A Personal List of Unsolved Problems
Concerning Lattice Gases
and Antiferromagnetic Potts Models*

Alan D. Sokal
Department of Physics
New York University
4 Washington Place
New York, NY 10003 USA
SOKAL@NYU.EDU

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Abstract
I review recent results and unsolved problems concerning the hard-core
lattice gas and the \( q \)-coloring model (antiferromagnetic Potts model at zero
temperature). For each model, I consider its equilibrium properties (unique-
ness/nonuniqueness of the infinite-volume Gibbs measure, complex zeros of the
partition function) and the dynamics of local and nonlocal Monte Carlo algo-
rithms (ergodicity, rapid mixing, mixing at complex fugacity). These problems
touch on mathematical physics, probability, combinatorics and theoretical com-
puter science.

[Pour M. Toubon] Je passe en revue des résultats récents et des problèmes
non résolus concernant le gaz sur réseau avec exclusion et le modèle de \( q \)-
coloriage (modèle de Potts antiferromagnétique à température nulle). Pour
chacun des deux modèles, je considère ses propriétés d’équilibre (unicité/non-
unicité de la mesure de Gibbs en volume infini, zéros complexes de la fonction de
partition) et la dynamique des algorithmes Monte Carlo locaux et non-locaux
(ergodicité, mélange rapide, mélange à fugacité complexe). Ces problèmes
touchent à la physique mathématique, à la probabilité, à la combinatoire et
t’à l’informatique théorique.

Running title: Lattice Gases and Potts Models

Key words: Hard-core lattice gas; \( q \)-coloring problem; antiferromagnetic Potts
model; independent-set polynomial; chromatic polynomial; Gibbs measure; phase
transition; Monte Carlo; rapid mixing.

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1 Introduction

In this paper I propose to review some recent results and to list some open problems concerning a pair of statistical-mechanical lattice models (defined precisely in Sections 2 and 3):

- Hard-core lattice gas with nearest-neighbor exclusion and fugacity \( w \) (= “independent-set model” in graph-theory language)

- \( q \)-coloring of the vertices of a graph

(These are zero-temperature models. More generally, one can study the hard-core lattice gas with a soft nearest-neighbor repulsion, and the antiferromagnetic Potts model at nonzero temperature.)

What these two models have in common is that they are “antiferromagnetic”: nearest neighbors prefer to be (in the \( q \)-coloring case have to be) in different states. Unlike ferromagnetic models, for which (roughly speaking) only one type of ordered phase is possible, in antiferromagnetic models the possible types of order can depend delicately on the parameters (e.g. \( w \) or \( q \)) and on the nature of the lattice (e.g. bipartite or not). This motivates studying these models on an arbitrary graph \( G = (V, E) \) — and not just on a regular lattice — in order to investigate which features of \( G \) correlate with which features of the phase transition. Here \( G \) will be either finite or countably infinite, depending on the question being investigated.

There is one other motivation for studying these models on arbitrary graphs: The hard-core lattice gas on a general graph \( G \) (with different fugacities \( w_i \in \mathbb{C} \) assigned to different vertices) is in fact the universal statistical-mechanical model in the sense that any statistical-mechanical model living on a vertex set \( V_0 \) can be mapped onto a gas of nonoverlapping “polymers” on \( V_0 \), i.e. a hard-core lattice gas on the intersection graph of \( V_0 \) [53, Section 5.7].

For each of these models, I will discuss the following questions:

- Equilibrium statistical mechanics
  - Uniqueness/nonuniqueness/properties of Gibbs measures in infinite volume
  - Complex zeros (in \( w \) or \( q \)) of the partition function in finite volume

- Monte Carlo algorithms (single-site, local and nonlocal)
  - Ergodicity (this is sometimes nontrivial at zero temperature)
  - Rapid mixing
  - Mixing at complex \( w \) or \( q \) (a new and perhaps crazy idea)

I want to stress that I’m not an expert on any of these things, so some of my questions may be naive and some of the “open problems” that I pose may already be solved.
2 Lattice Gas: Equilibrium Properties

Let \( G = (V, E) \) be a finite graph, and let \( w = \{w_x\}_{x \in V} \) be a set of (possibly complex) fugacities. The partition function of the hard-core lattice gas (= independent-set polynomial) on \( G \) is

\[
Z(w) = \sum_{A \subseteq V} \prod_{x \in A} w_x . \tag{2.1}
\]

(Recall that \( A \subseteq V \) is called an independent set if it does not contain any pair of adjacent vertices.) When the fugacities are nonnegative, an equilibrium probability distribution on the state space \( 2^V \) can be defined by

\[
\mu(A) = Z(w)^{-1} \prod_{x \in A} w_x \times \chi(A \text{ independent}) . \tag{2.2}
\]

When \( G \) is countably infinite and the fugacities are nonnegative, Gibbs measures can then be defined by the usual Dobrushin–Lanford–Ruelle prescription [26].

At small \( w \) we expect to have uniqueness of the Gibbs measure, exponential decay of correlations, analyticity, etc. Indeed, the Dobrushin uniqueness theorem [26, 59] easily implies the uniqueness of the infinite-volume Gibbs measure, and the exponential decay of correlations in this unique Gibbs measure, whenever \( 0 \leq w_x \leq (1 - \epsilon)/(d_x - 1 + \epsilon) \) for all vertices \( x \) [here \( \epsilon > 0 \), and \( d_x \) denotes the number of vertices adjacent to \( x \)]. In particular, when all vertices are assigned the same fugacity \( w \), this happens whenever \( 0 \leq w < 1/(\Delta - 1) \) [here \( \Delta = \max_{x \in V} d_x \) is the maximum degree of \( G \)].

A slightly better bound [4] can be obtained using the disagreement-percolation method: if the site percolation model on \( G \) with occupation probabilities \( p_x = w_x/(1 + w_x) \) has (with probability 1) no infinite occupied cluster, then the hard-core lattice gas with fugacities \( w \) has a unique Gibbs measure; moreover, the two-point covariances in the lattice gas are bounded above by the corresponding connection probabilities in the percolation model. In particular, if \( 0 \leq p_x \leq (1 - \epsilon)/(d_x - 1) \) for all vertices \( x \), then standard arguments (comparison to a branching process) show that the percolation model has (w.p. 1) no infinite occupied cluster and has exponential decay of connectivities. So we prove uniqueness and exponential decay for the lattice gas whenever \( 0 \leq w_x \leq (1 - \epsilon)/(d_x - 2 + \epsilon) \) for all vertices \( x \), or \( 0 \leq w < 1/(\Delta - 2) \) in case the fugacities are all equal.

It is natural to ask whether this result is sharp. The answer is almost certainly no: Vigoda [67, 68] improves \( 1/(\Delta - 2) \) to \( 2/(\Delta - 2) \), at least for regular lattices, as a byproduct of proving rapid mixing of Glauber dynamics (see Section 4 below).

\[\text{But I suspect that this result is not sharp either, and that the optimal result is:}\]

\[1\] For some lattices, the disagreement-percolation bound is better than \( 2/(\Delta - 2) \). For example, the triangular-lattice site-percolation model has \( p_c = 1/2 \) [49], which implies uniqueness of the triangular-lattice-gas Gibbs measure for for \( w < 1 \); but \( 2/(\Delta - 2) = 1/2 \).
Conjecture 2.1 For any countably infinite graph $G$ of maximum degree $\Delta$, the hard-core lattice gas on $G$ has a unique Gibbs measure whenever $0 \leq w_x \leq (1 - \epsilon) \times (\Delta - 1)^{\Delta-1}/(\Delta - 2)^{\Delta}$ \(\sim e/\Delta\) for large $\Delta$ for all vertices $x$, for some $\epsilon > 0$. [Perhaps this is true even with $\epsilon = 0$.]

Conjecture 2.1 is motivated by the fact that $w = (\Delta - 1)^{\Delta-1}/(\Delta - 2)^{\Delta}$ is the critical point for the complete rooted tree with branching factor $r = \Delta - 1$ \[53, 33, 7, 6, 65\]. It seems to be an open problem to prove Conjecture 2.1 even when $G$ is a non-regular tree and the $w_x$ are all equal.

On a finite graph $G$, the free energy $\log Z(w)$ and the correlation functions (which are derivatives of $\log Z$) are analytic functions of $w$ on any simply connected domain $D \subset \mathbb{C}$ where $Z(w)$ is nonvanishing. Moreover, by a standard Vitali argument \[59, pp. 417–418\], this analyticity can be carried over to the infinite-volume limit whenever this limit exists for real $w$ (e.g. for amenable transitive graphs). So it is of great interest to find sufficient conditions for the nonvanishing of $Z(w)$ which is trivial when $w \geq 0$, but not when $w$ is negative or complex. Shortly before his death, Dobrushin \[18, 19\] proved a beautiful theorem on the absence of zeros of $Z(w)$ at small complex fugacity:

**Theorem 2.2 (Dobrushin \[18, 19\])** Let $\{c_x\}_{x \in V}$ be an arbitrary set of nonnegative numbers, and define

$$R_x = (1 - e^{-c_x}) \exp \left( - \sum_{y \sim x} c_y \right)$$

where $y \sim x$ denotes that $y$ is adjacent to $x$. Then $Z(w)$ is nonvanishing in the closed polydisc $|w_x| \leq R_x$.

The proof is an extraordinarily simple 3-line induction on the number of vertices in $G$: see \[18, 19\], or see \[61, Section 3\] for an equally simple proof of a slightly stronger result.

**Corollary 2.3** If $G$ has maximum degree $\Delta$, then $Z(w)$ is nonvanishing in the closed polydisc $|w_x| \leq \Delta^\Delta / (\Delta + 1)^{\Delta+1}$ \(\sim 1/\epsilon\Delta\) for large $\Delta$.

**Remarks.** 1. Kotecký and Preiss \[38\] proved a result slightly weaker than Theorem 2.2, in which $1 - e^{-c_x}$ is replaced by $c_x e^{-c_x}$.

2. Corollary 2.3 is close to best possible: for the complete rooted tree with branching factor $r = \Delta - 1$ and depth $n$, $Z(w)$ has negative real zeros that tend to $w = -(\Delta - 1)^{\Delta-1}/\Delta^\Delta$ as $n \to \infty$ \[58, 38\]. Indeed, by an inductive argument closely related to (but more subtle than) Dobrushin’s, Shearer \[58\] improves Corollary 2.3 to the optimal radius $(\Delta - 1)^{\Delta-1}/\Delta^\Delta$. Alex Scott and I are investigating analogous improvements of Theorem 2.2. Note that this optimal radius is a factor $\approx e$ smaller than the interval at real positive $w$ that is obtained by the Dobrushin uniqueness theorem, and a factor $\approx e^2$ smaller than the interval proposed in Conjecture 2.1.
3. For any lattice gas with repulsive interactions — and in particular for one with hard-core exclusions — the Mayer expansion \( \log Z(w) = \sum c_n w^n \) has alternating signs: \((-1)^{|n|-1}c_n \geq 0\). It follows that the zero of \( Z(w) \) closest to the origin always lies on the negative real axis.

4. Theorem 2.2 (which can be generalized to soft-core repulsive interactions [61]) provides an extraordinarily simple proof of the convergence of the Mayer expansion for such lattice gases. Recall that the usual approach to proving convergence of the Mayer expansion [46, 57, 16, 11, 59, 12, 64] is to explicitly bound the expansion coefficients; this requires some rather nontrivial combinatorics (for example, an inequality of Penrose [46] together with the counting of trees). Once this is done, an immediate consequence is that \( Z \) is nonvanishing in any polydisc where the series for \( \log Z \) is convergent. Dobrushin’s brilliant idea was to prove these two results in the opposite order: first one proves, by an elementary induction on the cardinality of the state space, that \( Z \) is nonvanishing in some specified polydisc; it then follows immediately that \( \log Z \) is analytic in that polydisc, and hence that its Taylor series is convergent there. It is an interesting open question to know whether this approach can be made to work without the assumption of hard-core self-repulsion.

What if we ask about regions of \( w \)-space other than polydiscs centered at \( w = 0 \)?

**Question 2.4** What is the largest complex domain containing \( w = 0 \) on which \( Z(w) \) is zero-free for all graphs of maximum degree \( \Delta \)? [This question has two versions, depending on whether the \( w_x \) are assumed equal or unequal. In the latter version, one seeks domains \( D \) for which \( Z(w) \neq 0 \) whenever \( w_x \in D \) for all \( x \); but there need not exist a unique maximal such domain.]

I conjecture that there is a complex domain \( D_\Delta \) containing at least the interval \( 0 \leq w < 1/(\Delta - 1) \) of the real axis — and possibly even the interval \( 0 \leq w < (\Delta - 1)^{\Delta-1}/(\Delta - 2)^\Delta \) — on which \( Z(w) \) is zero-free for all graphs of maximum degree \( \Delta \). See also Section 3 regarding mixing at complex fugacity.

Another question is: Can we get sharper constraints on the location of the complex zeros of \( Z(w) \) for restricted classes of graphs \( G \)? A classic result of this kind is due to Heilmann and Lieb [34] (see also [27, 39]): if \( G \) is a line graph, then all the zeros of \( Z(w) \) are negative real. [The lattice gas on a line graph \( L(H) \) is identical to the matching polynomial (monomer-dimer-model partition function) on \( H \).] Now, it is well known that \( G \) is a line graph if and only if nine particular graphs \( G_1, \ldots, G_9 \) do not appear as induced subgraphs of \( G \) [29, pp. 73–77]. It turns out that for eight of these “forbidden induced subgraphs”\(^\text{,} \) all the zeros of \( Z(w) \) are negative real; the only one with non-real zeros is the claw \( K_{1,3} \). This suggests the conjecture:

**Conjecture 2.5** (Hamidoune [28], Stanley [66]) If \( G \) is claw-free (i.e. has no induced subgraph \( K_{1,3} \)), then all the zeros of \( Z(w) \) are negative real.
As vague evidence in favor of this conjecture, let us mention the following: (a) It implies the log concavity of the counts of independent sets, which is indeed true for claw-free graphs [28]. (b) It is implied by a plausible conjecture concerning a special symmetric function $X_G$ associated to $G$ [66, Corollary 2.10]. (c) The recent disagreement-percolation proof of complete analyticity for the monomer-dimer model [1] generalizes immediately to the hard-core lattice gas on any claw-free graph [3].

For possibly useful background on claw-free graphs, see [22]; see also [25]. For interesting results along vaguely related lines, see [51, 52].

Finally, one may ask: What happens when the fugacity $w$ is not small? In particular, one would like to understand the uniqueness or nonuniqueness of the infinite-volume Gibbs measure as a function of $w$, the nature of the large-$w$ Gibbs measures, and whether the phase transition(s) is/are first-order or second-order. On a bipartite graph with symmetry between the two sublattices, the mechanism driving the phase transition is clear: at large $w$, one sublattice becomes preferentially occupied and the other preferentially vacant. But this does not necessarily exhaust the possible Gibbs measures: for example, on the 3-regular tree there also exist Gibbs measures in which the density is not constant on each sublattice [3]. Moreover, the nonuniqueness of the Gibbs measure is not necessarily monotone in $w$ [3]. For general (non-bipartite) graphs, the situation is even worse, and the nature of the possible ordered phases seems poorly understood at present.

3 $q$-Coloring Model: Equilibrium Properties

Let $G = (V, E)$ be a finite graph and let $q$ be a positive integer. A map $\sigma: V \to \{1, 2, \ldots, q\}$ is called a proper $q$-coloring of $G$ in case $\sigma(x) \neq \sigma(y)$ for all pairs of adjacent vertices $x \sim y$. We define $\mu$ to be the uniform probability distribution on the set of proper $q$-colorings of $G$ (whenever this set is nonempty). When $G$ is countably infinite, Gibbs measures can then be defined by the usual Dobrushin–Lanford–Ruelle prescription [26]. The $q$-coloring problem is the zero-temperature limit of the antiferromagnetic $q$-state Potts model [72, 73].

When $q$ is large compared to the maximum degree $\Delta$, the conditional probability distribution of $\sigma(x)$ depends only weakly on $\{\sigma(y)\}_{y \sim x}$, so we expect to have uniqueness of the infinite-volume Gibbs measure and exponential decay of correlations. This is in fact the case:

**Theorem 3.1 (Kotecký [37], Salas and Sokal [55])** If $q > 2\Delta$, the hypotheses of the Dobrushin uniqueness theorem hold. Consequently, there is a unique infinite-volume Gibbs measure, and it has exponential decay of correlations.

More generally, for antiferromagnetic Potts models with $q > 2\Delta$, there is a unique infinite-volume Gibbs measure, with exponential decay of correlations, uniformly
down to and including zero temperature \[55\]. Otherwise put, zero temperature belongs to the high-temperature regime! The reason, of course, is the large ground-state entropy.

Salas and Sokal \[55\] have some improvements of this result for specific regular lattices (square, triangular, hexagonal, Kagomé), based on decimation and a computer-assisted proof. But their results are far from sharp.

**Problem 3.2** *Prove uniqueness of the infinite-volume Gibbs measure and exponential decay of correlations for \( q = 3 \) on the hexagonal lattice, \( q = 4, 5, 6 \) on the square lattice, etc.*

For the \( q = 4 \) square-lattice model, perhaps one could use the Ashkin-Teller representation plus antipercolation ideas.

It is natural to ask whether the borderline \( 2\Delta \) is sharp for some (perhaps irregular) lattice. The answer is most likely no: Vigoda \[69\] improves \( 2\Delta \) to \( \frac{11}{6}\Delta \), at least for regular lattices, as a byproduct of proving rapid mixing of a particular local dynamics (see Section 5 below). But I suspect that this result is not sharp either. Even for the \( \Delta \)-regular tree, the correct borderline is not known; all that is known is that there is a nonunique Gibbs measure whenever \( q \leq \Delta \) \[17\] and a unique Gibbs measure whenever \( q \geq \) a certain \( q_c(\Delta) \) that satisfies \( q_c(\Delta) \leq \frac{5}{7}\Delta - 1 \) and \( \limsup_{\Delta \to \infty} q_c(\Delta)/\Delta \leq 1.6296 \[1\]. For trees the Gibbs measure may well be unique as soon as \( q > \Delta \); and it is at least conceivable that this is the sharp borderline for general graphs.

By the Fortuin-Kasteleyn representation \[34, 24\], the \( q \)-state Potts model can be analytically continued to complex \( q \); indeed, on any finite graph the Potts-model partition function is a polynomial in \( q \) (see e.g. \[61, Section 1\] for a review). Specializing to the \( q \)-coloring problem, we conclude that \( P_G(q) = \#(\text{proper } q\text{-colorings of } G) \) is the restriction to \( \mathbb{Z}_+ \) of a polynomial in \( q \), which is called the chromatic polynomial of \( G \) \[13, 50, 17\]. It therefore makes sense to study the real or complex zeros of \( P_G(q) \). Here are some recent results:

**Theorem 3.3** *(Sokal \[61\])*  

(a) For a graph \( G \) of maximum degree \( \Delta \), all the (real or complex) zeros of \( P_G(q) \) lie in the disc \( |q| < C(\Delta) \), where \( C(\Delta) \) is the solution of a certain transcendental equation and satisfies \( C(\Delta) < 7.963907\Delta \).

(b) For a graph \( G \) of second-largest degree \( \Delta \), all the (real or complex) zeros of \( P_G(q) \) lie in the disc \( |q| < C(\Delta) + 1 \).

The proof is based on writing the Fortuin-Kasteleyn representation of \( P_G(q) \) as a gas of nonoverlapping polymers \( P \) with fugacity \( w(P) \sim q^{-(|P|-1)} \). When \( |q| \) is large enough, one can apply Theorem 2.2 to this polymer gas, and conclude that \( Z \neq 0 \).
Question 3.4

(a) What is the sharp bound $C_{opt}(\Delta)$? Might $2\Delta$ work? Is $C_{opt}(3) = 3$? What about regions of the $q$-plane other than discs centered at $q = 0$?

(b) Can “second-largest degree” be improved to “max flow”? (See [61, Section 7] for details.)

(c) Can one obtain a sublinear bound for suitable subclasses of graphs?

- For theta graphs $\Theta_{s_1,\ldots,s_p}$ [consisting of a pair of endvertices connected by $p$ internally disjoint paths of lengths $s_1,\ldots,s_p$] the answer is yes: there is a bound of order $p/\log p$.[4]

- For series-parallel graphs, I conjecture that the answer is yes (again $p/\log p$) for maximum degree, and no for second-largest degree or max flow; I am currently trying to prove these claims.

- For planar graphs, it is an open question.

Let $C$ be the (countably infinite) set consisting of the chromatic roots of all finite graphs, and let $\overline{C}$ be its closure. Jason Brown (unpublished) asked whether $\overline{C}$ has nonzero two-dimensional Lebesgue measure. The answer is yes, in the strongest possible sense: $\overline{C}$ is the whole complex plane! More precisely, one has:

**Theorem 3.5 (Sokal [63])** For theta graphs $\Theta^{(s,p)} \ (= p$ parallel-connected chains each consisting of $s$ edges in series$)$, the roots of their chromatic polynomials, taken together, are dense in the entire complex $q$-plane with the possible exception of the disc $|q - 1| < 1$.

For a brief discussion of the intuition behind the proof, see [62].

**Corollary 3.6 (Sokal [63])** There is a countably infinite family of (not-necessarily-planar) graphs whose chromatic zeros are, taken together, dense in the entire complex $q$-plane.

Indeed, it suffices to consider the union of the two families $\Theta^{(s,p)}$ and $\Theta^{(s,p)} + K_2$ and to recall that $P_{G+K_n}(q) = q(q - 1)\cdots(q - n + 1)P_G(q - n)$.[5]

Here $K_2 = \begin{array}{c}
\end{array}$ is the complete graph on two vertices. The join of two graphs, denoted $G_1 + G_2$, is obtained from the disjoint union $G_1 \cup G_2$ by adjoining an edge between each pair of vertices $x \in G_1$ and $y \in G_2$. 

[2] Here $K_2 = \begin{array}{c}
\end{array}$ is the complete graph on two vertices. The join of two graphs, denoted $G_1 + G_2$, is obtained from the disjoint union $G_1 \cup G_2$ by adjoining an edge between each pair of vertices $x \in G_1$ and $y \in G_2$. 

\[\]
4 Lattice Gas: Dynamics of Algorithms

The single-site heat-bath (Glauber) dynamics for the hard-core lattice gas on a finite graph \( G = (V, E) \) is defined as follows: Choose uniformly at random a vertex \( x \in V \); make \( x \) occupied with probability \( \frac{w_x}{1 + w_x} \) if all the neighbors of \( x \) are vacant, and make \( x \) vacant otherwise. This is easily seen to define an irreducible Markov chain satisfying detailed balance with respect to the Gibbs distribution \( \mu \).

We want to know: Under what conditions is this Markov chain rapidly mixing, in the sense that its mixing time \( \tau(\varepsilon) \) is bounded by a (hopefully low-order) polynomial in \( n \) (the number of vertices in \( G \))?\footnote{We use here the computer scientists’ definition of mixing time: Let \( \Delta_x(t) = \frac{1}{2} \sum_y |(P^t)_{xy} - \pi_y| \) be the distance to stationarity after time \( t \), starting in state \( x \); and define the (worst-case) mixing time \( \tau(\varepsilon) = \max_x \min_t \{ t : \Delta_x(t') \leq \varepsilon \text{ for all } t' \geq t \} \).}

The standard proof of the Dobrushin uniqueness theorem (see e.g. [59, Section 5.1]) shows also the \( O(n \log n) \) mixing of the Glauber dynamics whenever the Dobrushin hypothesis holds. In particular, this holds for the hard-core lattice gas whenever \( 0 \leq w < \frac{1}{\Delta - 1} \). This result can alternatively be derived by path-coupling arguments, which also show \( O(n^2 \log n) \) mixing at \( w = 1/(\Delta - 1) \) [21].

These results are, however, not optimal. By more intricate coupling arguments, Luby and Vigoda [42, 67, 68] have recently proven \( O(n \log n) \) mixing of the Glauber dynamics for \( 0 \leq w < \frac{2}{\Delta - 2} \), and \( O(n^3) \) mixing at \( w = \frac{2}{\Delta - 2} \).\footnote{One can also consider more general local dynamics, such as the single-edge heat-bath algorithm [41, 21] or the Dyer-Greenhill chain [21].}

The mixing properties of the Glauber (or any local) dynamics are closely related to the model’s equilibrium properties. Indeed, consider a model defined on the regular lattice \( \mathbb{Z}^d \), and suppose that there exists a local dynamics with mixing time \( O(L^{d+1-\epsilon}) \) on a cube of side \( L \), uniformly in the boundary condition. Then van den Berg [2] shows that there is a unique infinite-volume Gibbs measure. Conversely, suitable conditions of “weak dependence on boundary conditions” — which are stronger than uniqueness of the Gibbs measure, but which are implied by most uniqueness proofs — imply \( O(L^d \log L) \) mixing of the Glauber dynamics, uniformly in the boundary

\footnote{Dyer and Greenhill [21] earlier proved \( O(n \log n) \) mixing when \( 0 \leq w < 2/(\Delta - 2) \), and \( O(n^2 \log n) \) mixing when \( w = 2/(\Delta - 2) \), for a slightly more complicated dynamics that acts on a vertex \( v \) and its neighbors. By a comparison argument (see also [63]), they then deduced \( O(n^3 \log n) \) mixing when \( 0 \leq w < 2/(\Delta - 2) \), and \( O(n^4 \log n) \) mixing when \( w = 2/(\Delta - 2) \), for the Glauber dynamics. But the Luby-Vigoda direct analysis appears to give better bounds.}
I’d like to raise a general question: What is the relation between proofs of rapid mixing by coupling methods and by the Dobrushin uniqueness method? Otherwise put, suppose we try to translate the coupling proof of rapid mixing from probabilistic to analytic language: we conclude that the transition matrix \( P \) (acting on the quotient space modulo constant functions) has spectral radius \( \beta < 1 \), hence has norm \( \leq \beta + \epsilon < 1 \) in some norm or other — but which norm? I can give an answer in the usual situation where the coupling is Markovian, with a transition matrix \( Q(x, y \rightarrow x', y') \) satisfying \( \sum_{y'} Q(x, y \rightarrow x', y') = P(x \rightarrow x') \) for all \( y' \) and \( \sum_{x'} Q(x, y \rightarrow x', y') = P(y \rightarrow y') \) for all \( x' \), and where there is a Lyapunov function \( \Phi(x, y) \geq 0 \) satisfying

\[
E\left( \Phi(X_{t+1}, Y_{t+1}) \bigg| X_t, Y_t \right) \leq \beta \Phi(X_t, Y_t) .
\]

Then a simple calculation shows that

\[
\| Pf \|_{\text{Lip}(\Phi)} \leq \beta \| f \|_{\text{Lip}(\Phi)} ,
\]

where the Lipschitz seminorm is defined by

\[
\| f \|_{\text{Lip}(\Phi)} = \sup_{x \neq y} \frac{|f(x) - f(y)|}{\Phi(x, y)}. \]

This approach could perhaps be useful in trying to understand the circumstances under which the coupling method can or cannot give sharp bounds [14].

My reasons for wanting to translate a beautiful probabilistic proof into ugly analytic language are linked to my next topic, which is the mixing properties of Glauber dynamics at complex fugacity \( w \). (I know this sounds crazy, but please bear with me.) Since the elements of the Glauber transition matrix \( P \) are rational functions of \( w \), we can certainly extend them to complex \( w \). The matrix \( P \) continues to satisfy \( P1 = 1 \), but its rows \( P(x, \cdot) \) are complex measures with total variation norm \( > 1 \) whenever \( w \) is negative or complex. Nevertheless, it is easy to prove the following result:

**Theorem 4.1 (Sokal [65])** Let \( G \) be a finite graph, and suppose that at fugacity \( w \in \mathbb{C} \) the Glauber transition matrix \( P \) has spectral radius \( < 1 \) (acting on the quotient space modulo constant functions). Then \( Z(w) \neq 0 \).

This theorem thus provides a technique for proving the nonvanishing of \( Z(w) \) that is alternative to Theorem 2.2, and is inspired in part by old work of Israel [31].

The problem is: How to verify that \( \text{spr}(P) < 1 \)? One might hope to do this adapting the standard proof of the Dobrushin uniqueness theorem (see e.g. [59]); but surprisingly, this proof falls apart immediately as soon as \( w \) is even slightly negative or complex, if one employs (as usual) the total oscillation seminorm. (The proof fails in the strangest way: “dusting” a site \( i \) can cause the “dirt” on distant sites \( j \) to
be amplified exponentially!) But this does not mean that the Dobrushin uniqueness method is failing; it may mean only that we are not using the right seminorm. Indeed, for any finite graph \( G \) we clearly have \( \text{spr}(P) < 1 \) for all \( w \in [0, \infty) \), so by continuity this must hold also in some (\( G \)-dependent) complex neighborhood of \([0, \infty)\). Which one? In particular, can we find a complex domain in which \( \text{spr}(P) < 1 \) holds for all graphs \( G \) of maximum degree \( \Delta \)?

**Conjecture 4.2** There exists a complex domain \( D_\Delta \) containing the interval \([0, 1/(\Delta - 1)]\) such that \( \text{spr}(P) < 1 \) holds for all graphs \( G \) of maximum degree \( \Delta \) whenever \( w \in D_\Delta \). [As with Question 2.4, there are two versions of this conjecture, depending on whether or not the \( w \) are assumed equal.]

Indeed, it is not out of the question that \( 1/(\Delta - 1) \) can be replaced here by \( 2/(\Delta - 2) \) or even by \( (\Delta - 1)^{\Delta - 1}/(\Delta - 2)^\Delta \). Unfortunately, what I am thus far able to prove is much weaker, namely:

**Theorem 4.3** (Sokal [65]) Let \( \{c_x\}_{x \in V} \) be an arbitrary set of positive numbers, and define

\[
\tilde{R}_x = (e^{c_x} - 1) \exp \left( -\sum_{y \sim x} c_y \right) \tag{4.4}
\]

where \( y \sim x \) denotes that \( y \) is adjacent to \( x \). Then \( \text{spr}(P) < 1 \) holds in the open polydisc \( |w_x/(1 + w_x)| < \tilde{R}_x \). In particular, \( Z(w) \) is nonvanishing there.

**Corollary 4.4** (Sokal [65]) If \( G \) has maximum degree \( \Delta \), then \( \text{spr}(P) < 1 \) and \( Z(w) \neq 0 \) hold in the open polydisc

\[
\left| \frac{w_x}{1 + w_x} \right| < \frac{(\Delta - 1)^{\Delta - 1}}{\Delta^\Delta} \tag{4.5}
\]

Theorem 4.3 is strikingly similar to Theorem 2.2, but is strictly stronger [since \( \tilde{R}_x/(1 + \tilde{R}_x) > R_x \)]. Corollary 4.4 is very close to Shearer’s improvement of Corollary 2.3, but is slightly weaker (resp. stronger) than Shearer’s result when \( w < 0 \) (resp. \( w > 0 \)); it is thus almost but not quite sharp for \( w < 0 \). The proof of Theorem 4.3 uses an exponentially weighted seminorm on “Fourier coefficients” that is completely different from the total oscillation seminorm: Let \( \eta_x = 0, 1 \) be the occupation variable at site \( x \in V \); write \( f(\eta) = \sum_{X \subseteq V} a_X \prod_{x \in X} (1 - \eta_x) \) and define

\[
||f||_c = \sum_{X \subseteq V} \exp \left( \sum_{x \in X} c_x \right) |a_X| \tag{4.6}
\]

for each nonnegative vector \( c = \{c_x\}_{x \in V} \). The question is: How to interpolate smoothly between these two radically different seminorms, which work in different regions of \( w \)-space, in order to prove \( \text{spr}(P) < 1 \) for a domain \( D_\Delta \) containing both the disc (4.3) and the interval \([0, 1/(\Delta - 1)]\)?
5 \textit{q-Coloring Model: Dynamics of Algorithms}

The single-site heat-bath (Glauber) dynamics for the \(q\)-coloring model on a finite graph \(G = (V, E)\) is defined as follows: Choose uniformly at random a vertex \(x \in V\), and give \(\sigma(x)\) a new value (independent of the old one) from the uniform distribution over all colors different from \(\{\sigma(y)\}_{y \sim x}\). More generally, one can consider the single-edge heat-bath dynamics in which a pair of adjacent sites are simultaneously recolored conditional on their neighbors \([20]\), or a yet more complicated local dynamics (e.g. \([13, 69]\)). Finally, one can consider the Wang-Swendsen-Kotecký (WSK) nonlocal cluster dynamics \([70, 71]\), which is defined as follows: Choose uniformly at random a pair of distinct colors \(\alpha, \beta \in \{1, \ldots, q\}\); let \(G_{\alpha\beta}\) be the induced subgraph of \(G\) consisting of sites \(x\) for which \(\sigma(x) = \alpha\) or \(\beta\); then, independently on each connected component of \(G_{\alpha\beta}\), with probability \(\frac{1}{2}\) either leave that component alone or else interchange colors \(\alpha\) and \(\beta\) on it.

All these Markov chains are easily seen to satisfy detailed balance with respect to the uniform distribution over proper \(q\)-colorings. However, since we are at zero temperature, ergodicity (= irreducibility) is already a nontrivial question. The following results are known:

- Single-site dynamics is ergodic for \(q \geq \Delta + 2\) \([33]\), and can be nonergodic for \(q = \Delta + 1\) (consider \(G = K_{\Delta+1}\))
- Single-edge dynamics is ergodic for \(q \geq \Delta + 1\) \([20]\), and can be nonergodic for \(q = \Delta\) (consider \(G = K_{\Delta+1}\) minus a single edge)
- WSK dynamics is ergodic for \(q \geq \Delta + 1\) \([32]\)
- WSK dynamics is ergodic for all \(q\) if \(G\) is bipartite \([15, 23]\)
- WSK dynamics is ergodic for \(q = 4\) on subsets of the triangular lattice with free boundary conditions \([45]\)
- WSK dynamics is nonergodic for \(q = 3\) on \(3m \times 3n\) square lattices with periodic boundary conditions, whenever \(m, n\) are relatively prime \([40]\)
- WSK dynamics is nonergodic for \(q = 4\) on the \(6 \times 6\) triangular lattice with periodic boundary conditions, and for \(q = 3\) on the \(3 \times 3\) Kagomé lattice with periodic boundary conditions \([44]\)
- Whenever \(q \leq \Delta/2\) and \(q\) is sufficiently large, there exists a graph of maximum degree \(\Delta\) and chromatic number \(O(q/\log q)\) on which the WSK dynamics for \(q\)-colorings is nonergodic \([13]\)

\(\text{By a “}3 \times 3\ \text{Kagomé lattice” I mean one that is obtained from a} 3 \times 3\ \text{triangular lattice (= the Bravais lattice of the Kagomé) by placing 3 Kagomé sites on each triangular site. It thus has} 3 \times 3 \times 3 = 27\ \text{sites.}\)
All other cases are open (to the best of my knowledge). In particular, we would like to know for which values of \( n \) (if any) the WSK dynamics is ergodic for \( q = 4 \) on an \( n \times n \) periodic triangular lattice, or for \( q = 3 \) on an \( n \times n \) Kagomé lattice.

When the algorithm is ergodic, the next step is to investigate its mixing rate. Here is what is known:

(a) For the single-site heat-bath dynamics, the Dobrushin uniqueness argument proves \( O(n \log n) \) mixing whenever \( q > 2\Delta \) \[53\]. This result can alternatively be derived by coupling arguments, which also show \( O(n^3) \) mixing at \( q = 2\Delta \) \[33, 20\]. More generally, these results hold for the antiferromagnetic Potts model at inverse temperature \( \beta \) in case \( q > 2\Delta(1 - e^{-\beta}) \) \[33\].

(b) For the single-edge heat-bath dynamics, a path-coupling argument shows \( O(n \log n) \) mixing whenever \( q \geq 2\Delta \) \[20\].

(c) For a local algorithm involving simultaneous recoloring of a site and all its neighbors, a path-coupling argument shows \( O(n \log n) \) mixing for \( q = 5 \) when \( \Delta = 3 \), and for \( q = 7 \) when \( G \) is a 4-regular triangle-free graph \[13\]. This shows that the \( 2\Delta \) bound can be beaten. By a comparison argument, one also obtains rapid mixing of the single-site heat-bath dynamics, but the bounds are poor \([O(n^6 \log n) \) and \( O(n^7 \log n)\), respectively\].

(d) For a local algorithm involving WSK moves on components of size \( \leq 6 \) only, a path-coupling argument shows \( O(n \log n) \) mixing for \( q > \frac{11}{6}\Delta \), and polynomial-time mixing at \( q = \frac{11}{6}\Delta \) \[69\]. By a comparison argument, one also obtains \( O(n^2 \log n) \) mixing for \( q > \frac{11}{6}\Delta \), and polynomial-time mixing at \( q = \frac{11}{6}\Delta \), for the single-site heat-bath dynamics and for the single-cluster variant of the full WSK dynamics \[69\].

(e) For the full WSK algorithm, numerical data strongly suggest that there is constant-time mixing (i.e. the complete absence of critical slowing-down) for the \( q = 3 \) model on \( n \times n \) periodic square lattices (at least for \( n \) even), uniformly down to and including the zero-temperature critical point \[56, 23\]. It would be wonderful to be able to prove something!

(f) Łuczak and Vigoda \[13\] construct a family \( F_n \) of planar (hence 4-colorable!) graphs on which the WSK algorithm is torpidly mixing [i.e. has mixing time \( \gtrsim \exp(n^\delta) \) for some \( \delta > 0 \)] for arbitrarily large \( q \) [indeed, for any \( q = O(n^{\delta}) \)]. They also show that for each pair \((q, \Delta)\) satisfying \( 3 \leq q < \Delta/(20 \log \Delta) \), there exists a family \( G_{q,\Delta,n} \) of bipartite graphs of maximum degree \( \Delta \) on which the WSK algorithm is torpidly mixing.

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\[54\] Numerical experiments \[54\] suggest that WSK dynamics is nonergodic for \( q = 3 \) also on the \( 6 \times 6 \) Kagomé lattice (i.e. the one with \( 6 \times 6 \times 3 = 108 \) sites).
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