Non-ergodicity in Wang–Swenden–Kotecký Monte Carlo dynamics

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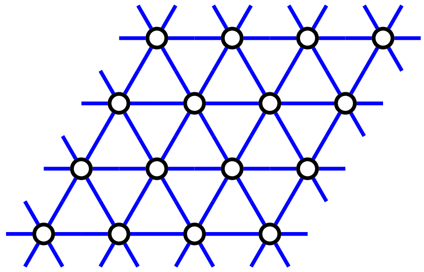
Summary

"A new Kempe invariant and the (non)-ergodicity of the Wang-Swendsen-Kotecký algorithm" [for the q-state antiferromagnetic Potts model]

1. The q-state Potts model
2. Markov Chain Monte Carlo methods: Ergodicity
3. The Wang-Swendsen-Kotecký algorithm for the q-state Potts antiferromagnet
4. The proof of non-ergodicity of WSK($q = 4$) at zero temperature for the triangular lattice on a torus
   - Kempe changes
   - Algebraic topology (Fisk)

The *standard* q-state Potts model

- G = Finite subset of a regular lattice with some boundary conditions



4×4 triangular lattice with toroidal bc's

- $\forall\, i \in V, \quad \sigma_i \in \{1, \ldots, q\}$ $\qquad q = 2, 3, \ldots \in \mathbb{Z}_+$

- $\boxed{\mathcal{H}(\sigma) = -J \sum_{\langle ij \rangle \in E} \delta_{\sigma_i,\sigma_j}}$ $\qquad \delta_{\sigma_i,\sigma_j} = \begin{cases} 1 & \sigma_i = \sigma_j \\ 0 & \sigma_i \neq \sigma_j \end{cases}$

- $J \in \mathbb{R}$ with $|J| \sim T^{-1}$ $\qquad \begin{cases} J > 0 & \text{Ferromagnetic} \\ J < 0 & \text{Antiferromagnetic} \end{cases}$

The *standard* q-state Potts model (2)

- Partition function $\qquad \boxed{Z_G(q,J) = \sum_{\sigma} e^{-\mathcal{H}(\sigma)}}$

- Free Energy $\qquad \boxed{f_G(q;J) \;=\; \frac{1}{|V|} \log Z_G(q,J)}$

$V \;=\;$ # spins ("Volume")

- Main goal: To obtain an explicit expression for $Z_G(q,J)$ or $f_G(q;J)$ for finite G, or …

- To obtain an explicit expression for the infinite-volume free energy

$$\boxed{f_{G_\infty}(q;J) \;=\; \lim_{n\to\infty} \frac{1}{|V_n|} \log Z_{G_n}(q;J)}$$

The *standard* q-state Potts model (3)

The Infinite-volume free energy is important

$$\boxed{f_{G_\infty}(q;J) \;=\; \lim_{n\to\infty} \frac{1}{|V_n|} \log Z_{G_n}(q;J)}$$

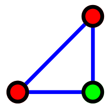
- Phase transition (= singularities in the free energy) cannot occur for finite systems if $J \in \mathbb{R}$

$$Z_G(q,J) \;=\; \sum_\sigma e^{J\sum\limits_{\langle ij\rangle} \delta_{\sigma_i,\sigma_j}} \;>\; 0$$

- $f_{G_\infty}(q;J)$ exists and is continuous in J for $J \in \mathbb{R}$
- The limit $J \to +\infty$ is not problematic: q ordered states.
- What about $J \to -\infty$??? [$T=0$ limit in the AF regime]

The $J \to -\infty$ limit on a triangular lattice

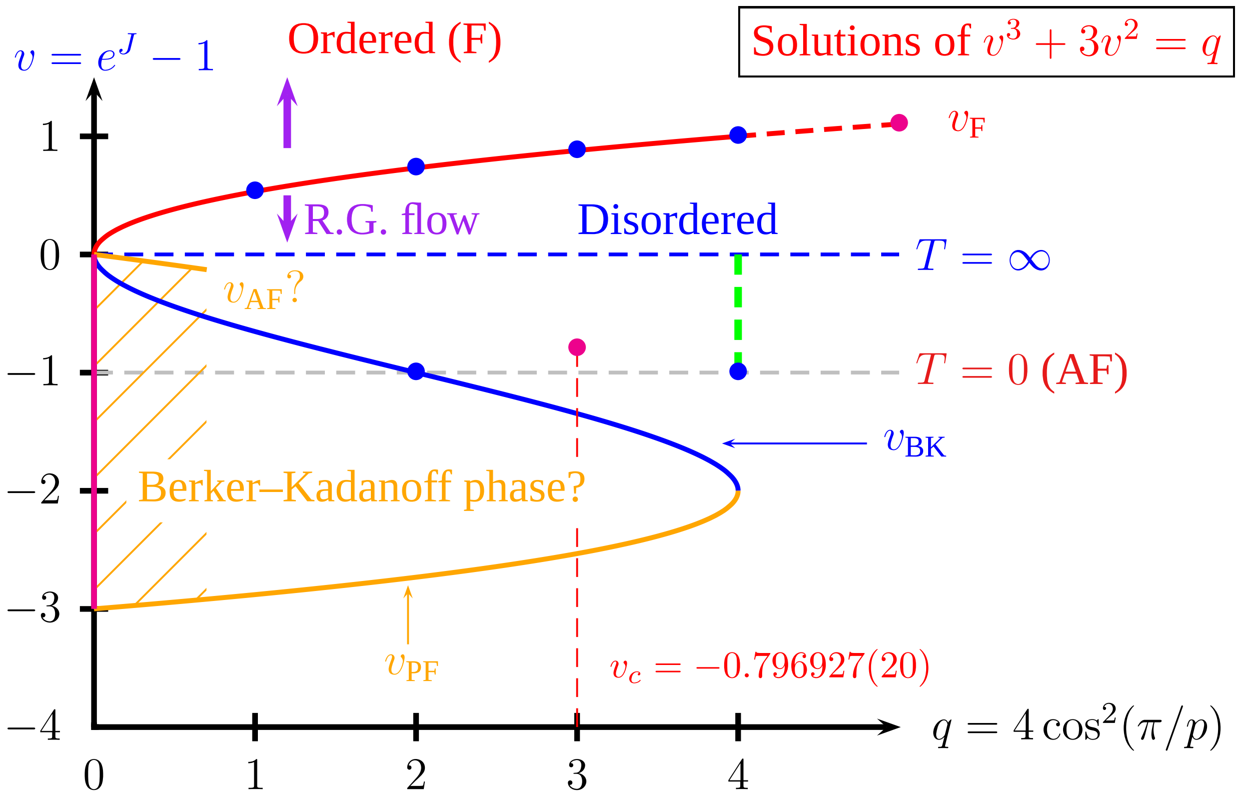
- If $q=2$: The allowed spin configurations (ground states) have on every triangle the following configuration



Frustration: many ground states and the energy is not minimized

- If $q \geq 3$: The allowed spin configurations correspond to proper colorings of G: $\sigma_i \neq \sigma_j$ if $i \sim j$
  - $q=3$: $3!$ ground states ($\sim$ ferromagnet at $T=0$)
  - $q \geq 4$: Many ground states with no frustration
    - The system is critical if $q=4$
    - The system is disordered if $q \geq 5$

Triangular-lattice Potts-model phase diagram



Markov-chain Monte Carlo simulations (1)

- We can use Monte Carlo simulations when we don't know how to obtain an explicit expression for the partition function/free energy.
- Important warning: This is Equilibrium Statistical Mechanics $\Rightarrow$ No time!!!
- Idea: Invent a stochastic process such that it converges to the probability measure of the Potts model

$$\boxed{\pi_{G,q,J}(\sigma) \;=\; \frac{1}{Z_G(q;J)}\, e^{-\mathcal{H}(\sigma)}}$$

- Problem: We ignore $Z_G(q;J)$!!!!

Markov-chain Monte Carlo simulations (2)

Goal: We want to obtain a discrete-time Markov chain $X_0, X_1, \ldots, X_t, \ldots$, such that:

- Each X_t takes values on the finite configuration space $\mathcal{S} = \{1, \ldots, q\}^V \ni \sigma$
- Is defined by an invented probability transition matrix P:

$$p_{\sigma,\sigma'} \;=\; P(\sigma \to \sigma') \;=\; \Pr(X_{t+1} = \sigma' \mid X_t = \sigma)$$

  The k-step transition probabilities are

$$p^{(k)}_{\sigma,\sigma'} \;=\; (P^k)_{\sigma,\sigma'} \;=\; \Pr(X_{t+k} = \sigma' \mid X_t = \sigma)$$

- Has the right unique stationary distribution limit:

$$\lim_{t\to\infty} p^{(t)}_{\sigma,\sigma'} \;=\; \pi_{G,q,J}(\sigma')$$

Markov-chain Monte Carlo simulations (3)

Probability transition matrix P:

$$\boxed{p_{\sigma,\sigma'} \;=\; P(\sigma \to \sigma') \;=\; \Pr(X_{t+1} = \sigma' \mid X_t = \sigma)}$$

(A) P is stationary w.r.t. $\pi_{G,q,J}$:

$$\sum_\sigma \pi_{G,q,J}(\sigma)\, p_{\sigma,\sigma'} \;=\; \pi_{G,q,J}(\sigma')$$

(A’) Detailed balance:

$$\pi_{G,q,J}(\sigma) p_{\sigma,\sigma'} \;=\; \pi_{G,q,J}(\sigma') p_{\sigma',\sigma}$$

(B) P is irreducible (or ergodic):
For all σ, σ', there exists a $n \in \mathbb{N}$ such that $p^{(n)}_{\sigma,\sigma'} > 0$

(C) P is aperiodic (period one, $D = 1$):
P has period D if $D = \gcd(\{k \geq 1 \mid p^{(k)}_{\sigma,\sigma} > 0\})$
P is ergodic and $p_{\sigma,\sigma} > 0$ for some $\sigma \Rightarrow P$ aperiodic

Markov-chain Monte Carlo simulations (4)

Theorem 1 *Consider an aperiodic irrducible Markov chain with finite state space* $\mathcal{S}$*. Then, for every* $\sigma, \sigma' \in \mathcal{S}$*, the limit*

$$\lim_{k\to\infty} p^{(k)}_{\sigma,\sigma'} \;=\; \pi(\sigma')$$

exists and it is independent of σ*. In addition,*

$$\sum_{\sigma} \pi(\sigma) \;=\; 1\,, \quad \text{and} \quad \sum_{\sigma} \pi(\sigma) p_{\sigma,\sigma'} \;=\; \pi(\sigma') \quad \text{for all } \sigma' \in \mathcal{S}.$$

Moreover, $v \;=\; \pi$ *is the only solution of*

$$\sum_{\sigma} v(\sigma) p_{\sigma,\sigma'} \;=\; v(\sigma')\,, \qquad v(\sigma) \geq 0\,, \qquad \sum_{\sigma} v(\sigma) \;=\; 1\,.$$

Markov-chain Monte Carlo simulations (5)

- $\pi(\sigma) \approx \Pr(X_t = \sigma)$ for $t \gg 1$, and independently of X_0.
- The system is essentially in equilibrium after $\tau_{\rm exp}$ MC steps
- Once in equilibrium, samples are correlated because X_{t+1} depends on X_t
- We obtain two statistically independent samples after $\tau_{\rm int}$ MC steps
- The bad news: Close to a second-order phase transition

$$\tau_{\rm exp} \;\approx\; \min(L,\xi)^{z_{\rm exp}}\,, \qquad \tau_{\rm int} \;\approx\; \min(L,\xi)^{z_{\rm int}}\,.$$

The Wang–Swendsen–Kotecký algorithm, 1989 (1)

Antiferromagnetic q–state Potts model

Step 1 Pick up uniformly at random two distinct colors $\mu \neq \nu \in \{1, 2, \ldots, q\}$

Step 2 Freeze all spins σ_i taking colors $\neq \mu, \nu$.

Step 3 Allow the remaining spins to take the values μ, ν

$$\Downarrow$$

We induce an AF Ising model and simulate it using the Anti-Swendsen-Wang algoritm (ASW)

The Wang–Swendsen–Kotecký algorithm, 1989 (2)

$$\begin{aligned} Z_G(q;J) &= \sum_\sigma \prod_{\langle ij \rangle} e^{-|J|\delta_{\sigma_i,\sigma_j}} = \sum_\sigma \prod_{\langle ij \rangle} \left[(1-p) + p(1-\delta_{\sigma_i,\sigma_j})\right] \\ p &= 1 - e^{-|J|} \in [0,1] \qquad \text{for } J \le 0 \\ \mu_{G,q,J}(\sigma) &= \frac{1}{Z_G(q;J)} \prod_{\langle ij \rangle} \left[(1-p) + p(1-\delta_{\sigma_i,\sigma_j})\right] \end{aligned}$$

We augment the state space by adding a variable $n_{ij} = 0, 1$ on every edge:

$$\mu(\sigma, n) = \frac{1}{Z_G(q;J)} \prod_{\langle ij \rangle} \left[(1-p)\delta_{n_{ij},0} + p(1-\delta_{\sigma_i,\sigma_j})\delta_{n_{ij},1}\right]$$

$n_{ij} = 1 \;\Rightarrow\;$ edge $\langle ij \rangle$ is occupied

The Wang–Swendsen–Kotecký algorithm, 1989 (3)

$$\mu(\sigma, n) \;=\; \frac{1}{Z_G(q;J)} \prod_{\langle ij \rangle} \left[(1-p)\delta_{n_{ij},0} + p(1-\delta_{\sigma_i,\sigma_j})\delta_{n_{ij},1} \right]$$

Step 4 Simulate $P_{\text{bond}} = \mu(n \mid \sigma)$
Independently for each edge $\langle ij \rangle$, take $n_{ij} = 0$ if $\sigma_i = \sigma_j$, and take $n_{ij} = 0, 1$ with probabilities $(1-p), p$ if $\sigma_i \neq \sigma_j$.

Step 5 Identify the clusters of sites connected with bonds $n_{ij} = 1$.

Step 6 Simulate $P_{\text{spin}} = \mu(\sigma \mid n)$
Independently for each connected cluster, either keep the original spin value or flip it ($\mu \leftrightarrow \nu$) with probability $1/2$.

The Wang–Swendsen–Kotecký algorithm, 1989 (4)

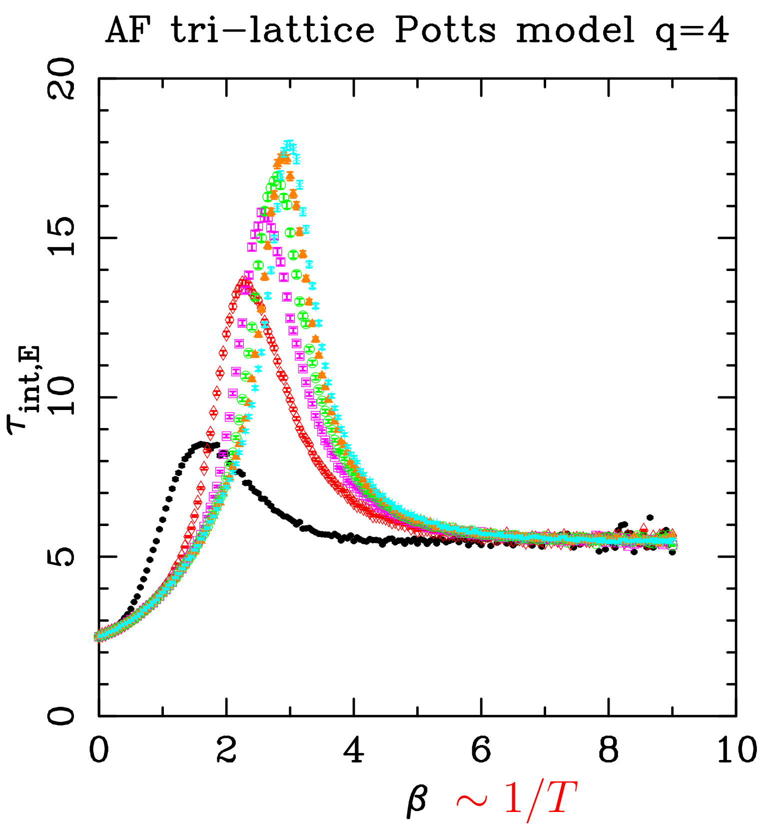
- The transition probability matrix $P = P_{\text{bonds}} \cdot P_{\text{spin}}$ leaves invariant $\mu_{G,q,J}$.
- It is ergodic for any $T \neq 0$: $J \in (-\infty, 0)$
- At $T = 0$ the ergodicity is a non-trivial question:
  - For bipartite lattices it is always ergodic for $q \geq 2$ [Burton-Henley, Ferreira-Sokal, Mohar]
  - For planar three-colorable lattices it is always ergodic for $q \geq 3$ [Mohar]

A practical situation

- Lattices are non-planar: we use periodic boundary conditions to minimize finite-size-effects (Torus)
- There are interesting models at $T = 0$ in the AF regime:
  - $q = 4$ on the triangular lattice (Non-bipartite)
- We want to consider a triangular lattice of linear size $(3L) \times (3N)$ with fully periodic boundary conditions

  $\Rightarrow$ Regular triangulation of the torus = $\boxed{T(3L, 3N)}$
  - Linear sizes multiples of 3 to ensure 3-colorability, and tripartiteness (physically important)
  - Regular graph with degree 6
  - In most applications, $L = N$

Autocorrelation time for $q = 4$



Kempe changes = Basic WSK moves at $T = 0$

- $\mathcal{S}$ is the space of proper q-colorings of G
- $\mu_{G,q,-\infty}$ is the uniform measure on $\mathcal{S}$

Algorithm:

Step 1 Pick up two distinct colors $\mu \neq \nu \in \{1, 2, \ldots q\}$

Step 2 Occupy all bonds $\langle ij \rangle$ with $\sigma_i = \mu$ and $\sigma_j = \nu$. Identify connected clusters of sites joined by occupied bonds.

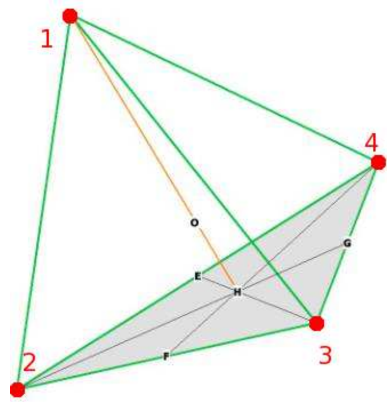
Step 3 For each connected cluster, either flip it or leave it unchanged with $p = 1/2$.

Note: Kempe moves contain single-spin-flip moves (Metropolis)

Degree of a 4–coloring (1)

Vector representation of the spin states:

$$\begin{aligned} \vec{e}^{\,(\alpha)} &\in \mathbb{R}^{q-1}, \qquad \alpha = 1, 2, \ldots, q \\ \vec{e}^{\,(\alpha)} \cdot \vec{e}^{\,(\beta)} &= \frac{q\delta_{\alpha,\beta} - 1}{q-1} \end{aligned}$$



For $q = 4$:

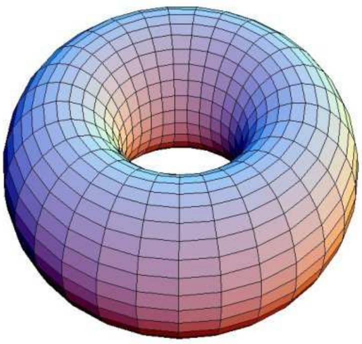
We have the surface of a tetrahedron in $\mathbb{R}^3$

$\Rightarrow \partial\Delta^3$ = Triangulation of the sphere S^2

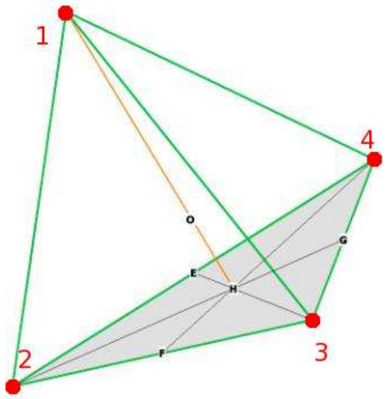
Degree of a 4–coloring (2)

A proper 4–coloring f of a triangulation T is a non-degenerate simplicial map

$$f \,:\, T \longrightarrow \partial\Delta^3$$



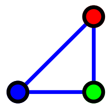
$\xrightarrow{f}$



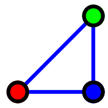
Si T is a closed orientable surface in $\mathbb{R}^3$, we can define an integer-valued function $\deg(f)$ (unique up to a sign)

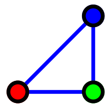
Degree of a 4–coloring (3)

- We first choose orientations for T and $\partial\Delta^3$ (e.g. clockwise)
- Given any triangular face t of $\partial\Delta^3$



we compute the number p (resp. n) of triangular faces of T mappring to t which have their orientation preserved (resp. reversed) by f





$p \rightarrow p+1 \qquad n \rightarrow n+1$

- $\deg(f) \;=\; p - n$
- $\deg(f)$ does NOT depend on the choice of t!!!

Properties of the degree of a 4–coloring

- Tutte's lemma: $\deg(f) \equiv \sum_{f(x)=a} d_x \pmod 2$ for $a = 1, 2, 3, 4$
- Corollary: The parity of a 4–coloring is a Kempe invariant

Tutte's lemma implies that any 4-coloring on $T(3L, 3N)$ has even degree!!! $\Rightarrow$ The invariant is useless

- Fisk's lemma: If T admits a 3–coloring, then $\deg(f) \equiv 0 \pmod 6$ for any 4-coloring f
  - $\deg(f) = 0, \pm 6, \pm 12, \pm 18$, etc
  - If g is a 3–coloring of T, $\deg(g) = 0$.

A new Kempe invariant

Theorem 2 *Let T be a 3–colorable triangulation of a closed orientable surface. If f and g are two 4–colorings of T related by a Kempe change, then*

$$\deg(g) \equiv \deg(f) \pmod{12}\,.$$

This is a useful Kempe invariant: there might be two ergodicity classes:

- Class #1: $\deg(f) \equiv 0 \pmod{12}$, which contains the 3–coloring of T
- Class #2: $\deg(f) \equiv 6 \pmod{12}$, which may be empty!!!

Note: $T(3L, 3N)$ is 3-colorable, and the torus is a closed and orientable surface

A new Kempe invariant (2)

Theorem 3 (Fisk) *Suppose the T is a triangulation of the sphere or torus. If T has a 3–coloring, then all 4–colorings with degree divisible by 12 are Kempe equivalent.*

Corollary 4 *Suppose the T is a triangulation of a 3–colorable torus. Then WSK for $q = 4$ is non-ergodic if and only of there exists a 4–coloring f with $\deg(f) \equiv 6 \pmod{12}$.*

But how can we prove that such 4–coloring exists for any triangulation $T(3L, 3N)$????

Existence of degree $\equiv 6 \pmod{12}$ 4-colorings

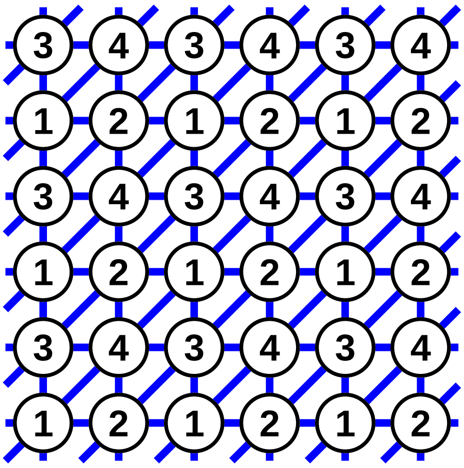
Theorem 5 *For any triangulation $T(3L, 3L)$ with $L \geq 2$, there exists a 4–coloring f with $\deg(f) \equiv 6 \pmod{12}$. Hence, the WSK dynamics for $q = 4$ on $T(3L, 3L)$ is non-ergodic.*

PROOF.

- Technically involved
- We have four cases: $L = 4k - 2$, $L = 4k - 1$, $L = 4k$, and $L = 4k + 1$ with $k \geq 1$
- Easiest case is $L = 4k - 2$: the sought 4-coloring is “trivial”
- For the other cases, we have an algorithmic proof that explicitly builds the 4–coloring.

Case $L = 4k - 2$

Smallest example $T(6,6)$: $|\deg(f)| = 18 \equiv 6 \pmod{12}$



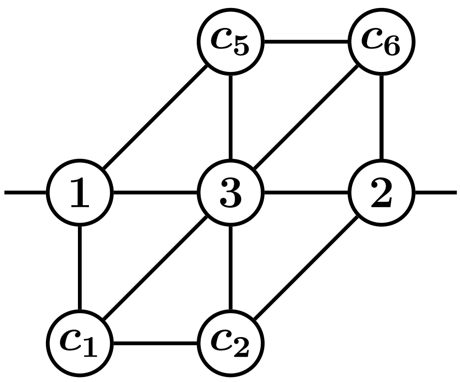
For $T(3(4k-2), 3(4k-2)) = T(6(2k-1), 6(2k-1))$, the periodical extension of the above 4-coloring has degree

$$\deg(f_{\text{extended}}) \;=\; (2k-1)^2 \deg(f) \;\equiv\; 6 \pmod{12} \;\blacksquare$$

What happens with $T(3, 3N)$?

Proposition 6 *The degree of any 4–coloring on any triangulation $T(3, 3L)$ or $T(3L, 3)$ with $L \geq 1$ is zero.*

PROOF. Look for $t = 123$. Focus on sites colored 3:



The 9 different and compatible 4-colorings have zero degree. $\blacksquare$

Existence of degree $\equiv 6 \pmod{12}$ 4-colorings (2)

Theorem 7 *For any triangulation $T(3L, 3N)$ with $L \geq 3$ and $N \geq L$ there exists a 4–coloring f with $\deg(f) \equiv 6 \pmod{12}$. Hence, the WSK dynamics for $q = 4$ on $T(3L, 3N)$ is non-ergodic.*

PROOF.

- By induction on $N \geq L$.
- The base case corresponds to $T(3L, 3L)$
- Given a "degree-6" 4-coloring on $T(3L, 3N)$ we can build a "degree-6" 4-coloring on $T(3L, 3(N+1))$ by gluing a "degree-0" 4-coloring on $T(3L, 3)$ with the same top-row coloring
- The 4-coloring on $T(3L, 3)$ is obtained algoritmically

Existence of degree $\equiv 6 \pmod{12}$ 4-colorings (3)

What happens for $T(6, 3N)$ with $N \geq 2$???

Proposition 8 *For any triangulation $T(6, 6k)$ with odd $k \geq 1$ there exists a 4–coloring f with $\deg(f) \equiv 6 \pmod{12}$. Hence, the WSK dynamics for $q = 4$ on $T(6, 6k)$ is non-ergodic.*

Proposition 9 *For the triangulation $T(6, 9)$ all 4-colorings have zero degree. Hence, the WSK dynamics for $q = 4$ on $T(6, 9)$ is ergodic.*

Conclusions

- Monte Carlo simulations are a great tool to investigate Statistical Mechanical systems; but one has to ensure its applicability.
- The WSK algorithm for the 4–state Potts antiferromagnet is not ergodic at $T = 0$ on most triangulations $T(3L, 3N)$ of the torus
- Open problems
  1. Find a procedure to test non-ergodicity in practice
  2. Invent a legal (and hopefully efficient) algorithm
  3. What happens for $q = 5, 6$ on the triangular lattice???