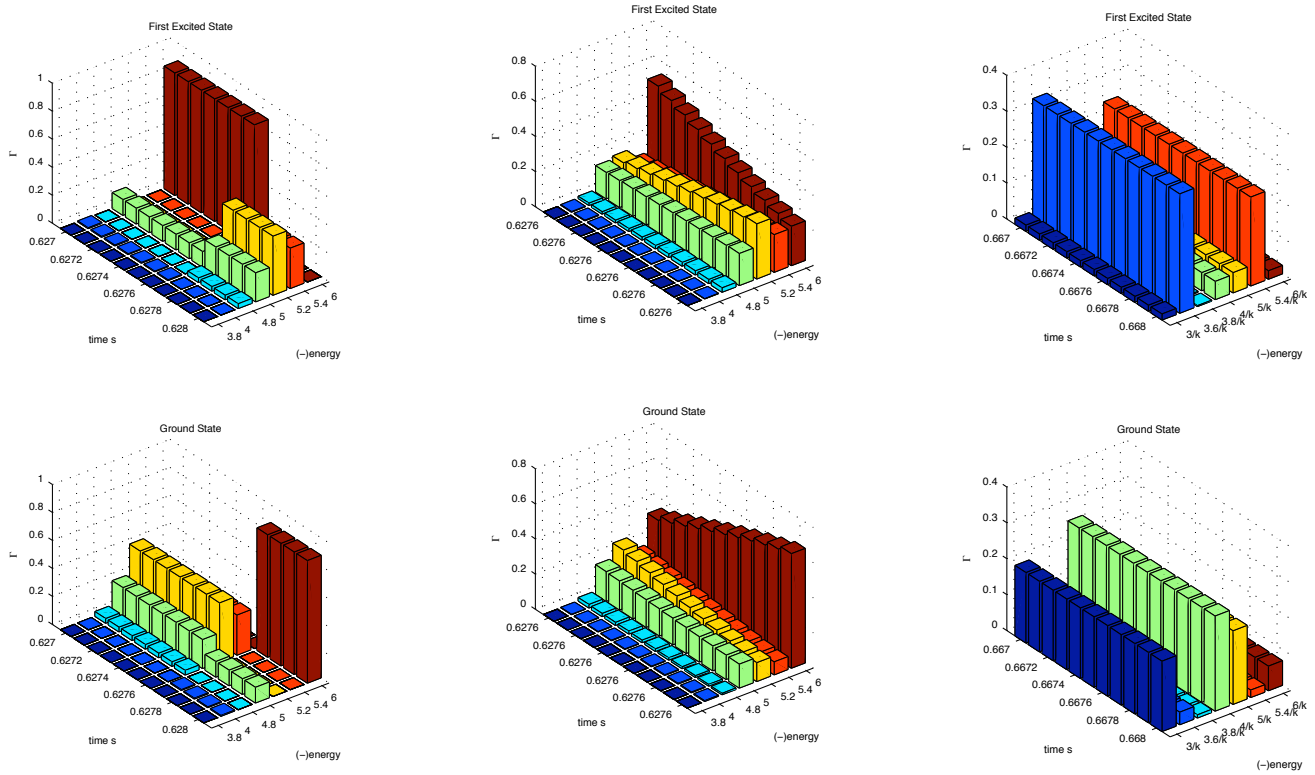


Figure 4: DESEV of the ground state and the first excited state of the MIS adiabatic algorithm with problem Hamiltonian $\mathcal{H}_1$ (left) and $\mathcal{H}_{10}$ (right) where $w_B = 1.8$. Notice the differences in the lowest few excited states. For $k = 1$, the $2nd$ and $3rd$ excited states are superpositions of $\triangle$s (vertex in V_B which constitutes the local optima); while for $k = 10$, the $2nd$ and $3rd$ excited states are superpositions of $\bullet$s (vertex in V_A which constitutes the global optimum). As a result, the first order phase transition from local minima to global minimum occurs for $k = 1$, which results in the $g_{\min} = 1.04 \times 10^{-5}$ at $s^* = 0.627$. For $k = 10$, such crossing no longer occurs, and $g_{\min} = 0.145$ at $s^* = 0.667$. See Figure 5 for the zoom-in.

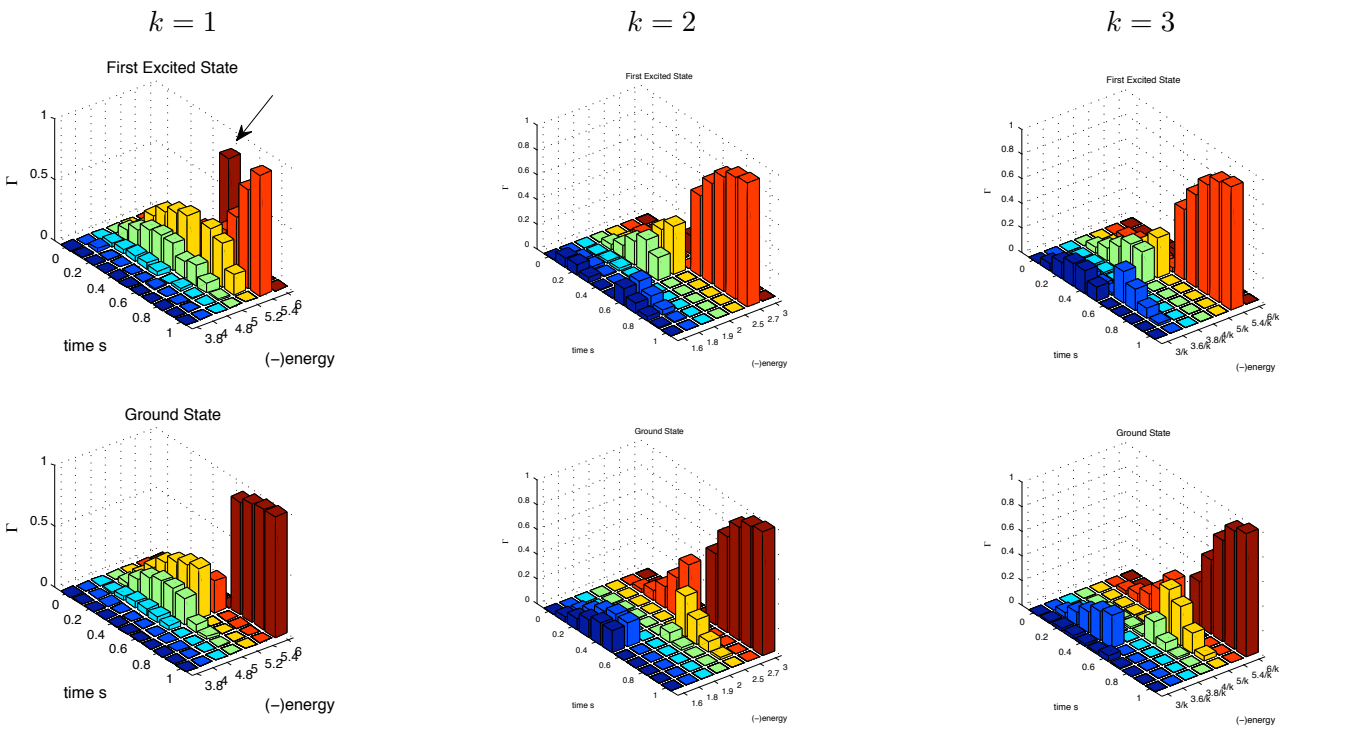
$k = 1 (s : 0.627 \ldots 0.628)$ $k = 1 (s : 0.62763 \ldots 0.62764)$ $k = 10 (s : 0.667 \ldots 0.668)$



$s^* = 0.62763727, g_{\mathsf{min}} = 1.04 \times 10^{-5}$ $s^* = 0.62763727, g_{\mathsf{min}} = 1.04 \times 10^{-5}$ $s^* = 0.66773072, g_{\mathsf{min}} = 1.45 \times 10^{-1}$

$k = 1$	3.8 $\lvert \bullet\bullet\triangle \rangle$	4 $\lvert \bullet\bullet\bullet\bullet \rangle$	4.8 $\lvert \triangle\!-\!\triangle\!-\!\triangle\!-\!\triangle\!-\!\triangle \rangle$	5 $\lvert \bullet\bullet\bullet\bullet\bullet \rangle + \lvert \triangle\!-\!\triangle\!-\!\triangle\!-\!\triangle \rangle$	5.2 $\lvert \triangle\triangle\triangle\!-\!\triangle \rangle$	5.4 $\lvert \triangle\triangle\triangle \rangle$	6 $\lvert \bullet\bullet\bullet\bullet\bullet\bullet \rangle$
$k = 10$	$3/k$ $\lvert \bullet\bullet\bullet \rangle$	$3.6/k$ $\lvert \triangle\triangle \rangle$	$3.8/k$ $\lvert \bullet\bullet\triangle \rangle$	$4/k$ $\lvert \bullet\bullet\bullet\bullet \rangle$	$5/k$ $\lvert \bullet\bullet\bullet\bullet\bullet \rangle$	$5.4/k$ $\lvert \triangle\triangle\triangle \rangle$	$6/k$ $\lvert \bullet\bullet\bullet\bullet\bullet\bullet \rangle$

Figure 5: Zoom around s^*.



$k = 1$	3.8 $\lvert\bullet\bullet\triangle\rangle$	4 $\lvert\bullet\bullet\bullet\bullet\rangle$	4.8 $\lvert\triangle\text{–}\triangle\text{–}\triangle\text{–}\triangle\text{–}\triangle\rangle$	5 $\lvert\bullet\bullet\bullet\bullet\bullet\rangle + \lvert\triangle\text{–}\triangle\text{–}\triangle\text{–}\triangle\rangle$	5.2 $\lvert\triangle\triangle\triangle\text{–}\triangle\rangle$	5.4 $\lvert\triangle\triangle\triangle\rangle$	6 $\lvert\bullet\bullet\bullet\bullet\bullet\bullet\rangle$
$k = 2$	1.6 $\lvert\triangle\triangle\text{–}\triangle\rangle$	1.8 $\lvert\triangle\triangle\rangle$	1.9 $\lvert\bullet\bullet\triangle\rangle$	2 $\lvert\bullet\bullet\bullet\bullet\rangle$		2.5 $\lvert\bullet\bullet\bullet\bullet\bullet\rangle$	2.7 $\lvert\triangle\triangle\triangle\rangle$	3 $\lvert\bullet\bullet\bullet\bullet\bullet\bullet\rangle$
$k \geq 3$	$3/k$ $\lvert\bullet\bullet\bullet\rangle$	$3.6/k$ $\lvert\triangle\triangle\rangle$	$3.8/k$ $\lvert\bullet\bullet\triangle\rangle$	$4/k$ $\lvert\bullet\bullet\bullet\bullet\rangle$		$5/k$ $\lvert\bullet\bullet\bullet\bullet\bullet\rangle$	$5.4/k$ $\lvert\triangle\triangle\triangle\rangle$	$6/k$ $\lvert\bullet\bullet\bullet\bullet\bullet\bullet\rangle$

Figure 6: DESEV of the ground state and the first excited state of the adiabatic algorithm with problem Hamiltonian $\mathcal{H}_k$ for $w_B = 1.8$, where $k = 1, 2, 3, 5, 10, 50$.