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IMPROVED MIXING BOUNDS FOR THE ANTI-FERROMAGNETIC POTTS MODEL ON $\mathbb{Z}^2$

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Abstract

We consider the anti-ferromagnetic Potts model on the the integer lattice $\mathbb{Z}^2$. The model has two parameters: q, the number of spins, and $\lambda = \exp(-\beta)$, where β is 'inverse temperature'. It is known that the model has strong spatial mixing if $q > 7$, or if $q = 7$ and $\lambda = 0$ or $\lambda > 1/8$, or if $q = 6$ and $\lambda = 0$ or $\lambda > 1/4$. The $\lambda = 0$ case corresponds to the model in which configurations are proper q-colourings of $\mathbb{Z}^2$. We show that the system has strong spatial mixing for $q \geqslant 6$ and any λ. This implies that Glauber dynamics is rapidly mixing (so there is a fully-polynomial randomised approximation scheme for the partition function), and also that there is a unique infinite-volume Gibbs state. We also show that strong spatial mixing occurs for a larger range of λ than was previously known for $q = 3$, $q = 4$ and $q = 5$.

1. *Introduction and statement of results*

1.1. *The anti-ferromagnetic Potts model*

We consider the anti-ferromagnetic Potts model on the integer lattice $\mathbb{Z}^2$. The set of spins is $Q = \{1, \ldots, q\}$. Configurations are assignments of spins to vertices, and $\Omega = Q^{\mathbb{Z}^2}$ is the set of all configurations. A region R is a (not necessarily connected) subset of vertices, and σ_R denotes the restriction of configuration σ to R. $\Omega_R = Q^R$ is the set of all such restrictions. If R is a finite region, then its vertex boundary, ∂R, is the set of vertices that are not in R, but are adjacent to R. A boundary configuration on ∂R is a function from ∂R to the set $\{0\} \cup Q$. The spin '0' corresponds to a 'free boundary' which does not influence the vertices in R. Let $E(R)$ denote the set of lattice edges that have at least one vertex in R. Given a region R and a boundary configuration $\mathcal{B}$ on ∂R, the energy of the configuration $\sigma_R \in \Omega_R$ is given by the Hamiltonian

$$H(\sigma) = \sum_{(i,j)\in E(R)} \beta\delta(\sigma_i, \sigma_j),$$

where $\beta \in \mathbb{R}$ is the 'inverse temperature' and

$$\delta(s, s') = \begin{cases} 1, & \text{if } s = s'; \\ 0, & \text{otherwise.} \end{cases}$$

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The *partition function* Z is equal to $\sum_{\sigma\in\Omega_R}\exp(-H(\sigma))$. The *finite-volume Gibbs measure* $\pi_{\mathcal{B}}$ is the distribution on Ω_R in which, for every $\sigma\in\Omega_R$, $\pi_{\mathcal{B}}(\sigma)=\exp(-H(\sigma))/Z$. If we let $\mathrm{mon}_\sigma(E(R))$ denote the number of monochromatic edges in $E(R)$ and take $\lambda=\exp(-\beta)$, it is apparent that $\pi_{\mathcal{B}}(\sigma)$ is proportional to $\lambda^{\mathrm{mon}_\sigma(E(R))}$.

In the zero-temperature case $\beta=\infty$, we have $\lambda=0$, and $\pi_{\mathcal{B}}$ is the uniform distribution on 'proper' colourings, which are configurations without monochromatic edges. In this paper we will focus on the situation in which the temperature is non-zero, so $\lambda\in(0,1]$.

For any $\Lambda\subseteq R$, $\pi_{\mathcal{B},\Lambda}$ denotes the distribution on configurations of Ω_Λ induced by $\pi_{\mathcal{B}}$.

1.2. *Strong spatial mixing*

If the parameters q and λ are chosen appropriately, then the anti-ferromagnetic Potts model has *strong spatial mixing*. Informally, this means that for any finite region R, if you consider two different boundary configurations $\mathcal{B}$ and $\mathcal{B}'$ on ∂R which differ at a single vertex y, then the effect that this difference has on a subset $\Lambda\subseteq R$ decays exponentially with the distance from Λ to y. The formal definition below is taken from [5] but has been adapted to the special case of the anti-ferromagnetic Potts model on $\mathbb{Z}^2$.

DEFINITION 1. The anti-ferromagnetic Potts model on $\mathbb{Z}^2$ has strong spatial mixing for parameters λ and q if there are constants η and $\eta'>0$ such that, for any non-empty finite region R, any $\Lambda\subseteq R$, any vertex $y\in\partial R$, and any pair of boundary configurations $(\mathcal{B},\mathcal{B}')$ of ∂R which differ only at y, we have

$$\mathrm{d_{TV}}(\pi_{\mathcal{B},\Lambda},\pi_{\mathcal{B}',\Lambda})\leqslant\eta|\Lambda|\exp(-\eta' d(y,\Lambda)),$$

where $d(y,\Lambda)$ is the lattice distance within R from the vertex y to the region Λ and $\mathrm{d_{TV}}$ denotes total variation distance.

We assume that y is not a free-boundary vertex in either configuration. That is, $\mathcal{B}_y\in Q$ and $\mathcal{B}'_y\in Q$.

Strong spatial mixing is an important property because of two, related, consequences. First, strong spatial mixing implies that there is a unique *infinite-volume Gibbs measure* on configurations in Ω. Qualitatively, there is one equilibrium, not many. Second, strong spatial mixing implies that *Glauber dynamics* can be used to efficiently sample configurations from π_B (for any finite region R and boundary configuration $\mathcal{B}$ on ∂R). We describe both of these consequences below, before stating our results.

1.3. *Uniqueness*

A measure μ on Ω is an infinite-volume *Gibbs measure* if, for any finite region R and any configuration σ, the conditional probability distribution $\mu(\cdot\mid\sigma_{\overline{R}})$ (conditioned on the configuration $\sigma_{\overline{R}}$ on all vertices other than those in R) is $\pi_{\sigma_{\partial R}}$. It is known that there is at least one infinite-volume Gibbs measure corresponding to any choice of the parameters q and λ. An important problem in statistical physics is determining for which parameters this is unique. Strong spatial mixing implies that there is a unique infinite-volume Gibbs measure [15, 19] with exponentially decaying correlations.

1.4. *Rapid mixing*

Suppose that R is a finite region of $\mathbb{Z}^2$, and that $\mathcal{B}$ is a boundary configuration on ∂R. We will consider the (heat-bath) Glauber dynamics for sampling from $\pi_{\mathcal{B}}$. This is a Markov chain $\mathcal{M}$ with state space Ω_R. A transition is made from a configuration $\sigma \in \Omega_R$ by choosing a vertex v uniformly at random from R, 'erasing' the spin at vertex v, and then choosing a new spin for vertex v from the conditional distribution, given $\sigma_{R-\{v\}}$ and $\mathcal{B}$. Here is a detailed description of the transition.

One step of the (heat-bath) Glauber dynamics Markov chain $\mathcal{M}$

1. Choose a vertex v uniformly at random from R.
2. For $i \in Q$, let n_i denote the number of neighbours of v which are assigned spin i (either in σ or in $\mathcal{B}$).
3. Choose a new spin c according to the distribution
$$\Pr(c = i) = \frac{\lambda^{n_i}}{\sum_{k \in Q} \lambda^{n_k}} \qquad \text{for } i \in Q.$$
4. Obtain the new configuration σ' from σ by assigning spin c to vertex v.

It is known (for example, see [5]) that $\mathcal{M}$ is ergodic, with unique stationary distribution $\pi_{\mathcal{B}}$. (It is easy to verify that $\mathcal{M}$ is ergodic for the positive temperature case $\lambda \in (0, 1]$ considered in this paper. Ergodicity is much more subtle in the zero-temperature case $\lambda = 0$. Here is an example that is not ergodic with $\lambda = 0$ and $q = 5$. The region R consists of two adjacent vertices u and v. The boundary configuration $\mathcal{B}$ assigns colours 3, 4 and 5 to the neighbours of u and the same colours to the neighbours of v. Now $\mathcal{M}$ is not ergodic since it cannot move between the configuration $(u, v) = (1, 2)$ and the configuration $(u, v) = (2, 1)$. However, the chain is ergodic if $q \geqslant 6$ (the maximum degree plus two), and it is ergodic if $q \geqslant 3$ if the boundary configuration is chosen appropriately (for example, the free boundary case). See, for example, the ergodicity proofs in [8, 14].)

It is also known that if the Potts model has strong spatial mixing (which is true for appropriate choices of q and λ, as we will see below) then $\mathcal{M}$ is rapidly mixing.

Before describing what is known about rapid mixing, we recall the definitions. Let P denote the transition matrix of $\mathcal{M}$, and let $P^t(\sigma, \sigma')$ be the t-step probability of moving from σ to σ'. For $\delta > 0$, the *mixing time* is defined as $\tau_{\mathcal{M}}(\delta) = \min\{t_0 : d_{tv}(P^t, \pi_{\mathcal{B}}) \leqslant \delta \text{ for all } t \geqslant t_0\}$. $\mathcal{M}$ is said to be *rapidly mixing* if $\tau_{\mathcal{M}}(\delta)$ is at most a polynomial in n and $\log(1/\delta)$, where n is the number of vertices in R.

It is well known that strong spatial mixing implies rapid mixing in our setting. The difficulty of the proof depends upon the precise bound on $\tau_{\mathcal{M}}(\delta)$ that is obtained. Dyer, Sinclair, Vigoda and Weitz give a nice simple combinatorial proof [5, Theorem 2.5] that strong spatial mixing implies that a certain 'heat-bath block dynamics' mixes in $O(n \log(n/\delta))$ time. Markov-chain comparison can now be applied in a standard way to show that Glauber dynamics mixes in $O(n(n + \log(1/\delta)))$ time (see, for example, [8, Section 7] or (for a slightly larger bound) [1]). In fact, it is known that strong spatial mixing implies $O(n \log(n/\delta))$ mixing of Glauber dynamics, giving a small improvement on the mixing-time bound. As is explained in [5], this can be proved using techniques from functional analysis [3, 15, 16, 18]. The idea is to bound the log-Sobolev constant of the block dynamics, and to translate this bound into a bound on the log-Sobolev constant of Glauber dynamics.

1.5. *Approximating the partition function*

We have seen in Section 1.4 that when the Potts model has strong spatial mixing, the Markov chain $\mathcal{M}$, which corresponds to heat-bath Glauber dynamics, is rapidly mixing. Thus, there is an efficient algorithm for sampling from the Gibbs distribution $\pi_{\mathcal{B}}$.

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Before stating our results in Section 1.6, we mention one consequence of rapid mixing. A *randomised approximation scheme* is an algorithm for approximately computing the value of a function f. The approximation scheme has a parameter $\varepsilon > 0$ which specifies the error tolerance. For concreteness, suppose that f is a function from Σ^* to $\mathbb{R}$. For example, for fixed values of q and λ, f might map an encoding of a region R and a boundary configuration $\mathcal{B}$ to the value of the partition function Z corresponding to R and $\mathcal{B}$. A *randomised approximation scheme* for f is a randomised algorithm that takes as input an instance $x \in \Sigma^*$ (for example, R and $\mathcal{B}$) and an error tolerance $\varepsilon > 0$, and outputs a number $z \in \mathbb{Q}$ (a random variable of the 'coin tosses' made by the algorithm) such that, for every instance x,

$$\Pr\left[\frac{f(x)}{1+\varepsilon} \leqslant z \leqslant (1+\varepsilon) f(x)\right] \geqslant \frac{3}{4}. \tag{1}$$

The randomised approximation scheme is said to be a *fully polynomial randomised approximation scheme*, or *FPRAS*, if it runs in time bounded by a polynomial in $|x|$ and ε^{-1}. Note that the quantity $\frac{3}{4}$ in Equation (1) could be changed to any value in the open interval $(\frac{1}{2}, 1)$ without changing the set of problems that have randomised approximation schemes.

Using ideas of Jerrum, Valiant and Vazirani [13], an efficient sampling algorithm for $\pi_{\mathcal{B}}$ can be turned into an FPRAS for the partition function. A straightforward proof is based on Dyer and Greenhill's extension [4] of [13].

In summary, if q and λ are chosen so that the Potts model has strong spatial mixing, then $\mathcal{M}$ is rapid mixing. This, in turn, gives an FPRAS for the partition function.

1.6. *Context and statement of results*

For $q = 2$ (see [15]) it is known that there is a critical point λ_c such that uniqueness (and strong spatial mixing) hold for $\lambda > \lambda_c$ but there are two Gibbs measures for $\lambda < \lambda_c$. (In one of these Gibbs measures, spin 1 is favoured at 'even-parity' vertices, and in the other, spin 2 is favoured.) The value of λ_c (see [17]) is $\lambda_c = \sqrt{2} - 1 \sim 0.41$.

Thus, we investigate the case $q > 2$. It is believed [17] that there is strong spatial mixing for every $\lambda \in (0, 1]$ for $q = 3$ and for every $\lambda \in [0, 1]$ for $q > 3$. The point $q = 3$, $\lambda = 0$ is excluded because, on physical grounds, this is believed to be a critical point. It is believed that at this point there is a unique infinite-volume Gibbs measure, but that the correlations only decay algebraically (for example, polynomially). Salas and Sokal used *Dobrushin uniqueness* to show that that strong spatial mixing occurs for every $\lambda \in [0, 1]$ for $q > 8$. As Jerrum points out [11, Section 5], Salas and Sokal's calculation applies whenever $q > 8(1 - \lambda)$, so it also applies to positive λ for smaller q. The result applies to a more general context than the one studied in this paper: it applies to the anti-ferromagnetic Potts model on any infinite graph. The generalised condition is $q > 2\Delta(1 - \lambda)$, where Δ is the maximum degree. Jerrum [11] considered the $\lambda = 0$ case and showed rapid mixing (in fact, $O(n \log(n/\delta))$ mixing) for Glauber dynamics when $q > 2\Delta$. (In fact, he considered a slightly different version of Glauber dynamics, but the difference is not important here.) Jerrum's result implies that of Salas and Sokal for $\lambda = 0$, since $O(n \log(n/\delta))$ mixing of Glauber dynamics implies strong spatial mixing [5, Theorem 2.3].

The results that we have just discussed give strong spatial mixing for $\lambda = 0$ and $q > 8$. In fact, better results are known for $\lambda = 0$. Salas and Sokal [17] used *decimation* to prove strong spatial mixing for $q \geqslant 7$. This is a machine-assisted proof. The $q = 7$ case is also implied by the work of Bubley, Dyer, Greenhill and Jerrum [2]. They gave a machine-assisted proof of $O(n \log(n/\delta))$ mixing for a block dynamics on 4-regular triangle-free graphs. As we

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mentioned above, this implies $O(n \log(n/\delta))$ mixing for Glauber dynamics, which, in turn, implies strong spatial mixing. A proof without machine assistance of strong spatial mixing for $q \geqslant 7$ is given by Goldberg, Martin and Paterson [8, Theorem 5]. Once again, the result applies more generally — in this case, to triangle-free graphs with maximum degree at most $\Delta \geqslant 3$ where $q > 1.76\Delta - 0.47$.

Achlioptas *et al*. [1] gave a machine-assisted proof of strong spatial mixing for $\lambda = 0$ and $q = 6$. Their method was to prove $O(n \log(n/\delta))$ mixing for a block dynamics, which implies spatial mixing as discussed above.

It is known that Glauber dynamics is rapidly mixing on rectangular regions when $q = 3$ and $\lambda = 0$. This is proved in the fixed-boundary case by Luby, Randall and Sinclair [14], and in the free-boundary case by Goldberg, Martin and Paterson [7]. The (polynomial) mixing-time bounds are not $O(n \log(n/\delta))$. Indeed, as mentioned above, it is not believed that strong spatial mixing holds for $\lambda = 0$ and $q = 3$.

The following proposition summarises the results that we have just discussed.

PROPOSITION 1. *Consider the anti-ferromagnetic Potts model on $\mathbb{Z}^2$ with parameters q and $\lambda \leqslant 1$. There is strong spatial mixing in the following cases.*

(i) $q \geqslant 8$ *and* $\lambda \geqslant 0$,

(ii) $q = 7$ *and* $\lambda = 0$ *or* $\lambda > 1/8 = 0.125$,

(iii) $q = 6$ *and* $\lambda = 0$ *or* $\lambda > 2/8 = 0.25$,

(iv) $q = 5$ *and* $\lambda > 3/8 = 0.375$,

(v) $q = 4$ *and* $\lambda > 4/8 = 0.5$, *and*

(vi) $q = 3$ *and* $\lambda > 5/8 = 0.625$.

Thus, in these cases, Glauber dynamics is rapidly mixing and there is a unique infinite-volume Gibbs measure.

The purpose of this work is to improve the results in Proposition 1. Our main objective was to extend the $q = 6$ and $q = 7$ results for $\lambda = 0$ to all temperatures. We state our results as two theorems, to separate the results that are proved without machine assistance (Theorem 2) from those that are proved with machine assistance. Theorem 3 subsumes Theorem 2.

THEOREM 2. *Consider the anti-ferromagnetic Potts model on $\mathbb{Z}^2$ with parameters q and $\lambda \leqslant 1$. There is strong spatial mixing in the following cases.*

(i) $q \geqslant 7$ *and* $\lambda \geqslant 0$,

(ii) $q = 6$ *and* $\lambda = 0$ *or* $\lambda > 1/7 \approx 0.1429$,

(iii) $q = 5$ *and* $\lambda > 2/7 \approx 0.2857$,

(iv) $q = 4$ *and* $\lambda > \frac{1}{2}(\sqrt{33} - 5) \approx 0.3723$, *and*

(v) $q = 3$ *and* $\lambda > \lambda_0$, *where* $\lambda_0 \approx 0.4735$ *is the real solution of* $\lambda^3 + 4\lambda - 2 = 0$.

Thus, in these cases, Glauber dynamics is rapidly mixing and there is a unique infinite-volume Gibbs measure.

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THEOREM 3. *Consider the anti-ferromagnetic Potts model on $\mathbb{Z}^2$ with parameters q and $\lambda \leqslant 1$. There is strong spatial mixing in the following cases.*

(i) $q \geqslant 6$ *and* $\lambda \geqslant 0$,

(ii) $q = 5$ *and* $\lambda \geqslant 0.127$,

(iii) $q = 4$ *and* $\lambda \geqslant 0.262$, *and*

(iv) $q = 3$ *and* $\lambda \geqslant 0.393$.

The bounds for $q = 5$, $q = 4$ and $q = 3$ can be further improved by more extensive machine calculation. These results will appear in the PhD thesis of one of the authors [10].

1.7. *The anti-ferromagnetic Potts model on general graphs*

In this paper we consider the anti-ferromagnetic Potts model on the integer lattice $\mathbb{Z}^2$. One reason for restricting attention to $\mathbb{Z}^2$ is that it is a natural lattice, of interest in statistical physics [15]. Another reason is that the model is known *not* to have good mixing properties on a general graph. As Welsh observes [20, 3.7.12], the partition function of the Potts model is a specialisation of the *Tutte polynomial* along the hyperbola $H_q = \{(x, y) : (x-1)(y-1) = q\}$. The *anti-ferromagnetic* Potts model (for real temperatures) corresponds to the additional constraint $0 \leqslant \lambda \leqslant 1$, which corresponds to a portion of the hyperbola in which $x - 1$ and $y - 1$ are negative. There is no FPRAS for the Tutte polynomial along this hyperbola unless NP = RP; see [20, 8.7.2].

Jerrum and Sinclair [12] considered the anti-ferromagnetic Ising model, which corresponds to the Potts model with $q = 2$. They used a reduction from MAXCUT (the problem of counting cut-sets of a specified size in a graph) to show that there is no FPRAS for the partition function unless NP=RP. Their proof applies for a particular value of λ, but the stretching and thickening technique of Jaeger, Vertigan and Welsh [9] can be used to show that there is no FPRAS for any fixed λ (see [6]). Welsh has shown that the same result holds for any $q \geqslant 3$; see [20, 8.7.2]. Thus, unless NP=RP, the anti-ferromagnetic model does not exhibit strong spatial mixing on a general graph. In this paper, we do not consider a general graph. Instead, we consider the integer lattice $\mathbb{Z}^2$.

2. *Recursive coupling*

2.1. *The recursive coupling tree*

The essence of proving strong spatial mixing lies in showing that, if you take an arbitrary region R and boundary configurations $\mathcal{B}$ and $\mathcal{B}'$ on ∂R that disagree on a single boundary vertex y, then there is a coupling of $\pi_{\mathcal{B}}$ and $\pi_{\mathcal{B}'}$ in which the probability of disagreement at a vertex decays exponentially with its distance from y. We will construct such a coupling using the recursive method of Goldberg, Martin and Paterson [8]. We start by describing the method.

Let R be a non-empty finite region. As in [8], we will find it convenient to work with the edge-boundary of R, rather than with the boundary ∂R of vertices surrounding R. Here is the notation that we will use. The *boundary* of the region R is the collection of edges that have exactly one endpoint in R. A *boundary configuration* B is a function from the set of edges in the boundary to the set $\{0\} \cup Q$. Given a configuration $\sigma \in \Omega_R$, the quantity $\text{mon}_\sigma(E(R))$ is the number of monochromatic edges in $E(R)$, where a boundary edge is said to be 'monochromatic' if its spin is the same as the spin that is assigned by σ to

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its endpoint. π_B is the Gibbs distribution in which the probability of σ is proportional to $\lambda^{\mathrm{mon}_\sigma(E(R))}$. We will be interested in studying how much π_B varies when we change the spin of a single edge of B. This small change to the boundary is formalised by the following notation.

DEFINITION 2. A *boundary pair* X consists of

- a non-empty finite region R_X,
- a distinguished boundary edge $s_X = (w_X, f_X)$ with $f_X \in R_X$, and
- a pair (B_X, B'_X) of boundary configurations which differ only on the edge s_X.

We require

- $B_X(s_X) \in Q$, and
- $B'_X(s_X) \in Q$, and
- any two perpendicular boundary edges that share a vertex $f \in \partial R_X$ have the same spin in at least one of the two configurations B_X and B'_X.

(Note that in the paper [8], this was referred to as a 'relevant boundary pair'. The reason for the terminology is that paper [8] also used the notion of a boundary pair in which the final condition above (the one about perpendicular boundary edges) is dropped. Note also that this condition depends upon the geometry of the lattice. In this paper we always work on the lattice $\mathbb{Z}^2$, and we always include all the conditions listed above, so we drop the word 'relevant' to simplify the terminology.)

A *coupling* Ψ of π_{B_X} and $\pi_{B'_X}$ is a distribution on $\Omega_{R_X} \times \Omega_{R_X}$ which has marginal distributions π_{B_X} and $\pi_{B'_X}$. For such a coupling Ψ, we define $1_{\Psi,f}$ to be the indicator random variable for the event that, when a pair of configurations is drawn from Ψ, the spin of f differs in these two configurations. For any boundary pair X we define Ψ_X to be some coupling of π_{B_X} and $\pi_{B'_X}$ minimizing $\mathbb{E}[1_{\Psi,f_X}]$. For every pair of spins c and c', let $p_X(c, c')$ be the probability that, when a pair of configurations (C, C') is drawn from Ψ_X, f_X has spin c in C and spin c' in C'.

We define a labelled tree T_X associated with each boundary pair X. We will use the tree to obtain an upper bound on the expected number of disagreements at any distance from w_X in a coupling of π_{B_X} and $\pi_{B'_X}$.

The tree T_X is constructed as follows. Start with a vertex r which will be the root of T_X. For every pair of spins $c \in Q$ and $c' \in Q$, $c \neq c'$, add an edge labelled $(p_X(c, c'), f_X)$ from r to a new node $r_{c,c'}$. If f_X has no neighbours in R_X, then $r_{c,c'}$ is a leaf. Otherwise, for some $k \in \{1, 2, 3\}$, let $e_1, \ldots, e_k$ be the edges from f_X to nodes in R_X. If $k = 3$, order these edges so that e_1 and e_3 are not perpendicular. For each $i \in \{1, \ldots, k\}$, let $X_i(c, c')$ be the boundary pair consisting of

- the region $R_X - f_X$;
- the distinguished edge e_i;
- the boundary configuration B of $R_X - f_X$ that
  - agrees with B_X on common edges,
  - assigns spin c' to $e_1, \ldots, e_{i-1}$, and
  - assigns spin c to $e_i, \ldots, e_k$; and
- the boundary configuration B' that agrees with B except that it assigns spin c' to e_i.

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Recursively construct $T_{X_i(c,c')}$, the tree corresponding to boundary pair $X_i(c, c')$. Add an edge with label $(1, \cdot)$ from $r_{c,c'}$ to the root of $T_{X_i(c,c')}$. That completes the construction of T_X.

We say that an edge e of T_X is *degenerate* if the second component of its label is '$\cdot$'. For edges e and e' of T_X, we write $e \to e'$ to denote the fact that e is an ancestor of e'. That is, either $e = e'$, or e is a proper ancestor of e'. Define the *level* of edge e to be the number of non-degenerate edges on the path from the root down to, and including, e. Suppose that e is an edge of T_X with label (p, f). We say that the *weight* $w(e)$ of edge e is p. Also the *name* $n(e)$ of edge e is f. The *likelihood* $\ell(e)$ of e is $\prod_{e':e'\to e} w(e)$. The *cost* $\gamma(f, T_X)$ of a vertex f in T_X is $\sum_{e:n(e)=f} \ell(e)$. For any $d \geqslant 1$, let $E_d(X)$ denote the set of level-d edges in T_X. Let $\Gamma_d(X) = \sum_{e\in E_d(X)} \ell(e)$. We use the following lemma, from [8].

Lemma 4 (*see* [8]). *Consider the anti-ferromagnetic Potts model on $\mathbb{Z}^2$ with parameters q and λ. Suppose that there is an $\varepsilon > 0$ such that, for every boundary pair X and every $d \geqslant 1$, we have $\Gamma_d(X) \leqslant (1-\varepsilon)^d$. Then the system has strong spatial mixing.*

Proof. The relevance of T_X for providing an upper bound on the quality of the coupling is established in [8, Lemma 12], which shows that there is a coupling Ψ of π_{B_X} and $\pi_{B'_X}$ such that, for all $f \in R_X$, $\mathbb{E}[1_{\Psi,f}] \leqslant \gamma(f, T_X)$ which is at most $\sum_{d\geqslant d(f,s_X)} \Gamma_d(X)$, where $d(f, s_X)$ is the lattice distance from f to s_X. (Thus, $d(f_X, s_X) = 1$ and if $f \in R_X$ is adjacent to f_X then $d(f, s_X) = 2$, and so on.) Following the proof of [8, Lemma 33], we find that

$$\mathbb{E}[1_{\Psi,f}] \leqslant \frac{1}{\varepsilon}(1-\varepsilon)^{d(f,s_X)}$$

and

$$\sum_{f\in R_X} \mathbb{E}[1_{\Psi,f}] \leqslant \frac{1-\varepsilon}{\varepsilon}.$$

Following the proof of [8, Lemma 34], we obtain similar conclusions, assuming that we start with a pair of boundary configurations on the boundary ∂R of *vertices* surrounding R, such that the pair differs only on a particular vertex v_X. In particular, there is a coupling Ψ such that

$$\mathbb{E}[1_{\Psi,f}] \leqslant \frac{6}{\varepsilon(1-\varepsilon)}(1-\varepsilon)^{d(f,v_X)}$$

and

$$\sum_{f\in R_X} \mathbb{E}[1_{\Psi,f}] \leqslant \frac{6}{\varepsilon}.$$

This implies strong spatial mixing [8, Corollary 21]. □

2.2. *Bounding the cost of level-d edges in the recursive coupling tree*

A key ingredient from the construction of T_X which affects $\gamma(f, T_X)$ is the quantity $\mathbb{E}[1_{\Psi_X, f_X}]$, which we denote $\nu(X)$. Thus, $\nu(X) = \min_\Psi \mathbb{E}[1_{\Psi,f_X}]$, where the minimum is over all couplings Ψ of π_{B_X} and $\pi_{B'_X}$.

In order to get good upper bounds on $\nu(X)$, Goldberg, Martin and Paterson [8] observed that $\nu(X)$ can be upper-bounded in terms of corresponding values for boundary pairs with smaller regions. They used the following lemma.

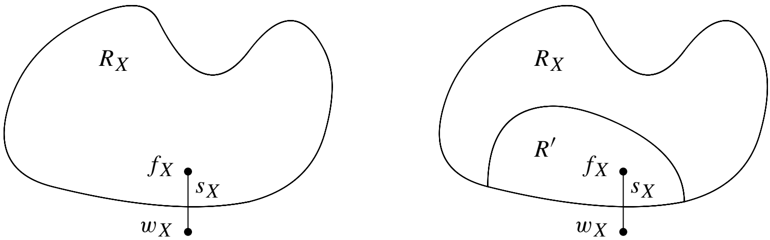
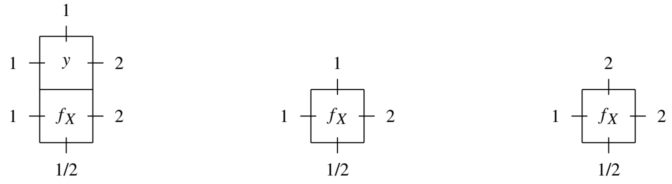


Figure 1: The application of Lemma 5.

LEMMA 5 (*see* [8]). *Suppose that* $\lambda = 0$. *Suppose that* X *is a boundary pair. Let* R' *be any subset of* R_X *which includes* f_X. *Let* χ *be the set of boundary pairs* $X' = (R_{X'}, s_{X'}, B_{X'}, B'_{X'})$ *such that* $R_{X'} = R'$, $s_{X'} = s_X$, $B_{X'}$ *agrees with* B_X *on common edges, and* $B'_{X'}$ *agrees with* B'_X *on common edges. Then* $\nu(X) \leqslant \max_{X' \in \chi} \nu(X')$.

Figure 1 is an illustration of how Lemma 5 is used to find an upper bound on $\nu(X)$. The basic idea is to pick a small subregion R' that contains the vertex f_X. Compute the maximum value of ν for that subregion, where we maximise over boundary configurations of R' that agree with the boundary configurations of R_X on the common overlap of these boundaries. This maximum value is an upper bound for $\nu(X)$.

An interesting feature of the positive-temperature Potts model is that this approach does not work. In particular, Lemma 5 does not apply to positive λ. For example, suppose that $q = 2$ and $\lambda = 1/2$. Consider a region R_X containing f_X and one of its neighbours, y, as illustrated below. (In this diagram and all subsequent diagrams we will denote vertices as squares, so that we have space to label them.) In the diagram, s_X is the edge between f_X and its lower neighbour (which is not pictured). The edge s_X is assigned spins 1 and 2 by the two boundary configurations B_X and B'_X. The rest of the boundary configurations are as shown (assigning spins 1, 1, 1, 2 and 2 clockwise around the picture). A calculation shows that $\nu(X) = 30/91$. However, if R' is chosen to be the region containing f_X only, then the corresponding boundary pairs X' (depicted to the right) both have $\nu(X') = 30/100 < 30/91$.



$\nu(X) = 30/91$ $\nu(X') = 30/100$ $\nu(X') = 30/100$

Our approach is to find an upper bound, $\mu(X)$, for $\nu(X)$ such that $\mu(X)$ can be upper-bounded using smaller regions along the lines of Lemma 5. Let X be a boundary pair. Recall that $E(R_X)$ is the set of lattice edges with at least one endpoint in R_X. For any subset $E \subseteq E(R_X) - \{s_X\}$ and any configuration $\sigma \in \Omega_{R_X}$, let $\text{mon}_\sigma(E)$ denote the number of monochromatic edges in E, where a boundary edge is considered to be monochromatic if its spin in B_X is the same as the spin assigned by σ to its endpoint. For $i \in Q$, let Ω_i be the set of configurations in Ω_{R_X} that assign spin i to vertex f_X. Let c_i be the total weight

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of these configurations, ignoring edge s_X:

$$c_i = \sum_{\sigma \in \Omega_i} \lambda^{\text{mon}_\sigma(E(R_X)-\{s_X\})}.$$

Let C contain the two spins assigned to s_X by the boundary configurations. That is, $C = \{B_X(s_X), B'_X(s_X)\}$, and let $c = \sum_{i \notin C} c_i$. We now define

$$\mu(X) = \max_{i \in C} \frac{(1-\lambda)c_i}{(1+\lambda)c_i + c}.$$

Lemma 6 below enables us to use $\mu(X)$ to find upper bounds for $\nu(X)$. The intuition behind the lemma is best understood from equations (2) and (3). Informally, (2) says that the disagreement probability $\nu(X)$ is at most the difference between the probability of seeing a certain colour in one distribution (with one boundary configuration) and the probability of seeing the same colour in the other distribution. A little manipulation gives equation (3), which shows that this quantity is at most $\mu(X)$. The remainder of the argument shows that $\mu(X)$ can be upper bounded using smaller regions.

(To see that it is plausible that $\mu(X)$ can be upper bounded using smaller regions, consider the boundary configuration B which is the same as the boundary configurations in X except that $B(s_X) = 0$, so s_X is a free boundary edge. Note that in the expression

$$\frac{(1-\lambda)c_i}{(1+\lambda)c_i + c} = \frac{1-\lambda}{1+\lambda+c/c_i},$$

from the definition of $\mu(X)$, c/c_i is the ratio of $\Pr_{\pi_B}(f_X \notin C)$ to $\Pr_{\pi_B}(f_X = i)$. By convexity, this ratio can be bounded by considering smaller regions (see the proof for details). Of course, the convexity argument allows some flexibility in the exact definition of $\mu(X)$ and the best thing is to define $\mu(X)$ so that it is as small as possible, subject to the constraint $\nu(X) \leqslant \mu(X)$.)

Lemma 6. *Suppose that X is a boundary pair. Let R' be any subset of R_X which includes f_X. Let χ be the set of boundary pairs $X' = (R_{X'}, s_{X'}, B_{X'}, B'_{X'})$ such that $R_{X'} = R'$, $s_{X'} = s_X$, $B_{X'}$ agrees with B_X on common edges, and $B'_{X'}$ agrees with B'_X on common edges. Then $\nu(X) \leqslant \max_{X' \in \chi} \mu(X')$.*

Proof. Without loss of generality (to simplify the notation), suppose that $B_X(s_X) = 1$, $B'_X(s_X) = 2$, and $c_1 \geqslant c_2$. We will show that

(i) $\nu(X) \leqslant \mu(X)$ and

(ii) $\mu(X) \leqslant \max_{X' \in \chi} \mu(X')$.

First, we show (i). Note that

$$\Pr_{\pi_{B_X}}(f_X = i) = \begin{cases} \dfrac{\lambda c_1}{\lambda c_1 + c_2 + c}, & i = 1; \\ \dfrac{c_i}{\lambda c_1 + c_2 + c}, & 2 \leqslant i \leqslant q, \end{cases}$$

$$\Pr_{\pi_{B'_X}}(f_X = i) = \begin{cases} \dfrac{\lambda c_2}{c_1 + \lambda c_2 + c}, & i = 2; \\ \dfrac{c_i}{c_1 + \lambda c_2 + c}, & i = 1, 3 \leqslant i \leqslant q. \end{cases}$$

Since $c_1 \geqslant c_2$ and $\lambda \leqslant 1$, the denominator in the expression for $\Pr_{\pi_{B'_X}}(f_X = i)$exceeds the denominator in $\Pr_{\pi_{B_X}}(f_X = i)$, so we can couple π_{B_X} and $\pi_{B'_X}$ in such a way that disagreement at f_X occurs only when the sample from $\pi_{B'_X}$ assigns spin 1 to f_X. Thus,

$$\begin{aligned}\nu(X) &\leqslant \Pr_{\pi_{B'_X}}(f_X = 1) - \Pr_{\pi_{B_X}}(f_X = 1) &(2)\\ &= \frac{c_1}{c_1 + \lambda c_2 + c} - \frac{\lambda c_1}{\lambda c_1 + c_2 + c}\\ &= \frac{c_1(1-\lambda)(c_2 + \lambda c_2 + c)}{(c_2 + \lambda c_1 + c)(c_1 + \lambda c_2 + c)}\\ &\leqslant \frac{(1-\lambda)c_1}{(1+\lambda)c_1 + c} \leqslant \mu(X). &(3)\end{aligned}$$

For part (ii), let $W = R_X - R'$. For $i \in Q$ and $\rho \in \Omega_W$, let $\Omega_{i,\rho}$ be the set of configurations $\sigma \in \Omega_{R_X}$ with $\sigma_{f_X} = i$ and $\sigma_W = \rho$. Let

$$c_{i,\rho} = \sum_{\sigma \in \Omega_{i,\rho}} \lambda^{\mathrm{mon}_\sigma(E(R_X) - \{s_X\})},$$

let $\hat{c}_\rho = \max(c_{1,\rho}, c_{2,\rho})$, and let $c_\rho = \sum_{i=3}^{q} c_{i,\rho}$. Then

$$\begin{aligned}\mu(X) &= \max\left(\frac{(1-\lambda)c_1}{(1+\lambda)c_1 + c}, \frac{(1-\lambda)c_2}{(1+\lambda)c_2 + c}\right)\\ &= \frac{1-\lambda}{1+\lambda+c/c_1} = \frac{1-\lambda}{1+\lambda+\left(\sum_{\rho\in\Omega_W} c_\rho\right)/\left(\sum_{\rho\in\Omega_W} c_{1,\rho}\right)}\\ &\leqslant \frac{1-\lambda}{1+\lambda+\left(\sum_{\rho\in\Omega_W} c_\rho\right)/\left(\sum_{\rho\in\Omega_W} \hat{c}_\rho\right)}\\ &= \frac{(1-\lambda)\sum_{\rho\in\Omega_W}\hat{c}_\rho}{(1+\lambda)\sum_{\rho\in\Omega_W}\hat{c}_\rho + \sum_{\rho\in\Omega_W} c_\rho} = \frac{\sum_{\rho\in\Omega_W}(1-\lambda)\hat{c}_\rho}{\sum_{\rho\in\Omega_W}((1+\lambda)\hat{c}_\rho + c_\rho)}\\ &\leqslant \max_{\rho\in\Omega_W} \frac{(1-\lambda)\hat{c}_\rho}{(1+\lambda)\hat{c}_\rho + c_\rho}\\ &= \max_{\rho\in\Omega_W}\left(\max\left(\frac{(1-\lambda)c_{1,\rho}}{(1+\lambda)c_{1,\rho} + c_\rho}, \frac{(1-\lambda)c_{2,\rho}}{(1+\lambda)c_{2,\rho} + c_\rho}\right)\right)\\ &= \max_{\rho\in\Omega_W} \mu(X'),\end{aligned}$$

where X' is the boundary pair in χ in which $B_{X'}$ and $B'_{X'}$ are induced by ρ. Note that X' is a boundary pair — in particular, it satisfies the condition about perpendicular edges. The last step follows from the observation that $c_{1,\rho}$, $c_{2,\rho}$ and c_ρ all contain the factor $\lambda^{\mathrm{mon}_\sigma(E(R_X) - E(R_{X'}))}$, which is constant for a fixed ρ, and can be cancelled out to obtain $\mu(X')$. □

3. *Proof of Theorem 2*

We start with a lemma, which we will use to obtain upper bounds on $\mu(X)$. The intuition behind the lemma is that if R_X is the region consisting of a single node f_X, then $\mu(X)$ is maximised by avoiding the colours of s_X in the rest of the boundary and otherwise spreading colours evenly over the boundary.

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LEMMA 7. *Suppose that X is a boundary pair in which R_X consists of a node f_X only. Let $v = 3 \mod (q-2)$ and $u = \lfloor 3/(q-2) \rfloor$. (So $u(q-2)+v = 3$.) Then*

$$\mu(X) \leqslant \frac{1-\lambda}{1+\lambda+v\lambda^{u+1}+(q-2-v)\lambda^{u}}.$$

In particular, if $q \geqslant 5$, then

$$\mu(X) \leqslant \frac{1-\lambda}{q-4(1-\lambda)}.$$

Proof. Without loss of generality, suppose that $B_X(s_X) = 1$, $B'_X(s_X) = 2$, and $c_1 \geqslant c_2$. Let $E = E(R_X) - s_X$, noting that $|E| \leqslant 3$. Let n_i be the number of edges in E that are assigned spin i by B_X. Note that $c_i = \lambda^{n_i}$, so the constraint $c_1 \geqslant c_2$ just says that $n_2 \geqslant n_1$.

Now we wish to choose B_X in order to maximise $\mu(X)$, or, equivalently, to minimise

$$Z = \frac{c}{(1-\lambda)c_1}.$$

First note that $n_1 = 0$ since Z can be reduced by recolouring edges coloured 1 with colour 2. Thus $c_1 = 1$.

Now we want to set $n_2, \ldots, n_q$ in order to minimise $c = \lambda^{n_3} + \ldots + \lambda^{n_q}$, where $n_3 + \ldots + n_q \leqslant 3$. Since $\lambda \leqslant 1$, we want to take $n_3 + \ldots + n_q = 3$.

Next, note that there is an optimal solution in which all n_j and n_k are within 1 of each other. To see this, consider a solution with $n_j > n_k + 1$. The boundary obtained by reassigning one of the j edges with spin k has a c-value which is at least as small, since the new c-value minus the old one is

$$-\lambda^{n_j} - \lambda^{n_k} + \lambda^{n_j-1} + \lambda^{n_k+1} = (1-\lambda)(\lambda^{n_j-1} - \lambda^{n_k}) \leqslant 0.$$

So the optimum value of c is $v\lambda^{u+1} + (q-2-v)\lambda^{u}$, which gives the first part of the lemma.

To derive the bound for $q \geqslant 5$, note that for $q \geqslant 6$ we have $u = 0$ and $v = 3$. For $q = 5$ we have $u = 1$ and $v = 0$. Both of these give the same bound. □

We now turn to the proof of Theorem 2. The cases $(q > 7)$, $(q = 7, \lambda = 0)$ and $(q = 6, \lambda = 0)$ follow from previous work (see Proposition 1). For each of the remaining cases we will use Lemma 7 to show that if X is a size-1 boundary pair, then $\mu(X) < 1/3$. This implies by Lemma 6 that every boundary pair X satisfies $\nu(X) < 1/3$ and there is an $\varepsilon > 0$ such that every boundary pair X satisfies

$$\nu(X) \leqslant (1-\varepsilon)\frac{1}{3}.$$

By induction on d (see [8, Lemma 18]), we get $\Gamma_d(X) \leqslant (1-\varepsilon)^d$. Hence, by Lemma 4 we have strong spatial mixing (and the theorem is proved).

We now consider the remaining cases. The second part of Lemma 7 applies for $q \geqslant 5$ where $q - 4(1-\lambda) > 3(1-\lambda)$; that is, $\lambda > 1 - q/7$. This finishes the cases with $q \geqslant 5$.

For $q = 4$ we use the first part of Lemma 7 with $u = 1$ and $v = 1$, and for $q = 3$ we use the first part of Lemma 7 with $u = 3$ and $v = 0$.

REMARK 1. Lemma 7 applies to the Potts model in a more general setting than the one considered in this paper. In particular, it applies to the Potts model on a general graph with maximum degree Δ. In the generalised version, the '3' in the definition of v and u becomes '$\Delta - 1$'. The final part of the lemma applies when $q \geqslant \Delta + 1$. It gives

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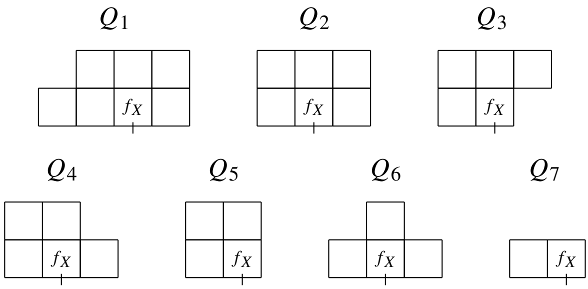
$\mu(X) \leqslant (1-\lambda)/(q-\Delta(1-\lambda))$, so, for example, we get the following result, which is slightly better than the condition derived by Salas and Sokal and discussed in Section 1.6.

THEOREM 8. *Consider the anti-ferromagnetic Potts model on a graph G with maximum degree Δ with parameters q and $\lambda \leqslant 1$. There is strong spatial mixing if $q > (1-\lambda)(2\Delta-1)$.*

4. *Proof of Theorem 3 for $q = 6$ and positive λ*

We will prove strong spatial mixing for $q = 6$ and $\lambda > 0$ by showing that there is an $\varepsilon > 0$ such that, for every boundary pair X and every $d \geqslant 1$, $\Gamma_d(X) \leqslant (1-\varepsilon)^d$. Then we apply Lemma 4. Following Goldberg, Martin and Paterson [**8**], we will consider the geometry of the lattice to derive a system of recurrences whose solution gives the desired bound. (The same proof technique applies to the $\lambda = 0$ case. However, we exclude $\lambda = 0$ because the result is already known [**1**], and excluding $\lambda = 0$ simplifies our presentation.)

We start by considering some particular boundary pairs. In particular, we will be interested in a boundary pair X such that R_X is one of the seven regions Q_1, Q_2, Q_3, Q_4, Q_5, Q_6, and Q_7 depicted below. As before, we denote vertices as squares in the diagrams and s_X is the edge between f_X and its lower neighbour. This edge is marked with a short line segment.



LEMMA 9. *Suppose that $q = 6$ and $\lambda \in (0, 1]$. Let $p_1 = 41/118$, $p_2 = 179/501$, $p_3 = 79/216$, $p_4 = 75/202$, $p_5 = 49/129$, $p_6 = 27/71$ and $p_7 = 3/7$. Define $q_i = p_i + \delta$ for $i \in \{1, \ldots, 7\}$ where $\delta = 1/1000$. Suppose that X is a boundary pair with region $R_X = Q_i$ above. Then $\mu(X) \leqslant q_i$.*

Proof. The lemma is proved by computation. For each region Q_i we have considered every boundary pair X which has $R_X = Q_i$. Each such boundary pair consists of a pair (B_X, B'_X) of boundary configurations which differ only on the edge s_X, obeying the requirements in Definition 2. For each such boundary pair, we calculated a rational function in λ, $\mu_X(\lambda)$, which gives an upper bound on $\mu(X)$ for any particular value of λ. The polynomials in the numerator and denominator of $\mu_X(\lambda)$ have integer coefficients. In order to find an upper bound on $\mu_X(\lambda)$ for $\lambda \in (0, 1]$, we partitioned the interval $[0, 1]$ into smaller intervals $[a, b]$. We then computed an upper bound for $\mu_X(\lambda)$ for $\lambda \in [a, b]$ by taking $\lambda = a$ for negative terms in the numerator and $\lambda = b$ for positive terms in the numerator. All terms in the denominator are positive, so we use $\lambda = a$. This computation was carried out exactly, with no approximations. Working through all the boundary pairs X and an appropriate collection of intervals $[a, b]$, we established the upper bounds given in the lemma. $\square$

REMARK 2. The value p_i defined in the statement of Lemma 9 is defined by

$$p_i = \max_{X : R_X = Q_i} \mu_X(0).$$

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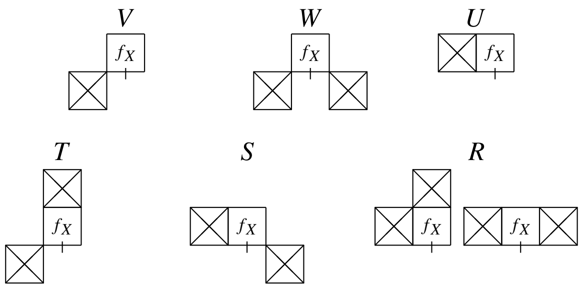
$\mu_X(\lambda)$ is in general not monotonic in λ. A simple non-monotonic example is the boundary pair consisting of a size-1 region with boundary $1, 2, 2$ where s_X is assigned spins 1 and 2. For this boundary pair, $c_1 = \lambda$, $c_2 = \lambda^2$ and $c_3 = c_4 = c_5 = c_6 = 1$, so

$$\mu_X(\lambda) = \frac{(1-\lambda)c_1}{(1+\lambda)c_1 + c} = \frac{(1-\lambda)\lambda}{(1+\lambda)\lambda + 4}.$$

Nevertheless, $\max_{X:R_X=Q_i} \mu_X(\lambda)$ seems to be monotonically decreasing in λ.

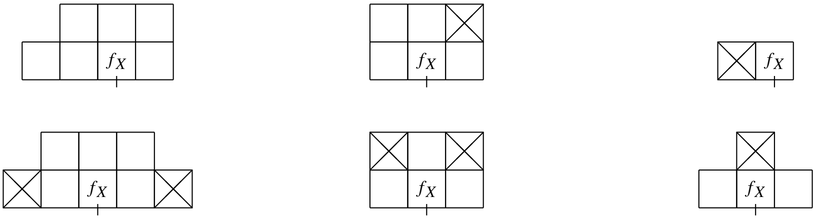
We now define some sets V, W, U, T, S, R of boundary pairs X. The sets depend only on the region R_X and the edge s_X, but not on the boundary configurations B_X and B'_X. The following diagram illustrates the sets.



A crossed-out square represents a vertex that is *not* in the region R_X. Squares that are not drawn represent vertices that are either in, or not in, the region R_X. As before, the edge s_X is marked with a short line segment. The diagrams may be rotated according to the symmetries of $\mathbb{Z}^2$. For example, a boundary pair X belongs to the set R if at least two of the neighbours of f_X are not in R_X. A boundary pair X belongs to the set U if the left or right neighbour of f_X (or both) is not in R_X. Obviously, these sets are not disjoint.

We will now define some recurrences. Let Γ_d denote the maximum, over boundary pairs X, of $\Gamma_d(X)$. Let V_d denote the maximum of $\Gamma_d(X)$ over boundary pairs $X \in V$; we use similar notation for the other sets.

Consider a boundary pair X. We will consider six cases below. Every boundary pair is covered by exactly one of the cases (up to symmetry). In the diagrams, an empty square represents a vertex in the region R_X. As before, a crossed-out square represents a vertex not in R_X, and all other vertices can be either in R_X or not in R_X.



To see that the cases cover all boundary pairs, note the that the left-most four diagrams cover all the cases in which all three neighbours of f_X are present. The lower central diagram applies if neither of the diagonal vertices is present in R_X. The diagram above that applies if just one of the diagonal vertices is present. The two diagrams to the left apply if both of the diagonal vertices are present.

We now add an inequality below each diagram, giving an upper bound on $\Gamma_d(X)$ for $d \geqslant 2$ when X is a boundary pair covered by the corresponding case. The inequality arises

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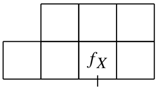
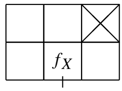
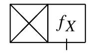
by considering the boundary pairs corresponding to the children of X in the tree T_X. The values q_1–q_7 are from Lemma 9.



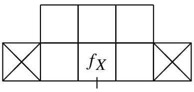
$\Gamma_d(X) \leqslant q_1(\Gamma_{d-1} + 2V_{d-1})$



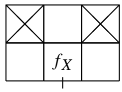
$\Gamma_d(X) \leqslant q_4(V_{d-1} + U_{d-1} + S_{d-1})$



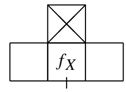
$\Gamma_d(X) \leqslant U_d$



$\Gamma_d(X) \leqslant q_2(\Gamma_{d-1} + 2T_{d-1})$



$\Gamma_d(X) \leqslant q_6(2S_{d-1} + R_{d-1})$



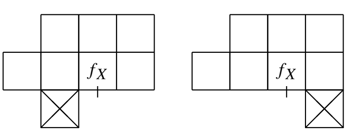
$\Gamma_d(X) \leqslant q_7(2W_{d-1})$

For example, consider a boundary pair X covered by the lower centre diagram. We will now show how to prove $\Gamma_d(X) \leqslant q_6(2S_{d-1} + R_{d-1})$. In the construction of T_X, for every pair of spins $c \in Q$, $c' \in Q$, $c \neq c'$, we introduce a child $r_{c,c'}$ of the root r. We construct three boundary pairs $X_1(c, c')$ (where the new distinguished edge goes left from f_X), $X_2(c, c')$ (where the new distinguished edge goes up from f_X) and $X_3(c, c')$ (where the new distinguished edge goes right from f_X). The boundary pair $X_1(c, c')$ is in S (this can be verified by consulting the diagram corresponding to S above), so $\Gamma_{d-1}(X_1(c, c')) \leqslant S_{d-1}$. Similarly, $X_3(c, c') \in S$, so $\Gamma_{d-1}(X_3(c, c')) \leqslant S_{d-1}$. Finally, $X_2(c, c') \in R$ (this can be verified by consulting the diagram corresponding to R above), so $X_2(c, c') \leqslant R_{d-1}$. Since $\nu(X)$ is the sum of the probabilities $p_X(c, c')$, we conclude that $\Gamma_d(X) \leqslant \nu(X)(2S_{d-1} + R_{d-1})$. Now we apply Lemma 6 and Lemma 9 to get $\nu(X) \leqslant \mu(X) \leqslant q_6$. Thus, we have shown that $\Gamma_d(X) \leqslant q_6(2S_{d-1} + R_{d-1})$. The other inequalities are derived similarly.

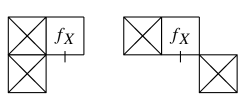
Putting all six cases together, we get the following inequality for $d \geqslant 2$:

$$\begin{aligned} \Gamma_d \leqslant \max(&q_1(\Gamma_{d-1} + 2V_{d-1}),\\ &q_2(\Gamma_{d-1} + 2T_{d-1}),\\ &q_4(V_{d-1} + U_{d-1} + S_{d-1}),\\ &q_6(2S_{d-1} + R_{d-1}),\\ &U_d,\\ &q_7(2W_{d-1})). \end{aligned} \tag{4}$$

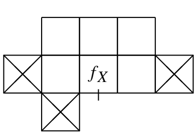
By re-considering similar scenarios with the additional assumption that $X \in V$, we derive a corresponding upper bound for V_d. The following seven cases cover all the boundary pairs in V.



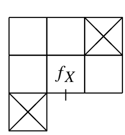
$\Gamma_d(X) \leqslant q_1(U_{d-1} + \Gamma_{d-1} + V_{d-1})$



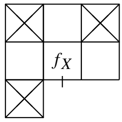
$\Gamma_d(X) \leqslant U_d$



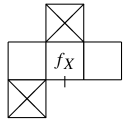
$\Gamma_d(X) \leqslant q_2(R_{d-1} + \Gamma_{d-1} + T_{d-1})$



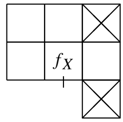
$\Gamma_d(X) \leqslant q_4(2U_{d-1} + S_{d-1})$



$\Gamma_d(X) \leqslant q_6(S_{d-1} + 2R_{d-1})$



$\Gamma_d(X) \leqslant q_7(S_{d-1} + W_{d-1})$

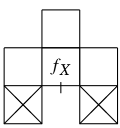


$\Gamma_d(X) \leqslant q_4(V_{d-1} + U_{d-1} + R_{d-1})$

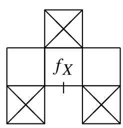
Putting these together, we get this inequality for $d \geqslant 2$:

$$\begin{aligned} V_d \leqslant \max(&q_1(U_{d-1} + \Gamma_{d-1} + V_{d-1}),\\ &q_2(R_{d-1} + \Gamma_{d-1} + T_{d-1}),\\ &q_4(2U_{d-1} + S_{d-1}),\\ &q_6(S_{d-1} + 2R_{d-1}),\\ &q_4(V_{d-1} + U_{d-1} + R_{d-1}),\\ &U_d,\\ &q_7(S_{d-1} + W_{d-1})). \end{aligned} \tag{5}$$

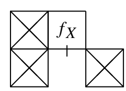
In a similar manner we can find an upper bound for W_d, and the following cases cover the boundary pairs in W.



$\Gamma_d(X) \leqslant q_6(2U_{d-1} + \Gamma_{d-1})$



$\Gamma_d(X) \leqslant q_7(2S_{d-1})$

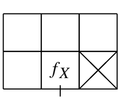


$\Gamma_d(X) \leqslant U_d$

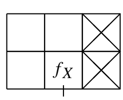
These cases give the following inequality for $d \geqslant 2$:

$$W_d \leqslant \max(q_6(2U_{d-1} + \Gamma_{d-1}), U_d, q_7(2S_{d-1})). \tag{6}$$

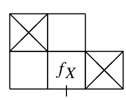
The following cases cover all boundary pairs in U, so we can find an upper bound for U_d.



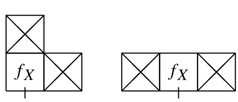
$\Gamma_d(X) \leqslant q_3(2V_{d-1})$



$\Gamma_d(X) \leqslant q_5(V_{d-1} + U_{d-1})$



$\Gamma_d(X) \leqslant q_7(S_{d-1} + U_{d-1})$



$\Gamma_d(X) \leqslant R_d$

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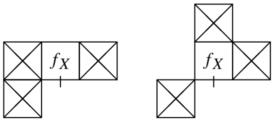
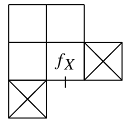
These give an upper bound on U_d for $d \geqslant 2$:

$$U_d \leqslant \max(q_3(2V_{d-1}), q_5(V_{d-1} + U_{d-1}), q_7(S_{d-1} + U_{d-1}), R_d). \tag{7}$$

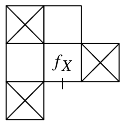
The following cases illustrate the situation for boundary pairs in S.



$\Gamma_d(X) \leqslant R_d$



$\Gamma_d(X) \leqslant q_5(U_{d-1} + V_{d-1})$

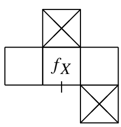


$\Gamma_d(X) \leqslant q_7(R_{d-1} + S_{d-1})$

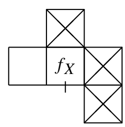
These give the following inequality for $d \geqslant 2$:

$$S_d \leqslant \max(R_d, q_5(U_{d-1} + V_{d-1}), q_7(R_{d-1} + S_{d-1})). \tag{8}$$

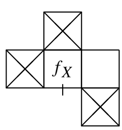
Now we derive a corresponding upper bound for T_d. The following cases cover all boundary pairs in T (apart from those in R).



$\Gamma_d(X) \leqslant q_7(W_{d-1} + S_{d-1})$



$\Gamma_d(X) \leqslant q_7(W_{d-1})$

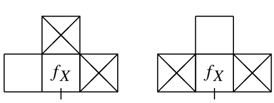


$\Gamma_d(X) \leqslant q_7(S_{d-1})$

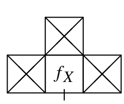
These give the following inequality for $d \geqslant 2$:

$$T_d \leqslant \max(R_d, q_7(W_{d-1} + S_{d-1})). \tag{9}$$

Finally, we derive an upper bound for R_d. The following cases cover all boundary pairs in R. Notice that the middle diagram below does not exactly match the set Q_7, but clearly we can use the value of q_7 to bound $\mu(X)$ also for this case.



$\Gamma_d(X) \leqslant q_7(W_{d-1})$



$\Gamma_d(X) = 0$ for $d \geqslant 2$

These give the following inequality for $d \geqslant 2$:

$$R_d \leqslant \max(0, q_7(W_{d-1})). \tag{10}$$

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We now set $\varepsilon = 1/1000$ and show that for every $d \geqslant 1$, we have $\Gamma_d \leqslant (1-\varepsilon)^d$. We define some rational numbers. Let $u = s = t = r = 7/10$ and $v = w = 92/100$. We will prove by induction on d that $\Gamma_d \leqslant (1-\varepsilon)^d$, $V_d \leqslant v(1-\varepsilon)^d$, $W_d \leqslant w(1-\varepsilon)^d$, $U_d \leqslant u(1-\varepsilon)^d$, $S_d \leqslant s(1-\varepsilon)^d$, $T_d \leqslant t(1-\varepsilon)^d$, and $R_d \leqslant r(1-\varepsilon)^d$.

The base case is $d = 1$. For any boundary pair X, we have $\Gamma_1(X) \leqslant \nu(X) \leqslant \mu(X)$, and from Lemma 7

$$\mu(X) \leqslant \frac{1-\lambda}{6-4(1-\lambda)} \leqslant \frac{1}{2}.$$

The base case then follows from the fact that

$$\frac{1}{2} \leqslant \min(1, v, w, u, s, t, r)(1-\varepsilon).$$

The inductive step follows from equations (4), (5), (6), (7), (8), (9) and (10).

First, we use inequality (10), the facts that $r \geqslant 0$ and $\varepsilon \leqslant 1$ (so $0 \leqslant r(1-\varepsilon)^d$), and the fact that $q_7 w \leqslant r(1-\varepsilon)$ to show that $R_d \leqslant r(1-\varepsilon)^d$. Similarly, we use the inductive hypothesis, inequality (9) and the facts that $r \leqslant t$ and $q_7(w+s) \leqslant t(1-\varepsilon)$ to show that $T_d \leqslant t(1-\varepsilon)^d$.

Next, we establish upper bounds on S_d and U_d. To show that $S_d \leqslant s(1-\varepsilon)^d$, we use the inductive hypothesis and inequality (8) together with the upper bound $R_d \leqslant r(1-\varepsilon)^d$ and the following facts: $r \leqslant s$, $q_5(u+v) \leqslant s(1-\varepsilon)$, and $q_7(r+s) \leqslant s(1-\varepsilon)$. To show that $U_d \leqslant u(1-\varepsilon)^d$, we use the inductive hypothesis and inequality (7), together with the upper bound $R_d \leqslant r(1-\varepsilon)^d$ and the following facts: $r \leqslant u$, $q_3 2v \leqslant (1-\varepsilon)u$, $q_5(v+u) \leqslant (1-\varepsilon)u$, and $q_7(s+u) \leqslant (1-\varepsilon)u$.

Finally, we establish upper bounds on W_d, V_d and Γ_d. All of these bounds use the inductive hypothesis and the upper bound $U_d \leqslant u(1-\varepsilon)^d$ along with $u \leqslant w$, $u \leqslant v$ and $u \leqslant 1$. To establish $W_d \leqslant w(1-\varepsilon)^d$, we use inequality (6) along with the following facts: $q_6(2u+1) \leqslant (1-\varepsilon)w$ and $q_7 2s \leqslant (1-\varepsilon)w$. To establish $V_d \leqslant v(1-\varepsilon)^d$, we use inequality (5) along with the following facts:

$$\begin{aligned}
q_1(u+1+v) &\leqslant v(1-\varepsilon);\\
q_2(r+1+t) &\leqslant v(1-\varepsilon);\\
q_4(2u+s) &\leqslant v(1-\varepsilon);\\
q_6(s+2r) &\leqslant v(1-\varepsilon);\\
q_4(v+u+r) &\leqslant v(1-\varepsilon);\\
q_7(s+w) &\leqslant v(1-\varepsilon).
\end{aligned}$$

Finally, to establish $\Gamma_d \leqslant (1-\varepsilon)^d$, we use Inequality (4) along with the following facts:

$$\begin{aligned}
q_1(1+2v) &\leqslant 1-\varepsilon;\\
q_2(1+2t) &\leqslant 1-\varepsilon;\\
q_4(v+u+s) &\leqslant 1-\varepsilon;\\
q_6(2s+r) &\leqslant 1-\varepsilon;\\
q_7(2w) &\leqslant 1-\varepsilon.
\end{aligned}$$

This concludes the proof of Theorem 3 for $q = 6$.

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5. *Proof of Theorem 3 for $q = 5$, $q = 4$ and $q = 3$*

The proof is the same as the proof for $q = 6$ in Section 4, except that for each value of q, we compute new values for $q_1, \ldots, q_7$ (as in Lemma 9). To find sufficiently small values we need to constrain the value of λ. If λ is too small, the values of $q_1, \ldots, q_7$ become too large. We do not repeat the values of λ already covered by Theorem 2.

LEMMA 10. *Suppose that $q = 5$ and $\lambda \in [0.127, 0.286]$. Let $p_1 = 7/20$, $p_2 = 9/25$, $p_3 = 19/50$, $p_4 = 2/5$, $p_5 = 2/5$, $p_6 = 2/5$ and $p_7 = 1/2$. Define $q_i = p_i + \delta$ for $i \in \{1, \ldots, 7\}$ where $\delta = 1/1000$. Suppose that X is a boundary pair with region $R_X = Q_i$. Then $\mu(X) \leqslant q_i$.*

LEMMA 11. *Suppose that $q = 4$ and $\lambda \in [0.262, 0.373]$. Let $p_1 = 7/20$, $p_2 = 19/50$, $p_3 = 19/50$, $p_4 = 19/50$, $p_5 = 2/5$, $p_6 = 19/50$ and $p_7 = 1/2$. Define $q_i = p_i + \delta$ for $i \in \{1, \ldots, 7\}$ where $\delta = 1/1000$. Suppose that X is a boundary pair with region $R_X = Q_i$. Then $\mu(X) \leqslant q_i$.*

LEMMA 12. *Suppose that $q = 3$ and $\lambda \in [0.393, 0.474]$. Let $p_1 = 873/2500$, $p_2 = 9/25$, $p_3 = 48/125$, $p_4 = 9/25$, $p_5 = 39/100$, $p_6 = 37/100$ and $p_7 = 1/2$. Define $q_i = p_i + \delta$ for $i \in \{1, \ldots, 7\}$ where $\delta = 1/1000$. Suppose that X is a boundary pair with region $R_X = Q_i$. Then $\mu(X) \leqslant q_i$.*

REMARK 3. Unlike Lemma 9, the values of p_i in the lemmas above are strict upper bounds on $\max_{X:R_X=Q_i} \mu_X(\lambda)$, where λ is the smallest value in the specified intervals above. Writing the exact values of $\max_{X:R_X=Q_i} \mu_X(\lambda)$ would require many more digits. Again, these values seem to be monotonically decreasing in λ.

We use computation in the same manner as for the proof of Lemma 9 to prove these lemmas. Following the proof of the $q = 6$ case of the theorem, and using the values of q_i in the lemmas above, we can then define new rational numbers v, w, u, t, s and r, and prove that $\Gamma_d(X) \leqslant (1 - \varepsilon)^d$.

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