Minor-Embedding in Adiabatic Quantum Computation: I. The Parameter Setting Problem

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Abstract

We show that the NP-hard quadratic unconstrained binary optimization (QUBO) problem on a graph G can be solved using an adiabatic quantum computer that implements an Ising spin-1/2 Hamiltonian, by reduction through *minor-embedding* of G in the quantum hardware graph U. There are two components to this reduction: *embedding* and *parameter setting*. The embedding problem is to find a minor-embedding G_{emb} of a graph G in U, which is a subgraph of U such that G can be obtained from G_{emb} by contracting edges. The parameter setting problem is to determine the corresponding parameters, qubit biases and coupler strengths, of the embedded Ising Hamiltonian. In this paper, we focus on the parameter setting problem. As an example, we demonstrate the embedded Ising Hamiltonian for solving the maximum independent set (MIS) problem via adiabatic quantum computation (AQC) using an Ising spin-1/2 system. We close by discussing several related algorithmic problems that need to be investigated in order to facilitate the design of adiabatic algorithms and AQC architectures.

1 Introduction

Adiabatic Quantum Computation (AQC) was proposed by Farhi et al.[15, 14] in 2000. The AQC model is based on the *adiabatic theorem* (see, e.g. [22]). Informally, the theorem says that if we take a quantum system whose Hamiltonian "slowly" changes from \mathcal{H}_{init} (initial Hamiltonian) to \mathcal{H}_{final} (final Hamiltonian), then if we start with the system in the *groundstate* (eigenvector corresponding to the lowest eigenvalue) of \mathcal{H}_{init} , then at the end of the evolution the system will be "predominantly" in the ground state of \mathcal{H}_{final} . The theorem is used to construct *adiabatic algorithms* for optimization problems in the following way: The initial Hamiltonian \mathcal{H}_{init} is designed such that the system can be readily initialized into its known groundstate, while the groundstate of the final Hamiltonian \mathcal{H}_{final} encodes the answer to the desired optimization problem. The complete (or *system*) Hamiltonian at a time t is then given by

$$\mathcal{H}(t) = \left(1 - s(\frac{t}{T})\right) \mathcal{H}_{\mathsf{init}} + s(\frac{t}{T}) \mathcal{H}_{\mathsf{final}}$$

for $t \in [0, T]$ where s increases monotonically from s(0) = 0 to s(1) = 1 and T is the total running time of the algorithm. If T is large enough, which is determined by the minimum spectral gap (the difference between the two lowest energy levels) of the system Hamiltonian, the adiabatic theorem guarantees the state at time t will be the groundstate of $\mathcal{H}(t)$, leading to the solution, the ground state of $\mathcal{H}(T) = \mathcal{H}_{final}$.

It is believed that AQC is advantageous over standard (the gate model) quantum computation in that it is more robust against environmental noise [11, 3, 4]. In 2004, D-Wave Systems Inc. undertook the endeavor to build an adiabatic quantum computer for solving NP-hard problems. Kaminsky and Lloyd [17] proposed a scalable architecture for AQC of NP-hard problems. Note that AQC is polynomially equivalent to the standard quantum computation, and therefore AQC is universal. Farhi et al. in their original paper [15] showed that AQC can be efficiently simulated by standard quantum computers. In 2004, Aharonov et al [1] proved the more difficult converse statement that standard quantum computation can be efficiently simulated by AQC. In this paper, however, we will focus on a subclass of Hamiltonians, known as *Ising models in a transverse field*, that are NP-hard but not universal for quantum computation. This subclass of Hamiltonians has been implemented by D-Wave Systems Inc.

D-Wave's quantum hardware architecture can be viewed as an undirected graph U with weighted vertices and weighted edges. See Figure 1 for an example. Denote the vertex set of U by V(U) and the edge set of U by



Figure 1: An example hardware graph: a 4×4 extended grid. Each qubit is coupled with its nearest and nextnearest neighbors.

E(U). Each vertex $i \in V(U)$ corresponds to a qubit, and each edge $ij \in E(U)$ corresponds to a coupler between qubit *i* and qubit *j*. In the following, we will use qubit and vertex, and coupler and edge interchangeably when there is no confusion. There are two weights, h_i (called the qubit *bias*) and Δ_i (called the *tunneling amplitude*), associated with each qubit *i*. There is a weight J_{ij} (called the coupler *strength*) associated with each coupler *ij*. In general, these weights are functions of time, i.e., they vary over the time, e.g., $h_i(t)$.

The Hamiltonian of the Ising model in a transverse field thus implemented is:

$$\mathcal{H}(t) = \sum_{i \in \mathsf{V}(G)} h_i(t)\sigma_i^z + \sum_{ij \in \mathsf{E}(G)} J_{ij}(t)\sigma_i^z\sigma_j^z + \sum_{i \in \mathsf{V}(G)} \Delta_i(t)\sigma_i^x$$

with $\sigma_i^z = I \otimes I \otimes \ldots \otimes \sigma^z \otimes \ldots \otimes I$ (the σ^z is in the *i*th position), similarly for σ_i^x and $\sigma_i^z \sigma_j^z$, where I is the 2×2 identity matrix, while σ^z and σ^x are the Pauli matrices given by

$$\sigma^{z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \text{ and } \sigma^{x} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

In general, the transverse field (i.e. $\sum_{i \in V(G)} \Delta_i \sigma_i^x$) encodes the initial Hamiltonian \mathcal{H}_{init} , while the other two terms encode the final Hamiltonian:

$$\mathcal{H}_{\text{final}} = \sum_{i \in \mathsf{V}(G)} h_i \sigma_i^z + \sum_{ij \in \mathsf{E}(G)} J_{ij} \sigma_i^z \sigma_j^z.$$
(1)

One can show (see Appendix) that the eigenvalues and the corresponding eigenstates of \mathcal{H}_{final} are encoded in the following energy function of Ising Model:

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

where $s_i \in \{-1, +1\}$, called a *spin*, and $h_i, J_{ij} \in \mathbb{R}$. In particular, the smallest eigenvalue of \mathcal{H}_{final} corresponding to the minimum of \mathcal{E} , and $\arg \min \mathcal{E}$ corresponds to its eigenvector (called *ground state*) of \mathcal{H}_{final} . When there is no confusion, we use the energy function of Ising model and Ising Hamiltonian interchangeably. Hereafter, we refer the problem of finding the minimum energy of the Ising Model or equivalently the groundstate of Ising Hamiltonian as the *Ising problem*. It can be shown that the Ising problem is equivalent to the problem of Quadratic Unconstrained Boolean Optimization (QUBO)(see [9] and references therein), which has been shown to be a common model for a wide variety of discrete optimization problems. More specifically, finding the minimum of \mathcal{E} in (2) is equivalent to finding the maximum of the following function (which is also known as quadratic pseudo-Boolean function [8]) of QUBO on the same graph:

$$\mathcal{Y}(x_1, \dots, x_n) = \sum_{i \in \mathsf{V}(G)} c_i x_i - \sum_{ij \in \mathsf{E}(G)} J_{ij} x_i x_j \tag{3}$$

where $x_i \in \{0, 1\}, c_i, J_{ij} \in \mathbb{R}$. The correspondence between the parameters, hs and cs will be shown in Section 2. Therefore, given an Ising/QUBO problem on graph G, one can thus solve the problem on an adiabatic quantum computer (using an Ising spin-1/2 system) if G can be embedded as a subgraph of the quantum hardware graph U. We refer this embedding problem as *subgraph-embedding*, to be defined formally in Section 3. In general, there are physical constraints on the hardware graph U. In particular, there is a *degree-constraint* in that each qubit can have at most a constant number of couplers dictated by hardware design. Therefore, besides the possible difficulty of the subgraph-embedding problem¹, the graphs that can be solved on a given hardware graph U through subgraph-embedding must also be degree-bounded. Kaminsky et al. [17, 18] observed and proposed that one can embed G in U through ferromagnetic coupling "dummy vertices" to solve Maximum Independent Set (MIS) problem ² of planar cubic graphs (regular graphs of degree-3)³ on an adiabatic quantum computer. In particular, they proposed an $n \times n$ square lattice as a scalable hardware architecture on which all n/3-vertex planar cubic graphs are embeddable. The notion of embedding here follows naturally from physicists' intuition that each *logical qubit* (corresponding to a vertex in the input graph) is mapped to a subtree of *physical qubits* (corresponding to vertices in the hardware graph) that are ferromagnetically coupled such that each subtree of physical qubits acts like a single logical qubit. For example, in Figure 2, the logical qubit 1 (in orange color) of the graph G is mapped to a subtree of physical qubits (labelled 1) of the square lattice. Informally, a minorembedding G_{emb} of a graph G in the hardware graph U is a subgraph of U such that G_{emb} is an "expansion" of G by replacing each vertex of G with a (connected) subtree of U, or equivalently, G can be obtained from G_{emb} by contracting edges (same color in Figure 2). In graph theory, G is called a (graph) minor of U (see for example [12]). The minor-embedding will be formally defined in Section 3. (Remark: The embedding in [17, 18] is a special case of minor-embedding, known as topological-minor embedding.)

¹Readers should be cautious not to confuse this embedding problem with the NP-complete subgraph isomorphism problem, in which both graphs are unknown. However, in our case, the hardware graph is known. For example, if the hardware graph is a complete graph, then the embedding problem will be trivial.

²MIS is a special case of QUBO and will be addressed in Section 5.

³In their earlier paper [17], it was said for graphs with degree at most 3, but the Ising Hamiltonian they used there was for regular graphs of degree-3.



Figure 2: $G_{emb}(right)$ is a minor-embedding of G(left) in the square lattice U. Each vertex (called a logical qubit) of G is mapped to a (connected) subtree of (same color/label) vertices (called physical qubits) of U. G is called a (graph) minor of U.

By reduction through minor-embedding, we mean that one can reduce the original Ising Hamiltonian on the input graph G to the embedded Ising Hamiltonian \mathcal{H}^{emb} on its minor-embedding G_{emb} , i.e., the solution to the embedded Ising Hamiltonian gives rise to the solution to the original Ising Hamiltonian. The intuition suggests that the reduction will be correct provided that the ferromagnetic coupler strengths used are sufficiently strong (i.e., large negative number). However, how strong is "strong enough"? In [17, 18], they do not address this question, i.e. what are the required strengths of these ferromagnetic couplers? In Section 4.1, we will show that it is not difficult to give an upper bound for the ferromagnetic coupler strengths might slow down the adiabatic algorithm. Furthermore, an adiabatic quantum computer is an analog computer and analog parameters can only be set to a certain degree of precision (a condition much more stringent than the setting of digital parameters). Hence, the allowed values of coupler strengths are limited. Therefore, from the computational point of view, it is important to derive as small (in terms of magnitude) as possible sufficient condition for these ferromagnetic coupler strengths. Furthermore, what should the bias for physical qubits be?

There are two components to the reduction: *embedding* and *parameter setting*. The embedding problem is to find a minor-embedding G_{emb} of a graph G in U. This problem is interdependent of the hardware graph design problem, which will be discussed in Section 6. The parameter setting problem is to set the corresponding parameters, qubit bias and coupler strengths, of the embedded Ising Hamiltonian. In this paper, we assume that the minor-embedding G_{emb} is given, and focus on the parameter setting problem (of the final Hamiltonian). Note that there are two aspects of efficiency of a reduction. One is how efficient one can reduce the original problem to the reduced problem. For example, here we are concerned how efficiently we can compute the minor-embedding and how efficiently we can compute the new parameters of the embedded Ising Hamiltonian. The other aspect concerns about the efficiency (in terms the running time) of the adiabatic algorithm for the reduced problem. In general, the latter depends on the former. For example, the running time of the adiabatic algorithm may depend

on a "good" embedding that is reduced to. According to the adiabatic theorem (see, e.g. [22]), the running time of the adiabatic algorithm depends on the minimum spectral gap (the difference between the two lowest energy levels) of the system Hamiltonian, which is defined by both initial Hamiltonian and final Hamiltonian. That is, the running time (and thus the efficiency of the reduction) will depend on both the initial Hamiltonian and the final Hamiltonian. In this paper, our focus is only on the final Hamiltonian, and therefore we are not able to address the running time of the adiabatic algorithm. Furthermore, the estimation of the minimum spectral gap of the (system) Hamiltonian is in general hard. Consequently, analytically analyzing the running time of an adiabatic algorithm is in general an open question.

Finally, let us remark that there is another different approach based on perturbation theory by Oliveira & Terhal [21] for performing the reduction. In particular, they employed perturbative gadgets to reduce a 2-local (system) Hamiltonian to a 2-local Hamiltonian on a 2-D square lattice, and were able to show (as in the pioneering work [19]) that the minimum spectral gap (and thus the running time) of the system Hamiltonian is preserved (up to a polynomial factor) after the reduction, for any given initial Hamiltonian. However, besides the ineffective embedding, as pointed out in [10], the method is "unphysical" as it requires that each parameter grows with the system size.

The rest of the paper is organized as follows. In Section 2, we recall the equivalences between the QUBO problem and the Ising problem. In Section 3, we introduce the minor-embedding definition and mention related work in graph theory. In Section 4, we derive the new parameters, namely values for the qubit bias and the sufficient condition for the ferromagnetic coupler strengths, for the embedded Ising Hamiltonian such that the original Ising problem can be correctly solved through the embedded Ising problem. In Section 5, we show the embedded Ising Hamiltonian for solving the (weighted) MIS problem. Finally, we conclude with several related algorithmic problems that need to be investigated in order to facilitate the design of efficient adiabatic algorithms and AQC architectures in Section 6.

2 **Equivalences Between QUBO and the Ising Problem**

In this section, we recall the equivalences between the problem of QUBO (maximization of \mathcal{Y} in Eq. (3)) and the Ising problem (minimization of \mathcal{E} in Eq. (2)). Notice that $x_i = \frac{s_i+1}{2}$, that is, $x_i = 1$ corresponds to $s_i = 1$, and $x_i = 0$ corresponds to $s_i = -1$. Using a change of variables, we have

$$\mathcal{Y}(x_1,\ldots,x_n) = \frac{1}{2} \sum_{i \in \mathsf{V}(G)} c_i - \frac{1}{4} \sum_{ij \in \mathsf{E}(G)} J_{ij} - \frac{1}{4} \left(\sum_{i \in \mathsf{V}(G)} \left(\sum_{j \in \mathsf{nbr}(i)} J_{ij} - 2c_i \right) s_i + \sum_{ij \in \mathsf{E}(G)} J_{ij} s_i s_j \right)$$

where $nbr(i) \stackrel{\text{def}}{=} \{j : ij \in E(G)\}$, the neighborhood of vertex *i*, for $i \in V(G)$. Therefore, $Max\mathcal{Y}(x_1, \ldots, x_n)$ in Eq. (3) is equivalent to $Min\mathcal{E}(s_1, \ldots, s_n)$ in Eq. (2) where $h_i = \sum_{j \in nbr(i)} J_{ij} - 2c_i$, or $c_i = 1/2(\sum_{j \in nbr(i)} J_{ij} - h_i)$ for $i \in V(G)$. See Figure 4 for the correspondences between parameters in QUBO and the Ising model.

3 **Minor-Embedding**

Definition 3.1. Let U be a fixed hardware graph. Given G, the minor-embedding of G is defined by

 $\phi: G \longrightarrow U$

such that



Figure 3: The correspondences between the parameters in QUBO and the Ising Model.

- each vertex in V(G) is mapped to a connected subtree T_i of U;
- there exists a map $\tau : V(G) \times V(G) \longrightarrow V(U)$ such that for each $ij \in E(G)$, there are corresponding $i_{\tau(i,j)} \in V(T_i)$ and $j_{\tau(j,i)} \in V(T_j)$ with $i_{\tau(i,j)}j_{\tau(j,i)} \in E(U)$.

Given G, if ϕ exists, we say that G is embeddable in U. In graph theory, G is called a minor of U. When ϕ is clear from the context, we denote the minor-embedding $\phi(G)$ of G by G_{emb} .

Equivalently, one can think of a minor G of U as a graph that can be obtained from a subgraph of U by contracting edges. See Figure 2 for an example.

In particular, there are two special cases of minor-embedding:

- Subgraph-embedding: Each T_i consists of a single vertex in U. That is, G is isomorphic to G_{emb} (a subgraph of U).
- Topological-minor-embedding: Each T_i is a chain (or path) of vertices in U.

Minors are well-studied in graph theory, see for example [12]. Given a *fixed* graph G, there are algorithms that find a minor-embedding of G in U in polynomial time of size of U, from the pioneering $O(|V(U)|^3)$ time algorithm by Robertson and Seymour [23] to recent nearly linear time algorithm of B. Reed (not yet published). However, it is worthwhile to reiterate that these algorithms are for *fixed* G, and their running times are *exponential* in the size of G. Here the minor-embedding problem is to find a minor-embedding of G (for any given G) while

fixing U. To the best of our knowledge, the only known work related to our minor-embedding problem was by Kleinberg and Rubinfeld [20], in which they showed that there is a randomized polynomial algorithm, based on a random walk, to find a minor-embedding in a given degree-bounded expander.

Our embedding problem might appear similar to the embedding problem from parallel architecture studies. However, besides the different physical constraints for the design of architectures, the requirements are very different. In particular, in our embedding problem, we do not allow for *load* > 1, which is the maximum number of logical qubits mapped to a single physical qubit. Also, we require *dilation*, which is the maximum number of stretched edges (through other qubits), to be exactly 1. However, all of the existing research on embedding problems for parallel processors [13], at least one of the conditions is violated (namely either load > 1 or dilation > 1). In this paper, our focus is on parameter setting such that the reduction is correct, and not on the minor-embedding algorithm and/or the related (minor-universal) hardware graph U design. These problems will be addressed in a subsequent paper.

4 Parameter Requirement for the Embedded Ising Hamiltonian

Let the QUBO problem, specified by \mathcal{Y} and G, be given as in Eq.(3), and the corresponding \mathcal{E} in Eq.(2). Suppose G_{emb} is a minor-embedding of G, and let \mathcal{E}^{emb} be the embedded energy function associated with G_{emb} :

$$\mathcal{E}^{\mathsf{emb}}(s_1,\ldots,s_N) \ = \ \sum_{i \in \mathsf{V}(G_{\mathsf{emb}})} h'_i s_i + \sum_{ij \in \mathsf{E}(G_{\mathsf{emb}})} J'_{ij} s_i s_j$$

where $|V(G_{emb})| = N$.

Our goal is to find out the requirement for new parameters, h's and J's, such that one can solve the original Ising problem on G by solving the embedded Ising problem on its embedding G_{emb} , or equivalently, such that there is an one-one correspondence between the minimum of \mathcal{E} (and thus the maximum of \mathcal{Y}) and the minimum of \mathcal{E}^{emb} .

As we mentioned in the introduction, the idea that we can solve the original Ising problem (i.e. finding the groundstate of the Ising Hamiltonian) on the input graph G by solving the new Ising problem on the embedded graph G_{emb} in U is that one can use ferromagnetic couplers to connect the physical qubits in each T_i of G_{emb} such that the subtree T_i will act as one logical qubit i of G.

Notation. First, we recall that $V(G_{emb}) = \bigcup_{i \in V(G)} V(T_i)$ and $E(G_{emb}) = \bigcup_{i \in V(G)} E(T_i) \cup \bigcup_{ij \in E(G)} i_{\tau(i,j)} j_{\tau(j,i)}$. We distinguish the edges within T_i s from the edges corresponding to the edges in the original graph. Denote the latter by $OE(G_{emb})$, that is, $OE(G_{emb}) = \bigcup_{ij \in E(G)} i_{\tau(i,j)} j_{\tau(j,i)}$. (The black edges in G_{emb} of Figure 2 correspond to $OE(G_{emb})$.) For convenience, $Onbr(i_k) \stackrel{\text{def}}{=} nbr(i_k) \cap OE(G_{emb})$ and $Enbr(i_k) \stackrel{\text{def}}{=} nbr(i_k) \setminus Onbr(i_k)$, $i_k \in V(T_i)$. Note $j_{\tau(j,i)} \in Onbr(i_k) \Leftrightarrow ij \in E(G)$.

The above intuition suggests that we use the same coupler strength for each original edge, i.e., $J'_{i_{\tau(i,j)}j_{\tau(j,i)}} = J_{ij}$ for $i_{\tau(i,j)}j_{\tau(j,i)} \in OE(G_{emb})$, and use ferromagnetic coupler strength, $F_i^e(<0)$, for each edge $e \in E(T_i)$, and redistribute the bias h_i of a logical qubit *i* to its physical qubits in T_i . That is, we choose h'_{i_k} for physical qubit $i_k \in V(T_i)$ such that $\sum_{i_k \in V(T_i)} h'_{i_k} = h_i$.

Therefore, we have

$$\mathcal{E}^{\mathsf{emb}}(s_1, \dots, s_N) = \sum_{i \in \mathsf{V}(G)} \left(\sum_{i_k \in \mathsf{V}(T_i)} h'_{i_k} s_{i_k} + \sum_{i_p i_q \in \mathsf{E}(T_i)} F_i^{pq} s_{i_p} s_{i_q} \right) + \sum_{i_j \in \mathsf{E}(G)} J_{i_j} s_{i_{\tau(i,j)}} s_{j_{\tau(j,i)}}$$
(4)

4.1 An Easy Upper Bound for the Ferromagnetic Coupler Strengths

In this section, we derive an easy upper bound for the ferromagnetic coupler strengths. The derivation is based on the *penalty or multiplier* method, in which a constrained optimization is reduced to an unconstrained one by replacing the corresponding expression into the objective function as a penalty term with a large multiplier.⁴ For example, this was used in the reduction from general (higher-order) unconstrained binary optimization to the quadratic one (see [8]).

Notice that by construction (i.e., G is a minor of G_{emb} and h'_{i_k} s are chosen such that $\sum_{i_k \in V(T_i)} h'_{i_k} = h_i$), minimization of \mathcal{E} in (2) is equivalent to

$$\min \mathcal{E}_{\text{constrained}}(s_1, \dots, s_N) = \sum_{i \in \mathsf{V}(G)} \sum_{i_k \in \mathsf{V}(T_i)} h'_{i_k} s_{i_k} + \sum_{i_j \in \mathsf{E}(G)} J_{i_j} s_{i_{\tau(i,j)}} s_{j_{\tau(j,i)}}$$
(5)
subject to
$$s_{i_p} s_{i_q} = 1 \text{ for all } i_p i_q \in \mathsf{E}(T_i), i \in \mathsf{V}(G)$$

where the condition $s_{i_p}s_{i_q} = 1$ for all $i_p i_q \in E(T_i)$ is equivalent to requiring the spins of physical qubits that correspond to the same logical qubit *i* to be of the same sign.

The corresponding unconstrained minimization is thus

$$\min \mathcal{E}'(s_1, \dots, s_N) = \sum_{i \in \mathsf{V}(G)} \sum_{i_k \in \mathsf{V}(T_i)} \left(h'_{i_k} s_{i_k} + \sum_{i_p i_q \in \mathsf{E}(T_i)} F_i^{pq}(s_{i_p} s_{i_q} - 1) \right) + \sum_{i_j \in \mathsf{E}(G)} J_{i_j} s_{i_{\tau(i,j)}} s_{j_{\tau(j,i)}}(6)$$

which is equivalent to solving Eq.(4) as $\sum_{i \in V(G)} \sum_{i_p i_q \in E(T_i)} F_i^{pq}$ is a constant. We are interested in how large (in terms of magnitude) F_i^{pq} s are sufficient to guarantee that the solution of Eq.(6) gives the solution to Eq.(5), and consequently to Eq.(2). The result is stated in the following theorem.

Theorem 4.1. Let $\mathcal{E}_{\text{constrained}}$ and \mathcal{E}' given as in Eq.(5) and Eq.(6). Suppose that for $i \in V(G)$,

$$F_i^{pq} < -\left(|h_i| + \sum_{j \in \mathsf{nbr}(i)} |J_{ij}|\right) \qquad \text{for } i_p i_q \in \mathsf{E}(T_i) \tag{7}$$

then we have $s_{i_p}^* s_{i_q}^* = 1$ for all $i_p i_q \in \mathsf{E}(T_i)$, $i \in \mathsf{V}(G)$, where $(s_{1_1}^*, \ldots, s_N^*) = \arg\min \mathcal{E}'$. Consequently,

$$\min \mathcal{E}_{\text{constrained}}(s_1, \ldots, s_N) = \min \mathcal{E}'(s_1, \ldots, s_N).$$

Proof. Let $(s_{1_1}^*, \ldots, s_N^*) = \arg \min \mathcal{E}'$. Suppose on the contrary. That is, there exists $f_p f_q \in \mathsf{E}(T_f)$, for some $1 \le f \le n$ such that $s_{f_p}^* s_{f_q}^* = -1$. Then we have

$$\mathcal{E}'(s_1^*, \dots, s_N^*) \ge -\left(\sum_{f_k \in \mathsf{V}(T_f)} |h'_{f_k}| + \sum_{j \in \mathsf{nbr}(f)} |J_{fj}|\right) - 2F_f^{pq} + \mathcal{E}'_{\mathsf{rest}}(s_1^*, \dots, s_N^*)$$

⁴This is closely related to the discrete Lagragian Multiplier method. However, the Lagragian multipliers are treated as unknown or iteratively solved with the Lagragian function.

where

$$\mathcal{E}'_{\mathsf{rest}}(s_1, \dots, s_N) = \sum_{i \in \mathsf{V}(G), i \neq f} \sum_{i_k \in \mathsf{V}(T_i)} \left(h'_{i_k} s_{i_k} + \sum_{i_p i_q \in \mathsf{E}(T_i)} F_i^{pq}(s_{i_p} s_{i_q} - 1) \right) + \sum_{i_j \in \mathsf{E}(G), i \neq f} J_{i_j} s_{i_{\tau(i,j)}} s_{j_{\tau(j,i)}}.$$

Thus, if Fs satisfy Eq.(??), we have

$$\mathcal{E}'(s_1^*,\ldots,s_N^*) > \sum_{f_k \in \mathsf{V}(T_f)} |h'_{f_k}| + \sum_{j \in \mathsf{nbr}(f)} |J_{fj}| + \mathcal{E}'_{\mathsf{rest}}(s_1^*,\ldots,s_N^*)$$

which is at least $\min \mathcal{E}'(s_1, \ldots, s_N) = \mathcal{E}'(s_1^*, \ldots, s_N^*)$, a contradiction. Consequently, we can conclude that $s_{i_p}^* s_{i_q}^* = 1$ for all $i_p i_q \in \mathsf{E}(T_i)$, $i \in \mathsf{V}(G)$, where $(s_{1_1}^*, \ldots, s_N^*) = \arg \min \mathcal{E}'$, implying the claimed equality of the minima.

4.2 A Tighter Bound for the Ferromagnetic Coupler Strengths

As we mentioned Section 1, it is desired to obtain tighter bounds for the ferromagnetic coupler strengths. In this section, we show that with a more careful analysis, we can reduce the bound by setting the qubit bias (h') appropriately.

For $i \in V(G)$, let

$$C_i \stackrel{\text{def}}{=} \sum_{j \in \mathsf{nbr}(i)} |J_{ij}| - |h_i|.$$

Observe that if $C_i < 0$, that is, $\sum_{j \in \mathsf{nbr}(i)} |J_{ij}| < |h_i|$. Then we have $s_i^* = -1$ for $h_i > 0$, and $s_i^* = +1$ for $h_i < 0$, where $(s_1^*, \ldots, s_n^*) = \arg \min \mathcal{E}$. Therefore, WLOG, for the rest of the paper, we will assume that $C_i \ge 0$.

Theorem 4.2. Let \mathcal{E} (\mathcal{Y} resp.) and G be given as in Eq.(2) (Eq.(3) resp.). Suppose G_{emb} is a minor-embedding of G, and let \mathcal{E}^{emb} be the energy of the embedded Ising Hamiltonian given in Eq.(4). Then for all $i \in V(G)$, if

$$h_{i_{k}}' = sign(h_{i}) \begin{cases} \sum_{j_{\tau(j,i)} \in \mathsf{Onbr}(i_{k})} |J_{ij}| - C_{i}/l_{i} & i_{k} \text{ is one of the } l_{i} \text{ leaves of } T_{i} \\ \sum_{j_{\tau(j,i)} \in \mathsf{Onbr}(i_{k})} |J_{ij}| & otherwise \end{cases}$$

and

$$F_i^e < -\frac{l_i - 1}{l_i}C_i \text{ for all } e \in \mathsf{E}(T_i),$$

where $C_i \ge 0$ (defined above) and $sign(h_i) = +1(-1 \text{ resp.})$ if $h_i \ge 0$ ($h_i < 0 \text{ resp.}$), we have $s_{i_p}^* s_{i_q}^* = 1$ for all $i_p i_q \in \mathsf{E}(T_i)$, $i \in \mathsf{V}(G)$, where $(s_{1_1}^*, \ldots, s_N^*) = \arg\min \mathcal{E}^{\mathsf{emb}}$. Consequently, there is one-one correspondence between $\arg\min \mathcal{E}^{\mathsf{emb}}$ and $\arg\min \mathcal{E}$ (and thus $\arg\max \mathcal{Y}$).

Furthermore, if we set $F_i^e = -\frac{l_i-1}{l_i}C_i - g_i/2$, for some $g_i > 0$, then the spectral gap (which is the difference between the two lowest energy levels) of the embedded Ising Hamiltonian will be the minimum of $\min_{i \in V(G)} g_i$ and the spectral gap of the original Ising Hamiltonian.

See Figure 4 for an example of the corresponding parameters in the embedded Ising Hamiltonian (for the topological-minor-embedding case).

In the following, we first explain the main idea behind, followed by the formal proof. For the illustration purpose, suppose $h_i > 0$, consider the simplest case in which all but one leaf is -1. Now, consider the energy

change if the leaf is flipping from +1 to -1. Our goal is to set Fs as small (in terms of the magnitude) as possible, such that the energy change is at least greater than zero. Note that the energy change $\Delta \mathcal{E}_{i_k} = 2(h'_{i_k} + 2(h'_{i_$ $\sum_{j\tau(i,j)\in\mathsf{Onbr}(i_k)} \delta_{j_{\tau(j,i)}} J_{ij} - F) \text{ where } \delta_{j_{\tau(j,i)}} \text{ depends on the sign of spin } s^*_{j_{\tau(j,i)}}. \text{ We would like to bound } \Delta \mathcal{E}_{i_k}$ without knowing the signs of $s^*_{j_{\tau(j,i)}}$ s. Observe that if Js are all positive, then the worst case we have $\Delta \mathcal{E}_{i_k} \geq$ $2(h'_{i_k} - \sum_{j_{\tau(i,j)} \in \mathsf{Onbr}(i_k)} J_{ij} - F). \text{ And in general } \Delta \mathcal{E}_{i_k} \geq 2(h'_{i_k} - \sum_{j_{\tau(i,j)} \in \mathsf{Onbr}(i_k)} J_{ij}^+ + \sum_{j_{\tau(i,j)} \in \mathsf{Onbr}(i_k)} J_{ij}^- - F),$ where $J_{ij}^+ > 0$ and $J_{ij}^- < 0$. Consequently, setting $F < h'_{i_k} - \sum_{j_{\tau(i,j)} \in \mathsf{Onbr}(i_k)} |J_{ij}|$ would imply $\Delta \mathcal{E}_{i_k} > 0$. One can then extend this argument to a segment that needs to be flipped, as illustrated in Figure 5.

Proof. It is easy to check that $\sum_{i_k \in V(T_i)} h'_{i_k} = sign(h_i)|h_i| = h_i$. We will first prove the theorem when G_{emb} is a topological-minor-embedding of G. That is, each T_i is a chain $(i_1, i_2, \ldots, i_{t_i})$ connected by consecutive vertices. Thus, the corresponding embedded energy function is given by

$$\mathcal{E}^{\mathsf{emb}}(s_1, \dots, s_N) = \sum_{i \in \mathsf{V}(G)} \left(\sum_{k=1}^{t_i} h'_{i_k} s_{i_k} + \sum_{k=1}^{t_i-1} F_i^{k(k+1)} s_{i_k} s_{i_{k+1}} \right) + \sum_{ij \in \mathsf{E}(G)} J_{ij} s_{i_{\tau(i,j)}} s_{j_{\tau(j,i)}}$$
(8)

In this case, we have $l_i = 2$. We prove by contradiction. Suppose NOT. That is, there exists $i \in V(G)$, and $1 \le k < t_i$ such that $s_{i_k}^* s_{i_{k+1}}^* = -1$. We distinguish two cases based on the value of h_i .

For $h_i > 0$, let p be the smallest index such that $s_{i_{p-1}}^* = -1$ and $s_{i_p}^* = +1$, and let q be the smallest index such that $s_{i_q}^* = +1$ and $s_{i_{q+1}}^* = -1$. That is, we have $s_{i_1}^* = \dots = s_{i_{p-1}}^* = -1$, $s_{i_p}^* = \dots = s_{i_q}^* = +1$. Note we have at least either p > 1 or q < n. (Otherwise they are all +1). Then we claim that by flipping the segment (i_p,\ldots,i_q) from +1s to -1s, the energy decreases, contradicting to the optimality. (Notice that the Fs within the segment do not change.) The energy change equals to

$$\begin{split} \Delta \mathcal{E}^{\mathsf{emb}} &= \mathcal{E}^{\mathsf{emb}}(\dots, -1, \dots, -1, \underbrace{+1, \dots, +1}_{k=1}, -1, \dots) - \mathcal{E}^{\mathsf{emb}}(\dots, -1, \dots, -1, \underbrace{-1, \dots, -1}_{k=1}, -1, \dots) \\ &\geq 2 \left(\sum_{k=p}^{q} h'_{i_{k}} - \sum_{k=p}^{q} \sum_{j_{\tau(j,i)} \in \mathsf{Onbr}(i_{k})} |J_{ij}| - F_{i}^{(p-1)p} - F_{i}^{q(q+1)} \right) \text{ (with convention that } F_{i}^{01} = F_{i}^{t_{i}(t_{i}+1)} = 0) \\ &\geq 2(-C_{i}/2 - F_{i}^{k(k+1)}) \text{ (where } k = p \text{ if } p > 1, k = q \text{ otherwise}) \end{split}$$

The argument for $h_i < 0$ is similar except that we will flip from -1 to +1 instead, and

$$\begin{split} \Delta \mathcal{E}^{\mathsf{emb}} &= \mathcal{E}^{\mathsf{emb}}(\dots, +1, \dots, +1, \underbrace{-1, \dots, -1}_{k=1}, +1, \dots) - \mathcal{E}^{\mathsf{emb}}(\dots, +1, \dots, +1, \underbrace{+1, \dots, +1}_{k=1}, +1, \dots) \\ &\geq 2\left(\sum_{k=p}^{q} -h'_{i_{k}} - \sum_{k=p}^{q} \sum_{j_{\tau(j,i)} \in \mathsf{Onbr}(i_{k})} |J_{ij}| - F_{i}^{(p-1)p} - F_{i}^{q(q+1)}\right) \\ &\geq 2(-C_{i}/2 - F_{i}^{k(k+1)}) \quad (\text{where } k = p \text{ if } p > 1, k = q \text{ otherwise}) \end{split}$$

Therefore, in both cases, if $F_i^{p(p+1)} < -C_i/2$, for all $1 \le p < t_i$, we have $\Delta \mathcal{E}^{\mathsf{emb}} > 0$, contradicting to the optimality. Hence all $s_{i_n}^*$ must be of the same sign.

For the general minor-embedding when T_i s are trees, we can similarly argue that for $h_i > 0$, if all but one leaf is positive (+1), then flipping them (from +1s to -1s) will decease the energy provided that $F_i < -\frac{l_i-1}{L}C_i$. Similarly, one can argue for the case when $h_i < 0$.

Notice that if we set $F_i = -\frac{l_i-1}{l_i}C_i - g_i/2$, then the energy change $\Delta \mathcal{E}^{\mathsf{emb}} \ge g_i$. In this case, the spectral gap of the embedded Ising Hamiltonian will be the minimum of $\min_{i \in \mathsf{V}(G)} g_i$ and the spectral gap of the original Ising Hamiltonian.

Remark. One can generally set $h'_{i_k} = sign(h_i)(\sum_{j_{\tau(j,i)} \in Onbr(i_k)} |J_{ij}| - C_{i_k})$ where C_{i_k} s are chosen such that $\sum_{i_k \in V(T_i)} C_{i_k} = C_i(=\sum_{j \in nbr(i)} |J_{ij}| - |h_i|)$, and set the *F*'s accordingly. This flexibility is useful when the precision for parameters is limited. (In the above theorem, we give an upper bound for the ferromagnetic coupler strengths. A natural question is how tight our bound is. Can one get an better bound without solving the original problem?)

5 Weighted Maximum Independent Set (WMIS) Problem

First, we formulate WMIS problem as a special case of QUBO in Section 5.1. Then, we apply Theorem 4.2 to set parameters for the embedded Ising Hamiltonian for the corresponding MIS problem in Section 5.2.

5.1 Formulate WMIS Problem As a Special Case of QUBO

Weighted MIS (WMIS). Given an undirected vertex-weighted graph G. Let $V(G) = \{1, 2, ..., n\}$, let $c_i \in \mathbb{R}^+$ be the weight of vertex *i*. WMIS seeks to find a wmis $(G) = S \subseteq V$ such that S is independent and the total weight of $S (= \sum_{i \in S} c_i)$ is maximized.

Theorem 5.1. If $J_{ij} \ge \min\{c_i, c_j\}$ for all $ij \in E(G)$, then the maximum value of

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

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

Proof of Theorem 5.1. Let $(x_1^*, \ldots, x_n^*) = \arg \max_{(x_1, \ldots, x_n) \in \{0,1\}^n} \mathcal{Y}(x_1, \ldots, x_n)$. Denote $S^* = \{i \in V(G) : x_i^* = 1\}$. We'll prove that if $J_{ij} > \min\{c_i, c_j\}$ for all $ij \in E(G)$, then S^* is an independent set.

Suppose on the contrary, that is, there exists an edge yz in the subgraph induced by S^* . WLOG, assume that $c_y < c_z$. Consider removing y from S^* . Let $S' = S^* \setminus \{y\}$. The weight change equals to $-c_y + \sum_{j \in \mathsf{nbr}(y) \cap S^*} J_{yj} \ge -c_y + J_{yz} > 0$, contradicting to the optimality of S^* .

The above theorem is a generalization of the known fact for unweighted case of MIS (see [8] and references therein). For the unweighted case of MIS, $c_i = 1$ for all $i \in V(G)$. Thus, it is sufficient to choose $J_{ij} = 1 + \epsilon$ for all $ij \in E(G)$ for some $\epsilon > 0$. Accordingly, the corresponding energy function of the Ising Model for MIS is $\mathcal{E}(s_1, \ldots, s_n) = \sum_{i \in V(G)} (\deg_i(1 + \epsilon) - 2) s_i - \sum_{ij \in E(G)} (1 + \epsilon) s_i s_j$.

Remark. If we choose J to be exactly 1 instead (as in [17, 18]), then we can only guarantee the size of the maximum independent set, but the returned set is not necessarily independent. For instance, when $G = K_4$, any (adjacent) two vertices also has the minimum energy of *one*.

Note that we thus can conclude that the Ising problem is NP-hard because WMIS is NP-hard. Indeed, Barahona [7] showed the NP-hardness of a special Ising problem through the reduction of MIS problem on cubic

graph (which remains NP-hard). Notice that for WMIS on a planar graph, there is a PTAS algorithm [5]. Recently, for the Ising problem on a planar graph, Bansal et al. [6] applied the same technique to obtain a PTAS algorithm in $O(n2^{36/\delta})$ where $(1 - \delta)$ is the approximation ratio. As another side note, conversely (to the fact that WMIS is a special case of QUBO), Boros et al (see e.g. [8]) has shown that a problem of QUBO on G can also be converted to a WMIS but on a different graph.

5.2 Embedded Ising Hamiltonian for Solving MIS

Let G be the graph of MIS problem and G_{emb} be the topological-minor-embedding of G in U. For the unweighted MIS, we have $C_i = \sum_{j \in nbr(i)} J_{ij} - h_i = 2$. Therefore, according to Theorem 4.2, it suffices to set $F_i < -C_i/2 = -1$. That is, the embedded Ising Hamiltonian for solving unweighted MIS is given as in Eq. (8), with

$$h'_{i_k} = \left\{ \begin{array}{ll} d_{i_k}J - 1 & k = 1, t_i \\ d_{i_k}J & 1 < k < t \end{array} \right.$$

where $d_{i_k} = |\mathsf{Onbr}(i_k)|$, and $J_{ij} \equiv J > 1$, $F_i^{k(k+1)} \equiv F < -1$. In particular, for degree-3 hardware graph U, by setting $J = 1 + \epsilon$, and $F = -(1 + \epsilon)$, for some $\epsilon > 0$, there are only 6 different parameter values, namely, $\{-(1 + \epsilon), 0, \epsilon, 1 + \epsilon, 1 + 2\epsilon, 1 + 3\epsilon\}$ in Eq. (8).

6 Discussion

In this paper, we introduce minor-embedding in AQC. In particular, we show that the NP-hard QUBO problem can be solved using an adiabatic quantum computer that implements Ising spin-1/2 Hamiltonians, through minorembedding reduction. There are two components to this reduction: embedding and parameter setting. Given a minor-embedding, we show how to derive the values for the corresponding parameters, in particular, a good upper bound (in terms of magnitude) for the ferromagnetic coupler strengths, of the embedded Ising Hamiltonian such that there is one-one correspondence between the groundstate of the original Ising Hamiltonian and the one of the embedded Ising Hamiltonian.

There are many algorithmic problems related to minor-embedding in AQC that remain to be addressed. In particular, the problems relate to the efficiency of the reduction. These problems in turn relate to the running time or complexity of quantum adiabatic algorithms. Recall that according to the adiabatic theorem, the running time of an adiabatic algorithm depends on the minimum spectral gap of the system Hamiltonian, which however might be as hard as solving the original problem. Despite several serious investigations, the power of AQC remains an open question [24, 25, 22, 16, 1]. How does the embedding reduction effect the time complexity of an adiabatic algorithm? In order to address this question, one will also need to specify the initial Hamiltonian. In [2], we show that for some special cases, how the embeddings, parameters, and initial Hamiltonian on the complexity of adiabatic algorithms remains to be investigated. In the following we state several main problems that need to investigate in order to facilitate the design of adiabatic algorithms and AQC architectures. Partial results to these problems will appear in our subsequent papers.

P1. Measurement for the minor-embedding. Define a measure for the minor-embedding such that a good minor-embedding corresponds to a reduced problem that admits an efficient adiabatic algorithm.

P2. Embedding-dependent initial Hamiltonian. Design an embedding-dependent initial Hamiltonian for a given minor-embedding such that the adiabatic algorithm for the reduced problem is at least as efficient as the adiabatic algorithm (with the best possible initial Hamiltonian) for the original problem.

P3. Hardware graph design. Given a family \mathcal{F} of graphs (which consists of classically hard instances), the problem is to design a hardware graph (called a \mathcal{F} -minor-universal graph) which is as small as possible (in terms of total number of vertices and edges) such that

- all known physical constraints are satisfied;
- all graphs in \mathcal{F} are embeddable;
- a good embedding of each graph in \mathcal{F} can be efficiently computed.

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Appendix

A Energy Function of the Ising Hamiltonian

In this section, we show that the energy function of the Ising Hamiltonian in Eq. (1) is given in Eq. (2). That is, replace each σ_i^z by the variable $s_i \in \{-1, +1\}$. The equivalence follows from two basics: (1) Eigenvalues and eigenvectors of σ^z : $\sigma^z |0\rangle = (+1)|0\rangle$, $\sigma^z |1\rangle = (-1)|1\rangle$, where $|0\rangle \stackrel{\text{def}}{=} [1,0]^{\dagger}$, $|1\rangle \stackrel{\text{def}}{=} [0,1]^{\dagger}$. (2) Tensor product property: $(A \otimes B)(|u\rangle \otimes |v\rangle) = A|u\rangle \otimes B|v\rangle$. More precisely, for $|z\rangle = |z_1\rangle \otimes \ldots \otimes |z_n\rangle$, $z_i \in \{0,1\}$, $i = 1, \ldots, n$.

$$\mathcal{H}_{\mathsf{final}}|z\rangle = \left(\sum_{i \in \mathsf{V}(G)} h_i \sigma_i^z + \sum_{ij \in \mathsf{E}(G)} J_{ij} \sigma_i^z \sigma_j^z \right) |z_1\rangle \otimes \ldots \otimes |z_n\rangle$$

$$= \sum_{i \in \mathsf{V}(G)} h_i |z_1\rangle \otimes \ldots \otimes (-1)^{z_i} |z_i\rangle \ldots \otimes |z_n\rangle + \sum_{ij \in \mathsf{E}(G)} J_{ij} |z_1\rangle \otimes \ldots \otimes (-1)^{z_i} |z_i\rangle \ldots \otimes |z_n\rangle$$

$$= \left(\sum_{i \in \mathsf{V}(G)} h_i (-1)^{z_i} + \sum_{ij \in \mathsf{E}(G)} J_{ij} (-1)^{z_i} (-1)^{z_j} \right) |z_1\rangle \otimes \ldots \otimes |z_n\rangle$$

Therefore, the energy function of $\mathcal{H}_{\mathsf{final}}$ is

$$\mathcal{E}(z_1, \dots, z_n) = \sum_{i \in \mathsf{V}(G)} h_i(-1)^{z_i} + \sum_{ij \in \mathsf{E}(G)} J_{ij}(-1)^{z_i}(-1)^{z_j}$$

where $z_i \in \{0, 1\}$, for i = 1, ..., n. Replace $(-1)^{z_i}$ by $s_i \in \{+1, -1\}$, we thus have Eq.(2).



Figure 4: The corresponding parameters in the embedded Ising Model. Bottom right, for J > 0; bottom left, for general J: $J_{i1} > 0$, $J_{i2} < 0$, $J_{i3} < 0$, and $c'_i = c_i - \sum_{j \in \mathsf{nbr}(i), J_{ij} < 0} J_{ij}$.



Figure 5: (a) For h > 0 and positive Js (denoted by J^+), the energy change $\Delta \mathcal{E} \ge 2(h - J^+ - J^+ - F)$ when flipping the leaf's spin from +1 to -1. (b) For h > 0, $\Delta \mathcal{E} \ge 2(h - J^+ + J^- - F)$ when flipping the leaf's spin from +1 to -1, where $J^+ > 0$, $J^- < 0$. (c) For h > 0, flip a segment from +1 to -1. (d) For h < 0, flip a segment from -1 to +1.