

# Absence of Phase Transition for Antiferromagnetic Potts Models via the Dobrushin Uniqueness Theorem

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We prove that the  $q$ -state Potts antiferromagnet on a lattice of maximum coordination number  $r$  exhibits exponential decay of correlations uniformly at all temperatures (including zero temperature) whenever  $q > 2r$ . We also prove slightly better bounds for several two-dimensional lattices: square lattice (exponential decay for  $q \geq 7$ ), triangular lattice ( $q \geq 11$ ), hexagonal lattice ( $q \geq 4$ ), and Kagomé lattice ( $q \geq 6$ ). The proofs are based on the Dobrushin uniqueness theorem.

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**KEY WORDS:** Dobrushin uniqueness theorem; antiferromagnetic Potts models; phase transition.

## 1. INTRODUCTION

Dobrushin's uniqueness theorem<sup>(1-4)</sup> provides a simple but powerful method for proving the uniqueness of the infinite-volume Gibbs measure, as well as the exponential decay of correlations in this unique Gibbs measure, for classical-statistical-mechanical systems deep in a single-phase region. The basic idea underlying this theorem is that if the probability distribution of a single spin  $\sigma_i$  depends "sufficiently weakly" on the remaining spins  $\{\sigma_j\}_{j \neq i}$ , then one can deduce (by a clever iterative argument) uniqueness of the Gibbs measure and exponential decay of correlations.

The principal applications of this method have been in two regimes:

1. *High temperature.* Here  $\sigma_i$  depends weakly on the  $\{\sigma_j\}_{j \neq i}$  because of the strong thermal fluctuations.

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2. *Large magnetic field.* Here  $\sigma_i$  tends to follow the magnetic field, no matter what the other spins are doing; so the probability distribution of  $\sigma_i$  again depends weakly on the  $\{\sigma_j\}_{j \neq i}$ .

However, Kotecký (cited in ref. 3, pp. 148–149, 457) has pointed out that Dobrushin's theorem is applicable also in a third regime:

3. *High entropy.* Here  $\sigma_i$  has so many states available to it (with equal or almost equal probability), no matter what the other spins are doing, that its probability distribution again depends weakly on the  $\{\sigma_j\}_{j \neq i}$ .

The simplest example of this situation is the antiferromagnetic  $q$ -state Potts model,<sup>(5-7)</sup>

$$\mathcal{H} = -J \sum_{x \sim y} \delta_{\sigma_x, \sigma_y} \quad (1.1)$$

with  $J = -\beta < 0$ , on a lattice in which each site has  $r$  nearest neighbors.<sup>2</sup> Even at zero temperature ( $J = -\infty$ ) the spin  $\sigma_i$  is required only to be different from all the neighboring spins  $\{\sigma_j\}_{j \sim i}$ . If  $q \gg r$ , then the probability distribution of  $\sigma_i$  depends only weakly on the values of the  $\{\sigma_j\}_{j \sim i}$ . It turns out that Dobrushin's theorem is applicable whenever  $q > 2r$  (see Section 3 below), as well as in some additional cases (see Sections 4 and 5). Thus, for  $q$  sufficiently large (how large depends on the lattice under consideration), the  $q$ -state Potts antiferromagnet has a unique Gibbs measure and exponential decay of correlations at all temperatures, including zero temperature: the system is disordered as a result of entropy.

More precisely, we expect that for each lattice  $\mathcal{L}$  there will be a value  $q_c(\mathcal{L})$  such that:

(a) For  $q > q_c(\mathcal{L})$  the model has exponential decay of correlations uniformly at all temperatures, including zero temperature.

(b) For  $q = q_c(\mathcal{L})$  the model has a critical point at zero temperature.

(c) For  $q < q_c(\mathcal{L})$  any behavior is possible. Often (though not always) the model has a phase transition at nonzero temperature, which may be of either first or second order.<sup>3</sup>

<sup>2</sup> We use the notation  $x \sim y$  to indicate that  $x$  is a nearest neighbor of  $y$ . The sum in (1.1) thus runs over all nearest-neighbor pairs of lattice sites (each pair counted once), and each spin takes values  $\sigma_x \in \{1, 2, \dots, q\}$ . The antiferromagnetic case corresponds to  $J = -\beta < 0$ .

<sup>3</sup> Exceptions to the usual behavior are, for example, the Ising model ( $q = 2$ ) on the triangular lattice ( $q_c = 4$ ), which has a zero-temperature critical point,<sup>(8)</sup> and the Ising model on the Kagomé lattice ( $q_c = 3$ ), which is noncritical at all temperatures, including zero temperature.<sup>(9)</sup>

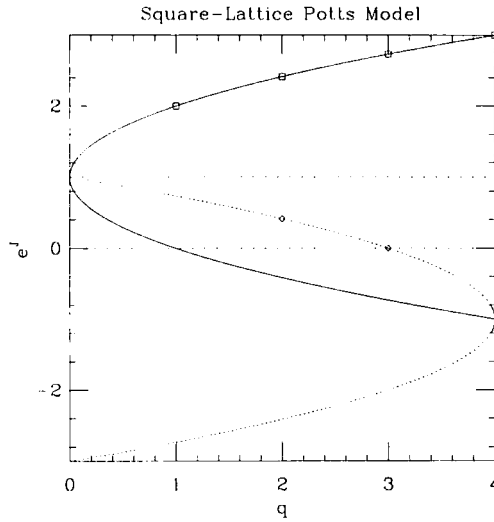


Fig. 1. Curves where the square-lattice Potts model has been solved: the self-dual curve  $(e^J - 1)^2 = q$  (solid curve), and  $(e^J + 1)^2 = 4 - q$  (dashed curve). The horizontal dotted lines correspond to  $e^J = 1$  (separating the ferromagnetic and antiferromagnetic regimes) and to  $e^J = 0$  (separating the antiferromagnetic regime from the unphysical region  $e^J < 0$ ). The squares show the known ferromagnetic critical points ( $q = 1, 2, 3, 4$ ) and the diamonds mark the known antiferromagnetic critical points ( $q = 2, 3$ ).

Here is what is believed to be true for the standard two-dimensional lattices:

*Square lattice.* Baxter<sup>(10, 11)</sup> has determined the exact free energy (among other quantities) for the square-lattice Potts model on two special curves in the  $(J, q)$  plane (see Fig. 1):

$$e^J = 1 \pm \sqrt{q} \tag{1.2}$$

$$e^J = -1 \pm \sqrt{4 - q} \tag{1.3}$$

Curve (1.2<sub>+</sub>) is known to correspond to the ferromagnetic critical point, and Baxter<sup>(11)</sup> has conjectured that curve (1.3<sub>+</sub>) corresponds to the antiferromagnetic critical point. For  $q = 2$  this gives the known exact value;<sup>(12)</sup> for  $q = 3$  it predicts a zero-temperature critical point ( $J_c = -\infty$ ), in accordance with previous belief,<sup>(13, 14),4</sup> and for  $q > 3$  it predicts that the

<sup>4</sup> Note also that the  $q = 3$  model is exactly soluble at zero temperature in an arbitrary magnetic field;<sup>(14-17)</sup> this might increase one's suspicions that the zero-temperature zero-field case is critical. Indeed, Henley<sup>(18)</sup> has some very interesting predictions for the critical exponents.

putative critical point lies in the unphysical region ( $e^{J_c} < 0$ ), so that the entire physical region  $-\infty \leq J \leq 0$  lies in the disordered phase. These predictions for  $q=3, 4$  have recently been confirmed by high-precision Monte Carlo simulation.<sup>(19)</sup> For some further interesting speculations, see refs. 20 and 21.

*Triangular lattice.* Baxter and collaborators<sup>(22-24)</sup> have determined the exact free energy (among other quantities) for the triangular-lattice Potts model on two special curves in the  $(J, q)$  plane (see Fig. 2):

$$(e^J - 1)^2 (e^J + 2) = q \quad (1.4)$$

$$e^J = 0 \quad \text{for } 0 < q < 4 \quad (1.5)$$

The uppermost branch of curve (1.4) is known to correspond to the ferromagnetic critical point,<sup>(22)</sup> and Baxter<sup>(23)</sup> has conjectured that (1.5) corresponds to the antiferromagnetic critical point. This prediction of a zero-temperature critical point is known to be correct for  $q=2$ ,<sup>(8)</sup> and there is heuristic analytical evidence that it is correct also for  $q=4$ .<sup>(18, 25)</sup>

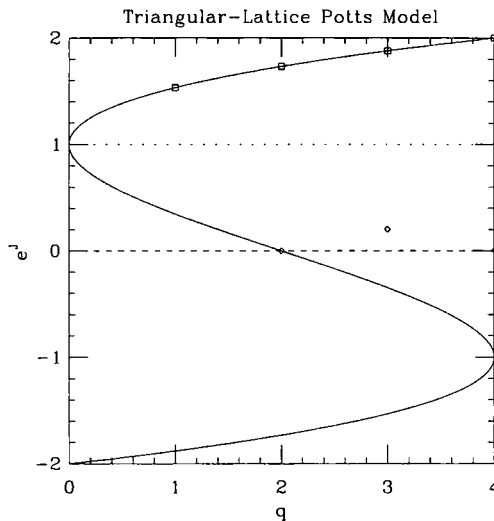


Fig. 2. Curves where the triangular-lattice Potts model has been solved:  $(e^J - 1)^2(e^J + 2) = q$  (solid curve), which has three branches; and the line  $e^J = 0$  (dashed line). The horizontal dotted line corresponds to  $e^J = 1$  (separating the ferromagnetic and antiferromagnetic regimes). The squares show the known ferromagnetic critical points ( $q=1, 2, 3, 4$ ) and the diamonds mark the known antiferromagnetic phase-transition points ( $q=2, 3, 4$ ). Note that the antiferromagnetic first-order transition for  $q=3$  does *not* lie on either of the exactly solved curves.

On the other hand, for  $q=3$  this prediction contradicts the rigorous result,<sup>(26)</sup> based on Pirogov–Sinai theory, that there is a low-temperature phase with long-range order and small correlation length. Indeed, a recent Monte Carlo study of the  $q=3$  model has found strong evidence for a first-order transition (to an ordered phase) at  $\beta \approx 1.594$ .<sup>(27)</sup> For  $q > 4$  one may expect that the triangular-lattice Potts model is noncritical even at zero temperature. Finally, the physical meaning of the two lower branches of (1.4) is mysterious. The lowermost branch of (1.4) lies entirely in the unphysical region  $e^J < 0$ . The middle branch is located in the antiferromagnetic region for  $0 < q < 2$  and in the unphysical region for  $q > 2$ ; at  $q=2$  it coincides with the antiferromagnetic critical point. For some further interesting speculations, see ref. 20.

*Hexagonal lattice.* This lattice is connected by duality<sup>(10)</sup> with the triangular lattice;<sup>5</sup> the image of (1.4)/(1.5) is

$$(e^J - 1)^3 - 3q(e^J - 1) - q^2 = 0 \quad (1.6)$$

$$e^J = 1 - q \quad \text{for } 0 < q < 4 \quad (1.7)$$

Curve (1.6) has three branches in the region  $q \geq 0$  (see Fig. 3): the uppermost branch (with  $0 \leq q < \infty$  and  $e^J \geq 1$ ) is the ferromagnetic critical point; the middle branch (with  $0 \leq q \leq 4$  and  $-1 \leq e^J \leq 1$ ) contains the antiferromagnetic Ising critical point ( $q=2$ ,  $e^J=2-\sqrt{3}$ ) and crosses the zero-temperature point  $e^J=0$  at  $q=(3+\sqrt{5})/2 \approx 2.618$ ; while the lowermost branch crosses the zero-temperature point  $e^J=0$  at  $q=(3-\sqrt{5})/2 \approx 0.382$ .<sup>6</sup> The meaning of this lowermost branch is mysterious, as is the meaning of (1.7). But the behavior of the middle branch suggests that it may be the antiferromagnetic critical curve: in this case there would be a zero-temperature critical point for  $q=(3+\sqrt{5})/2$  (if this assertion has any meaning<sup>7</sup>), and the

<sup>5</sup> Furthermore, the hexagonal-lattice Potts model *on the curve* (1.6) (and only there) can be mapped via the star–triangle transformation onto a triangular-lattice Potts model, which turns out to lie exactly on the curve (1.4).

<sup>6</sup> The middle branch is missing in ref. 20, p. 673, Fig. 8.

<sup>7</sup> The Potts models for noninteger  $q$  can be given a rigorous meaning via the mapping onto the Fortuin–Kasteleyn random-cluster model.<sup>(28–30)</sup> The trouble is that in the antiferromagnetic case ( $J < 0$ ) this latter model has negative weights, and so cannot be given a standard probabilistic interpretation. In particular, the existence of a good infinite-volume limit is problematic; the limit could depend strongly on the subsequence of lattice sizes and on the boundary conditions. The same is true of the “anti-Fortuin–Kasteleyn” representation, in which the coefficients are products of chromatic polynomials of clusters: again the weights can be negative for noninteger  $q$ , and the existence of the infinite-volume limit is problematic. Likewise, the ice-model representation<sup>(10, 31)</sup> has in general complex weights for  $0 < q < 4$ , even in the ferromagnetic case.

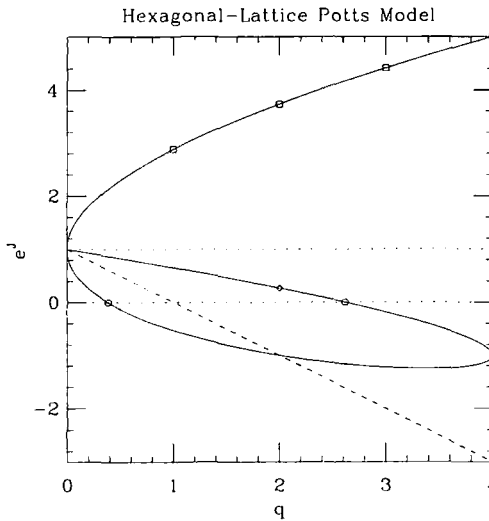


Fig. 3. Curves where the hexagonal-lattice Potts model has been solved:  $(e^J - 1)^3 - 3q(e^J - 1) = q^2$  (solid curve), which has three branches; and the line  $e^J = 1 - q$  (dashed line). The horizontal dotted lines correspond to  $e^J = 1$  (separating the ferromagnetic and antiferromagnetic regimes) and to  $e^J = 0$  (separating the antiferromagnetic regime from the unphysical region  $e^J < 0$ ). The squares show the known ferromagnetic critical points ( $q = 1, 2, 3, 4$ ) and the diamond marks the known antiferromagnetic critical point for  $q = 2$ . The open circles show the points where the two antiferromagnetic branches cross the  $e^J = 0$  line, namely  $q = (3 \pm \sqrt{5})/2$ .

model would be disordered even at zero temperature for  $q > (3 + \sqrt{5})/2$ . For some further interesting speculations, see ref. 21.

*Kagomé lattice.* This is not merely an academic example, as some condensed-matter systems (for instance, the insulator  $\text{SrCr}_{8-x}\text{Ga}_{4-x}\text{O}_{19}$ ) have the Kagomé lattice structure.<sup>(32,34)</sup> For  $q = 2$  this model has been solved exactly,<sup>(9)</sup> and there is no phase transition at any temperature. For  $q = 3$  the zero-temperature model can be mapped onto the zero-temperature four-state triangular-lattice Potts antiferromagnet<sup>(25)</sup> and so is expected to be critical.<sup>(18,35)</sup> For  $q > 3$  one may expect that this model is noncritical even at zero temperature.

In Table I we summarize the believed exact values of  $q_c(\mathcal{L})$  for these four lattices, along with the upper bounds that follow from our computer-assisted proofs. Clearly, our rigorous bounds still fall far short of what is believed to be true in most of the lattices considered here. Only for the hexagonal lattice are we somewhat close to the expected result.

The plan of this paper is as follows: In Section 2 we set the notation and recall the Dobrushin uniqueness theorem. In Section 3 we prove that

**Table I. Range of  $q$  for Which We Have Proven Exponential Decay of Correlations at Zero Temperature for Various Lattices<sup>a</sup>**

	Range of $q$				
	General	Hexagonal	Square	Kagomé	Triangular
Kotecký	$> 2r$	$\geq 7$	$\geq 9$	$\geq 9$	$\geq 13$
Single-site decimation		$\geq 5$	$\geq 7$	$\geq 7$	$\geq 11$
Cluster decimation		$\geq 4$		$\geq 6$	
Exact		$> 2.618\dots$	$> 3$	$> 3$	$> 4$

<sup>a</sup>The first row shows the result given by Kotecký (see ref. 3, pp. 148–149, 457) and slightly generalized here in Section 3. The second row gives our improved result using single-site decimation (Section 4), and the next row gives our further improvement using more sophisticated decimation schemes (Section 5). The last row (“Exact”) shows what is known or believed to be the right answer.

the Dobrushin uniqueness theorem is applicable to the  $q$ -state Potts anti-ferromagnet on a lattice of maximum coordination number  $r$ , uniformly at all temperatures (including zero temperature), whenever  $q > 2r$ . In Section 4 we improve this result for some common lattices (square, hexagonal, triangular, and Kagomé), using a single-site decimation scheme and a computer-assisted proof. Finally in Section 5 we improve our results for the hexagonal and Kagomé lattices using more sophisticated decimation schemes.

During the preparation of this paper we learned of the tragic death of Prof. R. L. Dobrushin, one of the founders of and main contributors to modern mathematical statistical mechanics. We dedicate this paper to his memory.

## 2. NOTATION AND PRELIMINARIES

### 2.1. Basic Setup

The basic framework for all our results is the Dobrushin–Lanford–Ruelle (DLR) approach to the equilibrium statistical mechanics of infinite-volume classical lattice systems. A pedagogical introduction to this theory can be found in ref. 36, Sections 2.1–2.3; detailed expositions can be found in the books of Preston,<sup>(37)</sup> Georgii,<sup>(3)</sup> and Simon.<sup>(4)</sup> Here we summarize very briefly the notation and the basic ideas. The central idea in the DLR theory is to define an *infinite-volume Gibbs measure* as a probability distribution for the infinite-volume system whose *conditional* probabilities for *finite* subsystems are given by the Boltzmann–Gibbs formula for the given formal Hamiltonian.

Consider a classical-statistical-mechanical system on a countably infinite lattice  $\mathcal{L}$ , with spin variables  $\sigma_i$  ( $i \in \mathcal{L}$ ) taking values in some state space  $E$ .<sup>8</sup> The equilibrium statistical mechanics of such a system is defined by a *specification*  $\Pi = \{\pi_A\}_{A \text{ finite } \subset \mathcal{L}}$ : here  $\pi_A(\sigma_A | \sigma_{A^c})$  gives the conditional probability distribution for the spin configuration  $\sigma_A \equiv \{\sigma_i\}_{i \in A}$  inside the finite set  $A$ , given the spin configuration  $\sigma_{A^c} \equiv \{\sigma_i\}_{i \in A^c}$  outside  $A$ . The  $\{\pi_A\}$  have to satisfy various consistency conditions.<sup>(3, 36, 37)</sup> We shall further assume that each kernel  $\pi_A$  is *quasilocal*:<sup>(3, 36)</sup> this is a very mild decay condition on the long-range interactions.

Usually the specification  $\{\pi_A\}$  is defined via an *interaction* (= “formal Hamiltonian”)  $\Phi = \{\Phi_A\}_{A \text{ finite } \subset \mathcal{L}}$ : here  $\Phi_A$  is, roughly speaking, the elementary contribution to the Hamiltonian coming from the finite set of spins  $A \subset \mathcal{L}$ . Thus, the Hamiltonian  $H_A^\Phi$  for volume  $A$  with external condition  $\sigma_{A^c}$  is

$$H_A^\Phi(\sigma_A | \sigma_{A^c}) = \sum_{\substack{A \text{ finite } \subset \mathcal{L} \\ A \cap A^c \neq \emptyset}} \Phi_A(\sigma_A, \sigma_{A^c}) \tag{2.1}$$

The kernel  $\pi_A$  is then, by definition, the corresponding Boltzmann–Gibbs measure:

$$\pi_A^\Phi(\sigma_A | \sigma_{A^c}) = Z_A^\Phi(\sigma_{A^c})^{-1} \exp[-H_A^\Phi(\sigma_A | \sigma_{A^c})] \prod_{i \in A} d\mu^0(\sigma_i) \tag{2.2}$$

where  $\mu^0$  is the *a priori* single-spin distribution. Under mild summability conditions on the interaction  $\{\Phi_A\}$ , it can be shown that (2.1)/(2.2) are well-defined and satisfy all the conditions for a specification, and furthermore that the  $\pi_A$  are quasilocal.<sup>(3, 36)</sup> (In this paper all interactions will be finite-range, so the requisite conditions will hold trivially.)

Finally, a probability measure  $\mu$  on the configuration space of the infinite-volume system is said to be an *infinite-volume Gibbs measure* for the specification  $\Pi$  if, for each finite subset  $A \subset \mathcal{L}$ , the conditional probability distribution  $\mu(\cdot | \sigma_{A^c})$  equals  $\pi_A(\cdot | \sigma_{A^c})$ . See refs. 3, 36, and 37 for details.

### 2.2. Dobrushin’s Uniqueness Theorem

Let us now focus on the kernels  $\pi_{\{i\}}$  ( $i \in \mathcal{L}$ ), which give the probability distribution of a *single* spin  $\sigma_i$  conditional on the remaining spins  $\{\sigma_k\}_{k \neq i}$ .

<sup>8</sup> In all the applications in this paper, the state space  $E$  will be the *finite* set  $\{1, \dots, q\}$ . However, the Dobrushin uniqueness theorem is valid in much greater generality.



Let us begin by fixing a site  $i \in \mathcal{L}$  and another site  $j \neq i$ . We shall define a quantity  $c_{ij}$  that measures the strength of direct dependence of  $\sigma_i$  on  $\sigma_j$ :

$$c_{ij} \equiv \sup_{\{\sigma\}, \{\tilde{\sigma}\} : \sigma_k = \tilde{\sigma}_k \forall k \neq j} d(\pi_{\{i\}}(\cdot | \{\sigma\}), \pi_{\{i\}}(\cdot | \{\tilde{\sigma}\})) \quad (2.3)$$

where

$$d(\mu_1, \mu_2) \equiv \sup_{A \subset E} |\mu_1(A) - \mu_2(A)| = \sup_{A \subset E} [\mu_1(A) - \mu_2(A)] \quad (2.4)$$

is half the variation distance between the probability measures  $\mu_1$  and  $\mu_2$ , and the supremum in (2.3) is taken over all pairs of configurations  $\{\sigma_k\}_{k \neq i}$  and  $\{\tilde{\sigma}_k\}_{k \neq i}$  that differ only at the site  $j$ . The matrix  $C = (c_{ij})_{i, j \in \mathcal{L}}$  is called *Dobrushin's interdependence matrix*. Please note that  $c_{ij}$  is a "worst-case" measure of the dependence of  $\sigma_i$  on  $\sigma_j$ , in the sense that it is defined via the *supremum* over all configurations of the spins  $\{\sigma_k = \tilde{\sigma}_k\}_{k \neq i}$ ,  $\sigma_j$  and  $\tilde{\sigma}_j$ . Finally, we define the *Dobrushin constant*

$$\alpha \equiv \sup_{i \in \mathcal{L}} \sum_{j \neq i} c_{ij} \quad (2.5)$$

We then have the following result:<sup>(1)</sup>

**Theorem 2.1** (Dobrushin uniqueness theorem). Let  $\Pi$  be a *quasilocal* specification whose Dobrushin constant  $\alpha$  is  $< 1$ . Then there is at most one infinite-volume Gibbs measure for  $\Pi$ .

For a proof, see ref. 3, Section 8.1, or ref. 4, Section V.I.<sup>9</sup>

**Remarks.** 1. Under very mild conditions on the specification  $\Pi$ —which always hold if, for example, the state space  $E$  is finite—it can be shown that there exists *at least one* infinite-volume Gibbs measure for  $\Pi$ . So the upshot of Dobrushin's uniqueness theorem is that there exists *exactly one* infinite-volume Gibbs measure for  $\Pi$ .

2. There is an extension of Dobrushin's uniqueness theorem that uses the Kantorovich–Rubinstein–Vasershtein–Ornstein distance corresponding to an arbitrary metric on the state space  $E$ , in place of the variation distance (2.4): see ref. 2 or ref. 4, Section V.3. This extension is particularly useful in studying continuous-spin systems. But in the Potts case it gains nothing, as the color-permutation symmetry of the Potts Hamiltonian ensures that the variation distance is in fact the "natural" distance.

<sup>9</sup> *Warning:* Simon<sup>(4)</sup> denotes by  $\rho_{ji}$  what we have called  $c_{ij}$ —note the reversal of indices!

The hypotheses of Theorem 2.1 imply also a strong result on the decay of correlations in the unique infinite-volume Gibbs measure. We need a few definitions: For any function  $f(\{\sigma\})$  and any site  $i$ , we define the *oscillation of  $f$  at  $i$* :

$$\delta_i(f) \equiv \sup_{\{\sigma\}, \{\sigma'\}: \sigma_k = \sigma'_k \ \forall k \neq i} |f(\{\sigma\}) - f(\{\sigma'\})| \tag{2.6}$$

We say that  $f$  has *finite total oscillation* if

$$A(f) \equiv \sum_{i \in \mathcal{L}'} \delta_i(f) < \infty \tag{2.7}$$

(In particular, any bounded function depending on only finitely many spins has finite total oscillation.) Finally, let  $C^n$  be the  $n$ th matrix power of Dobrushin's interdependence matrix  $C$ , and define

$$D_{ij} \equiv \sum_{n=0}^{\infty} (C^n)_{ij} \tag{2.8}$$

We then have:

**Theorem 2.2.** Let  $\Pi$  be a quasilocal specification satisfying the Dobrushin condition  $\alpha < 1$ . Then the unique infinite-volume Gibbs measure  $\mu$  satisfies

$$|\mu(fg) - \mu(f)\mu(g)| \leq \frac{1}{4} \sum_{i, j \in \mathcal{L}'} \delta_i(f) D_{ij} \delta_j(g) \tag{2.9}$$

for all functions  $f, g$  of finite total oscillation.

In particular, if  $\mathcal{L}'$  is a regular lattice and the interaction is of finite range (so that  $c_{ij} = 0$  whenever  $|i - j| > R$ ), then Dobrushin's condition  $\alpha < 1$  implies that  $D_{ij}$  decays *exponentially* as  $|i - j| \rightarrow \infty$ , so that Theorem 2.2 implies the *exponential decay of correlations* in the unique infinite-volume Gibbs measure. For proofs of Theorem 2.2 as well as these related results, see ref. 3, Section 8.2, or ref. 4, Section V.2.

**Remark.** The Dobrushin condition  $\alpha < 1$  is sufficient for uniqueness, but it is *not* necessary. A better result is given by the Dobrushin–Shlosman (DS) theory.<sup>(38–40)</sup> Instead of dealing with a single-spin volume  $A = \{i\}$ , they consider a general volume  $A$  and define the quantities

$$c_{A, j} \equiv \sup_{\{\sigma\}, \{\bar{\sigma}\}: \sigma_k = \bar{\sigma}_k \ \forall k \neq j} d(\pi_A(\cdot | \{\sigma\}), \pi_A(\cdot | \{\bar{\sigma}\})) \tag{2.10}$$

for every  $j \in A^c$ . The quantity  $c_{A,j}$  measures the dependence of the kernel  $\pi_A$  on the boundary spin  $\sigma_j$ . The Dobrushin criterion is replaced (for translation-invariant interactions) by

$$\gamma_A \equiv \frac{1}{|A|} \sum_{j \in A^c} c_{A,j} < 1 \tag{2.11}$$

If condition (2.11) holds for some volume  $A$ , then the infinite-volume Gibbs measure is unique.<sup>(38)</sup> When  $A = \{i\}$ , we recover Dobrushin’s Theorem 2.1. Those interactions satisfying condition (2.11) are called *completely analytical*. There are 12 different (but equivalent) characterizations of completely analytical interactions.<sup>(39, 40)</sup>

It would be very interesting to use DS theory to improve the bounds on  $q_c(\mathcal{L})$  given by the standard application of the Dobrushin criterion and to compare the results with our approach. An application of the DS criterion to the hard-square lattice gas has been worked out in ref. 41.

### 3. GENERAL PROOF OF UNIQUENESS FOR $q > 2r$

Let us now apply Dobrushin’s uniqueness theorem to a  $q$ -state Potts antiferromagnet defined by the (formal) Hamiltonian

$$\mathcal{H} = - \sum_{i \sim j} J_{ij} \delta_{\sigma_i \sigma_j} \tag{3.1}$$

with all couplings satisfying  $-\infty \leq J_{ij} \leq 0$ . We say that  $j$  is a nearest neighbor of  $i$  (denoted  $j \sim i$ ) in case  $J_{ij} \neq 0$ . We need to calculate the Dobrushin interdependence constants  $c_{ij}$ .

First, some preliminaries: Let  $\rho$  be a probability measure on the state space  $E$ , and let  $f \geq 0$  be any function on  $E$  such that  $\rho(f) \equiv \int f d\rho > 0$ . Then we define the probability measure  $\rho^{(f)}$  by

$$\rho^{(f)} = \frac{f\rho}{\rho(f)} \tag{3.2}$$

(“ $\rho$  weighted by  $f$  and then normalized”).

**Lemma 3.1.** Let  $0 \leq f, g \leq 1$ . Then

$$d(\rho^{(f)}, \rho^{(g)}) \leq \max \left[ \frac{\rho(1-f)}{\rho(f)}, \frac{\rho(1-g)}{\rho(g)} \right] \tag{3.3}$$

*Proof.* By definition,

$$d(\rho^{(f)}, \rho^{(g)}) = \sup_{A \subset E} \int_A \left[ \frac{g(x)}{\rho(g)} - \frac{f(x)}{\rho(f)} \right] d\rho(x) \tag{3.4}$$

Suppose (without loss of generality) that  $\rho(f) \leq \rho(g)$ . Then  $1/\rho(f) \geq 1/\rho(g)$ , so that

$$\frac{g(x)}{\rho(g)} - \frac{f(x)}{\rho(f)} \leq \frac{1-f(x)}{\rho(f)} - \frac{1-g(x)}{\rho(g)} \tag{3.5}$$

$$\leq \frac{1-f(x)}{\rho(f)} \quad [\text{since } g \leq 1] \tag{3.6}$$

But since  $f \leq 1$ , we have  $\int_A [1-f(x)] d\rho(x) \leq \int_E [1-f(x)] d\rho(x) \equiv \rho(1-f)$ . ■

**Remark.** If  $\rho(f) = \rho(g)$  and the supports of  $1-f$  and  $1-g$  are disjoint, then this estimate is sharp.

Let us now apply this lemma to compute the Dobrushin constant  $c_{ij}$  in the Potts antiferromagnet (3.1). We shall assume that the site  $i$  has at most  $r$  nearest neighbors. Fix two configurations  $\{\sigma_k\}_{k \neq i}$  and  $\{\tilde{\sigma}_k\}_{k \neq i}$  that differ only at the site  $j$ . Let  $\rho$  be the conditional probability distribution at site  $i$  in the presence of all of  $i$ 's neighbors *other than*  $j$ :

$$\rho(\sigma_i) = \left\{ \exp \left[ \sum_{k \neq i, j} J_{ik} \delta_{\sigma_i \sigma_k} \right] \right\} / \left\{ \sum_{\sigma=1}^q \exp \left[ \sum_{k \neq i, j} J_{ik} \delta_{\sigma \sigma_k} \right] \right\} \tag{3.7}$$

And let

$$f(\sigma_i) = \exp[J_{ij} \delta_{\sigma_i \sigma_j}] \tag{3.8a}$$

$$g(\sigma_i) = \exp[J_{ij} \delta_{\sigma_i \tilde{\sigma}_j}] \tag{3.8b}$$

The antiferromagneticity condition  $J_{ij} \leq 0$  guarantees that  $0 \leq f, g \leq 1$ , so we can apply Lemma 3.1. Because the site  $i$  has at most  $r-1$  nearest neighbors  $k \neq j$ , it follows that in the measure  $\rho$  there are at least  $q-r+1$  states with equal weight (namely, those states not equal to any of the  $\{\sigma_k\}_{k \neq i, j}$ ). Moreover, since all the  $J_{ik}$  are  $\leq 0$ , all the states that *are* equal to one or more of the  $\{\sigma_k\}_{k \neq i, j}$  have *smaller* weight. Hence the maximum weight given by  $\rho$  to any single state is  $\leq 1/(q-r+1)$ . Furthermore,  $1-f$  is nonzero on at most one state (namely,  $\sigma_j$ ) and is there  $\leq 1$ ; so we have  $\rho(1-f) \leq 1/(q-r+1)$ . The same holds for  $\rho(1-g)$ . Hence, by Lemma 3.1,

$$d(\rho^{(f)}, \rho^{(g)}) \leq \max \left[ \frac{\rho(1-f)}{\rho(f)}, \frac{\rho(1-g)}{\rho(g)} \right] \leq \frac{1}{q-r} \quad (3.9)$$

so that

$$c_{ij} \leq \frac{1}{q-r} \quad (3.10)$$

and consequently

$$\sum_{j \sim i} c_{ij} \leq \frac{r}{q-r} \quad (3.11)$$

If we now assume that *every* site in the lattice has at most  $r$  nearest neighbors, we can conclude that

$$\alpha \equiv \sup_{i \in \mathcal{L}} \sum_{j \sim i} c_{ij} \leq \frac{r}{q-r} \quad (3.12)$$

In particular, Dobrushin's condition  $\alpha < 1$  holds whenever  $q > 2r$ . Moreover, the bound (3.12) holds *uniformly* in the values of the couplings  $\{J_{ij}\}$ , provided only that they are antiferromagnetic. Therefore, Theorems 2.1 and 2.2 guarantee that for  $q > 2r$  there exists a unique infinite-volume Gibbs measure at all temperatures (including zero temperature), and that this unique infinite-volume Gibbs measure exhibits exponential decay of correlations uniformly in the temperature.

**Remarks.** 1. For the Potts antiferromagnet at *zero* temperature, i.e., when all nonzero  $J_{ij}$  equal  $-\infty$ , the bound (3.10) is sharp.

2. Kotecký (cited in ref. 3, pp. 148–149, 457) obtained the result (3.10)–(3.12) *at zero temperature*. But at nonzero temperature he obtained the weaker result  $c_{ij} \leq 2/(q-r)$  and hence  $\alpha \leq 2r/(q-r)$ , so that he proved uniqueness only for  $q > 3r$ .

3. Jerrum<sup>(43)</sup> has shown that the heat-bath dynamics (with random choice of site) for a *finite* Potts antiferromagnet at *zero* temperature is rapidly mixing (i.e., has an autocorrelation time which is bounded by a constant times the number of sites) whenever  $q > 2r$ . This result also follows immediately—for either random or sequential choice of site, and for either zero or nonzero temperature—from the proof of the Dobrushin uniqueness theorem combined with our bound (3.12). The point is that the heat-bath update at site  $i$  is given by  $\pi_{\{i\}}$ .

#### 4. IMPROVEMENTS VIA SINGLE-SITE DECIMATION

In this section we are going to improve on the bound  $q > 2r$ , using a computer-assisted proof that must be carried out separately for each lattice. For each of the four lattices we study (square, hexagonal, triangular, and

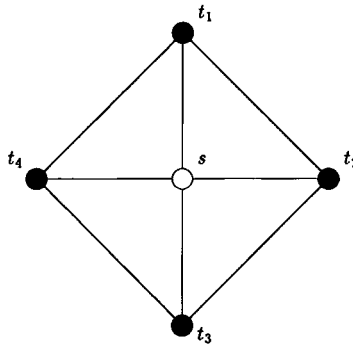


Fig. 4. Decimation for the square-lattice case. Once we sum over the spin  $s$  we obtain a new effective interaction among the spins  $t_j$  ( $j = 1, 2, 3, 4$ ).

Kagomé) we find that uniqueness holds for  $q > 2r - 2$ . But of course there is no guarantee that this result holds for general lattices!

We emphasize that our proof in this section is valid only at zero temperature ( $J = -\infty$ ). Presumably the result holds also for finite  $-\infty < J < 0$ , but we do not have any proof of this fact.

The idea of our proof is simple: decimate the original lattice and then apply Dobrushin’s criterion to the decimated lattice. This trick has also been used by other authors in a different context.<sup>(42)</sup>

The decimation step can be expressed in a general fashion. Consider a spin  $s$  that interacts with  $r$  nearest-neighbor spins  $t_1, \dots, t_r$ . (See Fig. 4 for the case of the square lattice, which has  $r = 4$ .) We have to perform the sum  $\sum_{s=1}^q \exp(J \sum_j \delta_{s, t_j})$ ; this will give us the statistical weight associated after decimation to the spin configuration  $(t_1, \dots, t_r)$ . The result is very simple for the antiferromagnetic model at zero temperature (that is,  $J = -\infty$ ):

$$\sum_{s=1}^q \exp\left(J \sum_{j=1}^r \delta_{s, t_j}\right) \stackrel{J=-\infty}{=} \sum_{s=1}^q \prod_{j=1}^r (1 - \delta_{s, t_j}) = q - C(t_1, \dots, t_r) \quad (4.1)$$

where  $C(t_1, \dots, t_r)$  is the number of distinct spin values (“colors”) we have in the configuration  $(t_1, \dots, t_r)$ . Thus, decimating the spin  $s$  will generate the  $r$ -body interaction (4.1) among the spins  $t_1, \dots, t_r$ .

In this section we will be considering only regular lattices, in which each site has the same number  $r$  of nearest neighbors.

### 4.1. Square Lattice

In this case the original lattice is bipartite, so we can sum over all the spins belonging to one of the two sublattices (for instance, the empty circles in Fig. 5). In this way we obtain a decimated lattice defined by the rest of

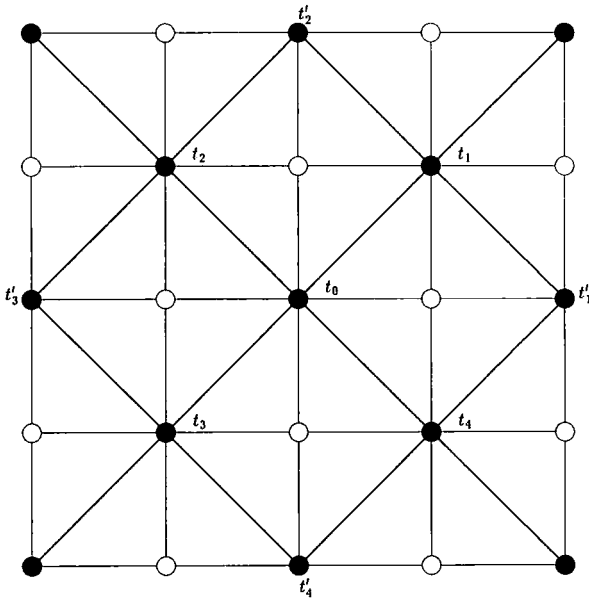


Fig. 5. Decimation for the square lattice. The empty circles represent the spins summed over; the solid circles represent the resulting decimated lattice. Each spin  $t_0$  of the decimated lattice interacts with eight spins: four nearest neighbors  $t_1, t_2, t_3, t_4$  and four next-to-nearest neighbors  $t'_1, t'_2, t'_3, t'_4$ .

the original spins (solid circles in Fig. 5). This decimated lattice is again a square lattice, but rotated 45 degrees with respect to the original one.

The previous discussion on the decimation procedure tells us that the interaction on the decimated lattice lives on the “plaquettes” (= squares): the statistical weight for each such square is given by (4.1). Each spin  $t_0$  on the decimated lattice (see Fig. 5) interacts with the other eight spins located on the four squares to which  $t_0$  belongs:  $(t_0, t_1, t'_2, t_2)$ ,  $(t_0, t_2, t'_3, t_3)$ ,  $(t_0, t_3, t'_4, t_4)$ , and  $(t_0, t_4, t'_1, t_1)$ . These eight spins fall into two classes: four nearest-neighbor spins  $t_1, t_2, t_3, t_4$  (which belong simultaneously to two of those squares), and four next-to-nearest neighbors  $t'_1, t'_2, t'_3, t'_4$  (which belong to only one of those squares). Thus, the quantity

$$c_{0,j} \equiv \sup_{\{t_i, \{t_j\} : t_k = t_j \forall k \neq j}} d(\rho_0(\cdot | \{t\}), \rho_0(\cdot | \{\tilde{t}\})) \tag{4.2}$$

will depend on whether the spin  $t_j$  is a nearest neighbor or a next-to-nearest neighbor of the spin  $t_0$ . In what follows,  $c_{0,nn}$  will denote this quantity evaluated at a nearest-neighbor spin  $t_j$ , and  $c_{0,nnn}$  will denote the same quantity evaluated at a next-to-nearest-neighbor spin  $t_j$ .

To obtain  $c_{0,j}$  we have to consider all the  $q^8$  distinct configurations  $\{t\}$  of the spins  $t_1, t_2, t_3, t_4, t'_1, t'_2, t'_3, t'_4$ , compute the conditional probability measure  $\rho_0(\cdot|\{t\})$  for each such configuration  $\{t\}$ , compute the variation distance between all pairs of such measures whose second arguments differ only by the value of the spin  $t_j$ , and finally take the maximum of those distances. In the original proof of Kotecký one could easily figure out which were the configurations which maximize (4.2). Here, this is more complicated due to the form of the four-body interaction (4.1). The important point is that for each fixed  $q$  there is only a *finite* number of configurations to look at. So we can write a computer algorithm to examine all the possible configurations and compute (4.2). We have written a FORTRAN code implementing these ideas. In this case, the number of configurations is manageable, but in order to streamline the computation we have exploited the color-permutation symmetry of the Potts Hamiltonian and have considered only those configurations that are not related by a mere relabeling of the colors. This list of configurations was generated by another FORTRAN code using a recursive algorithm.<sup>10</sup>

For each  $q$  we obtained  $c_{0,nn}$  and  $c_{0,nnn}$ . Given these values, it is easy to compute the quantity

$$\alpha \equiv \sum_{j \neq 0} c_{0,j} = 4c_{0,nn} + 4c_{0,nnn} \quad (4.3)$$

When  $\alpha < 1$ , Dobrushin's theorem states that the infinite-volume Gibbs measure is unique and that this measure exhibits exponentially decaying correlations. We performed this computation for  $q = 5, 6, 7, 8$ . [The case  $q = 4$  is very special. First, the statistical weight (4.1) associated to a plaquette with all the spins in different colors (i.e.,  $C = 4 = q = r$ ) is zero. Second and more important, there are configurations of the spins  $t_1, \dots, t_4, t'_1, \dots, t'_4$  for which *all* possible values of  $t_0$  are forbidden at  $T = 0$ , so that the probability measure  $\rho_0(\cdot|\{t\})$  at  $T = 0$  is ill-defined. In this case, we would have to compute  $\rho_0(\cdot|\{t\})$  at  $T > 0$  and then take the limit  $T \rightarrow 0$ . We are not going to consider such pathological cases in this paper.<sup>11</sup>]

The numerical results for  $q = 5, 6, 7, 8$  are displayed in Table II. Moreover, the general formulae for  $q \geq 6$  can be easily guessed. The method is as follows: First, we identify which are the configurations that

<sup>10</sup> Given a list of all the possible configurations (not related by a permutation of the colors) for  $n$  spins, it is very simple to construct the same list for  $n + 1$  spins. The starting point of the algorithm is trivial: for one spin there is only one such configuration.

<sup>11</sup> In any case, we shall see (empirically for our lattices) that Dobrushin's criterion is never satisfied when  $q = r + 1$ . As  $\alpha$  seems (again empirically) to be a decreasing function of  $q$ , Dobrushin's criterion would not hold when  $q = r$ .



**Table II. Numerical Results for the Square Lattice<sup>a</sup>**

$q$	$c_{0,nn}$	$c_{0,nnn}$	$\alpha$
5	0.3750	0.2353	2.4412
6	0.1899	0.1093	1.1967
7	0.1137	0.0636	0.7093 < 1
8	0.0756	0.0415	0.4683 < 1

<sup>a</sup> For each value of  $q$  we show the quantities  $c_{0,nn}$  and  $c_{0,nnn}$ . Finally, we give the value of the parameter  $\alpha = 4c_{0,nn} + 4c_{0,nnn}$ . When  $\alpha < 1$  there is a unique Gibbs measure at  $T = 0$ .

maximize  $c_{0,nn}$  for each value of  $q$ . There is (empirically) a value of  $q = q_{min}^{nn}$  such that whenever  $q \geq q_{min}^{nn}$  we always find the same maximizing configurations for  $c_{0,nn}$ . For these configurations we can compute exactly the value of  $c_{0,nn}$  for general  $q \geq q_{min}^{nn}$ . The same procedure can be carried out for  $c_{0,nnn}$ . For the square lattice we find that  $q_{min}^{nn} = 6$  and  $q_{min}^{nnn} = 5$ . The configurations found to maximize  $c_{0,nn}$  and  $c_{0,nnn}$  are depicted in Table III. From these patterns it is very easy to compute the general formulae:

$$c_{0,nn} = \frac{(q-3)^2(2q-7)}{q^5 - 16q^4 + 108q^3 - 391q^2 + 764q - 639} \quad \text{for } q \geq 6 \quad (4.4)$$

$$c_{0,nnn} = \frac{(q-3)^3}{q^5 - 16q^4 + 108q^3 - 389q^2 + 749q - 611} \quad \text{for } q \geq 5 \quad (4.5)$$

These results show that Dobrushin's condition  $\alpha < 1$  holds for  $q \geq 7$ . This value is two units smaller than the value obtained by Kotecký ( $q \geq 9$ ), although still far from the truth ( $q \geq 4$ , or more precisely,  $q > 3$ ).

**Table III. Configurations Which Maximize  $c_{0,nn}$  and  $c_{0,nnn}$  for the Square Lattice when  $q \geq 5$ <sup>a</sup>**

$c_{0,nn}$	$c_{0,nnn}$
<p style="text-align: center;"><math>q = 5</math></p>	<p style="text-align: center;"><math>q \geq 6</math></p>
<p style="text-align: center;"><math>q \geq 5</math></p>	

<sup>a</sup> Each distinct letter represents a distinct spin value. The spin  $t_0$  is denoted by an empty circle ( $\circ$ ). The spin  $t_j$  is the one that has two different spin values associated to it.

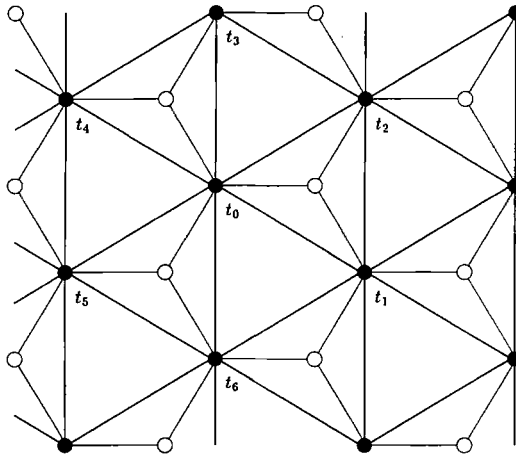


Fig. 6. Decimation for the hexagonal lattice. The original hexagonal lattice is drawn with thin lines; the empty circles represent the spins summed over; the triangular lattice resulting from decimation is drawn with solid circles and thick lines. Each spin  $t_0$  of the decimated lattice interacts with six nearest-neighbor spins  $t_1, \dots, t_6$ .

### 4.2. Hexagonal Lattice

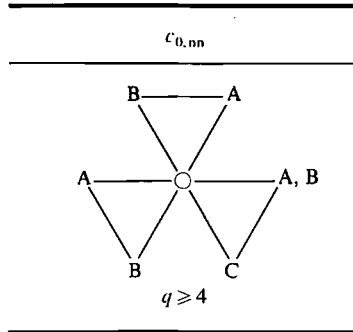
This lattice is also bipartite, so we can again sum over one of the two sublattices (empty circles in Fig. 6). By this decimation process we obtain a triangular lattice (solid circles in Fig. 6). The statistical weight (4.1) consists of three-body interactions living on the triangles that contain a decimated spin in their interior. To each spin  $t_0$  there correspond three such triangles:  $(t_0, t_1, t_2)$ ,  $(t_0, t_3, t_4)$ , and  $(t_0, t_5, t_6)$ ; so  $t_0$  interacts with six nearest-neighbor spins. All these spins are equivalent, so in this case we only have to compute one quantity  $c_{0,nn}$ . We then have  $\alpha = 6c_{0,nn}$ .

Table IV. Numerical Results for Hexagonal Lattice<sup>a</sup>

$q$	$c_{0,nn}$	$\alpha$
4	0.2667	1.6000
5	0.1233	$0.7397 < 1$
6	0.0699	$0.4192 < 1$

<sup>a</sup> For each value of  $q$  we compute the quantities  $c_{0,nn}$  and  $\alpha = 6c_{0,nn}$ .

**Table V. Configurations Which Maximize  $c_{0,nn}$  for the Hexagonal Lattice when  $q \geq 4$ <sup>a</sup>**



<sup>a</sup>The notation is as in Table III. Notice that, because the two outer spins within each triangle are equivalent, we can freely permute their values.

The numerical results for  $q = 4, 5, 6$  are contained in Table IV. The general form of  $c_{0,nn}$  can be guessed from the configuration which maximizes  $c_{0,nn}$  for  $q \geq 4$ ; this configuration is shown in Table V. The formula for  $c_{0,nn}$  is

$$c_{0,nn} = \frac{(q-2)^2}{q^4 - 9q^3 + 33q^2 - 59q + 43} \quad \text{for } q \geq 4 \quad (4.6)$$

We see that Dobrushin's condition  $\alpha < 1$  holds for  $q \geq 5$ . We again improve Kotecký's result ( $q \geq 7$ ) by two units. This should be compared to the believed exact result  $q \geq 3$  (more precisely,  $q > 2.618\dots$ ).

### 4.3. Triangular Lattice

This lattice is tripartite. We can decimate it by summing over all the spins belonging to one of the three sublattices (empty circles in Fig. 7). The result of the decimation process is a hexagonal lattice (solid circles in Fig. 7). From (4.1) we see that the interaction lives now on the hexagonal faces of this lattice, so each spin  $t_0$  interacts with the other 12 spins belonging to the three hexagons to which  $t_0$  belongs:  $(t_0, t_1, t'_1, t'_2, t'_3, t_2)$ ,  $(t_0, t_2, t'_4, t'_5, t'_6, t_3)$ , and  $(t_0, t_3, t'_7, t'_8, t'_9, t_1)$ . There are two types of neighboring spins: nearest-neighbor spins  $t_1, t_2, t_3$  (which belong to two different hexagons), and next-to-nearest neighbors  $t'_1, \dots, t'_9$  (which belong to

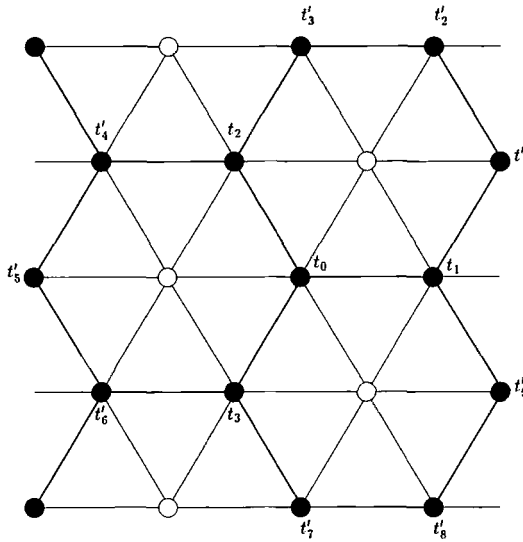


Fig. 7. Decimation for the triangular lattice. The original triangular lattice corresponds to both thin and thick lines; the empty circles represent the spins summed over; the hexagonal lattice resulting from decimation is drawn with solid circles and thick lines. Each spin  $t_0$  of the decimated lattice interacts with 12 spins: three nearest neighbors  $t_1, t_2, t_3$  and the nine next-to-nearest neighbors  $t'_1, \dots, t'_9$ .

only one hexagon).<sup>12</sup> For each type we have to compute the corresponding quantity (4.2). We again denote these  $c_{0, nn}$  and  $c_{0, nnn}$ , respectively. The quantity  $\alpha$  can be written as  $\alpha = 3c_{0, nn} + 9c_{0, nnn}$ .

There is one important point concerning this lattice. In the previous two examples the links of the decimated lattice did not coincide with those of the original lattice. However, in the triangular lattice the links of the decimated lattice are a *subset* of the links of the original lattice. This means that the statistical weight associated to a given hexagon is not given merely by (4.1); one has also the two-body interactions from the original Hamiltonian. For example, the weight associated at  $T=0$  to the hexagon  $(t_0, t_1, t'_1, t'_2, t'_3, t_2)$  is not  $q - C(t_0, t_1, t'_1, t'_2, t'_3, t_2)$ , but rather

$$\begin{aligned}
 & [q - C(t_0, t_1, t'_1, t'_2, t'_3, t_2)](1 - \delta_{t_0, t_1})(1 - \delta_{t_1, t'_1})(1 - \delta_{t'_1, t'_2}) \\
 & \times (1 - \delta_{t'_2, t'_3})(1 - \delta_{t'_3, t_2})(1 - \delta_{t_2, t_0})
 \end{aligned} \tag{4.7}$$

<sup>12</sup> Geometrically there are two classes of next-to-nearest-neighbor spins: those diametrically opposite to  $t_0$  (e.g.,  $t'_2$ ) and those not (e.g.,  $t'_1$  and  $t'_3$ ). But these two classes play identical roles in the interaction (4.1), which is invariant under permutations of  $t_1, \dots, t_r$ .

**Table VI. Numerical Results for Triangular Lattice<sup>a</sup>**

$q$	$c_{0,nn}$	$c_{0,nnn}$	$\alpha$
7	0.5714	0.2667	4.1143
8	0.3803	0.1233	2.2504
9	0.2832	0.0699	1.4784
10	0.2244	0.0446	1.0743
11	0.1852	0.0307	0.8324 < 1
12	0.1574	0.0224	0.6741 < 1

<sup>a</sup> Notation is as in Table II; here  $\alpha = 3c_{0,nn} + 9c_{0,nnn}$ .

When we take account of the three hexagons adjoining  $t_0$ , we have to include 15 factors  $1 - \delta_{t_k, t_j}$  in our statistical weight. However, only the three factors  $(1 - \delta_{t_0, t_1})(1 - \delta_{t_0, t_2})(1 - \delta_{t_0, t_3})$  are essential. This is because those delta functions whose arguments are both distinct from  $t_0$  are simply boundary conditions (their values are independent of  $t_0$ ). If their product is nonzero, they will factor out when computing  $\rho_0$ . If their product is zero,

**Table VII. Configurations Maximizing  $c_{0,nn}$  and  $c_{0,nnn}$  for the Triangular Lattice when  $q \geq 7$ <sup>a</sup>**

$c_{0,nn}$	$c_{0,nnn}$
$q \geq 7$	$q \geq 7$

<sup>a</sup> Notation is as in Table III. Notice that, as in Table V, we obtain equivalent configurations by permuting the outer spins within each hexagon (i.e., those spins that are not shared between two hexagons).

then we should go to  $T > 0$  [where the corresponding weight  $\exp(J\delta_{i_k, i_j})$  is nonzero], do the computation (and factor their contribution out), and take the limit  $T \rightarrow 0$ . At the end, the result would be the same as if we had omitted these factors from the very beginning.

The numerical results for  $7 \leq q \leq 12$  are displayed in Table VI. We find that there are two different types of configurations maximizing  $c_{0, nn}$ , and only one for  $c_{0, nnn}$ ; these patterns are depicted in Table VII. Using the configurations represented in Table VII, it is very easy to guess the general formulae for  $c_{0, nn}$  and  $c_{0, nnn}$ :

$$c_{0, nn} = \frac{(q - 5)^3}{q^4 - 21q^3 + 168q^2 - 609q + 847} \quad \text{for } q \geq 7 \quad (4.8)$$

$$c_{0, nnn} = \frac{(q - 5)^3}{q^4 - 21q^3 + 168q^2 - 608q + 841} \quad \text{for } q \geq 7 \quad (4.9)$$

We see that Dobrushin's condition  $\alpha < 1$  holds for  $q \geq 11$ , which is again an improvement of two units compared to Kotecký's result ( $q \geq 13$ ). Our result should be compared with the expected exact value  $q \geq 5$  (or more precisely,  $q > 4$ ).

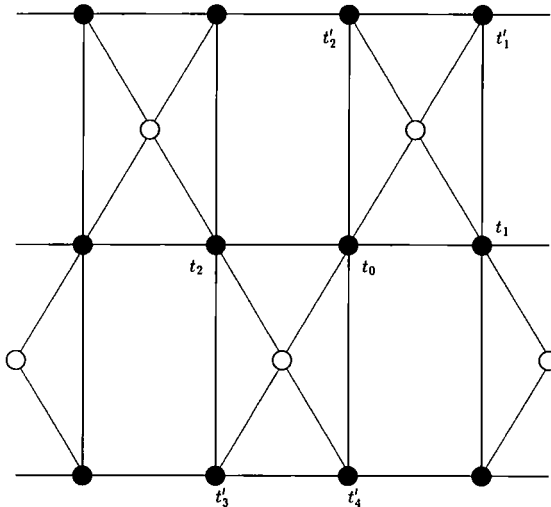


Fig. 8. Decimation for the Kagomé lattice. The original Kagomé lattice corresponds to all the diagonal and horizontal lines; the empty circles represent the spins summed over; the square lattice resulting from decimation is defined by the horizontal and vertical lines. Each spin  $t_0$  of the decimated lattice (solid circles) interacts with six spins: two nearest neighbors  $t_1, t_2$  and four next-to-nearest neighbors  $t'_1, t'_2, t'_3, t'_4$ . All these six spins live on the two "crossed" squares to which  $t_0$  belongs.

#### 4.4. Kagomé Lattice

In this case we sum over those spins situated on the top vertex of the up-pointing triangles (open circles in Fig. 8). After decimation we obtain a square lattice defined by the solid circles in Fig. 8. Obviously the interaction (4.1) lives on the “crossed” squares (i.e., those which have a decimated spin, indicated by an open circle, inside). Each spin  $t_0$  interacts with two such squares:  $(t_0, t_1, t'_1, t'_2)$  and  $(t_0, t_2, t'_3, t'_4)$ . Among the six spins with which  $t_0$  interacts, we can distinguish two types: two nearest-neighbor spins ( $t_1$  and  $t_2$ ), which are connected to  $t_0$  through an original link; and four next-to-nearest-neighbor spins ( $t'_1, t'_2, t'_3, t'_4$ ), which are connected to  $t_0$  through the plaquette interaction. We associate a different value of  $c_{0,j}$  to each type of spin ( $c_{0,nn}$  and  $c_{0,nnn}$ , respectively). The quantity  $\alpha$  is now equal to  $\alpha = 2c_{0,nn} + 4c_{0,nnn}$ .

As explained in the last subsection, we have to include in the statistical weight the delta functions corresponding to the surviving original links and involving the spin  $t_0$ . In this example there are two such factors:  $(1 - \delta_{t_0, t_1})(1 - \delta_{t_0, t_2})$ . The numerical results for  $q = 5, 6, 7, 8$  are displayed in Table VIII. The configurations which maximize  $c_{0,j}$  for each type of neighbor  $t_j$  are shown in Table IX. Using the configurations depicted in Table IX, it is easy to guess the general formulae for  $c_{0,nn}$  and  $c_{0,nnn}$ :

$$c_{0,nn} = \frac{q-3}{q^2-7q+13} \quad \text{for } q \geq 5 \quad (4.10)$$

$$c_{0,nnn} = \frac{q-3}{q^3-10q^2+35q-43} \quad \text{for } q \geq 5 \quad (4.11)$$

We see that Dobrushin's condition  $\alpha < 1$  holds for  $q \geq 7$ . Again we obtained an improvement of two units over Kotecký's result ( $q \geq 9$ ). Our bound  $q \geq 7$  should be compared to the exact result  $q \geq 4$  (or more precisely,  $q > 3$ ).

**Table VIII. Numerical Results for Kagomé Lattice<sup>a</sup>**

$q$	$c_{0,nn}$	$c_{0,nnn}$	$\alpha$
5	0.6667	0.2857	2.4762
6	0.4286	0.1304	1.3789
7	0.3077	0.0727	0.9063 < 1
8	0.2381	0.0459	0.6597 < 1

<sup>a</sup> Notation is as in Table II; here  $\alpha = 2c_{0,nn} + 4c_{0,nnn}$ .

**Table IX. Configurations Which Maximize  $c_{0,nnn}$  and  $c_{0,nnn}$  for the Kagomé Lattice when  $q \geq 5$ "**

$c_{0,nn}$	$c_{0,nnn}$
<p><math>q \geq 5</math></p>	<p><math>q \geq 5</math></p>

" Notation is as in Table III. In the diagrams a thick line represents a link belonging to the original lattice (and carrying an additional Kronecker delta term). On each square the two spins not connected to such a link can be freely interchanged.

## 5. FURTHER IMPROVEMENTS: CLUSTER DECIMATION

In this section we present slightly better results for the hexagonal and Kagomé lattices. The idea is simple: if using single-site decimation (Section 4) we obtained improved bounds, then it is natural to expect even better results if we decimate clusters of nearby spins. This is what happens in the proof presented in ref. 42, and it happens also in our case. Obviously, as we decimate larger clusters, the effective interaction among the remaining spins becomes more and more complicated (the effective interaction contains between 128 and 2410 terms for the three cases considered below); this fact limits the practical utility of this method. Nevertheless, we have been able to improve slightly our previous results in two cases: the hexagonal and Kagomé lattices. Our method will be explained in detail in the following subsections.

### 5.1. Hexagonal Lattice

The first step is to choose suitable clusters of spins to be summed over. In this example we selected a subset of the hexagonal faces of the original lattice (see Fig. 9). The remaining spins (solid circles) define the decimated lattice, which is again a hexagonal lattice. Each hexagonal face of this decimated lattice contains one hexagonal cluster of spins that were summed over (empty circles). It is important to notice that these clusters (of empty circles) do not have any nearest-neighbor interactions with other such clusters. So we can perform the sum over the six spins belonging to the



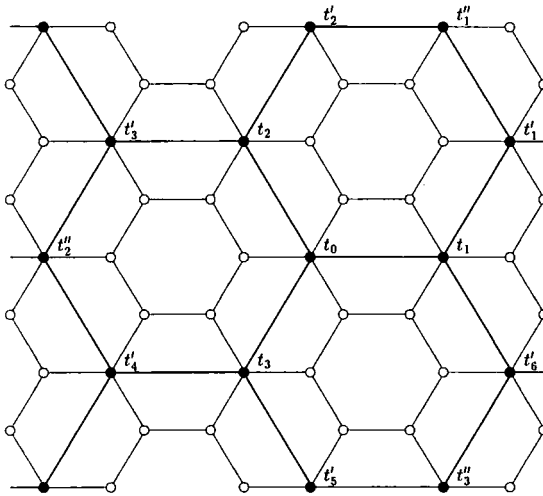


Fig. 9. More complex decimation for the hexagonal lattice. The original lattice is drawn with thin lines; the empty circles represent the spins summed over; the decimated lattice is drawn with solid circles and thick lines. Each spin  $t_0$  of the decimated lattice interacts with 12 spins: three nearest neighbors  $t_1, t_2, t_3$ , six second-nearest neighbors  $t'_1, \dots, t'_6$ , and three third-nearest neighbors  $t''_1, t''_2, t''_3$ .

cluster, and obtain an effective interaction among the six spins of the decimated lattice surrounding the cluster. However, this effective interaction is not as simple as the single-site-decimation interaction (4.1). To be able to handle it, we wrote a program in MATHEMATICA to do all the required sums. The final expression can be written as a certain linear combination of products of Kronecker delta functions. This turns to be very long and complicated, so we omit its form here.<sup>13</sup> We remark that this interaction has the property that even when  $q = 3 = r$ , every state of  $t_0$  gets nonzero weight, irrespective of the configuration of the neighboring spins; in particular, there is no ambiguity at  $T = 0$ , in contrast to what happens for the single-site-decimation interaction (4.1).

<sup>13</sup> Actually, we did not use this expression in our FORTRAN programs, as it is very memory- and time-consuming. Rather, we first classified all the possible configurations into classes with the same statistical weight. For the cases considered here, the number of classes is moderate (up to 36). The important point is that we can easily tell to which class a given configuration belongs, by measuring a few quantities (such as the number of distinct colors of the configuration). We then devise a simple formula that reproduces the correct statistical weight. The practical procedure depends on the lattice and type of decimation considered, but it is always faster and less memory-consuming than direct use of the formula computed with MATHEMATICA.

**Table X. Numerical Results for the Hexagonal Lattice when We Use Six-spin Decimation"**

$q$	$c_{0,1n}$	$c_{0,2n}$	$c_{0,3n}$	$\alpha$
3	0.5685	0.3904	0.2136	4.5985
4	0.1036	0.0292	0.0164	0.5356 < 1

"For each type of neighbor we show the corresponding value  $c_{0,j}$ . We also show  $\alpha = 3c_{0,1n} + 6c_{0,2n} + 3c_{0,3n}$ . When  $\alpha < 1$  there is a unique Gibbs measure at  $T = 0$ .

The effective interaction lives on the hexagonal faces of the decimated lattice. Each spin  $t_0$  interacts with three hexagons:  $(t_0, t_1, t'_1, t''_1, t'_2, t_2)$ ,  $(t_0, t_2, t'_3, t''_2, t'_4, t_3)$ , and  $(t_0, t_3, t'_5, t''_3, t'_6, t_1)$ . There are three types of neighbors: three nearest-neighbor spins  $t_1, t_2, t_3$  (which belong to two different hexagons), six second-nearest-neighbor spins  $t'_1, \dots, t'_6$  (which belong to only one hexagon and which are not diametrically opposite to  $t_0$ ), and three third-neighbor spins  $t''_1, t''_2, t''_3$  (which belong to only one hexagon and which are diametrically opposite to  $t_0$ ). We have to compute a different  $c_{0,j}$  for each type of neighbor: we denote these  $c_{0,1n}$ ,  $c_{0,2n}$ , and  $c_{0,3n}$ , respectively. The quantity (2.5) is now equal to  $\alpha = 3c_{0,1n} + 6c_{0,2n} + 3c_{0,3n}$ .

The numerical results for  $q = 3, 4$  are displayed in Table X. We see that Dobrushin's condition  $\alpha < 1$  is satisfied for  $q = 4$ , so we have improved by one unit the bound of Section 4. That is, we have proven that for the hexagonal lattice at zero temperature there is exponential decay of correlations for  $q \geq 4$ . The expected result is  $q > 2.618\dots$

## 5.2. Kagomé Lattice

In this case our chosen clusters will be a subset of the triangular faces of the Kagomé lattice (empty circles in Fig. 10); they are not connected by any nearest-neighbor interaction. The remaining spins (solid circles) define the decimated lattice, which turns out to be hexagonal. The triangular clusters are surrounded by the "deformed" hexagonal faces of the decimated lattice. In addition, there are hexagonal faces of the original lattice which belong also to the decimated lattice. The effective interaction coming from the decimation procedure lives on the "deformed" hexagonal faces only. It has again a very complicated form, and we had to use MATHEMATICA to compute it. When  $q = 4 = r$  we see that the effective interaction assigns a zero weight to a few configurations. However, there are no configurations of the neighboring spins for which *all* the possible values of  $t_0$  are forbidden, so there is no ambiguity at  $T = 0$  even in this case.

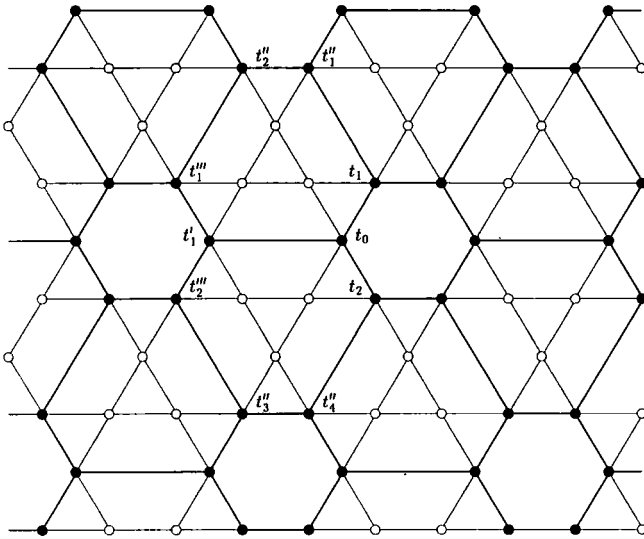


Fig. 10. More complex decimation for the Kagomé lattice. The original lattice corresponds to the whole set of circles (empty and solid) and the *nearest-neighbor* bonds between them; the empty circles represent the spins summed over; the decimated lattice is drawn with solid circles and thick lines. Each spin  $t_0$  of the decimated lattice interacts with nine spins: two nearest neighbors  $t_1, t_2$ , one second-nearest neighbor  $t'_1$ , four third-nearest neighbors  $t''_1, t''_2, t''_3, t''_4$ , and two fourth-nearest neighbors  $t'''_1, t'''_2$ .

From Fig. 10 we see that each spin  $t_0$  of the decimated lattice interacts with only two “deformed” hexagons. There are four types of neighboring spins: two nearest-neighbor spins  $t_1, t_2$  (which belong to only one hexagon), one second-nearest neighbor  $t'_1$  (which belongs to both hexagons), four third-nearest neighbors  $t''_1, t''_2, t''_3, t''_4$  (which belong to one hexagon and are not connected to  $t'_1$ ), and two fourth-nearest neighbors  $t'''_1, t'''_2$  (which belong to only one hexagon and are connected to  $t'_1$ ). Notice that, in addition to the effective interaction coming from the decimation procedure, we have to include the factors  $(1 - \delta_{t_0, t_1})(1 - \delta_{t_0, t_2})$  arising from the original two-body interaction, because the links  $\langle t_0, t_1 \rangle$  and  $\langle t_0, t_2 \rangle$  belong also to the original lattice. To each neighbor type we associate a different  $c_{0, j}$ : we denote these  $c_{0, 1n}, c_{0, 2n}, c_{0, 3n}$  and  $c_{0, 4n}$ , respectively. The quantity (2.5) takes the form  $\alpha = 2c_{0, 1n} + c_{0, 2n} + 4c_{0, 3n} + 2c_{0, 4n}$ .

In Table XI we show our numerical results for  $q = 4, 5, 6$ . We notice that the constants for the third and fourth nearest neighbors coincide in all cases. (However, we were unable to find an analytic proof of this result. In particular, there does not appear to be any symmetry that would yield this equality.) Dobrushin’s condition  $\alpha < 1$  holds for  $q = 6$ , improving the result

**Table XI. Numerical Results for the Kagomé Lattice when We Use Three-Spin Decimation<sup>a</sup>**

$q$	$c_{0,1n}$	$c_{0,2n}$	$c_{0,3n}$	$c_{0,4n}$	$\alpha$
4	1.0000	1.0000	0.6667	0.6667	7.0000
5	0.4949	0.1590	0.1003	0.1003	1.7504
6	0.2975	0.0581	0.0330	0.0330	0.8529 < 1

<sup>a</sup> Notation is as in Table X; here  $\alpha = 2c_{0,1n} + c_{0,2n} + 4c_{0,3n} + 2c_{0,4n}$ .

of Section 4 by one unit. So, there is no phase transition at zero temperature for the Kagomé lattice when  $q \geq 6$ , which should be compared with the expected result  $q > 3$ .

We have also tried to improve these results by considering decimation of hexagonal clusters (as we did in the previous subsection). After the decimation procedure we obtained a new Kagomé lattice (rotated 90 degrees). The values of  $\alpha$  for  $q = 4, 5$  were 3.83 and 1.07, respectively, which are smaller than the corresponding values reported in Table XI. However, in both cases  $\alpha > 1$ . Therefore, we are unable to prove exponential decay of correlations for  $q < 6$ .

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