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# Kempe reconfiguration and Potts antiferromagnets

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In collaboration with: Bojan Mohar (SFU) [and Alan Sokal (NYU/UCL)]:

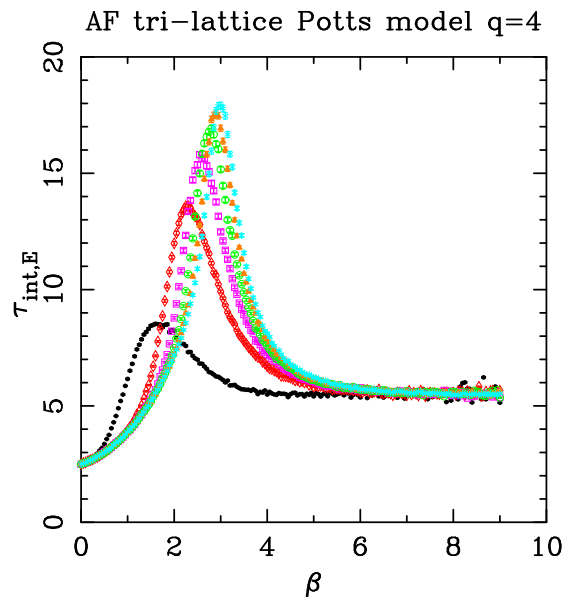
J. Phys. A **42** (2009) 225204; J. Stat. Mech. (2010) P05016.

Dedicated to the memory of Nathan Sokal

SIAM Conference on Discrete Mathematics DM16, Atlanta, June 6-10, 2016

# From spin systems physics to Kempe reconfiguration

'98 Alan Sokal-JS started a Monte-Carlo project for the antiferromagnetic 4-state Potts model on the triangular lattice with periodic boundary conditions (= on a torus).



$$\beta \sim \frac{1}{T}$$

- Critical point at  $T = 0$ .
- Disordered at all  $T > 0$ .
- Wang–Swendsen–Kotecký (WSK) algorithm.
- $L \times L$  triangular lattice.
- $L = 3$  ( $\bullet$ );  $L = 6$  ( $\diamond$ );  
 $L = 9$  ( $\square$ );  $L = 12$  ( $\circ$ );  
 $L = 15$  ( $\blacktriangle$ );  $L = 18$  ( $*$ ).

'02 We proved that at  $T = 0$ , WSK on a triangular lattice is irreducible (“ergodic”) for  $L = 3$ , and it’s **not** irreducible for  $L = 6$ .

## From spin systems physics to Kempe reconfiguration (2)

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- '05 We learned that studying the irreducibility of the  $T = 0$  WSK algorithm is equivalent to count the number of equivalence classes of colorings modulo Kempe moves.  
Bojan Mohar: “*Kempe equivalence of colorings*” preprint Jan 2005.  
B. Mohar joins the project.
- '06 Started to study seriously some Steve Fisk’s papers and algebraic topology. We found the right mathematical tools!
- '08 Proved that there are *at least* two Kempe equivalence classes for vertex 4-colorings on triangular graphs of sizes  $3L \times 3L$  with  $L \geq 2$  on a torus  $\Rightarrow$  WSK is not irreducible at  $T = 0$  on these graphs.

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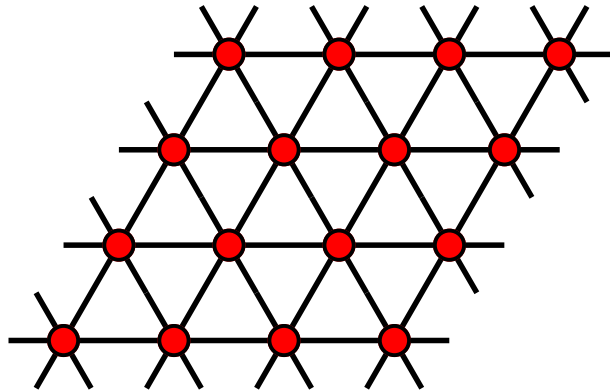
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Now, the gory details!

# The $q$ -state Potts model

- Let  $G = (V, E)$  be a graph. In Stat. Mech., it's chosen to be a **finite** subset of a **regular lattice**  $\mathcal{L}$  with **toroidal boundary conditions**.



$4 \times 4$  triangular lattice

- For all  $i \in V$ ,  $\sigma_i \in \{1, \dots, q\}$  with  $q = 2, 3, \dots \in \mathbb{N}$ .
- $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_{|V|}) \in \Omega = \{1, \dots, q\}^{|V|}$ .
- $\mathcal{E}(\boldsymbol{\sigma}) = -J \sum_{\{i,j\} \in E} \delta_{\sigma_i, \sigma_j}$ , with  $\delta_{\sigma_i, \sigma_j} = [\sigma_i = \sigma_j]$ .
- $J \in \mathbb{R}$  with  $|J| \sim \frac{1}{T}$   $\begin{cases} J > 0 & \text{Ferromagnetic,} \\ J < 0 & \text{Antiferromagnetic.} \end{cases}$

# The $q$ -state Potts model (2)

- Gibbs probability distribution:

$$\pi_{G,q,v}(\boldsymbol{\sigma}) = \frac{1}{Z_G(q,v)} e^{-\mathcal{E}(\boldsymbol{\sigma})},$$

where the **partition function**  $Z_G(q,v)$  is given by:

$$Z_G(q,v) = \sum_{\boldsymbol{\sigma} \in \Omega} e^{-\mathcal{E}(\boldsymbol{\sigma})}, \quad v = v(J) = e^J - 1 \geq -1.$$

- **Antiferromagnetic** regime:  $v \in [-1, 0)$ .
- At the  $T = 0$  limit in the AF regime ( $J \rightarrow -\infty$  or  $v = -1$ ):

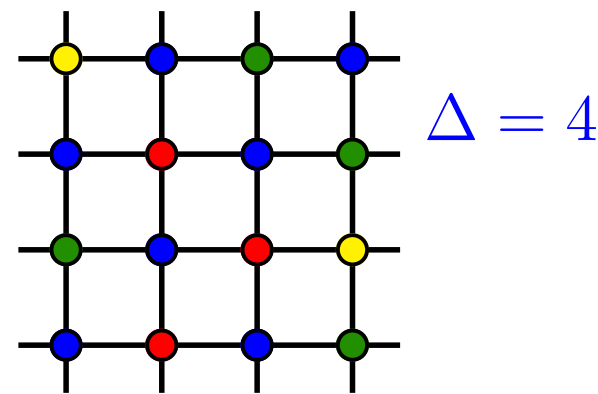
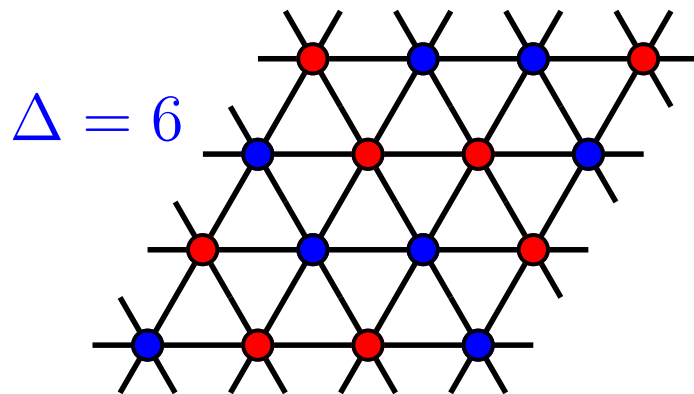
$$Z_G(q, -1) = P_G(q) = \# \text{ proper } q\text{-colorings of } G.$$

Now the sum in  $Z_G$  is over the set of proper  $q$ -colorings of  $G$ :

$\boldsymbol{\sigma} \in \mathcal{C}_q(G) \subset \Omega$  (but sometimes  $\mathcal{C}_q(G) = \emptyset!$ ).

# Potts antiferromagnets: why $T = 0$ is important?

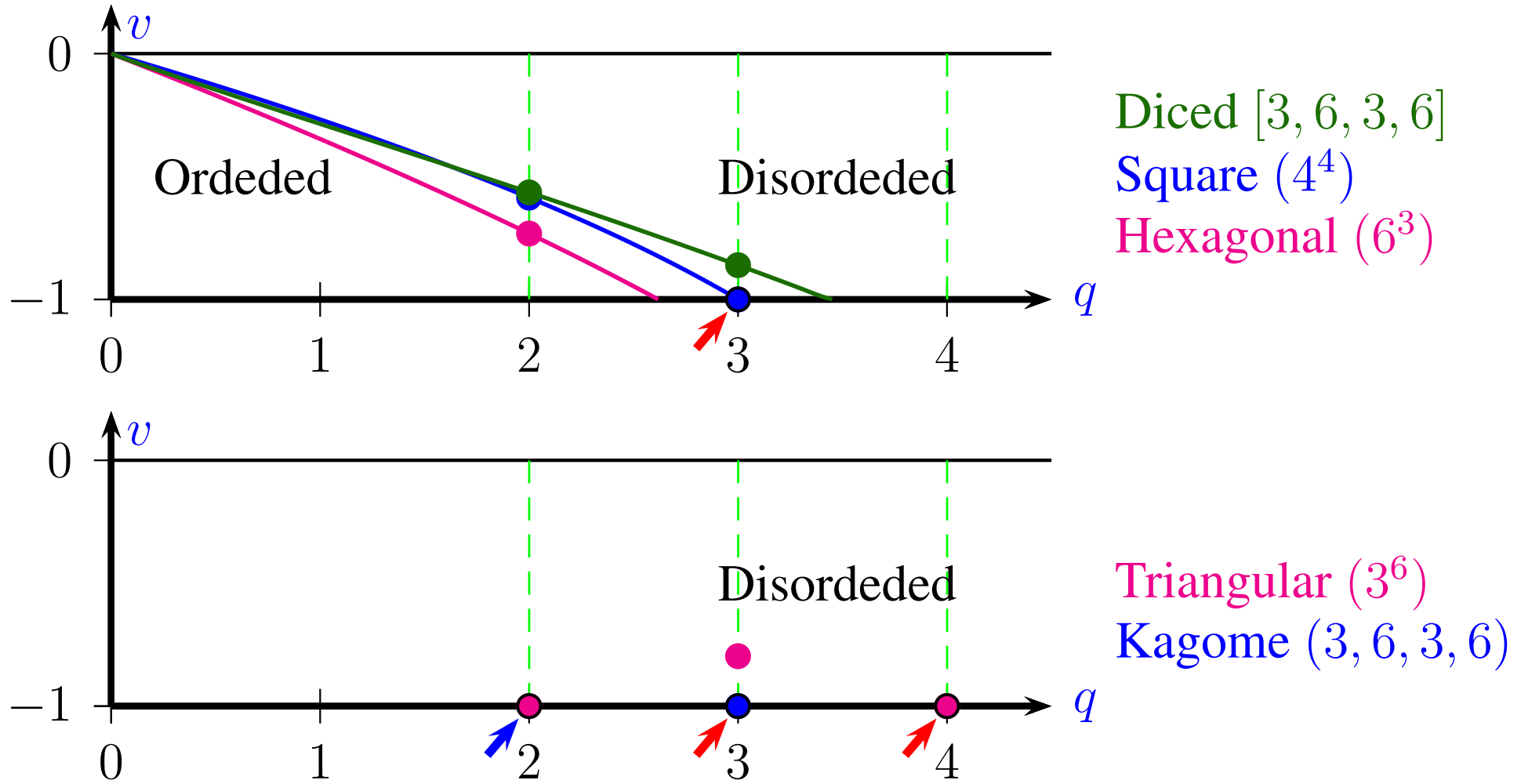
- **Universality** does **not** hold in general:  $d, q, \mathcal{L}$ . ( $d = 2$  in this talk)
- At  $T = 0$ , it may have **non-zero** ground-state entropy:
  1. **Frustration**: eg.  $q = 2$  on the triangular lattice ( $\mathcal{C}_2 = \emptyset$ ).
  2.  $q \gg \Delta = \max_{i \in V} d_i$ : eg.  $q = 4$  on the square lattice.



**Theorem 1 (Kotecký; Sokal-JS)** *If  $q > 2\Delta$ , there is a unique infinite-volume Gibbs measure, and it has exponential decay of correlations.*

# Potts antiferromagnets: why $T = 0$ is important? (2)

- $T = 0$  is a **critical point** for some AF Potts models on regular lattices: square, **triangular**, **kagome**, ...



- The study has to be done on a case-by-case basis!



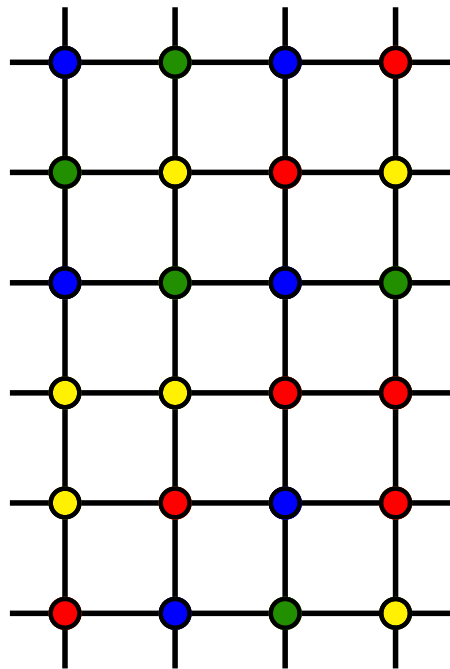
# Markov-chain Monte Carlo simulations

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- The  $q$ -state Potts model has not been yet solved analytically, except for the  $q = 2$  case ([Ising model](#)).
- Good playground for [Monte Carlo](#) methods: the algorithm of choice for [Potts antiferromagnets](#) is the [Wang–Swendsen–Kotecký \(WSK\)](#) one, which belongs to the class of [non-local cluster algorithms](#).
- Notation:
  - $\text{WSK}(G; q)$  = WSK algorithm for the  $q$ -state Potts antiferromagnet at  $T = 0$  on a graph  $G$ .
  - $\text{WSK}(\mathcal{L}; q)$  = WSK algorithm for the  $q$ -state Potts antiferromagnet at  $T = 0$  on a subset of the regular lattice  $\mathcal{L}$  embedded on a torus.

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

- Induce an AF Ising model, and use the (AF version of the) Swendsen–Wang (SW) algorithm for it.



AF 4-state Potts model

$G =$  Square lattice  $4 \times 6$  on a torus

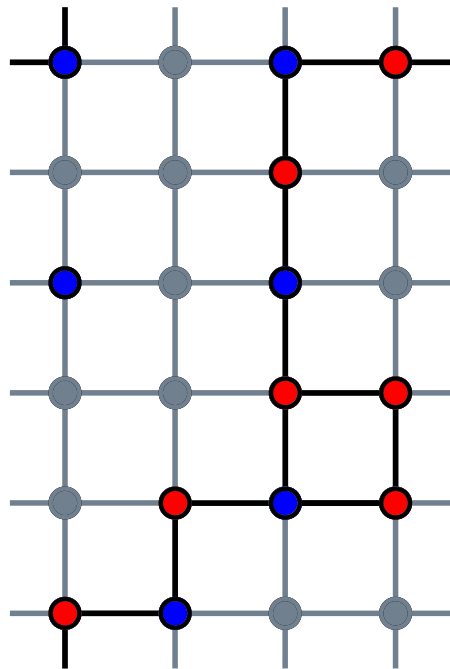
$T > 0$

1. Pick up uniformly at random 2 distinct colors  $\mu = \bullet$  and  $\nu = \bullet$ .
2. Freeze all spins  $\sigma_i$  taking colors  $\neq \mu, \nu$ , and allow the remaining spins to take the values  $\mu, \nu$ .

$\Rightarrow$  We induce an AF two-state (= Ising) model on  $G_{\mu, \nu}$

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

- We rewrite the partition function in a more convenient way:

$$Z_G(q, v) = \sum_{\sigma \in \Omega} \prod_{\{i,j\}} e^{J\delta_{\sigma_i, \sigma_j}} = \sum_{\sigma \in \Omega} \prod_{\{i,j\}} [(1 - p) + p(1 - \delta_{\sigma_i, \sigma_j})],$$

where  $p = 1 - e^J = -v \in [0, 1]$ .

- The Gibbs probability distribution takes the form:

$$\pi_{G,q,v}(\boldsymbol{\sigma}) = \frac{1}{Z_G(q, v)} \prod_{\{i,j\} \in E} [(1 - p) + p(1 - \delta_{\sigma_i, \sigma_j})].$$

- We augment the state space: we introduce  $n_{ij} \in \{0, 1\}$ :

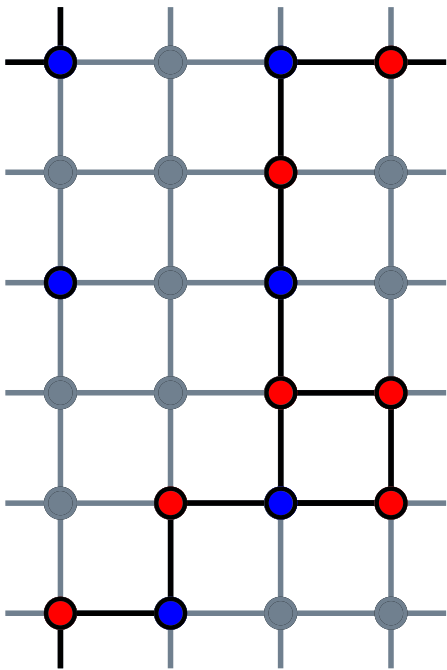
$$\pi(\boldsymbol{\sigma}, \mathbf{n}) = \frac{1}{Z_G(q, v)} \prod_{\{i,j\} \in E} [(1 - p) \delta_{n_{ij}, 0} + p(1 - \delta_{\sigma_i, \sigma_j}) \delta_{n_{ij}, 1}],$$

where  $n_{ij} = 1$  ( $n_{ij} = 0$ ) means that  $\{i, j\}$  is **occupied** (**empty**).

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

- We now simulate the joint probability distribution:

$$\pi(\boldsymbol{\sigma}, \mathbf{n}) = \frac{1}{Z_G(q, v)} \prod_{\{i,j\} \in E} [(1 - p) \delta_{n_{ij},0} + p (1 - \delta_{\sigma_i, \sigma_j}) \delta_{n_{ij},1}] .$$



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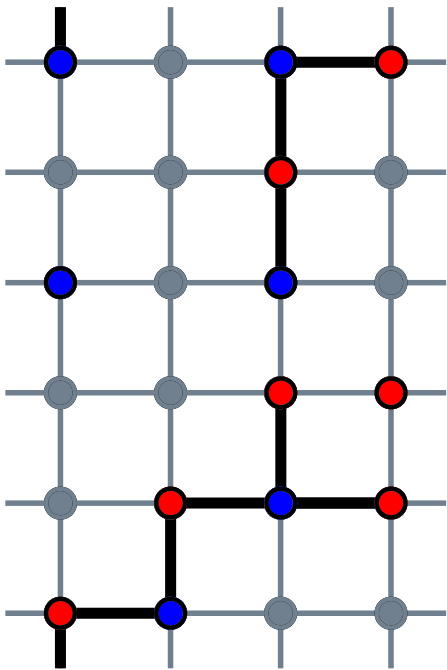
$T > 0 \quad \Rightarrow \quad 0 < p < 1$

3. Simulate  $P_{\text{bond}} = \pi(\mathbf{n} \mid \boldsymbol{\sigma})$ : *Independently* for each edge  $\{i, j\}$ , take  $n_{i,j} = 0$  if  $\sigma_i = \sigma_j$ , and take  $n_{ij} = 0$  or 1 with probabilities  $(1 - p)$  or  $p$  if  $\sigma_i \neq \sigma_j$ .

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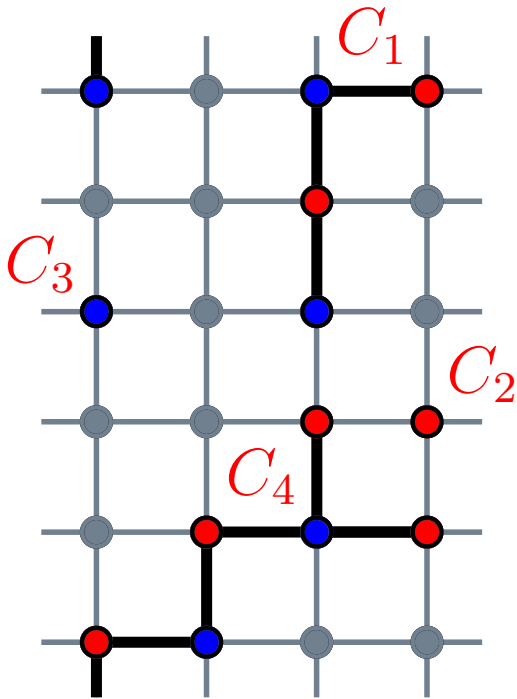
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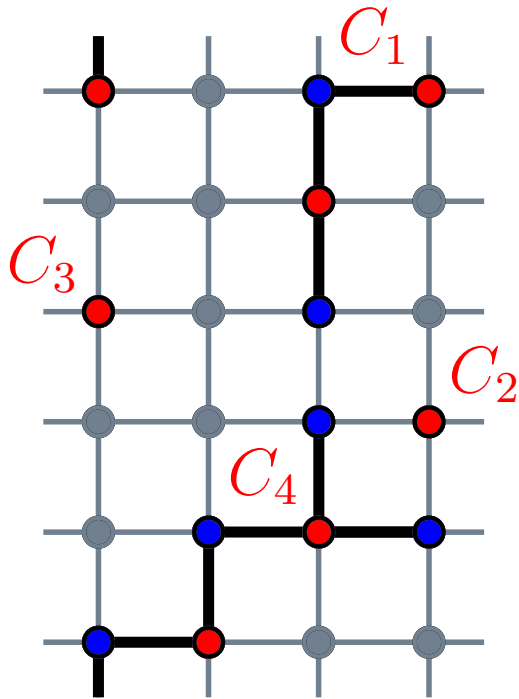
$T > 0 \Rightarrow 0 < p < 1$

4. Identify the clusters  $C_i$  of sites connected with bonds  $n_{ij} = 1$ .
5. Simulate  $P_{\text{spin}} = \pi(\boldsymbol{\sigma} \mid \boldsymbol{n})$ : *Independently* for each connected cluster, either keep the original spin value or flip it ( $\mu \leftrightarrow \nu$ ) with probability  $\frac{1}{2}$ .

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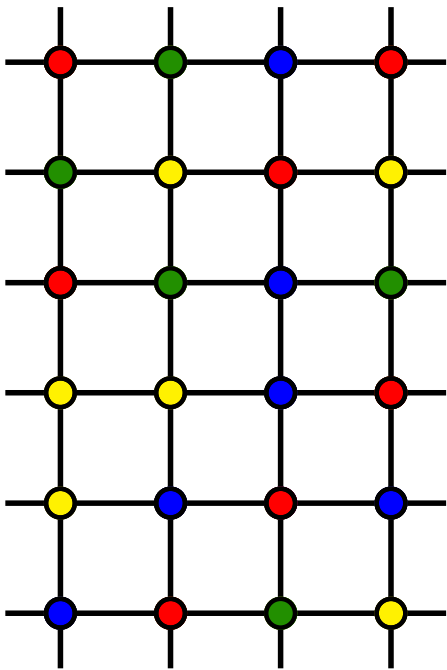
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AF 4-state Potts model

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$T > 0 \quad \Rightarrow \quad 0 < p < 1$

6. We have a new spin configuration and we repeat the process as many time as needed.

# The Wang–Swendsen–Kotecký algorithm, 1989 (5)

- The transition probability matrix  $P_{\text{WSK}} = P_{\text{bond}} \cdot P_{\text{spin}}$  leaves invariant  $\pi_{G,q,v}$  for all  $T \geq 0$  or  $v \in [0, 1]$ .
- It is irreducible for any  $T > 0$  or  $v \in [0, 1)$ .
- At  $T = 0$ , we only consider proper  $q$ -colorings and WSK reduces to Kempe chains:
  1. Pick up at random two distinct colors  $\mu \neq \nu$ .
  2.  $G_{\mu,\nu}$  is the subgraph of  $G$  induced on vertices of colors  $\mu$  or  $\nu$ .
  3. The connected components  $K_i$  of  $G_{\mu,\nu}$  are the Kempe components.
  4. Flip or keep the colors in each  $K_i$  with probability  $\frac{1}{2}$ .
- The irreducibility of WSK at  $T = 0$  is a highly non-trivial issue.
- For non-frustrated systems, single-site moves are a proper subset of Kempe moves.

# Irreducibility of the WSK algorithm

- Some notation:
  - The set of proper  $q$ -colorings of the graph  $G$  is  $\mathcal{C}_q(G)$ .
  - Two colorings are Kempe equivalent if there is a sequence of Kempe moves that transform one into the other.
  - The number of equivalence classes of  $q$ -colorings of  $G$  modulo Kempe equivalence is  $\kappa(G; q)$ .
- *Reminder:*  $\text{WSK}(G; q)$  is irreducible if and only if  $\kappa(G; q) = 1$ .
- Intuitively,  $\text{WSK}(G; q)$  is irreducible if  $q \gg 1$ :

**Theorem 2 (Las Vergnas–Meyniel, Jerrum, Mohar)** *Let  $\Delta$  be the maximum degree of a graph  $G$ , and let  $q \geq \Delta + 1$  be an integer. Then  $\kappa(G; q) = 1$ , or  $\text{WSK}(G; q)$  is irreducible. If  $G$  is connected and contains a vertex of degree  $< \Delta$ , then  $\kappa(G; \Delta) = 1$ , or  $\text{WSK}(G; \Delta)$  is irreducible.*

## Irreducibility of the WSK algorithm (2)

Lattice $\mathcal{L}$	$\Delta$	WSK( $\mathcal{L}; q$ ) irreducible for
Hexagonal	3	$q \geq 4$
Square, kagome	4	$q \geq 5$
Triangular, diced	6	$q \geq 7$

- But for  $q \geq \Delta + 1$ , these Potts models are **disordered at  $T = 0$ !!**

**Theorem 3 (Burton–Henley, Ferreira–Sokal, Mohar)** *Let  $G$  be a bipartite graph and  $q \geq 2$  an integer. Then  $\kappa(G; q) = 1$ , or WSK( $G; q$ ) is irreducible.*

- This solves the problem for bipartite lattices on the torus (square, hexagonal, diced, ...).
- For non-bipartite graphs, we need to work harder!

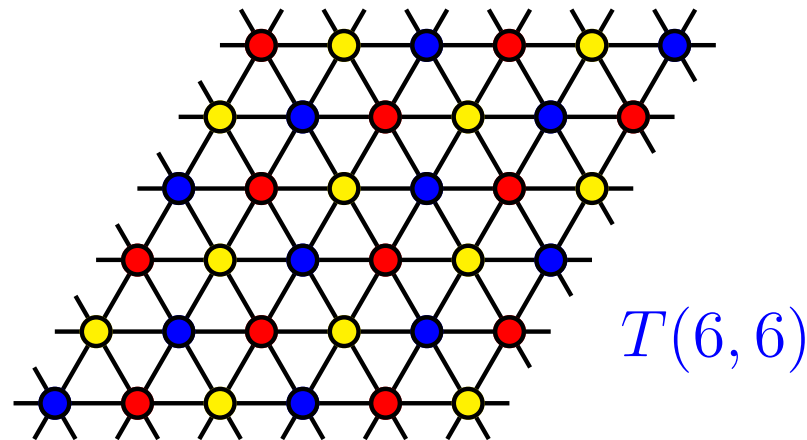
# Irreducibility of the WSK algorithm (3)

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- For non-bipartite lattices we have several **open problems**:
  - Kagome lattice with  $q = 2, 3, 4$ .
  - Triangular lattice with  $q = 2, 3, 4, 5, 6$ .
- For  $q = 2$ , the AF Potts model on both lattices is **frustrated**:  $\mathcal{C}_2 = \emptyset$ .
- $q = 3$  for a 3-colorable **triangular lattice is trivial**: the 3-coloring is *unique* modulo global color permutations.
- The most interesting cases are  $q = 4$  for the **triangular** lattice, and  $q = 3$  for the **kagome** lattice: we expect these systems to be **critical** at  $T = 0$ .
- The other cases:  $q = 4$  for the **kagome** lattice, and  $q = 5, 6$  for the **triangular** lattice are less important: we expect these systems to be **disordered** at  $T = 0$ .

# Non-irreducibility of WSK(tri; 4)

- For each  $L \geq 1$ ,  $T(3L, 3L)$  is the 3-colorable 6-regular triangulation that is a subset of the triangular lattice of linear size  $3L$  and embedded on the torus.

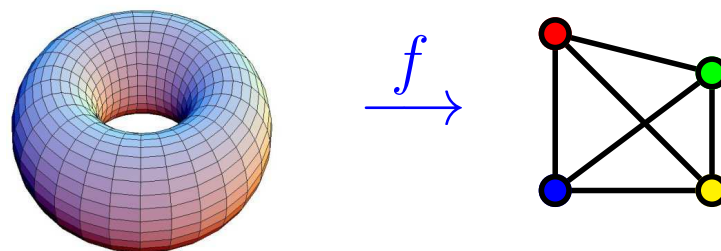


**Theorem 4 (Mohar-JS)** For any triangulation  $G = T(3L, 3L)$  with  $L \geq 2$ ,  $\kappa(G; 4) > 1$ , or equivalently  $WSK(G; 4)$  is not irreducible.

- The proof is based on [algebraic topology](#) [Fisk '73–'77].
- But it's specific to  $q = 4 \dots$

# Degree of a 4-coloring

- A proper 4-coloring  $f$  of a triangulation  $T$  is a non-degenerate simplicial map  $f : T \rightarrow \partial\Delta^3 \simeq S^2$ .



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

- We choose orientations for  $T$  and  $\partial\Delta^3$  (eg. clockwise), and fix a face  $t$  of  $\partial\Delta^3$ , eg.

- $p$  (resp.  $n$ ) = # faces of  $T$  mapping to  $t$  with their orientation preserved (resp. reversed) by  $f$ : resp.

- $\deg(f) = p - n$ , and it doesn't depend on the choice of  $t$ .

## Non-irreducibility of WSK(tri; 4) (2)

**Theorem 5 (Fisk, '73)** *Let  $T$  be a 3-colorable triangulation of a closed orientable surface. If  $f$  is a 4-coloring of  $T$ , then  $\deg f \equiv 0 \pmod{6}$ .*

**Theorem 6 (Fisk, '77)** *Let  $T$  be a 3-colorable triangulation of the torus. Then all 4-colorings  $f$  of  $T$  such that  $\deg f \equiv 0 \pmod{12}$  are Kempe equivalent.*

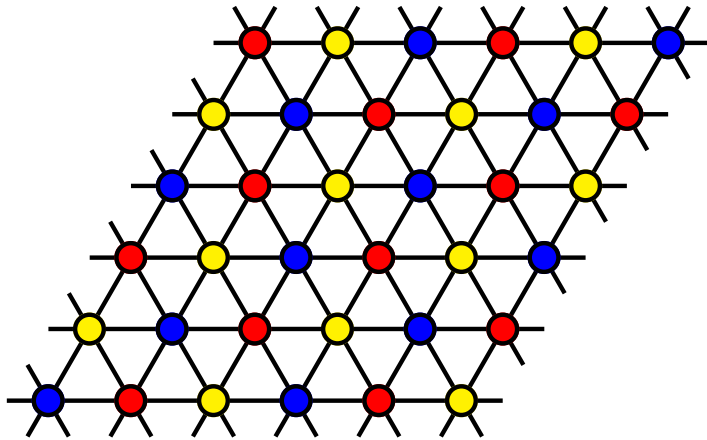
**Theorem 7 (Mohar-JS)** *Let  $T$  be a 3-colorable triangulation of a closed orientable surface. If  $f$  and  $g$  are two 4-colorings of  $T$  related by a Kempe move, then  $\deg f \pmod{12} = \deg g \pmod{12}$ .*

- There might be (at least) 2 Kempe equivalence classes on the torus:
  1. One with  $\deg f \equiv 0 \pmod{12}$ . It's **non-empty**: it contains the 3-coloring of  $T$ .
  2. At least one with  $\deg f \equiv 6 \pmod{12}$ ; but it **might be empty**!

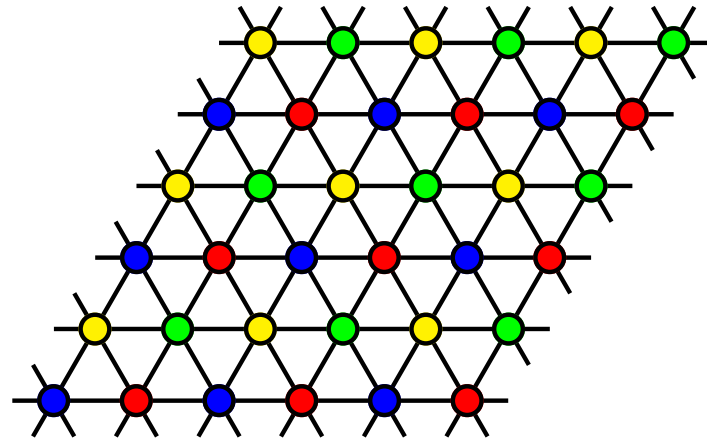


# Non-irreducibility of WSK(tri; 4) (3)

**Corollary 8** *Let  $T$  be a 3-colorable triangulation of the torus. Then  $\kappa(T; 4) > 1$  if and only if there exists a 4-coloring  $f$  such that  $\deg f \equiv 6 \pmod{12}$ .*



$$\deg f \equiv 0 \pmod{12}$$

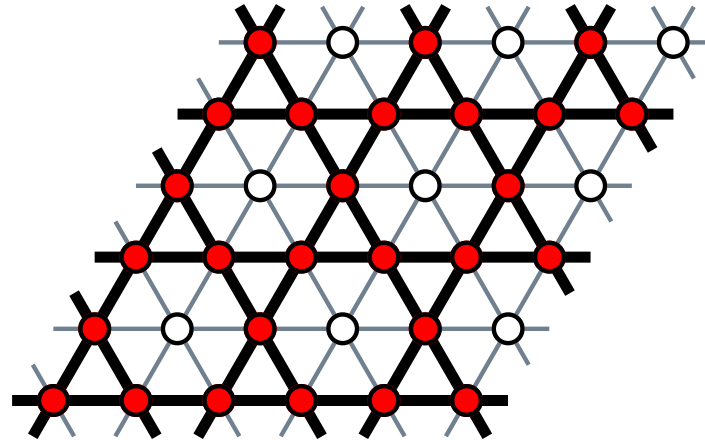


$$|\deg g| = 18 \equiv 6 \pmod{12}$$

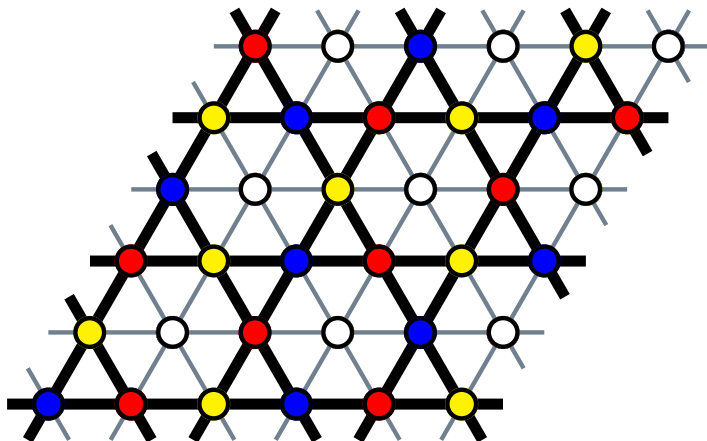
- For any  $G = T(3L, 3L)$  with  $L \geq 2$ , we find a 4-coloring  $f$  with  $\deg f \equiv 6 \pmod{12}$ . Then,  $\kappa(G; 4) \geq 2$ , or **WSK( $G; 4$ ) is not irreducible**.
- **WSK( $T(3L, 3L); 4$ )** includes **single-site dynamics** (eg. Metropolis).
- This method does not tell us anything about  $q = 5, 6!$

# Non-irreducibility of WSK(kag; 3)

- A kagome graph is the medial graph  $T'(3L, 3L)$  of the triangulation  $T(3L, 3L)$ . Note that  $T'(3L, 3L) \subset T(6L, 6L)$ .



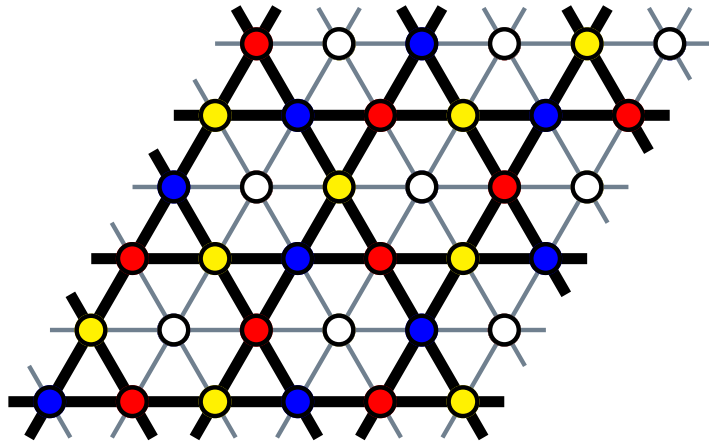
- 3-colorings of  $T'(3L, 3L)$  are **constrained** 4-colorings of  $T(6L, 6L)$ :



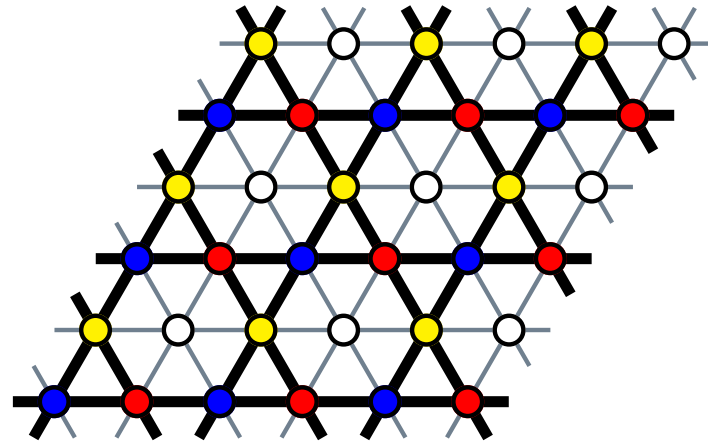
We **fix** the color white to the vertices of  $T(6L, 6L)$  not in  $T'(3L, 3L)$

# Non-irreducibility of WSK(kag; 3) (2)

- We can use the methods used in the proof for the non-irreducibility of  $WSK(T(3L, 3L); 4)$  for  $L \geq 2$ .



$$\deg f \equiv 0 \pmod{12}$$



$$|\deg g| = 18 \equiv 6 \pmod{12}$$

**Theorem 9 (Mohar-JS)** For any kagome graph  $G = T'(3L, 3L)$  with  $L \geq 1$ ,  $WSK(G; 3)$  is not irreducible.

# Irreducibility of WSK(kag; 4)

**Theorem 10 (McDonald-Mohar-Scheide '12)** *If  $G$  is a graph with maximum degree  $\Delta = 3$ , then all 4-edge-colorings of  $G$  are Kempe equivalent.*

- **Edge-coloring:** we color the edges of  $G$  such that all edges incident to a vertex have distinct colors.
- Given  $G = T(3L, 3L)$ , then its **dual graph**  $G^* = T^*(3L, 3L)$  is a subset of the **hexagonal lattice on the torus**. The line graph of  $G^*$  is also the kagome graph  $T'(3L, 3L)$ .
- The hexagonal graph  $T^*(3L, 3L)$  is 3-regular ( $\Delta = 3$ ).
- There is a bijection between the 4-edge-colorings of  $T^*(3L, 3L)$  and the 4-vertex-colorings of its line graph  $T'(3L, 3L)$ .

**Corollary 11** *For any kagome graph  $G = T'(3L, 3L)$  with  $L \geq 1$ ,  $WSK(G; 4)$  is irreducible.*

# Irreducibility of WSK(tri; 6) and WSK(kag; 4)

**Theorem 12 (Bonamy–Bousquet–Feghali–Johnson '15)** *Let  $k \geq 4$  be a positive integer. If  $G$  is a connected non-complete  $k$ -regular graph, then the set of  $k$ -colorings of  $G$  is a Kempe class.*

- The triangulations  $T(3L, 3L)$  for  $L \geq 1$  are 6-regular, connected and non-complete graphs.

**Corollary 13** *For any triangulation  $G = T(3L, 3L)$  with  $L \geq 1$ ,  $\kappa(G; 6) = 1$ , or equivalently  $\text{WSK}(G; 6)$  is irreducible.*

- The kagome graphs  $T'(3L, 3L)$  for  $L \geq 1$  are 4-regular, connected and non-complete graphs.

**Corollary 14** *For any kagome graph  $G = T'(3L, 3L)$  with  $L \geq 1$ ,  $\kappa(G; 4) = 1$ , or equivalently  $\text{WSK}(G; 4)$  is irreducible.*

# Conclusions

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- The WSK algorithm for the AF  $q$ -state Potts model reduces at  $T = 0$  to Kempe moves.  $\text{WSK}(G; q)$  is irreducible  $\Leftrightarrow \kappa(G; q) = 1$ .
- For any bipartite graphs,  $\kappa(G; q) = 1$  for any  $q \geq 2$ .
- For non-bipartite graphs on a torus:  $\text{WSK}(\text{tri}; 4)$ , and  $\text{WSK}(\text{kag}; 3)$  are not irreducible (critical points at  $T = 0$ ).
- For non-bipartite graphs on a torus:  $\text{WSK}(\text{tri}; q)$  for  $q \geq 6$ , and  $\text{WSK}(\text{kag}; q)$  for  $q \geq 4$  are irreducible (disordered at  $T = 0$ ).
- Open problems:
  - Invent new, legal, and efficient algorithms for  $\text{WSK}(\text{tri}; 4)$  and  $\text{WSK}(\text{kag}; 3)$  (worm algorithm, Liu–Deng–Garoni '11)
  - What happens to  $\text{WSK}(\text{tri}; 5)$ ? Conjecture: it's irreducible.

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Thanks for your attention!