A PTAS for the Classical Ising Spin Glass Problem on the Chimera Graph Structure

Rishi Saket*

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Abstract

We present a polynomial time approximation scheme (PTAS) for the minimum value of the classical Ising Hamiltonian with linear terms on the Chimera graph structure as defined in the recent work of McGeoch and Wang [MW13]. The result follows from a direct application of the techniques used by Bansal, Bravyi and Terhal [BBT09] who gave a PTAS for the same problem on planar and, in particular, grid graphs. We also show that on Chimera graphs, the trivial lower bound is within a constant factor of the optimum.

1 Introduction

The classical Ising spin glass problem is defined as follows. Given a graph $G(V, E)$ along with real numbers $d_u$ for all vertices $u$ and $c_{uv}$ for all edges $(u, v)$, the classical Ising spin glass problem is to the minimize the following Hamiltonian,

$$H(S) := \sum_{(u,v) \in E} c_{uv} S_u S_v + \sum_{u \in V} d_u S_u,$$

over all $\{-1, 1\}$ assignments to the vertices given by $S = \{S_u \in \{-1, 1\}\}_{u \in V}$. It is useful to note that $E_S[H(S)] = 0$, and thus the optimum of $H(S)$ is non-positive.

The Ising spin glass problem is used to model the interactions in physical spin systems and its minimum value is a measure of the ground state-energy of the system. As such this computational problem has received significant attention from both, the algorithmic and complexity perspectives. For a detailed discussion on this problem we refer the reader to the related work of Bansal, Bravyi and Terhal [BBT09] who gave a PTAS for this problem on planar graphs. In this work we focus on the approximability of this problem on the Chimera graph structure which we formally define below.

The Chimera Graph Structure. We shall work with the Chimera graph structure as defined in [MW13], with a different notation for convenience. For a positive integer $r$, the Chimera graph $G_r$ is constructed as follows.

Vertices $V$. The set of vertices $V$ consists of the integer tuples $\{(i, j, k, l) \in \mathbb{Z}^4 \mid 1 \leq i, j \leq r, 1 \leq k \leq 4, l = 0, 1\}$. The indices $i$ and $j$ specify the location in a $r \times r$ grid, $k$ indicates one of four possible vertices, and $l$ specifies the layer in which the vertex belongs. The number of vertices is $8r^2$.

*IBM T. J. Watson Research Center. Email: rsaket@us.ibm.com
Edges $E$. The edge set is a disjoint union of $E_0$, $E_1$, and $E_{01}$, where $E_0$ is the set of edges in layer 0, $E_1$ is the set of edges in layer 1, and $E_{01}$ is the set of edges across the the two layers. These sets of edges are defined as follows:

$E_0$: For any $1 \leq i \leq r - 1$, $1 \leq j \leq r$, and $1 \leq k \leq 4$, $E_0$ contains an edge between $(i, j, k, 0)$ and $(i + 1, j, k, 0)$.

$E_1$: For any $1 \leq i \leq r$, $1 \leq j \leq r - 1$, and $1 \leq k \leq 4$, $E_1$ contains an edge between $(i, j, k, 1)$ and $(i, j + 1, k, 1)$.

$E_{01}$: For any $1 \leq i \leq r$, $1 \leq j \leq r$, $1 \leq k_0 \leq 4$ and $1 \leq k_1 \leq 4$, $E_{01}$ contains an edge between $(i, j, k_0, 0)$ and $(i, j, k_1, 1)$.

Note that $E_0$ is a disjoint collection of $4r (r - 1)$-length paths, one each for a fixed pair of values for $j$ and $k$. Similarly, $E_1$ is a disjoint collection of $4r (r - 1)$-length paths, one each for a fixed pair of values for $i$ and $k$. Also, $E_{01}$ is a disjoint collection of $r^2 K_{4,4}$ graphs, one for each value of $(i, j)$ with the bipartition given by the sets $\cup_{k=1}^4 \{(i, j, k, 0)\}$ and $\cup_{k=1}^4 \{(i, j, k, 1)\}$.

Note that the Chimera graph structure is non-planar as it contains the $K_{4,4}$ graph, as well as a $K_{r,r}$ minor. Thus, the results of Bansal et al. [BBT09] are not directly applicable. However, utilizing the symmetries in the above construction we are able to adapt the techniques of [BBT09] to prove the following algorithmic results.

Our Results. This work shows the existence of a polynomial time approximation scheme (PTAS) for the classical Ising spin glass problem on the Chimera graph structure. Formally we prove the following theorem.

Theorem 1.1. Given a Chimera graph structure $G_r$ on $n = 8r^2$ vertices, the Hamiltonian $H(S)$ can be approximated to $(1 - \varepsilon)$ of its minimum value in time $O \left( n \cdot 2^{\frac{22}{17}} \right)$.

The above result is obtained by noting that the graph $G_r$ can be disconnected into constant width strips by removing a small fraction of edges from $E_0$ (or $E_1$). This allows the application of the partitioning technique used by Bansal et al. [BBT09] for their PTAS on grid graphs. The analysis requires a straightforward lower bound on the magnitude of the optimum value of $H(S)$ in terms of sum of the absolute values of the bilinear coefficients in $H(S)$ corresponding to edges in $E_0$.

A somewhat more involved analysis yields the following result which shows that the trivial lower bound is within a constant factor of the optimum.

Theorem 1.2. Let $H^*$ be the optimum value of $H(S)$ on the Chimera graph structure. Then, $H^* \leq -(C/(3C + 4)) \left[ \sum_{(u,v) \in E} |c_{uv}| + \sum_{u \in V} |d_u| \right]$, for some constant $C > \frac{\ln(1+\sqrt{2})}{\pi}$. In particular, the approximation factor is $(3C + 4)/C < 17.26$.

The above result is obtained by extending the straightforward lower bound used to prove Theorem 1.1 with a complementary bound obtained via the Grothendieck constant.

2 PTAS on Chimera Graphs

Let $G_r = G(V, E)$ be the Chimera graph on $n = 8r^2$ vertices and $H(S)$ be the Hamiltonian given in Equation (1) for some real values $\{c_{uv}\}_{(u,v) \in E}$ and $\{d_u\}_{u \in V}$. Recall that $E$ is the disjoint union, $E = E_0 \cup E_1 \cup E_{01}$. For convenience we split $H(S)$ as,

$$H(S) := M_0(S) + M_1(S) + M_{01}(S) + D(S), \quad \text{(2)}$$
where,

\[ M_l(S) := \sum_{(u,v) \in E_l} c_{uv} S_u S_v, \quad l = 0, 1, \]

\[ M_{01}(S) := \sum_{(u,v) \in E_{01}} c_{uv} S_u S_v, \]

\[ D(S) := \sum_{u \in V} d_u S_u. \]

We also define the following quantities.

\[ A_l := \sum_{(u,v) \in E_l} |c_{uv}| \text{ for } l = 0, 1. \]

\[ A_{01} := \sum_{(u,v) \in E_{01}} |c_{uv}|. \]

\[ B := \sum_{u \in V} |d_u|. \quad (3) \]

The following lemma follows from the structure of \( G \).

**Lemma 2.1.** Let \( H^* \) be the minimum value of \( H(S) \). Then, \( H^* \leq -(A_0 + A_1) \).

**Proof.** From the construction of \( G_r \) we have that \( E_0 \) is a disjoint collection of \( 4r \) \((r-1)\)-length paths in layer 0. Similarly, \( E_1 \) is a disjoint collection of \( 4r \) \((r-1)\)-length paths in layer 1. Thus, \( E_0 \cup E_1 \) is a disjoint collection of \( 8r \) \((r-1)\)-length paths. Thus, there exists an assignment \( S' \) such that \( M_0(S') = -A_0 \) and \( M_1(S') = -A_1 \). We can ensure that \( M_{01}(S') \leq 0 \), otherwise the values assigned to all the vertices in layer 0 i.e. all vertices of the form \((i,j,k,0)\) can be flipped which changes the sign of \( M_{01}(S') \) while preserving \( M_0(S') \) and \( M_1(S') \). Thus, we can ensure that \( M_0(S) + M_1(S) + M_{01}(S) \leq -(A_0 + A_1) \). Now, if \( D(S') \) is positive, then \( S' \) can be flipped for all vertices to ensure that \( H(S') \leq -(A_0 + A_1) \). \( \square \)

Let us define a *strip* graph with \( m \) levels and width \( b \) as any graph which has \( m \) levels of \( b \) vertices each such that all edges between levels are between adjacent levels. The levels may have edges within them. To be precise, a vertex in level \( j \) may have edges only to other vertices in levels \( j, (j-1) \) or \( (j+1) \). Bansal et al. [BBT09] showed that the problem of minimizing the Hamiltonian on \( m \times b \) strip graphs can be solved using dynamic programming in time \( O(m4^b) \). The dynamic program computes for level \( j \) and each of the \( 2^b \) assignments to the vertices in that level, the value of the best solution with that assignment to level \( j \) for the Hamiltonian on the subgraph induced by levels \( 1, \ldots, j \). Going from level \( j \) to \( j+1 \) requires \( O(4^b) \) operations, a constant number for each pair of assignments to levels \( j \) and \( j+1 \). Thus, the total time taken is \( O(m4^b) \). Our goal in designing the PTAS is to describe a way to decompose the graph \( G \) into strip graphs with constant width while not losing much in the objective value. This is similar to the decomposition in [BBT09] for grid graphs with a slightly different analysis.

Recalling the structure of \( G_r \), for any \( i = 1, \ldots, r \) let,

\[ E_{i0} := \{(i,j,k,0), (i',j,k,0)\} \mid i' = \{i-1, i+1\} \cap \{1, \ldots, r\}, 1 \leq j \leq r, 1 \leq k \leq 4. \]
In other words, $E_{i0}$ consists of all edges within layer 0 which are incident on the vertices $(i,j,k,0)$. Let $T$ be a large positive integer which we shall set later. For any $k = 0, 1, \ldots, T - 1$, let,

$$E^k_0 := \bigcup_{i \equiv k \mod T, 1 \leq i \leq r} E_{i0},$$

$$A^k_0 := \sum_{(u,v) \in E^k_0} |c_{uv}|,$$

$$H_k(S) := \sum_{(u,v) \in E^k_0} c_{uv}S_uS_v,$$

$$H_{\text{sub},k}(S) := H(S) - H_k(S).$$

Since every edge in $E_0$ is present in exactly 2 of the subsets $E^k_0$, we obtain by averaging that there is a $k^*$ such that $A^{k^*_0} \leq (2/T)A_0$. Further, it can be seen that $H_{\text{sub},k}(S)$ is the Hamiltonian on a disjoint collection of at most $r/T$ strip graphs of dimensions $r \times 8T$ and at most $r/T$ strip graphs of dimensions $r \times 8$. To complete the analysis we first assume because of symmetry that $A^1_0 \geq A^0_0$. Thus, by Lemma 2.1, the minimum value of $H(S)$ is at most $-2A_0$. Let $S'$ be the assignment that minimizes the value of $H_{\text{sub},k^*}(S')$, and $S^{\text{opt}}$ the assignment that minimizes the value of $H(S)$. We have,

$$H_{\text{sub},k^*}(S') \leq H_{\text{sub},k^*}(S^{\text{opt}}) \leq H(S^{\text{opt}}) + A^{k^*_0} \leq H(S^{\text{opt}}) + (2/T)A_0 \leq (1 - 1/T)H(S^{\text{opt}}),$$

and,

$$H(S') \leq H_{\text{sub},k^*}(S') + A^{k^*_0} \leq (1 - 1/T)H(S^{\text{opt}}) + (2/T)A_0 \leq (1 - 2/T)H(S^{\text{opt}}).$$

Since $H(S') \geq H(S^{\text{opt}})$, from the above we get that $H(S')$ is a $(1 - 2/T)$ approximation to $H(S^{\text{opt}})$. We now set $T = 2/\varepsilon$ to obtain a $(1 - \varepsilon)$ approximation to $H(S^{\text{opt}})$. To compute the value $H(S')$, we compute the assignment $S'$ that minimizes $H_{\text{sub},k}(S)$ for each $k = 0, 1, \ldots, T - 1$, and take the one that gives the minimum value of $H(S')$. For each $k$, this involves minimizing the Hamiltonian on at most $(2r/T + 2)$ strip graphs of $r$ levels and width at most $8T$. As discussed above, the computation time for one such strip graph is $O(r4^{8T})$ which adds up to $O(r2^44^{8T}/T)$ time for all the strip graphs for one value of $k$. Thus, the total computation time to obtain a $(1 - \varepsilon)$ approximation is $O \left( r^24^\frac{12}{4T} \right) = O \left( n^\frac{12}{4T} \right)$.

3 A constant factor bound

In this section we prove Theorem 1.2. The key ingredient is the following lemma which bounds the bilinear quadratic form on $K_{4,4}$ in terms of the sum of the absolute values of the coefficients.
Lemma 3.1. Let \( G(U, V, E) \) be a \( K_{4,4} \) graph with \( U = \{u_1, \ldots, u_4\} \) and \( V = \{v_1, \ldots, v_4\} \) giving the bipartition and \( E = U \times V \) the edge set. There is a universal constant \( C > 0 \) such that for any real numbers \( \{c_{ij} \mid 1 \leq i, j \leq 4\} \),
\[
\min_S \sum_{1 \leq i, j \leq 4} c_{ij} S_u^i S_v^j \leq -C \sum_{1 \leq i, j \leq 4} |c_{ij}|, \tag{4}
\]
where \( S = \{S_u \mid u \in U\} \cup \{S_v \mid v \in V\} \) is a \( \{-1, 1\} \) assignment to the vertices of \( G \). In particular, the above holds for some \( C > \frac{\ln(1+\sqrt{2})}{2} \).

Proof. Let us first assign unit vectors \( x_i \) for vertices \( u_i \) and \( y_j \) for vertices \( v_j \) \( (1 \leq i, j \leq 4) \). The seminal work of Grothendieck [Gro53] implies the following:
\[
\max_{x_i, y_j \in S} \sum_{1 \leq i, j \leq 4} c_{ij} \langle x_i, y_j \rangle \leq K \max_S \sum_{1 \leq i, j \leq 4} c_{ij} S_u^i S_v^j. \tag{5}
\]
Here \( K \) is a universal constant for which the above inequality holds for any \( K_t, t \), wherein our case \( t = 4 \). Determining the exact value of \( K \) has been a major open question. The work of Krivine [Kri77] showed that \( K \leq \frac{\pi}{2 \ln(1+\sqrt{2})} \) and in more recent work Braverman, Makarychev, Makarychev and Naor [BMMN11] showed that in fact \( K < \frac{\pi}{2 \ln(1+\sqrt{2})} \). The following claim helps to leverage the above inequality.

Claim 3.2. There exists a set of unit vectors vectors \( \{x_i \mid 1 \leq i \leq 4\} \cup \{y_j \mid 1 \leq j \leq 4\} \) such that,
\[
\sum_{1 \leq i, j \leq 4} c_{ij} \langle x_i, y_j \rangle \geq \left(\frac{1}{2}\right) \sum_{1 \leq i, j \leq 4} |c_{ij}|. \tag{6}
\]

Proof. We first set the vectors \( \{x_i \mid 1 \leq i \leq 4\} \) to be a set of 4 orthonormal vectors. For \( j = 1, 2, 3, 4 \) we let the unit vector \( y_j = (1/2) \sum_{i=1}^4 \text{sgn}(c_{ij}) x_i \). It is easy to check that this setting of the vectors satisfies the inequality in the claim.

Using the above claim in conjunction with Equation (5) along with the bound on the value of \( K \) we obtain,
\[
\max_S \sum_{1 \leq i, j \leq 4} c_{ij} S_u^i S_v^j \geq C \sum_{1 \leq i, j \leq 4} |c_{ij}| \tag{7}
\]
Reversing the signs of the assignments to the vertices in \( U \), we complete the proof of the lemma.

The following lemma provides a bound on the minimum value of \( H(S) \).

Lemma 3.3. Let \( H^* \) be the minimum value of \( H(S) \). Then \( H^* \leq A_0 + A_1 - CA_{01} \).

Proof. Since the set of edges \( E_{01} \) is a disjoint collection of \( r^2 \) \( K_{4,4} \) graphs, using Lemma 3.1 one can set the assignment \( S \) such that \( M_{01}(S) \leq -CA_{01} \). The maximum values of \( M_0(S) \) and \( M_1(S) \) are \( A_0 \) and \( A_1 \) respectively. Also, by flipping the sign of \( S \) if necessary, one can simultaneously ensure that \( D(S) \) is non-positive.
Combining the above lemma with Lemma 2.1 we obtain,

\[(C + 2)H^* \leq -(C + 1)(A_0 + A_1) + A_0 + A_1 - CA_{01},\]
\[\Rightarrow (C + 2)H^* \leq -C(A_0 + A_1 + A_{01}),\]
\[\Rightarrow \left(\frac{C + 2}{C}\right)H^* \leq -(A_0 + A_1 + A_{01}).\] (8)

Moreover, an appropriate assignment of \(S\) ensures that \(D(S) = -B\). Thus, we also have the following bound,

\[H^* \leq A_0 + A_1 + A_{01} - B.\]

Combining the above with Equation (8) yields,

\[\left(\frac{2(C + 2)}{C} + 1\right)H^* \leq -2(A_0 + A_1 + A_{01}) + (A_0 + A_1 + A_{01} - B),\]
\[\Rightarrow H^* \leq -\left(\frac{C}{3C + 4}\right)(A_0 + A_1 + A_{01} + B)\]

which completes the proof of Theorem 1.2.

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