Dynamic critical behavior of the WSK algorithm for 2D Potts antiferromagnets

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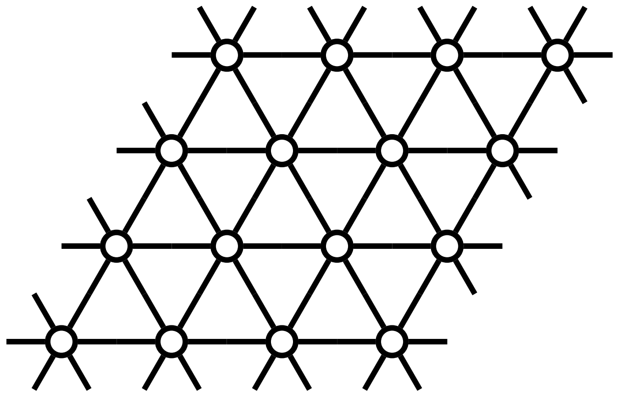
J. Stat. Mech. (2010) P05016.

The q-state Potts model

- $G = (V, E) =$ Finite subset of a regular lattice $\mathcal{L}$ with toroidal boundary conditions (and aspect ratio $= 1$).



4×4 triangular lattice

- $\forall\, i \in V\,, \quad \sigma_i \in \{1, \ldots, q\}, \qquad q = 2, 3, \ldots \in \mathbb{N}.$
- $\mathcal{H}(\sigma) = -J \sum_{\langle ij \rangle \in E} \delta_{\sigma_i, \sigma_j}, \qquad \delta_{\sigma_i, \sigma_j} = \begin{cases} 1 & \sigma_i = \sigma_j \\ 0 & \sigma_i \neq \sigma_j \end{cases}$
- $J \in \mathbb{R}$ with $|J| \sim T^{-1}$ $\qquad \begin{cases} J > 0 & \text{Ferromagnetic} \\ J < 0 & \text{Antiferromagnetic} \end{cases}$

The q-state Potts model (2)

- Spin probability distribution:

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

- Partition function (Fortuin–Kasteleyn '69): If $G = (V,E)$,

$$Z_G(q,v) \;=\; \sum_{\sigma} e^{-\mathcal{H}(\sigma)} \;=\; \sum_{A\subseteq E} v^{|A|}\, q^{k(A)}\,.$$

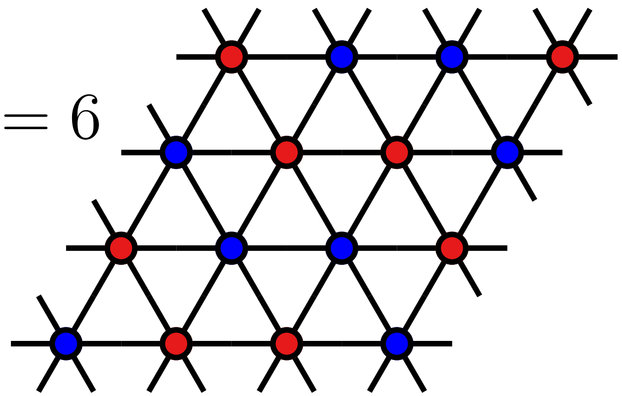
  - $v \;=\; e^J - 1 \;\geq\; -1$.
    - Antiferromagnetic regime: $v \in [-1,0]$.
  - $Z_G(q,v)$ is a polynomial in q, v: $\;\Rightarrow\;$ $(q,v) \in \mathbb{R}^2$.
  - At $v = -1$ ($J \to -\infty$):

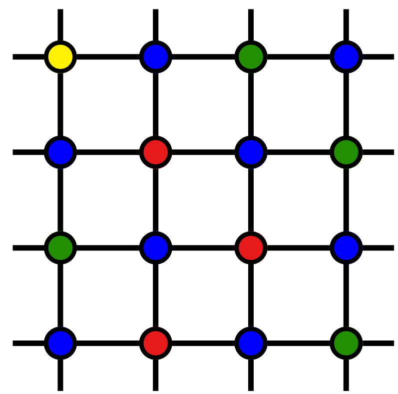
$$Z_G(q,-1) \;=\; P_G(q) \;=\; \#\text{ proper } q\text{–colorings of } G.$$

Potts antiferromagnets

- Universality does not hold in general: $d, q, \mathcal{L}$.
- At $T = 0$, it may have non-zero ground-state entropy:
  1. Frustration: eg. $q = 2$ on the triangular lattice.
  2. $q \gg \Delta$: eg. $q = 4$ on the square lattice.

$\Delta = 6$



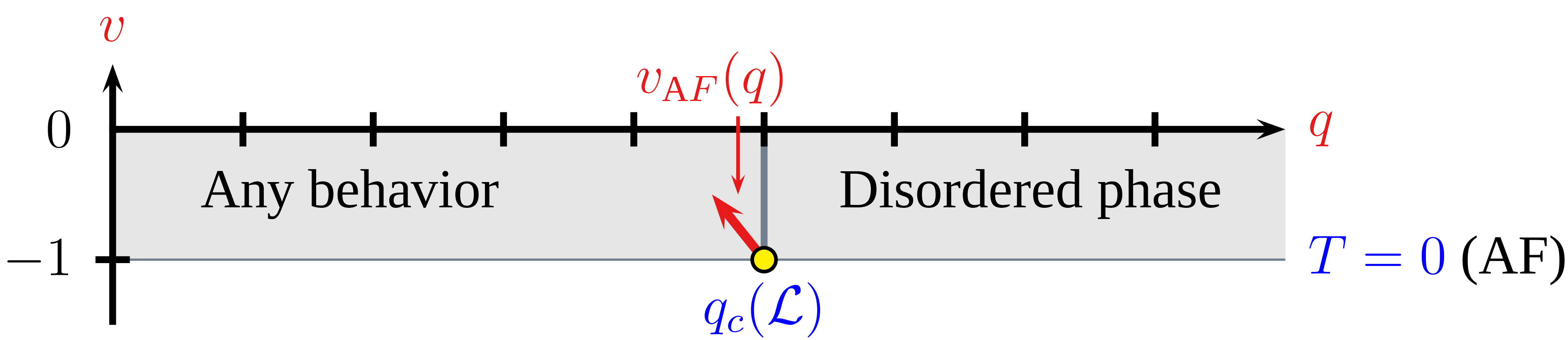


$\Delta = 4$

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

Potts antiferromagnets (2)

- Some models at $T = 0$ can be mapped onto a height model:
  - Critical points: eg. $q = 2, 4$ on the triangular lattice.
  - Long-range order: eg. $q = 3$ on the diced lattice.
- We expect some sort of universality for antiferromagnets:
  For each regular lattice $\mathcal{L}$, there is a number $q_c(\mathcal{L}) \in \mathbb{R}$



- Goal: compute $q_c(\mathcal{L})$ for the commonest lattices $\mathcal{L}$.

Markov-chain Monte Carlo simulations

- We want to invent a discrete-time Markov chain $X_0, X_1, \ldots, X_t \ldots$ such that it converges to $\pi_{G,q,v}(\sigma)$.
- Probability transition matrix P:

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

1. P is stationary with respect to $\pi_{G,q,v}$:

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

   Detailed balance: $\pi_{G,q,v}(\sigma) p_{\sigma,\sigma'} \;=\; \pi_{G,q,v}(\sigma') p_{\sigma',\sigma}$

2. P is ergodic: $\forall\, \sigma, \sigma'$, there exists a $n \in \mathbb{N}$ such that $p^{(n)}_{\sigma,\sigma'} = (P^n)_{\sigma,\sigma'} = \Pr(X_{t+n} = \sigma' \mid X_t = \sigma) > 0$.

- Then, there is a unique limit, and it is the right one:

$$\boxed{\lim_{t\to\infty} p^{(t)}_{\sigma,\sigma'} \;=\; \pi_{G,q,v}(\sigma')} \qquad \text{(independently of } X_0\text{).}$$

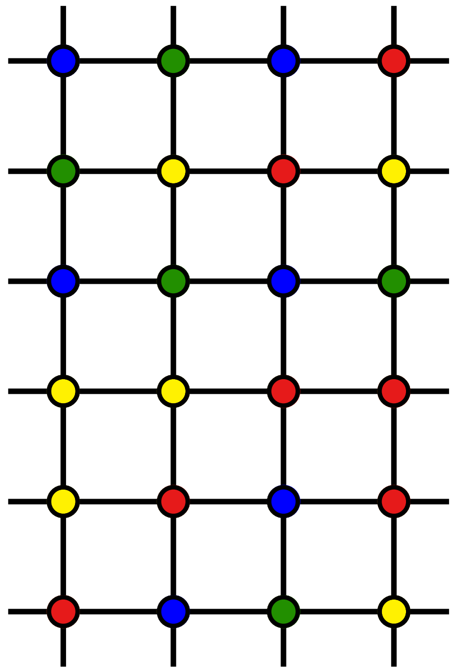
Markov-chain Monte Carlo simulations (2)

- $\pi(\sigma) \approx \Pr(X_t = \sigma)$ for $t \gg 1$, and independently of X_0.
- How to measure the efficiency of a Monte Carlo algorithm?
  - $\tau_{\rm exp}$: # MC step the system needs to be essentially in equilibrium $\approx \pi_{G,q,v}$.
  - $\tau_{\rm int}$: once in equilibrium, # MC steps we need to produce two statistically independent samples.
  - Critical slowing down: Close to a second-order phase transition

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

  - Dynamic critical exponents: $z_{\rm exp}$, $z_{\rm int}$.

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



Antiferromagnetic q–state Potts model

eg. $q = 4$

4×6 square lattice on a torus

$T > 0$

1. Pick up uniformly at random 2 distinct colors μ, ν:
   eg. $\mu =$ ● and $\nu =$ ●.
2. Freeze all spins σ_i taking colors $\neq \mu, \nu$, and allow the remaining spins to take the values μ, ν.
   $\Rightarrow$ We induce an AF Ising model on $G_{\mu,\nu}$ $\Rightarrow$ aSW

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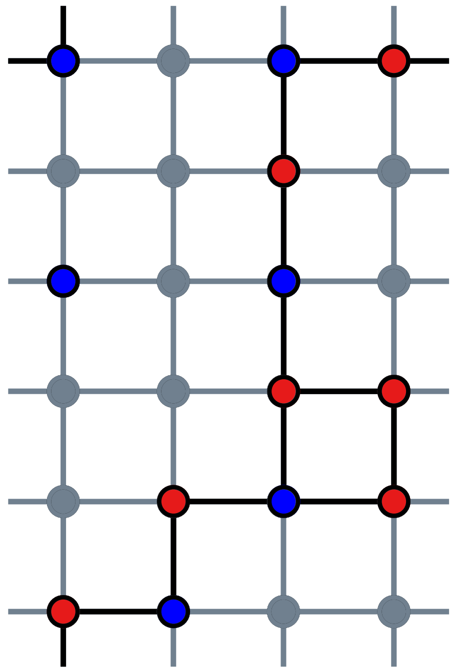

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   $\Rightarrow$ We induce an AF Ising model on $G_{\mu,\nu}$ $\Rightarrow$ aSW

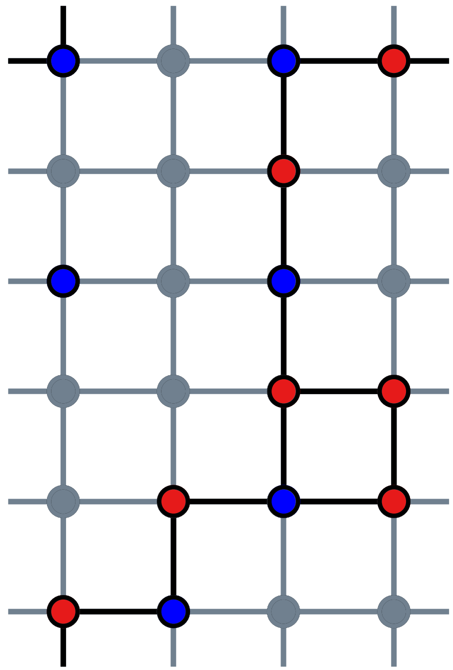
The Wang–Swendsen–Kotecký algorithm, 1989 (2)

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

We augment the state space: $n_{ij} = 0, 1$ on every edge $\langle ij \rangle$.

$$
\begin{aligned}
\pi(\sigma, n) &= \frac{1}{Z_G(q,v)} \prod_{\langle ij \rangle} \left[(1-p)\delta_{n_{ij},0} + p(1-\delta_{\sigma_i,\sigma_j})\delta_{n_{ij},1} \right] \\
n_{ij} &= \begin{cases} 1 & \text{edge } \langle ij \rangle \text{ is occupied} \\ 0 & \text{edge } \langle ij \rangle \text{ is empty} \end{cases}
\end{aligned}
$$

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



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

3. Simulate $P_{\text{bond}} = \pi(n \mid \sigma)$:
   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 $\sigma_i \neq \sigma_j$.

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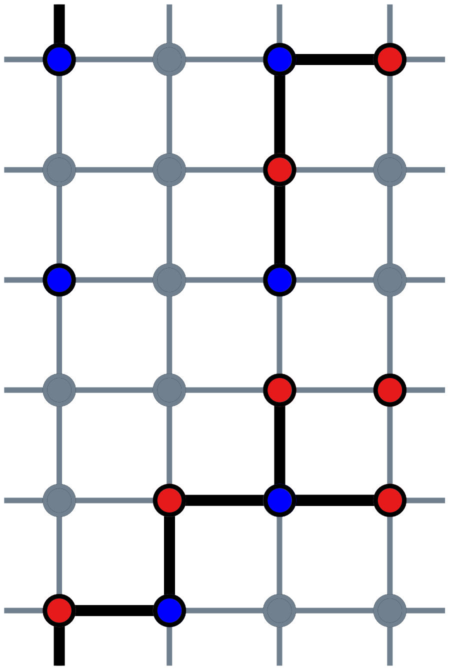

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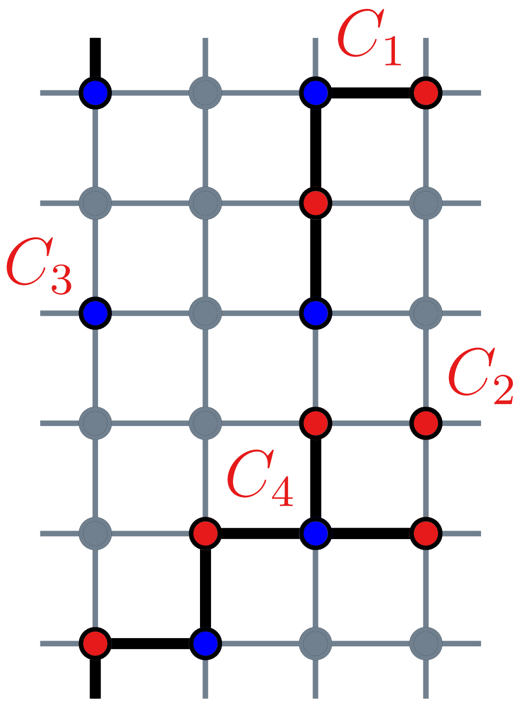

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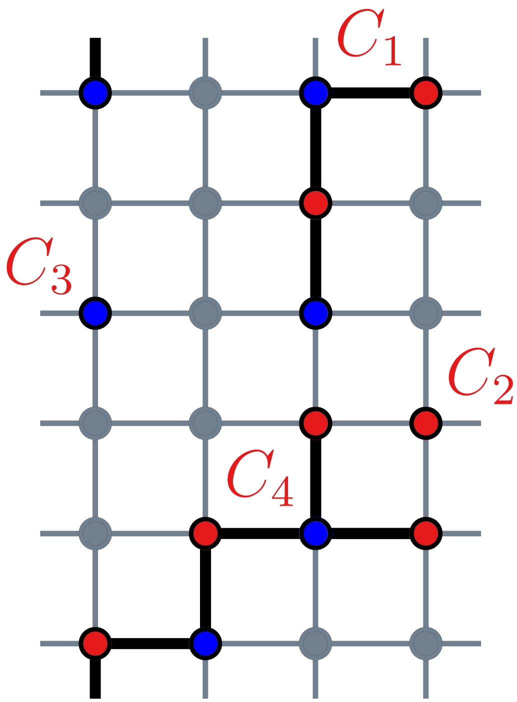
4. Identify the clusters of sites connected with bonds $n_{ij} = 1$.
5. Simulate $P_{\text{spin}} = \pi(\sigma \mid n)$: Independently for each connected cluster, either keep the original spin value or flip it ($\mu \leftrightarrow \nu$) with probability $\frac{1}{2}$.

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



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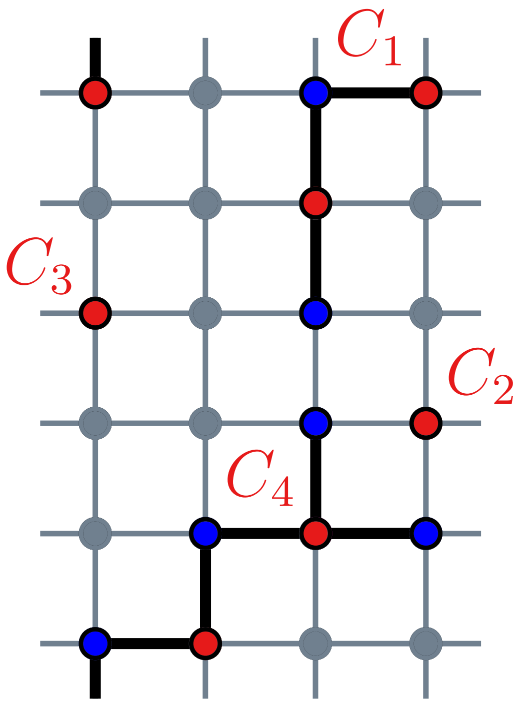

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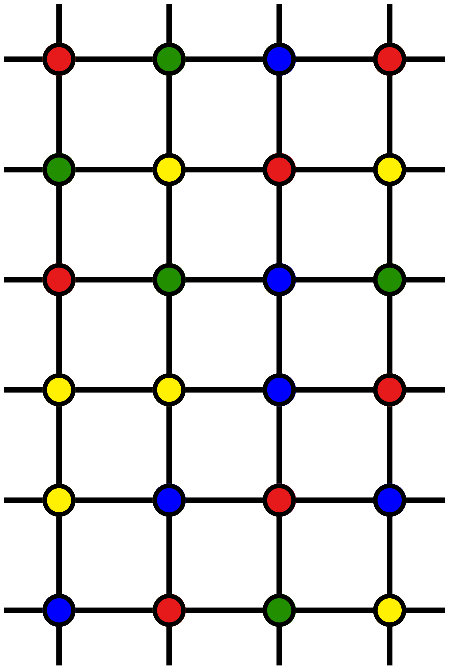


Antiferromagnetic q–state Potts model

eg. $q = 4$

4×6 square lattice on a torus

$T > 0$

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

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

1. The transition probability matrix $P = P_{\text{bond}} \cdot P_{\text{spin}}$ leaves invariant $\pi_{G,q,v}$ for all $T \geq 0$ ($v \geq -1$).
2. It is ergodic for any $T > 0$ ($v > -1$).

- However, at $T = 0$:
  - All edges in $G_{\mu,\nu}$ have $n_{ij} = 1$ ($p = -v = 1$).
  - WSK reduces to the Kempe chain in graph theory.
  - The ergodicity of WSK is a highly non-trivial question.
  - For non-frustrated systems ($q \geq \chi(G)$), WSK contains single-site moves.

Ergodicity of the WSK algorithm

$\mathrm{WSK}(G, q)$ is ergodic at $T = 0$ when $q \gg 1$:

Theorem 2 (Jerrum, Mohar) *Let Δ be the maximum degree of a graph G, and let $q \geq \Delta + 1$ be an integer. Then WSK(G, q) is ergodic. If G is connected and contains a vertex of degree $< \Delta$, then WSK(G, Δ) is ergodic.*

Lattice	Δ	$\mathrm{WSK}(G, q)$ ergodic for
Hexagonal	3	$q \geq 4$
Square, kagomé	4	$q \geq 5$
Diced, triangular	6	$q \geq 7$

But $\Delta + 1 \; > \; q_c(\mathcal{L}) \Rightarrow$ Disordered systems!!

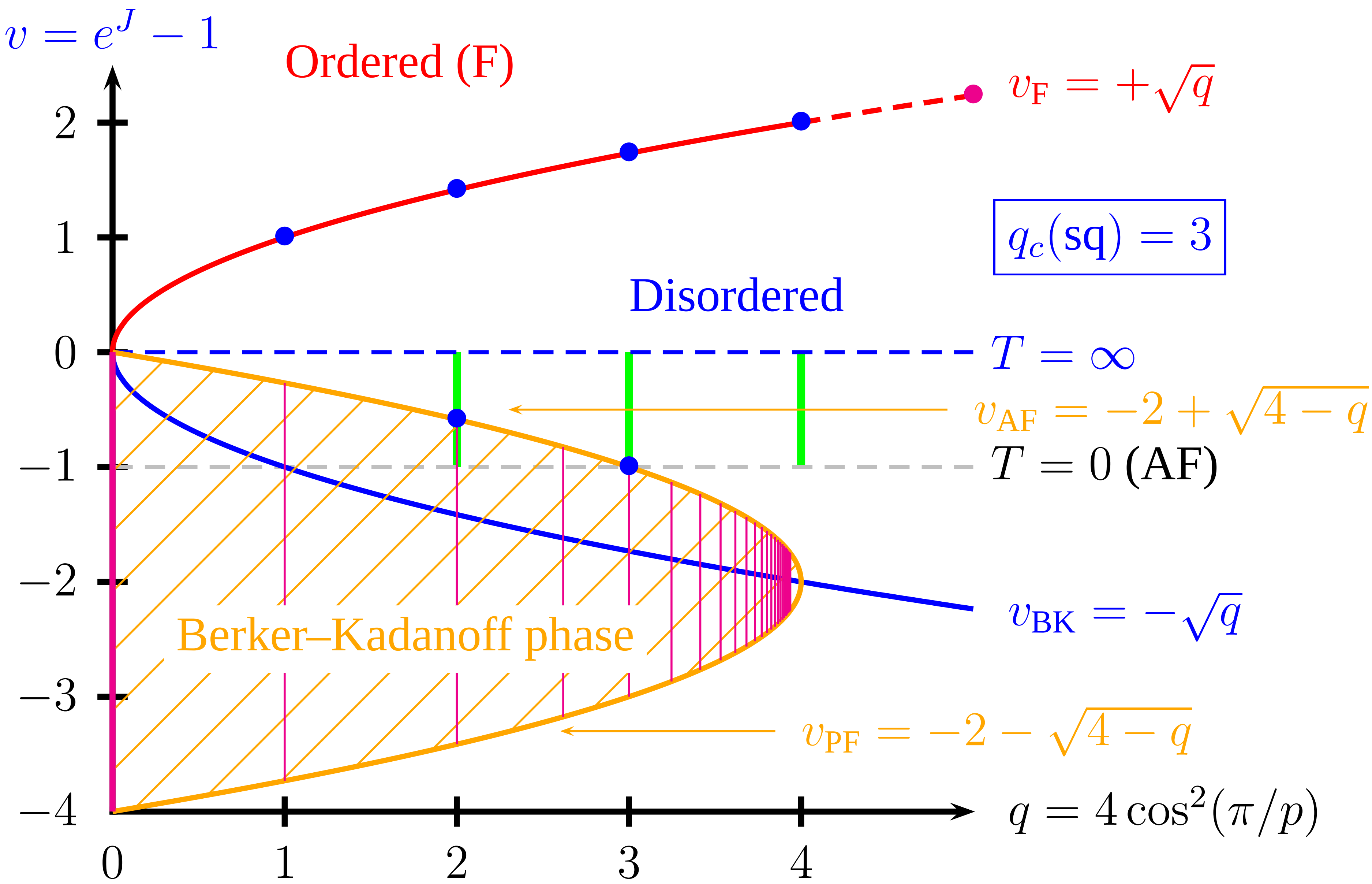
Ergodicity of the WSK algorithm (2)

Theorem 3 (Burton-Henley, Ferreira-Sokal, Mohar) *WSK*(G,q) *is ergodic for any bipartite graph* G *and any integer* $q \geq 2$*.*

For non-bipartite graphs, we know the answer only for planar graphs:

Theorem 4 (Mohar) *Let* G *be a 3–colorable planar graph, then WSK*(G,q) *is ergodic for any integer* $q \geq 4$*.*

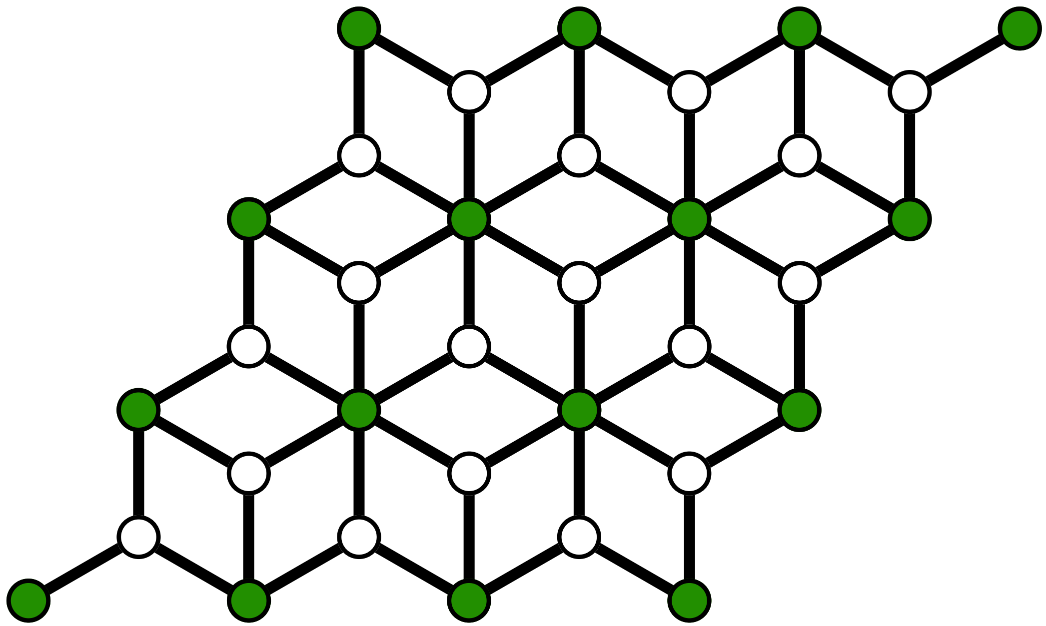
Square-lattice Potts-model phase diagram



WSK on the square lattice

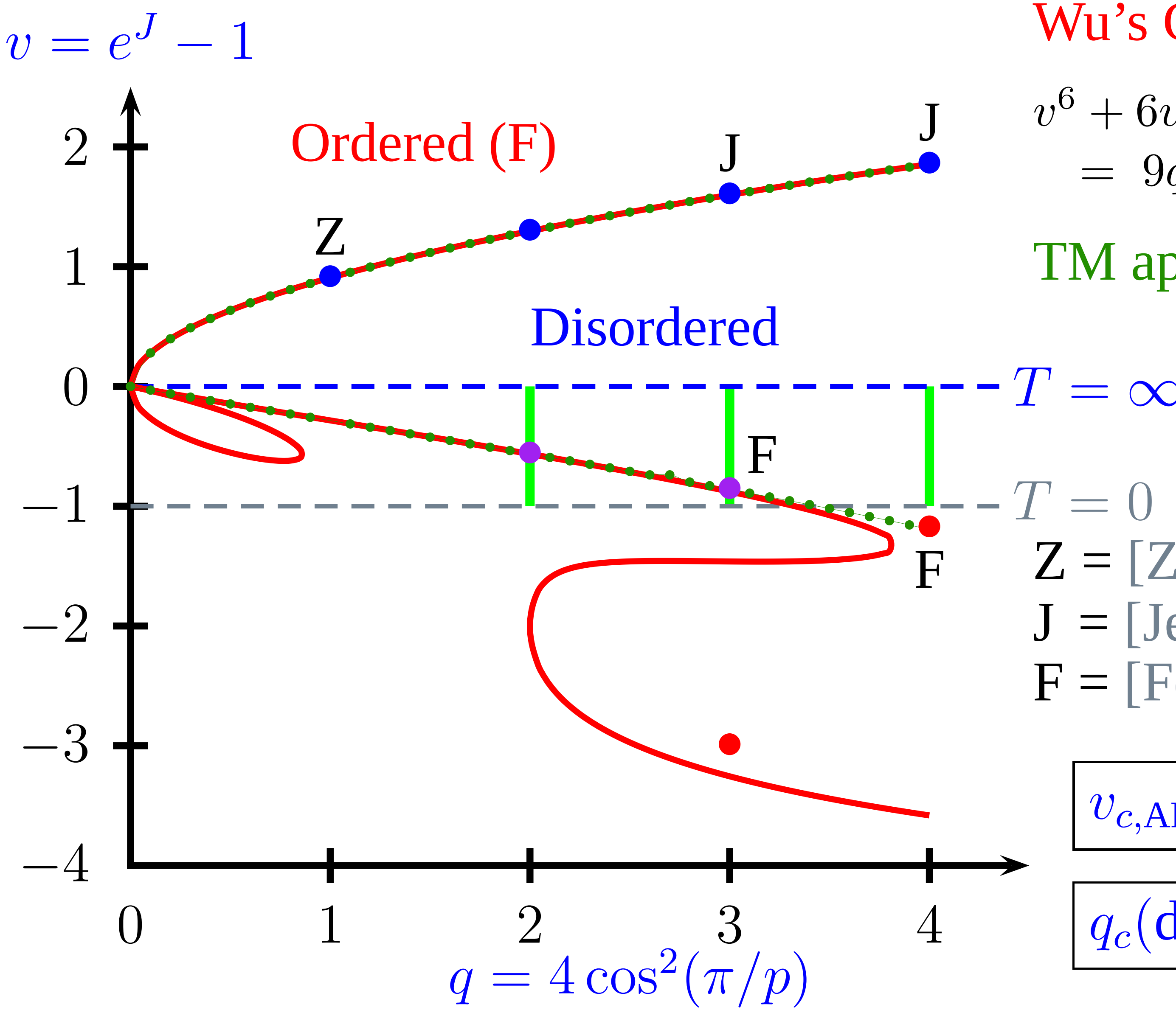
- $q = 2$: WSK is equivalent to SW.
- $q = 3 = q_c(\text{sq})$: The model is critical at $T = 0$.
  - WSK(sq,3) has NO critical slowing down!: $z_{\text{int}} = 0$. [Ferreira-Sokal '96, Sokal-JS '98]:
    - $\tau_{\text{int},\mathcal{M}^2_{\text{stagg}}} \lesssim 5$ and $\tau_{\text{int},\mathcal{E}} \lesssim 4$ uniformly in $L, T > 0$.
    - $\tau_{\text{int}} \lesssim 8$ uniformly in L at $T = 0$.
  - $\nu = 2, \quad \left(\frac{\gamma}{\nu}\right)_{\text{stagg}} = \frac{5}{3}, \quad \left(\frac{\gamma}{\nu}\right)_{\text{u}} = \frac{2}{3}.$
- $q \geq 4$: The model is disordered at all temperatures $T \geq 0$.
  - WSK(sq,4) has no critical slowing down [Ferreira-Sokal] $\tau_{\text{int},\mathcal{M}^2_{\text{stagg}}} \lesssim 2.6$ and $\tau_{\text{int},\mathcal{E}} \lesssim 3.5$ uniformly in $L, T > 0$.

Diced-lattice Potts model



- Dual of kagomé.
- Non-regular bipartite quadrangulation.

Diced-lattice Potts-model phase diagram



Wu's Conjecture '79

$$v^6 + 6v^5 + 12v^4 + 2qv^3 = 9qv^2 + 6q^2v + q^3$$

TM approach [Jacobsen-JS]

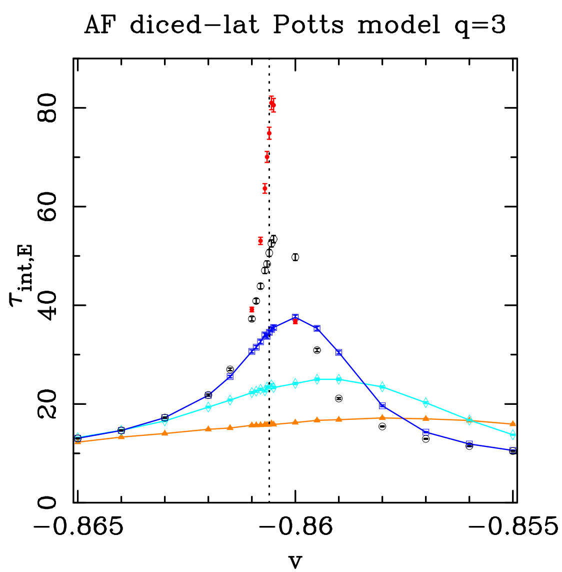
Z = [Ziff-Suding '97]
J = [Jensen *et al.* '97]
F = [Feldman *et al.* '98]

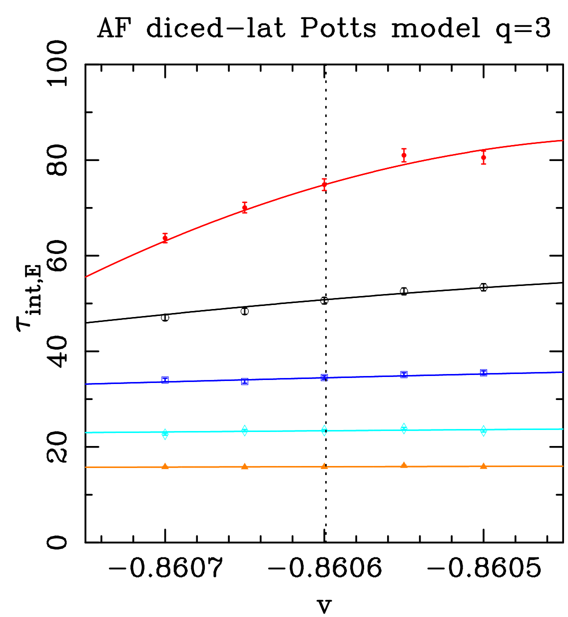
$$\boxed{v_{c,\mathrm{AF}}(3) = -0.860599(4)}$$

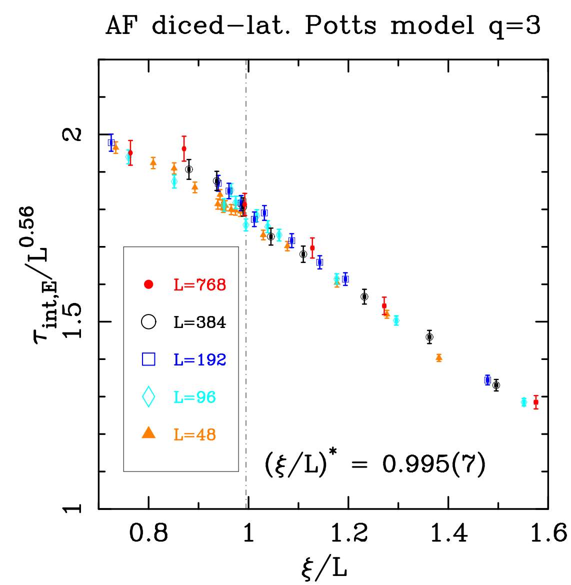
$$\boxed{q_c(\text{diced}) \approx 3.45}$$

WSK on the diced lattice

- $q = 2$: WSK is equivalent to SW.
- $q = 3$: The model has a critical point at $v_c = -0.860599(4)$, and has long-range order for $v < v_c$.
  - WSK(diced,3) has critical slowing down: $z_{\mathrm{int},\mathcal{E}} = 0.56(1)$.







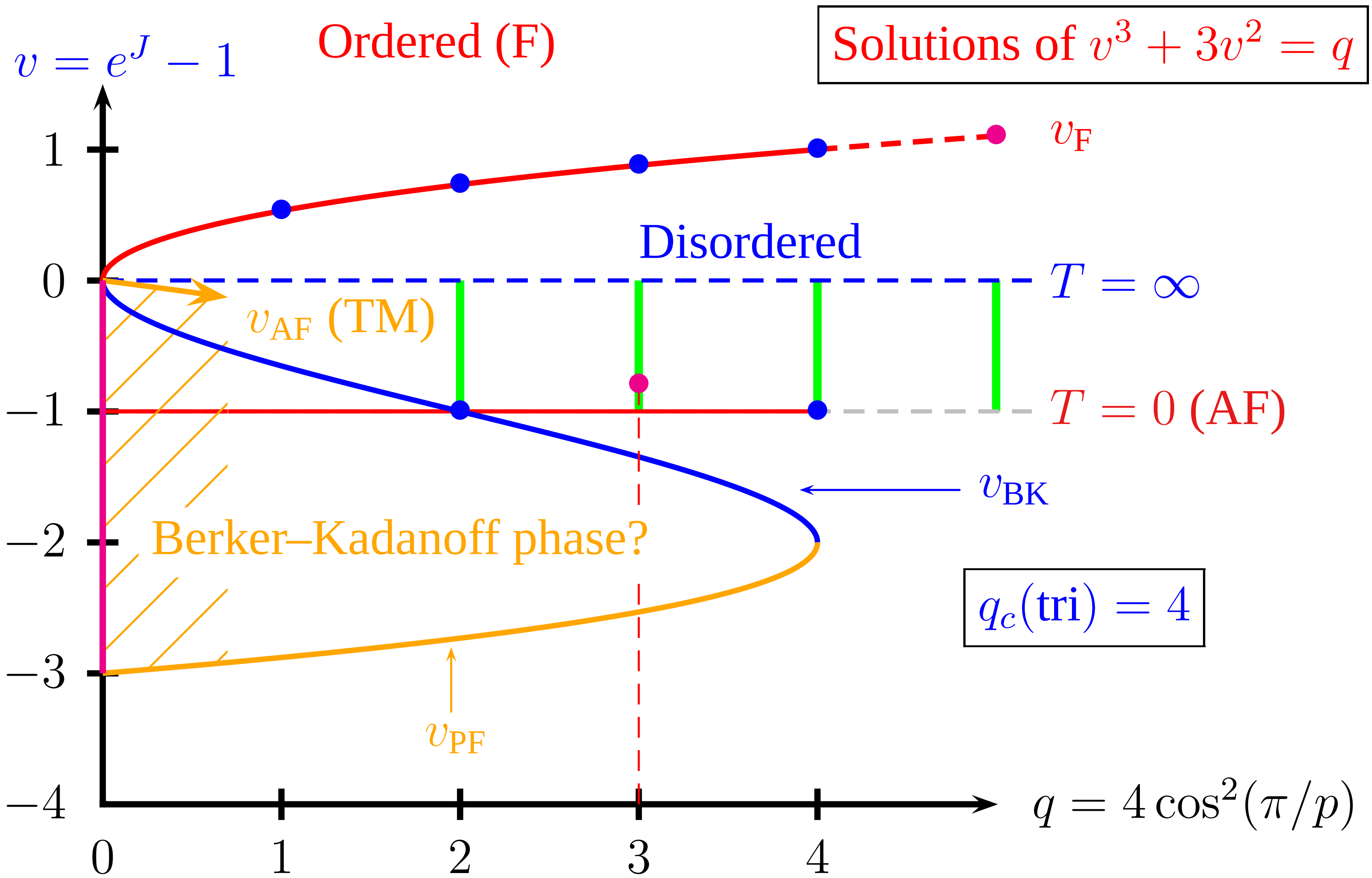
WSK on the diced lattice (2)

- $q = 3$. The critical point at $v_c = -0.860599(4)$:
  - Ferromagnetic 3–state Potts model universality class.
    - $\nu = \frac{5}{6}, \quad \left(\frac{\gamma}{\nu}\right)_{\text{stagg}} = \frac{26}{15}.$
  - SW for ferro 3–state Potts model [Sokal-JS '97]:

    $z_{\text{int},\mathcal{E}} = 0.515(6) \lesssim 0.56(1)$.
- $q \geq 4$: The model is disordered at all $T \geq 0$.
  - WSK(diced,4) has no critical slowing down

    $\tau_{\text{int},\mathcal{E}} \lesssim 5$ uniformly in $L, T \geq 0$.

Triangular-lattice Potts-model phase diagram



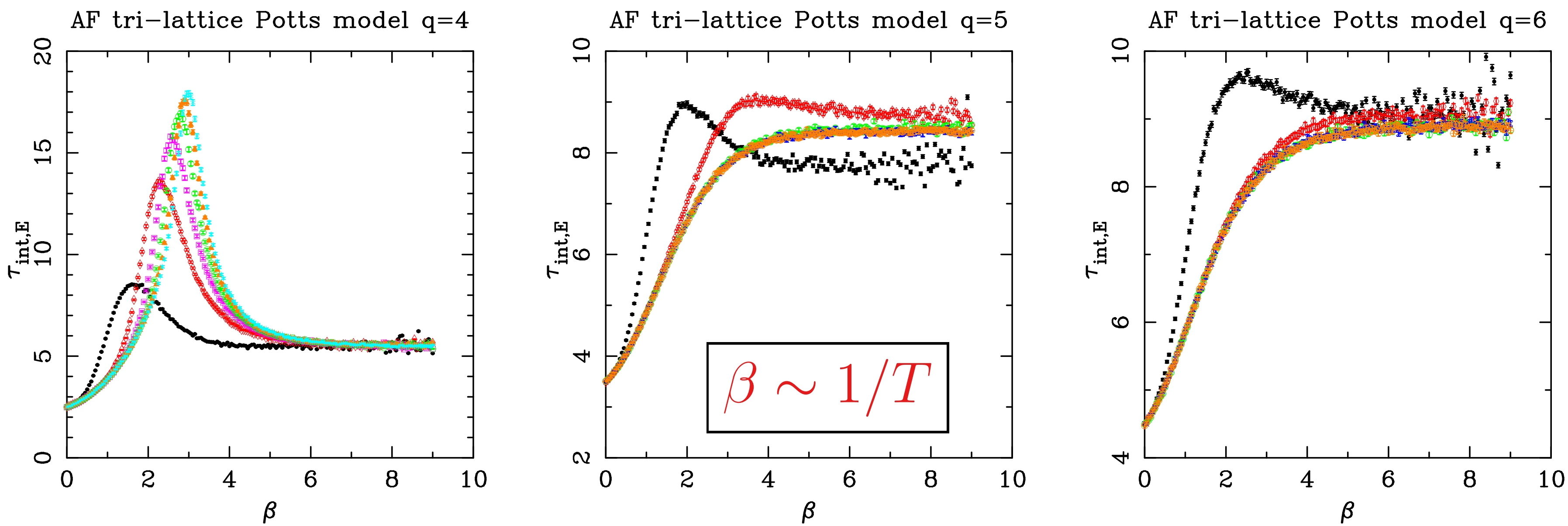
WSK on the triangular lattice

- $q = 2$: The system is critical at $T = 0$, and disordered for any $T > 0$.
  - Frustration: WSK is *not* ergodic at $T = 0$ (one cluster).
- $q = 3$: The model has a weak first–order phase transition [Adler *et al*. '95] at finite temperature:

$$v_c = \begin{cases} -0.79691(3) & \text{[Adler } \textit{et al}.\text{]} \ \textbf{(MC)} \\ -0.796927(20) & \text{[Chang } \textit{et al}.\text{ '04]} \ \textbf{(TM)} \end{cases}$$

  - WSK$(G, 3)$ is ergodic at $T = 0$ on any 3–colorable triangulation G.
  - We expect $\tau_{\text{int}} \sim e^{AL^{d-1}}$.

Autocorrelation time for $q = 4, 5, 6$



- Moore and Newman ('00) proved that WSK(T,4) is ergodic on any 3–colorable triangulation of S^2 or the projective plane.

$$z_{\mathrm{exp}} \;=\; 0.74(2)$$

- We expect logarithmic corrections at $T = 0$ (the height model is at the roughening transition).

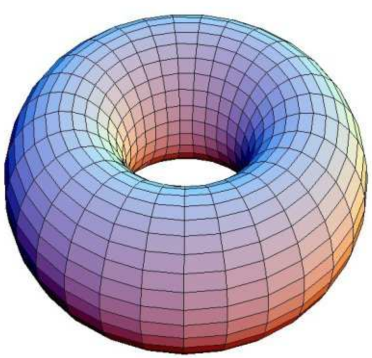
- Predictions: $\left(\frac{\gamma}{\nu}\right)_{\mathrm{stagg}} = \frac{5}{3}, \quad \left(\frac{\gamma}{\nu}\right)_{\mathrm{u}} \;=\; 1$ [Henley '93].

Non-ergodicity for $q = 4$

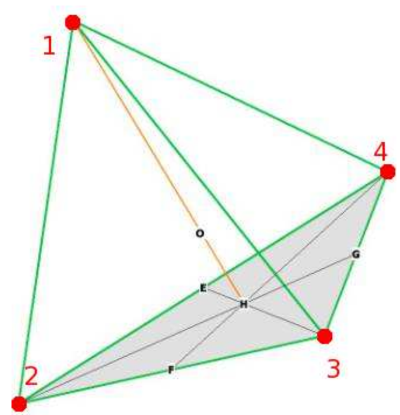
Theorem 5 *For any triangulation $T = T(3L, 3L)$ of the torus with $L \geq 2$, the corresponding WSK$(T, 4)$ algorithm is not ergodic.*

The proof is based on algebraic topology [Fisk '73–'77].

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



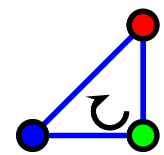
$\xrightarrow{f}$

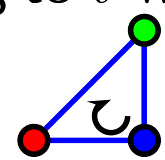


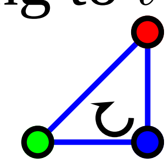
$$\boldsymbol{e}^{(\alpha)} \in \mathbb{R}^{q-1}$$
$$\alpha = 1, \ldots, q$$
$$\boldsymbol{e}^{(\alpha)} \cdot \boldsymbol{e}^{(\beta)} = \frac{q\delta_{\alpha\beta} - 1}{q - 1}$$

Degree of a 4–coloring

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

- We choose orientations for T and $\partial\Delta^3$ (e.g. clockwise).
- Fix a triangular face t of $\partial\Delta^3$, e.g., 

  p = # faces of T mapping to t with their orientation preserved by f: 

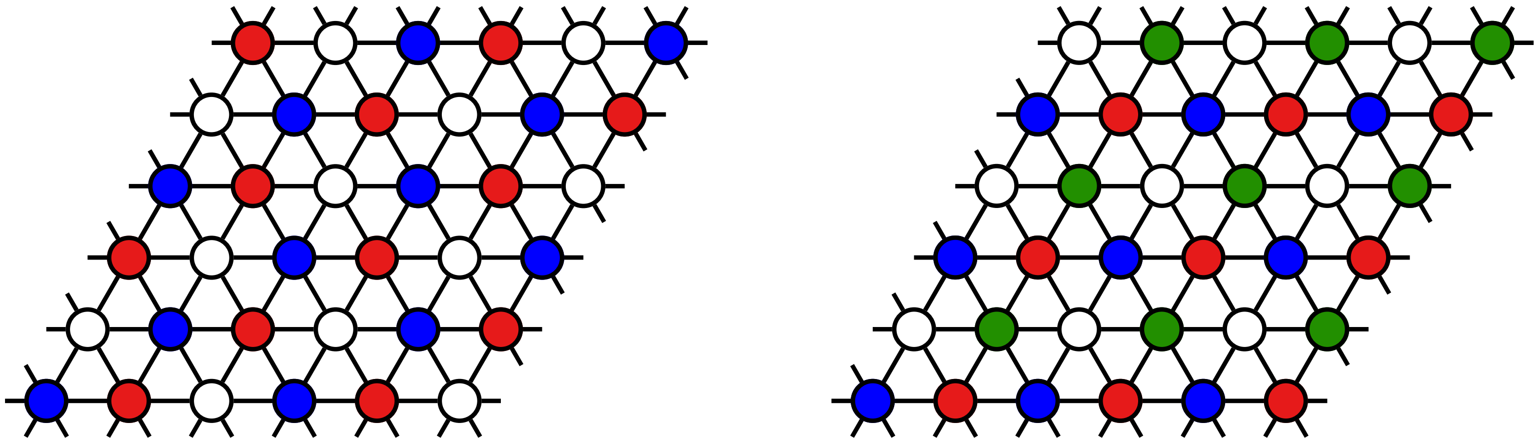
  n = # faces of T mapping to t with their orientation reversed by f: 
- $\deg(f) \; = \; p - n$.
- $\deg(f)$ does NOT depend on the choice of t!!!

Non-ergodicity for $q = 4$ (2)

- For any 3–colorable triangulation of the torus:
  - $\deg f \equiv 0 \pmod 6$ [Fisk '73].
  - Under a WSK move, $\deg f \pmod{12}$ is invariant.
- There might be (at least) two ergodicity classes:
  - One with $\deg f \equiv 0 \pmod{12}$: $\deg f = 0, \pm 12$, etc (non-empty: it contains the 3–coloring of T).
  - One with $\deg f \equiv 6 \pmod{12}$: $\deg f = \pm 6, \pm 18$, etc (might be empty!!!).

They can't be connected via WSK moves!

Non-ergodicity for $q = 4$ (3)



$\deg f \equiv 0 \pmod{12}$ $\qquad$ $|\deg g| = 18 \equiv 6 \pmod{12}$

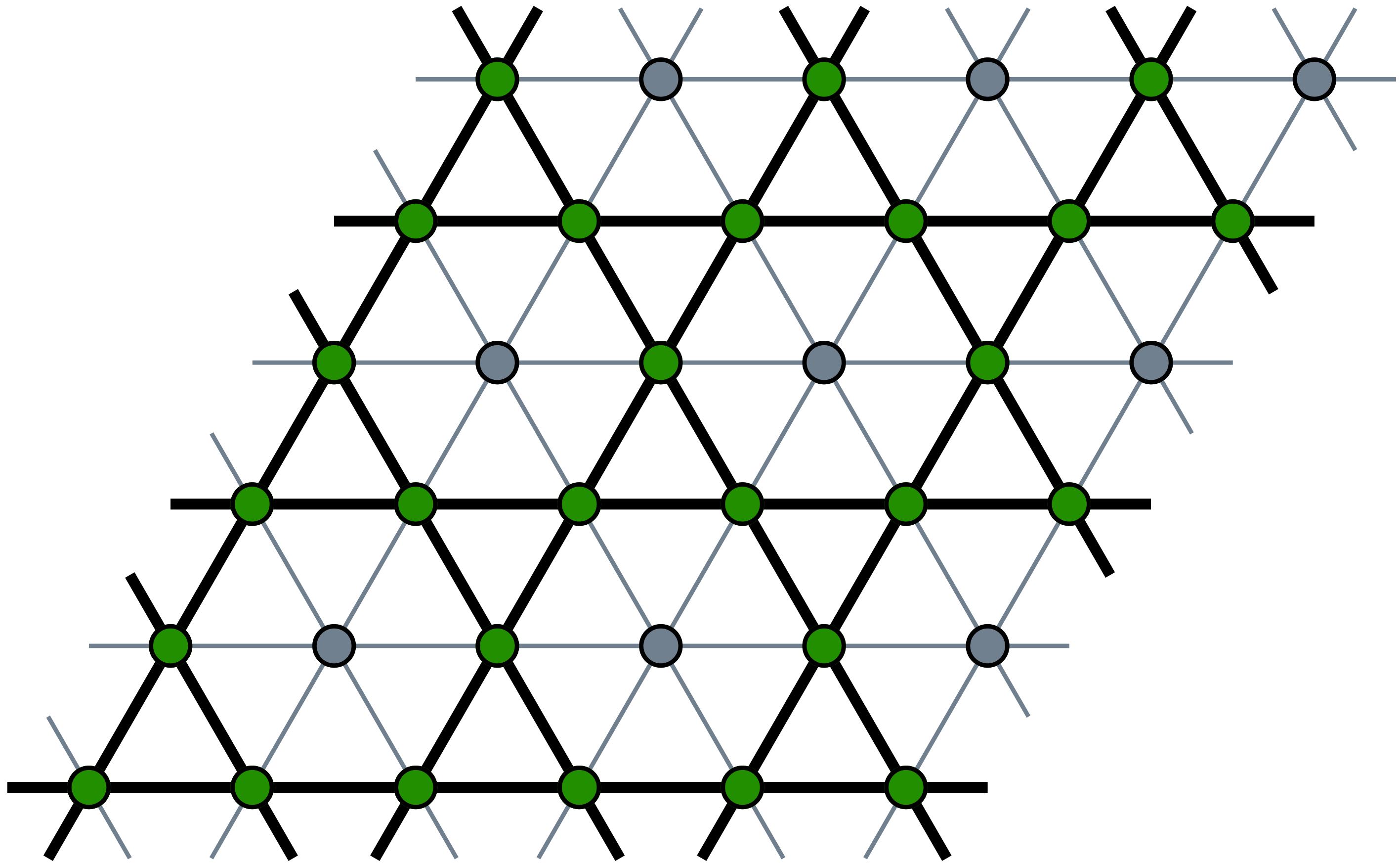
- On any $T(3L, 3L)$, we find two 4–colorings f, g such that

$$\deg f - \deg g \equiv 6 \pmod{12}.$$

$\Rightarrow$ WSK(T,4) is not ergodic at $T = 0$.

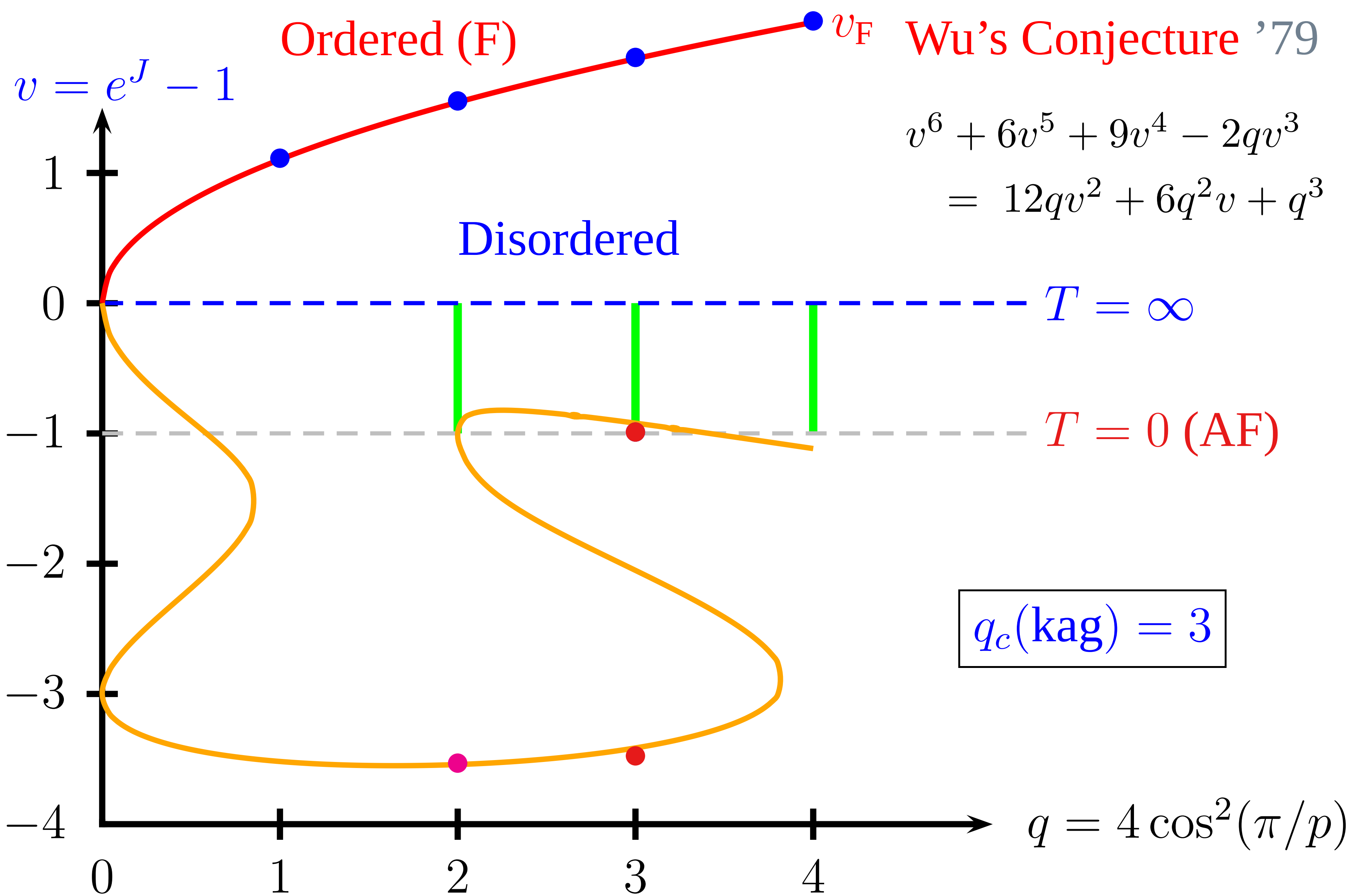
- WSK$(T, 4)$ includes single-site dynamics.
- This method does not tell us anything about $q = 5, 6$!!!

Kagomé-lattice Potts model



- Medial $T'(3L, 3L)$ of the triangular lattice $T(3L, 3L)$.
- $T'(3L, 3L) \subset T(6L, 6L)$.

Kagomé-lattice Potts-model phase diagram

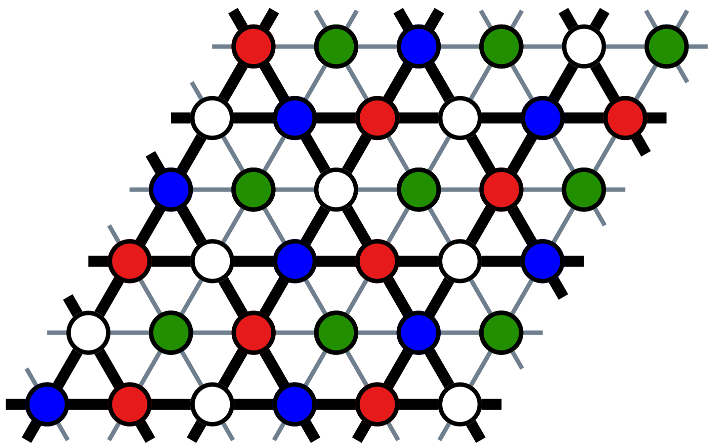


WSK on the kagomé lattice

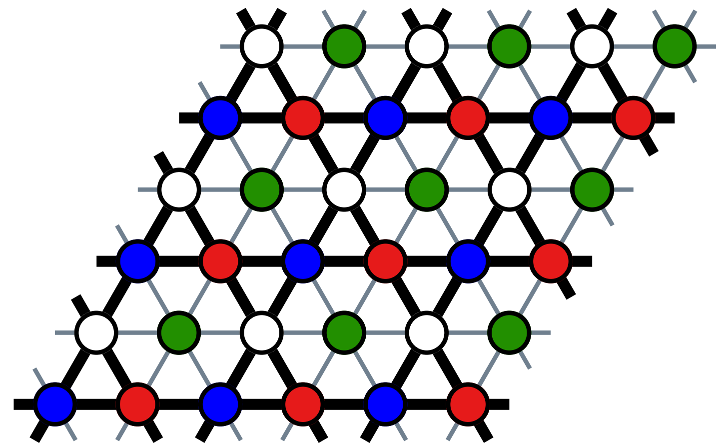
- $q = 2$: The system is disordered $\forall\, T \geq 0$ [Kano-Naya ’53].
  - Frustration: WSK is not ergodic at $T = 0$ (one cluster).
- $q = 3$: At $T = 0$, the model is “equivalent” to the $T = 0$ 4–state AF model on the triangular lattice.
  - Each 4–coloring on the triangular lattice induces a 3–coloring on the kagomé lattice.
    The reverse is not true in general on the torus!!
  - Huse and Rutenberg (’92):
    - There is a height representation at $T = 0$, and the height model is at the roughening transition (logs!).
    - Path–flipping algorithm $\equiv$ WSK (non-ergodic?)
    - Prediction: $\left(\frac{\gamma}{\nu}\right)_{\text{stagg}} = \frac{2}{3}$.

WSK on the kagomé lattice (2)

- $q = 3$: A 3–coloring on the kagomé lattice $T'(3L, 3L)$ can be regarded as a constrained 4–coloring on $T(6L, 6L)$.



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



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

Theorem 6 *For any kagomé graph $G = T'(3L, 3L)$ on the torus with $L \in \mathbb{N}$, the corresponding WSK$(G, 3)$ algorithm is not ergodic.*

WSK on the kagomé lattice (3)

- $q = 4$: The system is disordered for all $T \geq 0$.

Theorem 7 (McDonald-Mohar-Scheide) *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.
- The hexagonal lattice has $\Delta = 3$.
- The 4–edge–colorings of the hexagonal lattice are equivalent to 4–colorings of its line graph $=$ kagomé lattice.

Corollary 8 *For any kagomé graph $G = T'(3L, 3L)$ on the torus with $L \in \mathbb{N}$, the corresponding WSK$(G, 4)$ algorithm is ergodic.*

Conclusions

- For bipartite lattices, WSK is ergodic and efficient:
  - Square lattice with $q = 3$: $z_{\rm int} = 0$.
  - Diced lattice with $q = 3$: $z_{{\rm int},\mathcal{E}} = 0.56(1)$.
- For non-bipartite lattices, WSK is non-ergodic at $T = 0$ in the most interesting cases:
  - Triangular lattice with $q = 4$.
  - Kagomé lattice with $q = 3$.
- Open problems:
  - Invent new, legal, and hopefully efficient algorithms for the above models (worm algorithm?)