Cycle Basis Markov Chains for the Ising Model *

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Abstract

A very challenging problem from statistical physics is computing the partition function of the ferromagnetic Ising model, even in the relatively simple case of no applied field. In this case, the partition function can be written as a function of the subgraphs of the underlying graph in which all vertices have even degree. In their seminal work, Jerrum and Sinclair showed that this quantity can be approximated by a rapidly converging Markov chain on all subgraphs. However, their chain frequently leaves the space of even subgraphs. Our aim is to devise and analyze a new class of Markov chains that do not leave this space, in the hopes of finding a faster sampling algorithm.

We define Markov chains by viewing the even subgraphs as a vector space (often called the cycle space) whose transitions are defined by the addition of basis elements. The rate of convergence depends on the basis chosen, and our analysis proceeds by dividing bases into two types, short and long. The classical single-site update Markov chain known as Glauber dynamics is a special case of our short cycle basis Markov chains. We show that for any graph and any long basis, there is a temperature for which the corresponding Markov chain requires an exponential time to mix. Moreover, we show that for d-dimensional grids with $d \geq 2$—those of the most physical importance—all fundamental bases (a natural class of bases derived from spanning trees) are long. For the 2-dimensional grid on the torus, we show that there is a temperature for which the Markov chain requires exponential time for any chosen basis.

1 Introduction

Estimating the partition function Z of the ferromagnetic Ising model with zero applied field is a fundamental problem in statistical physics [8, 11, 1]. A common approach to estimating Z is to sample spin configurations from the Gibbs distribution using a Markov chain. The behavior of the classical single-site update Markov chain $\mathcal{M}_{\mathrm{GD}}$, known as Glauber dynamics, has received intense study from the physics and computer science communities. It is believed to be rapidly mixing at all temperatures on the 2-dimensional square grid with a fixed plus boundary condition [16], but is known to require exponential time to mix at low temperatures if the lattice has free or periodic boundary conditions [21, 22]. This critical slowing down is closely related to the existence of multiple Gibbs states—where spin configurations are dominated by either plus spins or minus spins—since the local nature of $\mathcal{M}_{\mathrm{GD}}$ makes it difficult to move between the two regimes.

When local Markov chains are inefficient, it is natural to seek nonlocal algorithms. Swendsen and Wang introduced a promising algorithm that appears to work well in practice, although rigorous bounds have been found in only limited cases [2, 3, 7, 13]. Jerrum and Sinclair introduced the first fully-polynomial randomized approximation scheme (*fpras*) for the Ising model [9], which was extended to an efficient random sampler by Randall and Wilson [20]. Jerrum and Sinclair appealed to the high-temperature expansion of Z, which reduces the problem, in the case of no applied field, to sampling even subgraphs of a graph G according to $\pi'(X) = \lambda^{|E(X)|}/Z'$ for some $\lambda \in [0, 1]$. Their *fpras* is based on a Markov chain that is polynomially-mixing at all temperatures. However, the running time of this algorithm is large, partly because the Markov chain spends a lot of time outside the set of even subgraphs.

In this paper we consider whether it is possible to design a faster algorithm by restricting to even subgraphs. We present a new class of Markov chains for sampling even subgraphs based on cycle bases. This

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class, called the Cycle Basis Markov chains, contains $\mathcal{M}_{\mathrm{GD}}$ and generalizes it to nonlocal chains.

In Section 2, we describe in detail the relationship between the Ising model and even subgraphs and provide background on both cycle bases and mixing times of Markov chains. In Section 3, we formally define our Markov chains and state the main results of the paper. Section 4 is devoted to the proofs of two of the main results, and Section 5 is devoted to the proof of the third. Finally, in Section 6, we discuss future directions.

2 Preliminaries

2.1 The Ising model Given a graph $G = (V, E)$ with $|V| = n$ and $|E| = m$, a *spin configuration* $\sigma = \sigma(G)$ is an assignment of spins in $\{+1, -1\}$ to the elements of V. In this paper we assume no external field has been applied, so the energy of σ is given by the Hamiltonian $H(\sigma) = -J \sum_{(x,y)\in E} \sigma_x \sigma_y$, where J is the interaction energy. The probability assigned to state σ is given by the Gibbs distribution, defined as $e^{-\beta H(\sigma)}/Z$, where $\beta = 1/(k_{\mathcal{B}} T)$ is proportional to inverse temperature and $k_{\mathcal{B}}$ is Boltzmann's constant. The normalizing constant $Z = \sum_\sigma \exp(-\beta H(\sigma))$ is also called the partition function.

Following the notation of [9], let $\lambda = \tanh(\beta J)$ and $\mu = \tanh(\beta B)$. The high-temperature expansion is defined by $Z = AZ'$, where $A = 2^n \cosh(\beta J)^m$ is an easily computed constant, and $Z' = \sum_{X \subseteq E} \lambda^{|E(X)|}$, where the sum is taken over all subsets X of $E(G)$ that induce an even subgraph (defined in Section 2.2). We will sample from the distribution $\pi'(X) = \lambda^{|E(X)|}/Z'$.

2.2 Cycle bases We now provide some elementary algebraic graph theory to formally introduce the topic of cycle bases, which have a long history in combinatorics [15], and are used both in theory and applications [10]. The interested reader can find more background information in [5].

The *symmetric difference* of two subgraphs Y_1 and Y_2 of a graph G, written $Y_1 \oplus Y_2$, is the subgraph of G that contains precisely those edges in exactly one of Y_1 and Y_2. One may consider this operation as addition of subgraphs over the field $\mathbb{F}_2 = \{0, 1\}$. Let $\mathcal{E} = \mathcal{E}(G)$ be the set of subgraphs with no vertices of odd degree—the *even subgraphs* of G. Since the symmetric difference of two elements in $\mathcal{E}$ is again in $\mathcal{E}$, we may view $\mathcal{E}$ as a vector space over $\mathbb{F}_2$, called the *cycle space* of G. Every maximal set of linearly independent even subgraphs is a *cycle basis* of G. All cycle bases have size $m - n + k$, where m is the number of edges in G, n is the number of vertices, and k is the number of components. Further, every $Y \in \mathcal{E}$ has a unique basis representation. We assume for simplicity that $k = 1$ so that G is connected.

As an example, let T be a spanning tree of G and $e \notin E(T)$. Then $T + e$ has a unique cycle. The set of such cycles over all $e \notin E(T)$ is a cycle basis called a *fundamental cycle basis*. Such bases are easy to find computationally, as spanning trees can be found easily (see e.g. [4]).

2.3 Markov chains Let P be the transition matrix of a Markov chain $\mathcal{M}$ with stationary distribution π. The state space of $\mathcal{M}$ is often referred to as Ω. We will use this notation in this subsection only; everywhere else, the state space is the vector space of even subgraphs, $\mathcal{E}$.

It is common to measure the distance between the t-step probability distribution and the stationary distribution π in terms of the total variation distance $\|P^t(X, \cdot), \pi\|_{tv} = \frac{1}{2}\sum_{Y\in\Omega} |P^t(X, Y) - \pi(Y)|$. Then the efficiency of the Markov chain $\mathcal{M}$ can be described by its *mixing time* $\tau = \tau(1/4) = \max_{X\in\Omega} \min\{t : \|P^t(X, \cdot), \pi\|_{tv} \le 1/4\}$. We say that a Markov chain is *rapidly mixing* if $\tau = O(p(n))$ for some polynomial p, where n is the size of each configuration — for us, n is the number of vertices in the graph G.

In this paper, we provide lower bounds on the mixing time that are exponential in n^δ for some constant $\delta > 0$. Consider the *conductance* of a Markov chain $\mathcal{M}$, defined as $\Phi_{\mathcal{M}} = \min_{\substack{S\subset\Omega \\ \pi(S)\le 1/2}} \phi_S$, where

$$\phi_S = \frac{1}{\pi(S)} \sum_{x\in S, y\notin S} \pi(x) P(x, y) \tag{2.1}$$

is the *conductance of a set* S. The existence of a set S for which ϕ_S is very small prevents the chain from mixing rapidly (see, e.g. [12, Theorem 7.3]):

THEOREM 2.1. $\tau \ge (4\Phi_{\mathcal{M}})^{-1}$.

3 Algorithm and Results

3.1 Cycle basis Markov chains Given any cycle basis $\mathcal{B}$ of G, we can define $\mathcal{M}(\mathcal{B})$ as in Algorithm 1.

Algorithm 1 Cycle Basis Markov chain $\mathcal{M}(\mathcal{B})$

`Starting at any` $Y \in \mathcal{E}$`, iterate the following:`

`Choose` $B \in \mathcal{B}$ `uniformly at random.`

`With probability` $\frac{1}{2}\min\left(1, \frac{\pi'(Y\oplus B)}{\pi'(Y)}\right)$`, move to` $Y \oplus B$.

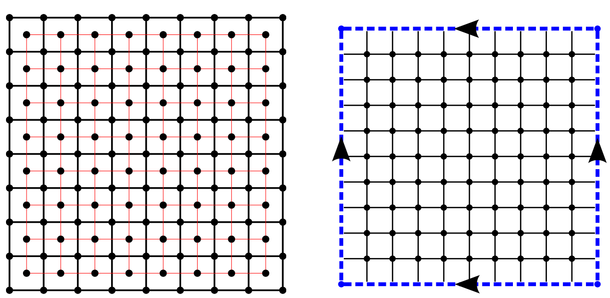
`With all remaining probability, stay at` Y.

Clearly, $\mathcal{M}(\mathcal{B})$ connects the state space $\mathcal{E}$. The transition probabilities are chosen to ensure that

$\mathcal{M}(\mathcal{B})$ converges to the stationary distribution π' [12, 17]. Notice π' satisfies the *detailed balance condition*: $\pi'(x)P(x,y) = \pi'(y)P(y,x)$ for all $x, y \in \Omega$. When $\lambda = 1$, π' is the uniform distribution and $\mathcal{M}(\mathcal{B})$ is a uniform random walk on the hypercube $\{0,1\}^{m-n+k}$, which is rapidly mixing [12, p. 67–68]. In this paper, we will be interested in what happens when λ is small.

More generally, $\mathcal{M}(\mathcal{B})$ can sample from any state space that is comprised of all subgraphs with *any* fixed set of odd-degree vertices, since moves of $\mathcal{M}(\mathcal{B})$ do not change the parity of the degree of any vertex. Subgraphs with a fixed set of odd-degree vertices are important in a variety of applications in statistical physics and computing, such as the Ising model with an external field (not considered here), as well as perfect matchings, Eulerian orientations, and 3-colorings [14]. For example, to sample perfect matchings using $\mathcal{M}(\mathcal{B})$, one could restrict to subgraphs in which every vertex has odd degree and reject moves that increase degrees above one. This idea generalizes an approach that has been proven to be fast on the 2-dimensional lattice [14].

Although $\mathcal{M}(\mathcal{B})$ is defined for all graphs, the graphs of the most physical interest are square, d-dimensional lattices with side length s (i.e. the cartesian product of d s-paths), which we denote $G_d(s)$, and those same lattices with periodic boundary conditions (i.e. the cartesian product of d s-cycles), denoted $G_d^p(s)$. Note that $G_2(s)$ is planar and $G_2^p(s)$ is toroidal. See Figure 1.



(a) Edges of $G_2(s)$ are thick and black, its planar dual, $G_2(s-1)$, has thin and red edges

(b) $G_2^p(9)$ in its standard embedding on the torus

Figure 1

In two dimensions, there is a correspondence between spin configurations with fixed boundary conditions and subgraphs with a particular set of odd degree vertices associated with those boundary conditions. In particular, consider $G_2(s)$ and its planar dual, minus the vertex representing the infinite face, $G_2(s-1)$. See Figure 1a. Spin configurations with a fixed plus boundary on $G_2(s)$ are in bijection with even subgraphs of $G_2(s-1)$. See Figure 2. Let $\mathcal{F}$ be the faces of $G_2(s-1)$ that are bounded by 4-cycles in the embedding in Figure 1a, and define the *facial basis* $\mathcal{B}_{\mathcal{F}}(s-1)$ as the set of 4-cycles bounding elements of $\mathcal{F}$. These cycles induce a basis of $\mathcal{E}$,[1] and moreover, $\mathcal{M}(\mathcal{B}_{\mathcal{F}}(s-1))$ is precisely $\mathcal{M}_{\mathrm{GD}}$; flipping a spin in $G_2(s)$ is equivalent to taking the symmetric difference with an element of $\mathcal{B}_{\mathcal{F}}(s-1)$. Thus, $\mathcal{M}_{\mathrm{GD}}$ on $G_2(s)$ is a cycle basis Markov chain.[2]

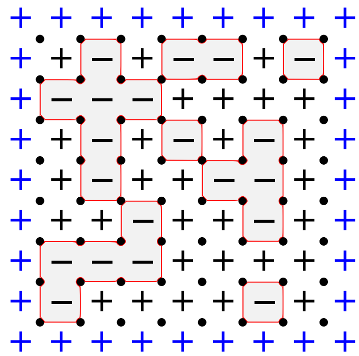


Figure 2: Spin configurations on $G_2(s)$ with plus boundary; even subgraphs on $G_2(s-1)$

3.2 Our results Given any cycle basis $\mathcal{B}$ of a graph G, every $Y \in \mathcal{E}$ has a unique representation

$$Y = \alpha_1 C_1 \oplus \alpha_2 C_2 \oplus \cdots \oplus \alpha_{m-n+1} C_{m-n+1}, \tag{3.2}$$

where $\alpha_i \in \{0,1\}$ and $C_i \in \mathcal{B}$. Define the *support* of Y in $\mathcal{B}$ as $\mathrm{supp}_{\mathcal{B}}(Y) = \{C_i \in \mathcal{B} : \alpha_i = 1\}$. When $\mathcal{B}$ is clear, we will simply write $\mathrm{supp}(Y)$. The *length* of $\mathcal{B}$ is the maximum of $|E(B)|$ over all $B \in \mathcal{B}$ such that $B \in \mathrm{supp}(X)$ for some 4-cycle X in G.[3]

THEOREM 3.1. *Let $\mathcal{B}$ be a cycle basis of length L of a graph G with maximum degree Δ. Then for $\lambda < \Delta^{-3}/2$, the mixing time of $\mathcal{M}(\mathcal{B})$ is $\Omega(2^{L/2})$.*

Recall that in order to be rapidly mixing, the Markov chains must mix in time by some polynomial in n, the number of vertices of the graph. Theorem 3.1 proves this cannot hold for cycle bases with length at least n^δ for some constant $\delta > 0$ (we call these bases "long"). In Theorem 3.2, we prove that fundamental cycle bases of $G_d(s)$ and $G_d^p(s)$ have length $\Omega(s)$, which implies:

[1] All 2-connected planar graphs have a cycle basis contained in the set of facial cycles.

[2] On the 2-dimensional lattice, even subgraphs arise as contours separating spin-types, and cycle basis Markov chains on the planar dual are a natural extension of $\mathcal{M}_{\mathrm{GD}}$. In the remainder of the paper, even subgraphs arise as a consequence of the high-temperature expansion, which works on all graphs.

[3] This definition can be generalized to allow X to be any even subgraph with a constant number of edges. As our aim is studying the d-dimensional grid, we choose 4-cycles for simplicity.

THEOREM 3.2. *Let $\mathcal{B}$ be a fundamental cycle basis of $G \in \{G_d(s), G_d^p(s)\}$. If $\lambda < 1/(16d^3)$, then the mixing time of $\mathcal{M}(\mathcal{B})$ is at least $2^{\Omega(s)}$.*

For short bases (those with length less than s) of $G_2^p(s)$, Theorem 3.1 does not yield a slow mixing proof. So instead, we show that these Markov chains are slowly mixing for a different reason, namely that they behave like $\mathcal{M}_{\mathrm{GD}}$.

THEOREM 3.3. *Suppose $\mathcal{B}$ is a cycle basis of $G_2^p(s)$ of length $L < s$. Then whenever $\lambda < .004$, the mixing time of the Markov chain $\mathcal{M}(\mathcal{B})$ is at least $2^{\Omega(s)}$.*

Recall that, for $G_2(s)$, $\mathcal{M}(\mathcal{B}_{\mathcal{F}}(s))$ is believed to be rapidly mixing at all temperatures (as it corresponds to $\mathcal{M}_{\mathrm{GD}}$), and its mixing time is known to be at most $O(s^{\log s})$ for small λ [16]. In contrast, Theorems 3.1 and 3.3 imply that for small λ, the mixing time of $\mathcal{M}(\mathcal{B})$ is $2^{\Omega(s)}$ for *every* cycle basis $\mathcal{B}$ of $G_2^p(s)$. Moreover, Theorem 3.2 suggests that fundamental cycle bases are not ideal, as they create chains that require exponential time to mix even as $\mathcal{M}(\mathcal{B}_{\mathcal{F}}(s))$ could be rapidly mixing.

3.3 Techniques and consequences We use graph theory and linear algebra to analyze the structure of *all* cycle bases of the grid. We then use insights from statistical physics, such as Peierls arguments, to demonstrate the existence of a bad cut in the state space which prevents $\mathcal{M}(\mathcal{B})$ from mixing rapidly. For long cycle bases witnessed by $B \in \mathcal{B}$, we prove that $\mathcal{M}(\mathcal{B})$ cannot easily move between subgraphs whose support includes B and those that do not. For short cycle bases on $G_2^p(s)$, we first use topological graph theory to argue that subgraphs with noncontractible cycles in their support are exponentially unlikely. The remaining subgraphs are in bijection with spin configurations and inherit the bottleneck of $\mathcal{M}_{\mathrm{GD}}$. However, as these bases are nonlocal, the argument requires careful examination of the stationary distribution and we appeal to results of [18] to upper-bound the probability that a spin configuration has a density of +1 spins that is *close* to 1/2.

We consider the definition of $\mathcal{M}(\mathcal{B})$ and the insight that cycle bases can be used to understand local Markov chains, such as $\mathcal{M}_{\mathrm{GD}}$, to be significant contributions of this paper. For each negative result, we make use of the structure of the vector space $\mathcal{E}$. We believe that positive results may stem from this perspective as well. For example, while our results suggest that changing the cycle basis from $\mathcal{B}_{\mathcal{F}}(s)$ will not overcome the critical slowing down of $\mathcal{M}_{\mathrm{GD}}$, we may be able to modify these Markov chains slightly (by adding transitions) to yield better algorithms. See Section 6.

4 Long cycle bases

We begin this section by showing that any long cycle in a cycle basis $\mathcal{B}$ is unlikely to be used as a move in the Markov chain $\mathcal{M}(\mathcal{B})$ for all graphs with bounded maximum degree $\Delta = \Delta(G)$. Afterwards, we bound the mixing time in terms of the length of the basis to prove Theorem 3.1. Finally, we show that all fundamental cycle bases of $G_d(s)$ and $G_d^p(s)$ are of length $\Omega(s)$.

LEMMA 4.1. *Suppose $B \in \mathcal{B}$ has L edges and $\lambda < \Delta^{-3}/2$. Then*

$$\sum_{Y \in \mathcal{E}} \pi'(Y) P(Y, Y \oplus B) \le 2^{-L/2+2}. \tag{4.3}$$

Proof. For any transition $(Y, Y \oplus B)$, either Y or $Y \oplus B$ contains at least half of $E(B)$. Since detailed balance provides $\pi'(Y)P(Y, Y \oplus B) = \pi'(Y \oplus B)P(Y \oplus B, Y)$, we may assume, without loss of generality, that Y has at least half of $E(B)$. Further, $\pi'(Y)P(Y, Y \oplus B) \le \pi'(Y)$.

Enumerate the edges of B in some canonical way (such as in order along each edge-disjoint cycle in B) from an arbitrary (fixed) starting edge $e_1 \in E(B)$ and let $|E(Y) \cap E(B)| = \{e_{i_1}, e_{i_2}, \ldots, e_{i_t}\}$ with increasing indices. Since $Y \in \mathcal{E}$, each component is 2-connected, and hence each edge of Y is in a cycle. Let C_1 be a cycle in Y containing e_{i_1}, and for $j \in \{2, 3, \ldots, t\}$, let C_j be a cycle in $Y \bigoplus_{k=1}^{j-1} C_k$ containing e_{i_j}. (Note: if $e_{i_j} \in E(C_k)$ for $k < j$, then C_j is empty.) Define the map g by $g(Y) = Y \bigoplus_{k=1}^{t} C_k$. Notice that $E(g(Y)) \cap E(C) = \emptyset$. Since the C_k are edge-disjoint cycles in Y, $\pi'(Y) = \lambda^M \pi'(g(Y))$, where $M = \sum_{k=1}^{t} |C_k| \ge L/2$. See Figure 3.

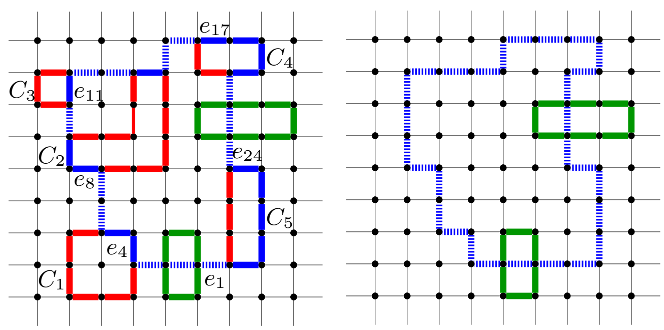


Figure 3: On the left is Y and the right is $g(Y)$. Bold edges are in the graph, blue edges are in C, and red edges are in a C_k. With the labeling of $E(C)$ proceeding clockwise from e_1 we have $e_{i_1} = e_4$, $e_{i_2} = e_8$, $e_{i_3} = e_{11}$, $e_{i_4} = e_{17}$, and $e_{i_5} = e_{24}$.

Next, we show that no element of the image of g has too many preimages. To this end, let H be in the image of g and let $g_M^{-1}(H)$ denote those subgraphs Y

such that $g(Y) = H$ and $|E(Y)| = |E(H)| + M$. Any such preimage Y of H can be recorded by a walk W of length $M + L \le 3M$, which proceeds as follows. Start at e_1. Walk along $E(B)$ in the ordering fixed above by recording the character "$*$" until e_{i_1} is traversed, which, as above, is the first edge in $E(B) \cap E(Y)$. Walk along $C_1 - e_{i_1}$ by recording a character in $[\Delta - 1]$ that describes the edge incident with the most recently seen vertex v in W according to a fixed ordering on the edges incident with v. After returning to e_{i_1} (not recording it the second time), continue this process of recording the edges of $E(B) \setminus E(Y)$ with "$*$"s and the edges of the C_k with characters in $[\Delta - 1]$ until all of $E(B) \cup \bigcup_i E(C_i)$ have been recorded in W. Clearly, each element of $g_M^{-1}(H)$ can be recorded in this manner, and, as each edge in W is described by an element of $\{1, 2, \ldots, \Delta - 1, *\}$, it is clear that $|g_M^{-1}(B)| \le \Delta^{M+L} \le \Delta^{3M}$.

Putting everything together,

$$
\begin{aligned}
\sum_{Y \in \mathcal{E}} \pi'(Y) P(Y, Y \oplus B) & \\
&\le 2 \sum_{Y : |E(Y) \cap E(C)| \ge L/2} \pi'(Y) \\
&= 2 \sum_{B} \sum_{M=L/2}^{m} \sum_{Y \in g_M^{-1}(H)} \pi'(Y) P(Y, Y \oplus H) \\
&= 2 \sum_{H} \sum_{M=L/2}^{m} \sum_{Y \in g_M^{-1}(H)} \pi'(B) \lambda^M \\
&\le 2 \sum_{M=L/2}^{m} \lambda^M \sum_{H} \pi'(H) \Delta^{3M} \\
&\le 2 \sum_{M=L/2}^{m} \left(\lambda \Delta^3\right)^M \sum_{H} \pi'(H) \\
&< 2 \sum_{M=L/2}^{m} \frac{1}{2^M} \quad < \quad 2^{-L/2+2},
\end{aligned}
$$

since $\lambda \Delta^3 < 1/2$.

Next, we show that long cycle bases are slowly mixing for small enough λ, proving Theorem 3.1.

Proof of Theorem 3.1. Suppose X is a four-cycle and $B \in \operatorname{supp}(X)$ has L edges. Define $S_1 = \{Y \in \mathcal{E} \mid B \notin \operatorname{supp}(Y)\}$ and let $S_2 = \mathcal{E} \setminus S_1$. Define the map $f : S_1 \to S_2$ by $f(Y) = Y \oplus X$. Clearly f is a bijection. Moreover, $\lambda^{-4} \ge \pi'(Y)/\pi'(f(Y)) \ge \lambda^4$, and so

$$
\pi'(S_1) = \sum_{Y \in S_1} \pi'(Y) \le \frac{1}{\lambda^4} \sum_{Y \in S_1} \pi'(f(Y)) = \frac{\pi'(S_2)}{\lambda^4}.
$$

Similarly, $\pi'(S_1) \ge \lambda^4 \pi'(S_2)$. Hence, $\pi'(S_1)$ and $\pi'(S_2)$ are each at least $\frac{\lambda^4}{1+\lambda^4}$. By Lemma 4.1,

$$
\begin{aligned}
\sum_{Y \in S_1, Y' \in S_2} \pi'(Y) P(Y, Y') &= \sum_{Y \in S_1} \pi'(Y) P(Y, Y \oplus B) \\
&= \frac{1}{2} \sum_{Y \in \Omega} \pi'(Y) P(Y, Y \oplus B) \\
&\le 2^{-L/2+1}.
\end{aligned}
$$

So $\phi_{S_i} \le \frac{\lambda^4+1}{\lambda^4} 2^{-L/2+1}$ for $i \in \{1, 2\}$ and $\Phi_{\mathcal{M}(\mathcal{B})} = O(2^{-L/2})$. The result follows from Theorem 2.1. $\square$

4.1 Fundamental cycle bases of grids

In this section, we prove Theorem 3.2, which states that fundamental cycle bases of a grid yield Markov chains $\mathcal{M}$ with exponential mixing time at low temperatures. It suffices to show that fundamental cycle bases of a grid satisfy the conditions of Theorem 3.1 with $L \ge s$. Let T be a spanning tree of G. Let $xy \in E(G)$. If $xy \notin E(T)$, define C_{xy} as the unique cycle in $T + xy$. Otherwise, define $C_{xy} = \emptyset$. Recall the fundamental cycle basis of G associated to T is the set $\{C_{xy} : xy \notin E(T)\}$. The following proposition is easy to prove.

Proposition 4.1. *Let $\mathcal{B}$ be a fundamental cycle basis of a graph G. Then for any even subgraph F of G,* $\operatorname{supp}(F) = \{C_{x_1x_2} : (x_1, x_2) \in E(F) \setminus T\}$.

Let C_{xy} be a long cycle in $\mathcal{B}$. Proposition 4.1 implies that every even subgraph containing xy contains C_{xy} in its support. When $G \in \{G_d(s), G_d^p(s)\}$, every edge is in a 4-cycle. Thus, in order to prove Theorem 3.2, we need only show that every fundamental cycle basis of $G_d(s)$ and $G_d^p(s)$ contains a long cycle. Before completing the proof, we need two lemmas about spanning trees. For a tree T on n vertices, we say an edge $e \in E(T)$ *equitably divides* T if each of the two components of $T - e$ has at least $(n-1)/\Delta$ vertices. Lemma 4.2, which is well-known, shows that every tree has such an edge. We include a proof for completeness.

Lemma 4.2. *Let T be a tree with maximum degree Δ_T. There is an edge whose removal splits T into T_1 and T_2 such that $|E(T_1)|$ and $|E(T_2)|$ are at least $|E(T)|/\Delta_T - 1$, and this is best possible.*

Proof. Pick an arbitrary vertex v_0 as the root of T. Define the sequence $v_0, v_1, \ldots, v_t$ as follows: for $i \ge 1$, v_i is a child of v_{i-1} whose subtree is largest, and t is the smallest index such that v_t has at most $\frac{\Delta_T - 1}{\Delta_T} |E(T)|$ vertices in its subtree. The edge e we desire is the edge between v_{t-1} and v_t. Let T_1 be the subtree with v_t and T_2 the other.

By definition, T minus the subtree of v_t has at least $\frac{1}{\Delta_T}|E(T)|$ edges, so by removing e, we see the condition for T_2 is satisfied. For T_1, we have two cases. First, assume $t = 1$. Then the subtree of v_0 that includes v_1 has at least $\frac{1}{\Delta_T}|E(T)|$ edges since it is biggest, and removing e yields the desired bound for T_1. Otherwise, we know that the subtree of v_{t-1} has more than $\frac{\Delta_T - 1}{\Delta_T}|E(T)|$ edges. Since the subtree of v_t is the largest of the at most $\Delta_T - 1$ subtrees of v_{t-1}, we again get our desired bound for T_1.

For $A \subseteq V$, let the *boundary* of A, denoted $\partial(A)$, be the set of edges with exactly one end in A.

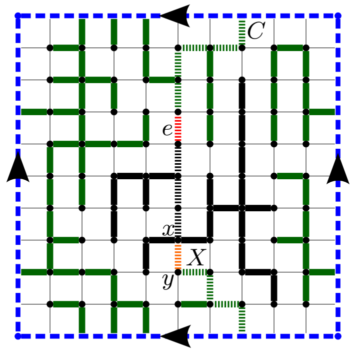
LEMMA 4.3. *Let T be a spanning tree of $G \in \{G_d(s), G_d^p(s)\}$ and let e be an edge that equitably divides T. Let A be the smaller component of $T-e$. Then there exists an $x \in A$ and an edge $xy \in \partial(A)$ such that the distance in G between x and the endpoints of e is at least $\lfloor s/6 \rfloor$.*

Proof. Recall $n = |V(G)|$. Since e equitably divides T, Lemma 4.2 yields $|A| \geq (n-1)/\Delta_T \geq (n-1)/\Delta = (n-1)/2d > n/3d$, as long as $n > 3$. On the other hand, since A is the smaller component of $T-e$, $|A| \leq n/2$. Let v be the endpoint of $e = uv$ contained in A. Consider the ball B_R of radius $R = \lfloor s/6 \rfloor$ in G centered at v (all vertices whose distance in G is at most R). We will show that there exists a vertex $x \in A \setminus B_R$ and an edge $xy \in \partial(A)$.

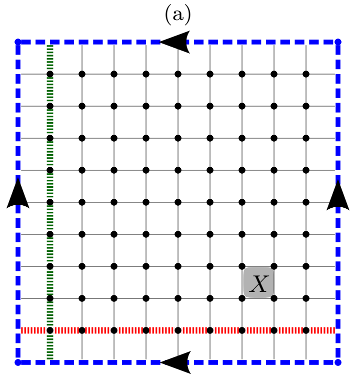
Since $G \in \{G_d(s), G_d^p(s)\}$, the ball B_R is contained in a hypercube H of side-length $2R$. Moreover, if $V(H)$ is the set of vertices of G inside of H, then $G \setminus V(H)$ is connected. Notice $|H| \leq n/3^d < n/(3d) < |A|$. This implies that there exists a vertex $x_1 \in A \setminus V(H)$. If $G \setminus V(H)$ were contained in A then $|A| \geq |G \setminus V(H)| \geq n - |H| > n - |A|$, and so $|A| > n/2$, a contradiction. Hence, there exists a vertex $y_1 \in (G \setminus V(H)) \setminus A$ and a path from x_1 to y_1 contained only in $G \setminus V(H)$. Somewhere along this path there must be an edge xy such that $x \in A \setminus V(H)$ and $y \in (G \setminus V(H)) \setminus A$. This is the edge we seek.

Figure 4a depicts a spanning tree T of $G_2^p(9)$ that is equitably divided into black (the set A) and green by the red edge e. The orange edge $xy \in \partial(A)$ creates a fundamental cycle $C = C_{xy}$, which is dashed. The 4-cycle X plays a role in the proof of Theorem 3.2, which appears next.

Proof of Theorem 3.2. Let $G \in \{G_d(s), G_d^p(s)\}$. By Theorem 3.1, it suffices to show that $\mathcal{B}$ contains a cycle C with $|C| = \Omega(s)$ and a 4-cycle X with $C \in \text{supp}(X)$. Let T be the spanning tree defining $\mathcal{B}$. By Lemma 4.2, T has an edge e such that the two components of $T-e$ each



(a)



(b) $\mathcal{B}_{\mathcal{F}}^p$

Figure 4

have at least $(n-1)/\Delta$ vertices. Let A be the smaller component of $T - e$. Every edge in $\partial(A) - e$ creates a fundamental cycle using the edge e. By Lemma 4.3, there exists an $x \in A$ and an edge $xy \in \partial(A)$ such that the distance in G between x and e is at least $\lfloor s/6 \rfloor$. Define $C = C_{xy}$. Then C has length at least $\lfloor s/6 \rfloor$ and contains e. The edge e is contained in a 4-cycle X, and $C \in \text{supp}(X)$ by Proposition 4.1. ☐

5 Short Cycle Bases of $G_2^p(s)$

Let H be a graph embedded in the torus. Recall that the dual of an embedded graph is a (multi-)graph such that the faces (respectively, faces sharing an edge) correspond to vertices (respectively, edges)—see, e.g. [19]. We denote the toroidal dual of H by H^*. If $F \subseteq E(H)$, denote by F^* the subset of $E(H^*)$ that corresponds to F. A cycle C in H is *contractible* if it bounds a disc. The subgraph of H embedded inside of this disc is called the *interior* of C, denoted $\text{int}(C)$, whereas the complement is the *exterior*, $\text{ext}(C)$. Noncontractible cycles do not have interiors. For more on topological graph theory, we refer the reader to [19].

In this section, we will only consider the graph $G_2^p(s)$, $s \geq 5$, embedded on the torus in the standard way (see Figure 1b), and hence refer to this graph simply as G. For a cycle basis $\mathcal{B}$ of G, let $\mathcal{N}$ be the set of elements of $\mathcal{B}$ that contain a noncontractible cycle as a subgraph, and let $\overline{\mathcal{N}} = \mathcal{B} \setminus \mathcal{N}$. Recall that any basis has size $m - n + 1$, where $m = |E(G)|$ and $n = |V(G)|$. Since $|E(G)| = 2n$ for the grid, we have $|\mathcal{N}| + |\overline{\mathcal{N}}| = |\mathcal{B}| = n + 1$. Define $S_{\mathcal{N}} = \{Y \in \mathcal{E} : \mathrm{supp}(Y) \cap \mathcal{N} \neq \emptyset\}$.

In Section 5.1, we show that although the size of $S_{\mathcal{N}}$ is large, $\pi'(S_{\mathcal{N}})$ is exponentially small. The remaining subgraphs are in bijection with spin configurations, as seen in Section 5.2. We then use ideas from the analysis of $\mathcal{M}_{\mathrm{GD}}$ to find a bottleneck which prevents $\mathcal{M}(\mathcal{B})$ from mixing rapidly.

5.1 $\mathcal{N}$ in support implies small weight We say that a cycle basis of G is *short* if its length is less than s (recall the definition of length from Section 3.2). The canonical example of a short cycle basis is the facial cycle basis $\mathcal{B}^p_{\mathcal{F}}$ of G, pictured in Figure 4b. It consists of two noncontractible s-cycles, one horizontal and the other vertical, and all-but-one of the facial 4-cycles. The 4-cycle X bounding the shaded face is not in $\mathcal{B}^p_{\mathcal{F}}$. Notice that $\mathrm{supp}_{\mathcal{B}^p_{\mathcal{F}}}(X)$ is all of the other facial 4-cycles. The two s-cycles do not count towards the length of $\mathcal{B}^p_{\mathcal{F}}$ because they are not in the support of any 4-cycle.

We start with a simple lemma.

LEMMA 5.1. *If $\mathcal{B}$ is a short cycle basis of G, then $|\mathcal{N}| = 2$.*

Proof. Noncontractible cycles on the torus have homotopy types, and can thus be seen as elements of the fundamental group of the torus, $\mathbb{Z} \times \mathbb{Z}$ [6, p. 34]. Since the $(1, 0)$ and $(0, 1)$ homotopy types cannot be generated by a single element of the group, and since each are even subgrpahs, $\mathcal{B}$ must have more than one element with a noncontractible cycle. Hence $|\mathcal{N}| \geq 2$.

Now let X be a 4-cycle in G. Since $\mathcal{B}$ is short, $\mathrm{supp}(X) \cap \mathcal{N} = \emptyset$. Therefore, all of the 4-cycles in G lie in the subspace generated by $\overline{\mathcal{N}}$. Since every set of $n - 1$ facial 4-cycles is linearly independent, it must be the case that $|\overline{\mathcal{N}}| \geq n - 1$. Hence, $|\mathcal{N}| \leq 2$. $\square$

Next, we show that if $Y \in \mathcal{E}$ satisfies $\mathrm{supp}(Y) \cap \mathcal{N} \neq \emptyset$ then the toroidal dual of Y is not bipartite.

LEMMA 5.2. *Let $\mathcal{B}$ be a short cycle basis of G and let $Y \in \mathcal{E}$. If Y^* is bipartite then* $\mathrm{supp}(Y) \cap \mathcal{N} = \emptyset$.

Proof. We can 2-color the vertices of Y^*, and hence the faces of the embedding of Y, with 1's and 0's so that any two faces of the embedding of Y that share an edge e have the same color if and only if $e \notin Y$. Let S be the set of 4-cycles in the interior of color-1 faces. Since $\mathrm{supp}(X) \cap \mathcal{N} = \emptyset$ for every $X \in S$ and $\mathrm{supp}(Y) = \bigcup_{X \in S} \mathrm{supp}(X)$, we find $\mathrm{supp}(Y) \cap \mathcal{N} = \emptyset$.

Before proceeding with the proof of the main result of this section, Lemma 5.4, we need a few simple propositions, the first of which is proven in [5]. A *bond* in G is a minimal edge-cut, and the size of a bond is the number of edges it contains.

PROPOSITION 5.1. *Every edge-cut is the disjoint union of bonds.*

PROPOSITION 5.2. *If $H \in \mathcal{E}$, then H has no odd-size bonds.*

Proof. By way of contradiction, let F be an odd-size bond in H and let H_1 and H_2 be the components of $H - F$. Since $|F|$ is odd, there are an odd number of vertices in $V(H_1)$ that are incident with an odd number of edges in F, say V_1. Since H is even, the set of odd-degree vertices in the graph induced by $V(H_1)$ is precisely V_1, contrary to the fact that graphs have an even number of vertices of odd degree.

LEMMA 5.3. *Let $H \in \mathcal{E}$. If H^* is nonbipartite, then H contains a noncontractible cycle.*

Proof. Let $F \subset E(H)$ be such that F^* is the edgeset of an odd-cycle C in H^*. Suppose first that F is a cutset in H. By Proposition 5.1, F is the disjoint union of bonds. One such bond must have odd size since $|F|$ is odd, contrary to Proposition 5.2. See Figure 5a.

So we may assume F is not a cutset in G. Thus, C is nonseparating, and hence noncontractible. Let $e = v_1v_2 \in F$. Since H has no loops, $v_1 \neq v_2$. Cut the torus along C, creating a cylinder with boundaries C_1 and C_2. Let $c_i = e \cap C_i$ for $i \in \{1, 2\}$. Since F is not a cutset, $H - F$ has a path P with ends v_1 and v_2. Extend this path to a simple path P' in the cylinder by adding the portions of e from v_1 to c_1 and from v_2 to c_2. Clearly, P' does not separate the cylinder. Hence $P' = P \cup e$ is a nonseparating cycle in the torus, and hence a noncontractible cycle in H. See Figure 5b.

We now combine the previous results to show that the total weight in π' of even subgraphs with noncontractible cycles in their basis representation is small.

LEMMA 5.4. *If $\lambda < 2^{-7}$ then $\pi'(S_{\mathcal{N}}) \leq 2^{-s/2+1}$.*

Proof. Let $Y \in S_{\mathcal{N}}$. By Lemma 5.2, the toroidal dual of Y is nonbipartite. By Lemma 5.3, Y contains a noncontractible cycle as a subgraph. As noncontractible cycles in G have length at least s, the proof of Lemma 4.1 implies the result.

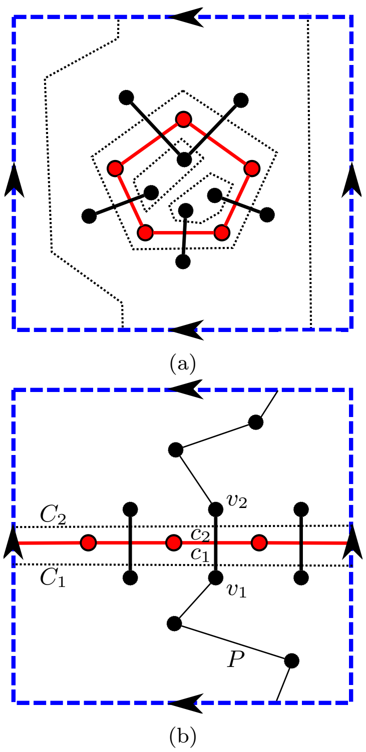


Figure 5: Cycle C is in red. The bold black edges are F.

5.2 Bottleneck among spin configurations Lemma 5.4 allows us to focus on even subgraphs whose support misses $\mathcal{N}$. Let $\mathcal{F}$ be the set of faces of G in the embedding depicted in Figure 1b, and define a bijection between these subgraphs and half of the spin configurations of G^* as follows. For any cycle basis $\mathcal{B}$ of G and any $Y \in \mathcal{E} \setminus S_{\mathcal{N}}$, define a spin configuration $\mathcal{I}_Y^{\mathcal{B}}$ of G^* by $\mathcal{I}_Y^{\mathcal{B}}(F) = (-1)^{q_Y^{\mathcal{B}}(F)}$ for each $F \in \mathcal{F}$, where $q_Y^{\mathcal{B}}(F)$ is the number of basis elements $B \in \mathrm{supp}(Y)$ such that F is a face of $\mathrm{int}(B)$. In other words, $\mathcal{I}_Y^{\mathcal{B}}$ assigns $+1$ or -1 to the faces of G, where the -1's generalize our previous notion of interior to subgraphs in $\mathcal{E} \setminus S_{\mathcal{N}}$. We choose the -1's instead of the $+1$'s to coincide with the plus boundary conditions on $G_2(s)$, as in Figure 2. For any edge e incident with faces $F_1, F_2 \in \mathcal{F}$, we have $\mathcal{I}_Y^{\mathcal{B}}(F_1) \neq \mathcal{I}_Y^{\mathcal{B}}(F_2)$ if and only if $e \in E(Y)$. Denote by $\mathbf{1}_{\mathcal{B}}(Y)$ the set of faces F of G with $\mathcal{I}_Y^{\mathcal{B}}(F) = 1$. Note, if C is a contractible cycle, $\mathbf{1}_{\mathcal{B}}(C)$ is either the faces of $\mathrm{ext}(C)$ or of $\mathrm{int}(C)$. For example, in $\mathcal{B}_{\mathcal{F}}^p$, $\mathbf{1}_{\mathcal{B}_{\mathcal{F}}^p}(X)$ is the faces of $\mathrm{ext}(X)$ for every 4-cycle $X \in \mathcal{B}_{\mathcal{F}}^p$, whereas $\mathbf{1}_{\mathcal{B}_{\mathcal{F}}^p}(X)$ is the faces of $\mathrm{int}(X)$ for the 4-cycle not in $\mathcal{B}_{\mathcal{F}}^p$.

The main idea of the proof of Theorem 3.3 is that $\mathcal{M}(\mathcal{B})$ cannot easily move between subgraphs Y with $|\mathbf{1}_{\mathcal{B}}(Y)|$ large and subgraphs with $|\mathbf{1}_{\mathcal{B}}(Y)|$ small—in order for $\mathcal{M}(\mathcal{B})$ to do so for a short basis $\mathcal{B}$, it must go through configurations with $|\mathbf{1}_{\mathcal{B}}(Y)| \approx n/2$. Given any constant $c > 0$, define $\mathcal{S}_c$ as the set of $Y \in \mathcal{E}$ such that $c \leq |\mathbf{1}_{\mathcal{B}}(Y)|/n \leq 1 - c$. The following theorem in [18] shows that these configurations are exponentially unlikely to appear.

Theorem 5.1. (MRS) *Given $c > 0$, let $\lambda < 5^{-3/(2c)}$. Then $\pi'(\mathcal{S}_c(G_2^p(s))) = 2^{-\Omega(s)}$.*

In order for Theorem 5.1 to imply that $\mathcal{M}(\mathcal{B})$ is slowly mixing, it must be the case that configurations Y with $|\mathbf{1}_{\mathcal{B}}(Y)|$ large and those with $|\mathbf{1}_{\mathcal{B}}(Y)|$ small are both fairly likely. To prove this, we identify in Lemma 5.5 a 4-cycle X such that symmetric difference with X is a bijection between these sets that nearly preserves weight.

Lemma 5.5. *For any cycle basis $\mathcal{B}$ of G, there exists a 4-cycle X for which $\mathbf{1}_{\mathcal{B}}(X) = \{F_X\}$, where $F_X \in \mathcal{F}$ is the face bounded by X.*

Proof. We proceed by induction on the number k of 4-cycles that are not in $\mathcal{B}$. As there is a linear dependency among $\mathcal{F}$, $k \geq 1$. When $k = 1$, $\mathcal{B}$ is precisely $\mathcal{B}_{\mathcal{F}}^p$, and the unique 4-cycle not in $\mathcal{B}$ satisfies the requirements of the lemma. So suppose $\mathcal{B}$ has exactly $k+1 \geq 2$ 4-cycles not in it.

Since there are at most $n-2$ 4-cycles in $\mathcal{B}$, there must be a 4-cycle $X_1 \notin \mathcal{B}$ such that $\mathrm{supp}(X_1)$ contains some $Y \in \mathcal{B}$ with $|E(Y)| > 4$. Let F_1 be the face bounded by X_1. If $\mathbf{1}_{\mathcal{B}}(X_1) = \{F_1\}$, then we are done. If not, it must be that $\mathbf{1}_{\mathcal{B}}(X_1) = \mathcal{F} - F_1$. Replace Y by X_1 in $\mathcal{B}$ to obtain a new basis $\mathcal{B}'$. By the inductive hypothesis, there exists a 4-cycle X_2 bounding the face F_2 for which $\mathbf{1}_{\mathcal{B}'}(X_2) = \{F_2\}$. We may assume that $X_1 \in \mathrm{supp}_{\mathcal{B}'}(X_2)$, since otherwise $\mathbf{1}_{\mathcal{B}'}(X_2) = \mathbf{1}_{\mathcal{B}}(X_2)$, and we are done.

Therefore, $\mathrm{supp}(X_1 \oplus X_2)$ is the same in both $\mathcal{B}$ and $\mathcal{B}'$, since it only uses basis cycles in $\mathcal{B} \cap \mathcal{B}'$. So for all $F \in \mathcal{F} \setminus \{F_1, F_2\}$, we have $\mathcal{I}_{X_1 \oplus X_2}^{\mathcal{B}}(F) = \mathcal{I}_{X_1 \oplus X_2}^{\mathcal{B}'}(F) = -1$. Since $\mathcal{I}_{X_1}^{\mathcal{B}}(F) = -1$ if and only if $F = F_1$, it must be that $\mathcal{I}_{X_2}^{\mathcal{B}}(F) = -1$ for all $F \in \mathcal{F} - F_2$, and so $\mathbf{1}_{\mathcal{B}}(X_2) = \{F_2\}$.

For example, the face F_X bounded by the 4-cycle X in $\mathcal{B}_{\mathcal{F}}^p$ depicted in Figure 4b meets the criterion of Lemma 5.5. This 4-cycle is special because, by taking the symmetric difference of $Y \in \mathcal{E}$ with X, all of the spins in the dual graph flip except for one (corresponding to F_X), and $\pi'(Y)$ does not differ significantly from $\pi'(Y \oplus X)$. Lemma 5.5 shows that this four-cycle is a property of the graph that cannot be overcome by changing the basis. We now proceed with the proof of Theorem 3.3.

Proof of Theorem 3.3. By Lemma 5.5, there exists a 4-cycle X for which $\mathbf{1}_{\mathcal{B}}(X) = \{F_X\}$, where F_X is the face bounded by X. For any even subgraph Y, define $N(Y)$ to be the number of faces $F \neq F_X$ of G such that $\mathcal{I}_Y^{\mathcal{B}}(F) = 1$. Let S_1 be the subset of $\mathcal{E} \setminus S_{\mathcal{N}}$ such that $N(Y) < n/2$ and let $S_2 = (\mathcal{E} \setminus S_{\mathcal{N}}) \setminus S_1$. Define the map $f : S_1 \to S_2$ by $f(Y) = Y \oplus X$. Then $\lambda^4 \leq \pi'(f(C))/\pi'(C) \leq \lambda^{-4}$. This implies $\lambda^4 \leq \pi'(S_1)/\pi'(S_2) \leq \lambda^{-4}$. By Lemma 5.4, $\pi'(S_{\mathcal{N}}) = 2^{-s/2+1}$. Therefore, $\pi'(S_1)$ and $\pi'(S_2)$ are each at least

$$\frac{\lambda^4}{(1+\lambda^4)}\left(1 - 2^{-s/2+1}\right) \geq \frac{\lambda^4}{2(1+\lambda^4)}. \tag{5.4}$$

Lastly, we show that $\sum_{Y \in S_1, Y' \in S_2} \pi'(Y)P(Y,Y')$ is small. Let (Y, Y') be such a transition with nonzero probability, where $Y' = Y \oplus B$ for some $B \in \mathcal{B}$. Since $\mathcal{B}$ is short, $|E(B)| \leq s$. Notice $s = \sqrt{n}$, since n is the number of vertices of the grid. This implies that B can change the number of spins by at most $n/16$, and so $n/2 > N(Y) \geq n/2 - n/16 = 7n/16$. Therefore $Y \in \mathcal{S}_{7/16}$. By Theorem 5.1, if $\lambda \leq .004 < 5^{-24/7}$, then $\pi'(\mathcal{S}_{7/16}) = 2^{-\Omega(s)}$. This implies $\sum_{Y \in S_1, Y' \in S_2} \pi'(Y)P(Y,Y') = 2^{-\Omega(s)}$. Then for each $i \in \{1, 2\}$,

$$\begin{aligned}
\phi_{S_i} &= \frac{1}{\pi'(S_i)} \sum_{Y \in S_1} \Big(\sum_{Y' \in S_{\mathcal{N}}} \pi'(Y)P(Y,Y') + \\
&\qquad + \sum_{Y' \in S_2} \pi'(Y)P(Y,Y') \Big) \\
&\leq \frac{1}{\pi'(S_i)} \left(\pi'(S_{\mathcal{N}}) + 2^{-\Omega(s)} \right) \\
&\leq \frac{2(1+\lambda^4)}{\lambda^4} \left(2^{-s/2+1} + 2^{-\Omega(s)} \right) \;=\; 2^{-\Omega(s)}.
\end{aligned}$$

The result now follows from Theorem 2.1. ☐

6 Conclusions and Future Work

Using insights from this paper, we may be able to modify $\mathcal{M}(\mathcal{B})$ slightly to yield much better algorithms, by adding additional transitions. In particular, each of our slow mixing results relies on the existence of a short cycle $X \notin \mathcal{B}$, which, if added to the set of allowable transitions, may create a rapidly mixing Markov chain. For example, adding the special 4-cycle to the set of allowable moves of $\mathcal{M}(\mathcal{B}^p_{\mathcal{F}})$ is similar to allowing $\mathcal{M}_{\text{GD}}$ to flip all spins at once. While this move is contrived in the context of spin configurations, adding this 4-cycle is natural in the context of cycle bases. We believe this new perspective of the state space as a vector space will be useful in designing and analyzing generalizations of these algorithms.

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