Treating the Independent Set Problem by 2D Ising Interactions with Adiabatic Quantum Computing

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Abstract

We construct a nearest-neighbor Hamiltonian whose ground states encode the solutions to the NP-complete problem INDEPENDENT SET in cubic planar graphs. The Hamiltonian can be easily simulated by Ising interactions between adjacent particles on a 2D rectangular lattice. We describe the required pulse sequences. Our methods could help to implement adiabatic quantum computing by "physically reasonable" Hamiltonians like short-range interactions.

1 Introduction

Adiabatic quantum computation has been proposed as a general way of solving computationally hard problems on a quantum computer [Fea01]. Adiabatic quantum algorithms proposed so far work by applying a time-dependent Hamiltonian

$$H(t) = (1 - \frac{t}{T})H_B + \frac{t}{T}H_P \tag{1}$$

that interpolates linearly from an initial Hamiltonian H_B to the final Hamiltonian H_P . The Hamiltonians are chosen such that the ground

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states of H_B are easily prepared and the ground states of the final Hamiltonian H_P encode the solutions to the problem [Fea01].

The running time of the algorithm is denoted by T. If H(t) varies sufficiently slowly, i.e., T is sufficiently high, then one hopes that the final state of the quantum computer will be close to the ground state of the final Hamiltonian H_P , so a measurement will yield a solution to the problem with high probability. The adiabatic theorem is the justification for this hope. However, it is not clear whether all necessary conditions for adiabatic evolution are satisfied. For instance, it is not clear whether the gap between the ground states and first excited states of H(t) is sufficiently high for all t.

The adiabatic method can only succeed if the Hamiltonian H(t) changes slowly. But how slow is slow enough? Unfortunately, this question has proved difficult to analyze in general. Some numerical evidence suggests the possibility that the adiabatic method might efficiently solve computationally interesting instances of hard combinatorial problems, outperforming classical algorithms [Fea01]. Whether adiabatic quantum computing provides a definite speedup over classical methods for certain problems remains an interesting open question.

Our objective in this paper is not to explore the computational power of the adiabatic quantum computing, but rather to investigate how to implement the adiabatic time evolution starting from "physically reasonable" Hamiltonians like short-range interactions.

A Hamiltonian can be considered as physically reasonable only if it is "local". One way to describe locality is a follows. Let $\mathcal{H} := \mathbb{C}^2$ denote the Hilbert space of a single qubit and $\mathcal{H}^{\otimes n}$ the joint Hilbert space of *n* qubits. $\mathbf{L}(\mathcal{H}^{\otimes s})$ denotes the set of linear operators from $\mathcal{H}^{\otimes s}$ to $\mathcal{H}^{\otimes s}$. Let $A \in \mathbf{L}(\mathcal{H}^{\otimes s})$ be an arbitrary operator and $S \subseteq \{1, \ldots, n\}$ with |S| = s. We denote by $A[S] \in \mathbf{L}(\mathcal{H}^{\otimes n})$ the embedding of the operator A into the Hilbert space $\mathcal{H}^{\otimes n}$, i.e., the operator that acts as A on the qubits specified by S.

An operator $H: \mathcal{H}^{\otimes n} \to \mathcal{H}^{\otimes n}$ is called an *s*-local Hamiltonian if it is expressible in the form

$$H = \sum_{j} H_j[S_j], \qquad (2)$$

where each term $H_j \in \mathbf{L}(\mathcal{H}^{\otimes |S_j|})$ is a Hermitian operator acting on a set $S_j, |S_j| \leq s$.

A Hamiltonian is local if it can be expressed as a sum of terms, where each term acts on a bounded number of qubits. Indeed, in this case, the corresponding time evolution can be approximately simulated by a universal quantum computer [NC00].

For a direct physical implementation of the continuously varying Hamiltonian H(t) we require a stronger locality condition. Physical interactions are usually pair-interactions, unless one considers effective Hamiltonians. The system Hamiltonian can be thus decomposed as

$$H = \sum_{k < l} H_{kl} + \sum_{k} H_k \,, \tag{3}$$

 H_{kl} is a Hermitian operator acting on the joint Hilbert space of particle k and l and H_k is the free Hamiltonian of particle k. Furthermore, the interaction strength is decreasing with the distance. Therefore, we do not want to propose a scheme that relies on "weak" interaction terms among distant particles. We thus require that each particle is coupled to only a few other particles in its direct neighborhood.

One of the most simple nontrivial examples are the Ising interactions on a 2D lattice. Our resource is the Ising Hamiltonian on an $r \times s$ rectangular lattices, i.e.,

$$H_{\text{Ising}} = \sum_{(k,l)\in L} \sigma_z^{(k)} \sigma_z^{(l)} , \qquad (4)$$

where L are the edges of a rectangular lattice, i.e., a graph of order rs obtained by placing vertices at the coordinates $\{(i, j) \mid 0 \le i < r, 0 \le s < J\}$ with edges joining just the pairs at unit distance.

Let L' be a subgraph of L. We construct a final Hamiltonian

$$\hat{H}_P = \sum_{(k,l)\in L'} w_{kl} \,\sigma_z^{(k)} \sigma_z^{(l)} + \sum_k w_k \sigma_z^{(k)} \quad \text{with } w_{kl}, w_k \in \mathbb{Z} \,, \quad (5)$$

such that its ground states encode the solution to the NP-complete problem "independent set". Clearly, such Hamiltonians satisfy the locality condition. The aim of our paper is to show how such Hamiltonians can be constructed using planar orthogonal embeddings of graphs and how they can be obtained efficiently from the 2D Ising model Hamiltonian H_{Ising} . Together with the choice of a local initial Hamiltonian

$$\hat{H}_B = \sum_k \sigma_x^{(k)} \tag{6}$$

our results allow to simulate efficiently the adiabatic quantum evolution according to

$$\hat{H}(t) = (1 - \frac{t}{T})\hat{H}_B + \frac{t}{T}\hat{H}_P.$$

2 Independent set problem

The idea to consider the INDEPENDENT SET problem is motived by [KL02, RAS02]. The INDEPENDENT SET problem [GJ79] is defined as follows:

- INSTANCE: Graph G = (V, E), positive integer $v \le |V|$.
- QUESTION: Does G contain an independent set whose cardinality is at least v, i.e., a subset $V' \subseteq V$ such that $|V'| \ge v$ and such that no two vertices in V' are joined by an edge in E?

The INDEPENDENT SET problem remains NP-complete for cubic planar graphs [GJS76]. A graph is called *cubic* if all vertices have degree 3, i.e., all vertices are connected to exactly three vertices. A graph is called *planar* if it can be drawn in the plane such that the edges do not intersect. An example of a planar cubic graph is shown in Figure 1.

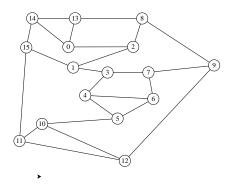


Figure 1: Planar cubic graph

We consider a method that determines the maximal cardinality of independent set of a planar cubic graph. Let us recall how the solution to the maximum independent set can be encoded in the ground states of a pair-interaction Hamiltonian H_P .

Theorem 1 (Planar spin glass within a magnetic field)

Let G = (V, E) be a cubic planar. Determining the energy of the ground states of the corresponding Hamiltonian

$$H_P = \sum_{(k,l)\in E} \sigma_z^{(k)} \sigma_z^{(l)} + \sum_{k\in V} \sigma_z^{(k)}$$
(7)

is equivalent to determining the maximum cardinality of independent sets of G.

Proof. This has been shown in [Bar82] (see also [WB03]). We include the proof here for completeness. We associate a variable $X_k \in \{0, 1\}$ to each vertex $k \in V$. There is an independent set whose cardinality is at least v if and only if there is an assignment to the variables $\{X_k \mid k \in V\}$ such that

$$L = \sum_{k \in V} X_k - \sum_{(k,l) \in E} X_k X_l \ge v.$$
(8)

This is seen as follows. If V' is an independent set whose cardinality is at least v, then the assignment $X_k = 1$ for $k \in V'$ and $X_k = 0$ for $k \in V \setminus V'$ fulfills inequality (8).

Now let X_1, \ldots, X_n be an assignment that fulfills inequality (8). If $V' = \{k \mid X_k = 1\}$ is not an independent set, then we must have $|V'| \ge v + p$, where $p := \sum_{(k,l)\in E} X_k X_l > 0$ is the "penalty" for V' not being an independent set. Let $(\tilde{k}, \tilde{l}) \in E$ with $X_{\tilde{k}} = X_{\tilde{l}} = 1$. By removing \tilde{k} from V' (i.e. setting $X_{\tilde{k}} := 0$) the cardinality of V' drops by 1, while p drops by at least 1. After repeating this several times, we end up with an independent set whose cardinality is at least v.

Setting $S_k = 2X_k - 1$ for all $k \in V$ and observing that $|E| = \frac{3}{2}|V|$ for all cubic graphs, we obtain

$$L = -\frac{1}{4} \sum_{k \in V} S_k - \frac{1}{4} \sum_{(k,l) \in E} S_k S_l + \frac{1}{8} |V| \,. \tag{9}$$

For $E = -4L + \frac{1}{2}|V|$ we see that there exists an independent set whose cardinality is at least k if and only if there is an assignment of values to the variables $S_k \in \{-1, 1\}$ (corresponding to the eigenvalues of σ_z) such that

$$E = \sum_{k \in V} S_k + \sum_{(k,l) \in E} S_k S_l \le \frac{1}{2} |V| - 4v.$$
 (10)

Now it is clear that determining the minimal energy E is equivalent to determining the maximal cardinality v of independent sets of G. \Box

In adiabatic quantum computing the initial Hamiltonian is chosen as

$$H_B = \sum_{k \in V} \sigma_x^{(k)} \tag{11}$$

and the time-dependent Hamiltonian as

$$H(t) = (1 - \frac{t}{T})H_B + \frac{t}{T}H_P.$$
 (12)

This Hamiltonian H_P does not necessarily satisfy the locality conditions.

3 "Planar orthogonal" Hamiltonians

Due to the lattice structure of our resource Hamiltonian we need to embed our graph into this structure. This can be done using *planar* orthogonal embeddings of graphs [KW01]. This idea is inspired by [KL02, RAS02]. We shall be concerned with embedding graphs into a 2D rectangular lattice.

Definition 1 (Planar orthogonal embedding)

A planar orthogonal embedding Γ of a graph G = (V, E) is a mapping that

- maps vertices $k \in V$ to lattice points $\Gamma(k)$ and
- edges $(k, l) \in E$ to paths in the lattice such that the images of their endpoints $\Gamma(k)$ and $\Gamma(l)$ are connected and such that the paths do not share any vertices (besides the endpoints).

Note that the map inserts "dummy vertices" if necessary to create the paths connecting the vertices Γ_k and Γ_l . A planar orthogonal embedding is shown in Figure 2.

Every planar graph with maximum degree 3 admits a planar orthogonal embedding on an $\lfloor n/2 \rfloor \times \lfloor n/2 \rfloor$. The algorithm presented in [Kan96] computes efficiently such planar orthogonal embeddings of graphs. We used AGD (Libary of Algorithms for Graph Drawing) to compute the embedding [AGD02].

In the proposal of [KL02] the Hamiltonian H_P is considered. The planar orthogonal embedding gives a regular wiring among the qubits. This means that the couplings are not spatially local. In contrast, we need a Hamiltonian \hat{H}_P that contains only nearest-neighbor interactions. This is necessary that it can be simulated by H_{Ising} . The idea is to use the dummy vertices as wires that propagate the state of a (real) vertex spin to the neighborhood of another vertex. This can be achieved by constructing a path of adjacent dummy vertices,

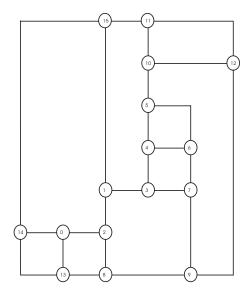


Figure 2: Planar orthogonal embedding of the graph in Fig. 1

each interacting with its neighbor by a strong ferromagnetic coupling. Furthermore, the first dummy at one end of this "dummy path" is strongly ferromagnetically coupled to a vertex and the last dummy at the other end is in the neighborhood of another real vertex, coupled to it via a usual antiferromagnetic interaction. The interaction strength is chosen in such a way that it is always energetically better when all dummies have the same state as the real vertex to which they are connected to than to have a mismatch along the "ferromagnetic path".

Formally, this construction is as follows:

- The dummy vertices have no local σ_z term.
- The vertices $\Gamma(k)$ have σ_z as local Hamiltonians.
- Let $(k, l) \in E$ be an edge of G.

If Γ_k and Γ_l are adjacent, then the coupling between Γ_k and Γ_l is chosen to be antiferromagnetic, i.e., $\sigma_z \otimes \sigma_z$.

Otherwise there are m dummy vertices v_1, \ldots, v_m such that the path $(\Gamma_k, v_1, \ldots, v_m, \Gamma_l)$ connects the vertices Γ_k and Γ_l . The couplings between Γ_k and v_1 and v_i and v_{i+1} for $i = 1, \ldots, m-1$ are chosen to be ferromagnetic with coupling strength c, i.e., $-c \sigma_z \otimes \sigma_z$. The coupling between v_m and Γ_l is chosen to be antiferromagnetic, i.e., $\sigma_z \otimes \sigma_z$.

The corresponding "planar orthogonal Hamiltonian" is shown in Figure 3. The filled circles correspond to dummy vertices that do not have any local Hamiltonian. The circles with indices correspond to the original vertices of G. They have σ_z as local Hamiltonians. The thin lines correspond antiferromagnetic interactions and the thick lines to ferromagnetic interactions. The idea behind this construction is that

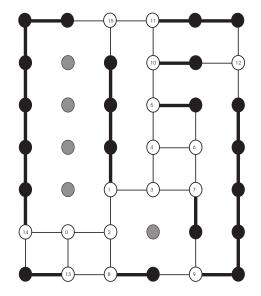


Figure 3: Hamiltonian corresponding to the planar orthogonal embedding in Fig. 2

there is a direct one-to-one correspondence between the ground states of H_P and \hat{H}_P . The same is true for the first excited states. This can be seen as follows:

Let $(k, l) \in E$ be an edge of G and $(\Gamma_1, v_1, \ldots, v_m, \Gamma_l)$ be the path on the lattice connecting Γ_k and Γ_l . The variables $S_{\Gamma_k}, S_1, \ldots, S_m \in \{0, 1\}$ indicate whether the corresponding qubit is spin up or spin down.

A ground state satisfies the condition that S_1, \ldots, S_m are all equal to S_{Γ_k} . To show this we define the number of mismatches along the path to be the number of occurrences of $S_{\Gamma_k} \neq S_1$, $S_i \neq S_{i+1}$ for $i = 1, \ldots, m-1$. This number is denoted by δ .

Then the minimal possible energy (due to the couplings along the path) is

$$c(-m+\delta) - 1. \tag{13}$$

If we remove the mismatches (by setting $S_i := S_{\Gamma_k}$ for i = 1, ..., m) then the maximal possible energy is

$$-cm+1. \tag{14}$$

By choosing c = 3 minimal energy can be achieved only if the states of all dummy vertices are equal to the state of the qubit corresponding to Γ_k .

For adiabatic quantum computing it is important that the gap between the ground and first excited states of the Hamiltonian at all times is sufficiently large. We show that the modification of H_P to \hat{H}_P does not decrease this gap.

The gap between the ground and the first excited states of H_P is smaller or equal to 8. This is seen as follows. Let $S_1, \ldots, S_n \in \{-1, +1\}$ be an assignment corresponding to a ground state of H_P . Pick any vertex k and let l_1, l_2, l_3 be at the three vertices connected to k. By flipping S_k the energy can increase by at most 8 because the relevant Hamiltonian is

$$\sigma_z^{(k)} + \sum_{i=1}^3 \sigma_z^{(k)} \sigma_z^{(l_i)}$$

By choosing c = 9 it is seen that the first excited states of \hat{H}_P satisfy the condition that the states all of dummy vertices are equal to the vertex of Γ_k .

4 Simulating "planar orthogonal" Hamiltonians

To implement the time-evolution according to the Hamiltonian \hat{H}_P we make use of the concepts of simulating Hamiltonians that has been used in nuclear magnetic resonance for a long time [EBW87]. These techniques rely on the so-called average Hamiltonian approach. The idea is to conjugate the natural time evolution by unitary control operations u_j , i.e., the total evolution is

$$u_k \exp(-iHt_k)u_k^{\dagger} \dots u_2^{\dagger} \exp(-iHt_2)u_2^{\dagger}u_1 \exp(-iHt_1)u_1^{\dagger},$$

where the system evolves in an undisturbed way during periods of length t_1, t_2, \ldots, t_k . If these periods are short compared to the time

scale of the natural evolution, the total dynamics is approximatively the same as the evolution according to the average Hamiltonian

$$\overline{H} := \sum_{j} \frac{t_j}{t} u_j H u_j^{\dagger}$$

with $t := \sum_{j} t_{j}$. Usually, the control operations on n particles are assumed to be of the form

$$u := v_1 \otimes v_2 \otimes \cdots \otimes v_n$$

where v_j is a unitary acting on particle j. The design of simulation schemes for Hamiltonians with n particles interacting via pairinteractions leads to non-trivial combinatorial problems (e.g. [LCYY00, DNBT01, WJB02, JWB02]). An experimental proposal for simulating dynamics in optical systems is presented in [JVD⁺02].

Starting from the Ising Hamiltonian H_{Ising} , we can implement the Hamiltonian \hat{H}_P with time overhead (slow-down) 2c + 1 and 16 time steps by interspersing the time evolution according to H_{Ising} by local operations in $X \otimes X \otimes \cdots \otimes X$, where $X = \{\mathbf{1}, \sigma_x\}$.

Following the ideas of [LCYY00, WJB02] we construct a selective decoupling scheme based on Hadamard matrices. Due to the special form of H_{Ising} it is sufficient to use the Hadamard matrix of size 4 only.

Our scheme consists of 4 subroutines that implement the following couplings of \hat{H}_P :

- 1. horizontal $\sigma_z \otimes \sigma_z$,
- 2. vertical $\sigma_z \otimes \sigma_z$,
- 3. horizontal $-c \sigma_z \otimes \sigma_z$, and
- 4. vertical $-c \sigma_z \otimes \sigma_z$

The indices i, j enumerate the rows and the columns of the lattice. We denote the columns of the Hadamard matrix of size 4

by W(0,0), W(0,1), W(1,0) and W(1,1).

Let $v = (v_1, v_2, v_3, v_4) \in \{-1, 1\}^4$ be a column vector. We use the abbreviation

"apply v at (i, j)"

to denote the following control sequence with 4 equally long time steps: at the beginning and the end of the *s*th time step we apply σ_x on the qubit at position (i, j) if $v_s = -1$ and do nothing if $v_s = 1$, where time step *s* runs from 1 to 4.

Let $v, v' \in \{-1, 1\}^4$. One easily checks that applying v and v' at adjacent lattice points changes $\sigma_z \otimes \sigma_z$ to $\langle v, v' \rangle \sigma_z \otimes \sigma_z$, where $\langle v, v' \rangle$ denotes the inner product of v and v'. This is the key observation for constructing the selective decoupling scheme.

In the first and second subroutines the length of the 4 time steps is chosen to 1/4. Let us consider the first subroutine. The vertical couplings are automatically removed if we apply in rows with even indices only W(0,0) and W(1,0) and in rows with odd indices W(1,0) and W(1,1). The choice between W(a,0) and W(a,1) depends on which horizontal interactions should remain or be switched off. Explicitly, this choice is as follows. Choose W(a,0) for the leftmost spin. If the interaction between the spins (j-1) and j should remain, then apply the same W(a, b) to j as to (j-1). Otherwise (i.e. the coupling should be switched off) apply the second possible W(a, b') to j.

The second subroutine is obtained from the first subroutine by exchanging the roles of rows and columns of the lattice.

In the third and fourth subroutines the length of the 4 time steps is chosen to c/4. The third subroutine is obtained from the first subroutine by apply $(-1)^{j}v$ instead of v to the spin j. Finally, the fourth subroutine is obtained from the third subroutine by exchanging the roles rows and columns of the lattice.

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