Markov-chain Monte Carlo algorithms for studying cycle spaces, with some applications to graph colouring

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April 20, 2011
Monash Discrete Maths Seminar

Collaborators/References

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   Phys. Rev. Lett. 99, 110601 (2007).

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  - Using worm algorithm instead

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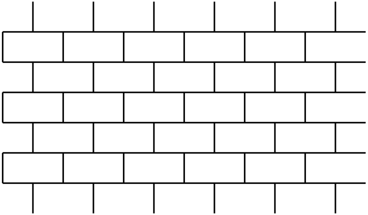

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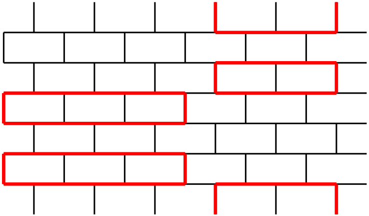

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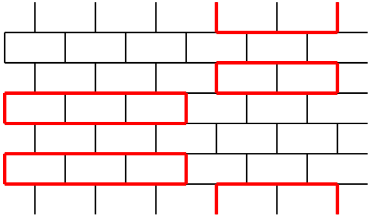

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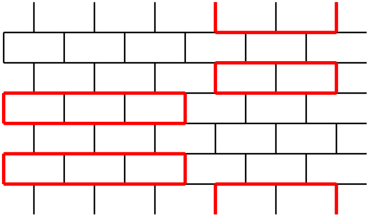

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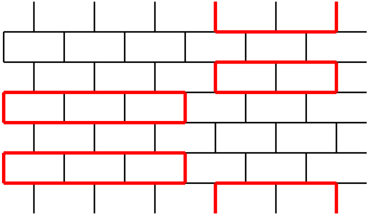

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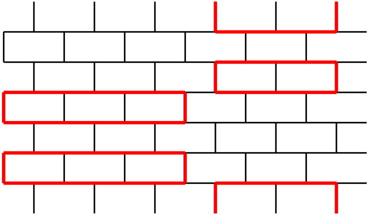

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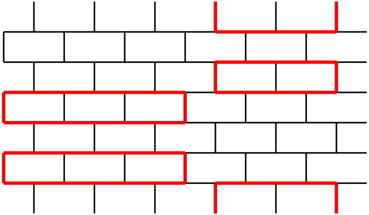

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- If G is large its infeasible to calculate $Z_{G,n,x} = \sum_{A \in \mathcal{C}(G)} n^{c(A)} x^{|A|}$
- So how can we sample from $\phi_{G,n,x}(\cdot)$?

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Theorem (Ergodic Theorem)

If P is irreducible with stationary distribution π then for any initial distribution

$$\frac{1}{N}\sum_{n=1}^{N} f(X_n) \xrightarrow[N\to\infty]{} \sum_{s\in S} \pi(s) f(s) \qquad a.s.$$

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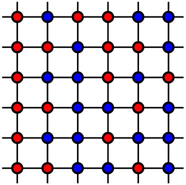

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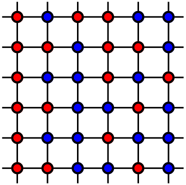

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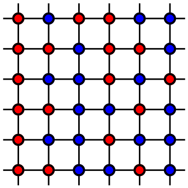

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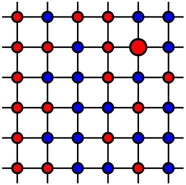

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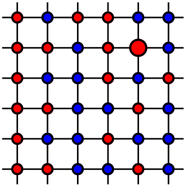

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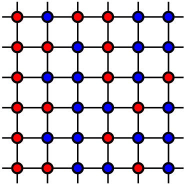

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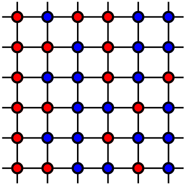

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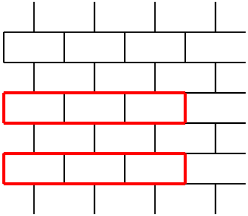
Worm chains

- Local moves on $\mathcal{C}(G)$ not so obvious



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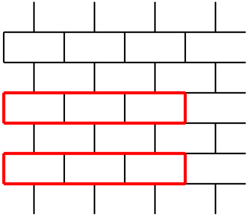

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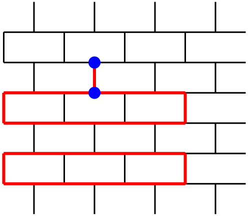

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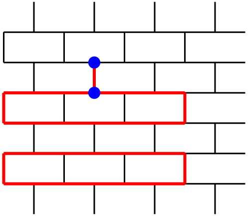

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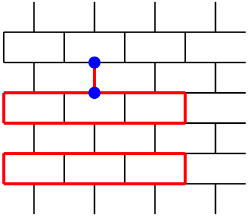

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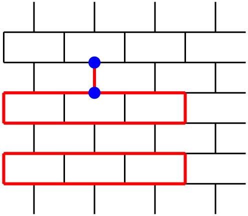

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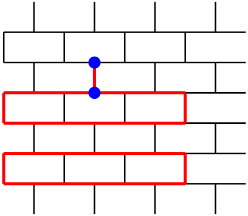

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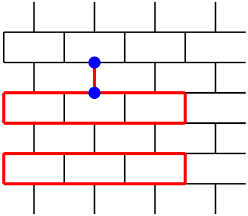

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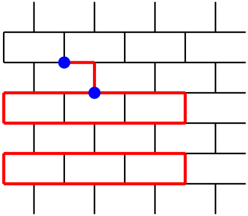

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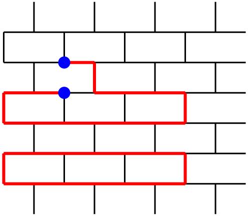

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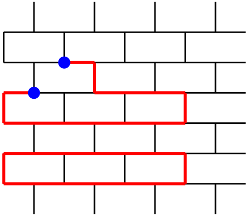

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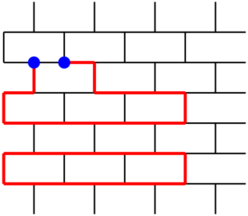

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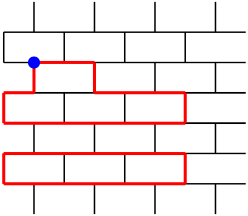

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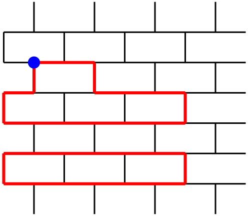

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  - Get new chain, $\overline{P}_{n,x}$, in detailed balance with $\overline{\pi}_{n,x}$

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- Consider an irreducible P on a finite state space $\mathcal{S}$
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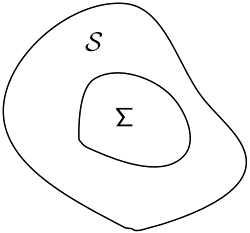

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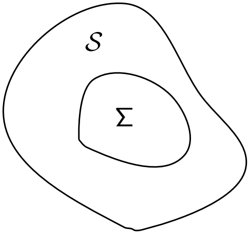

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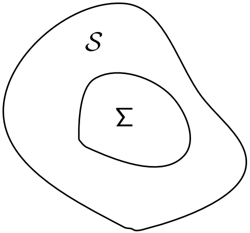

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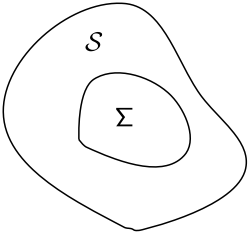

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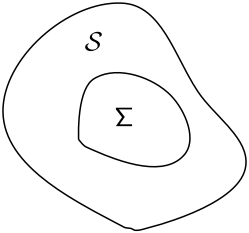

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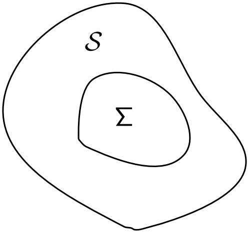

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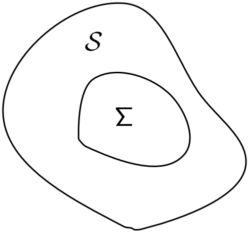

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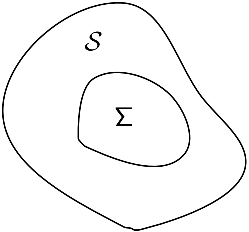

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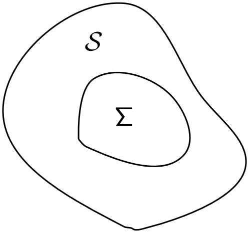

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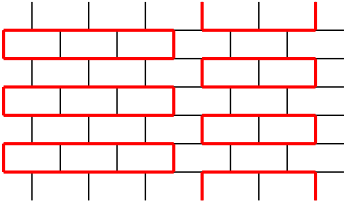

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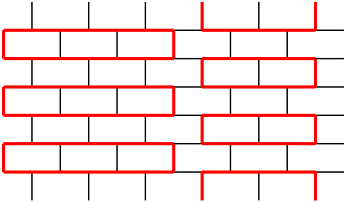

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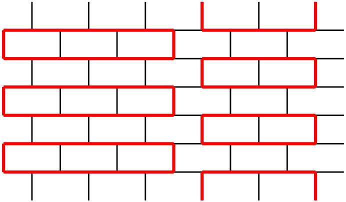

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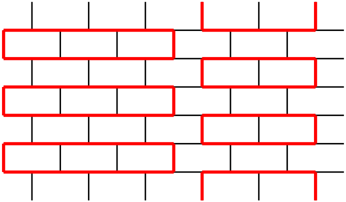

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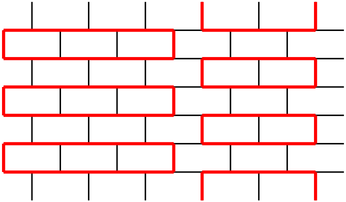

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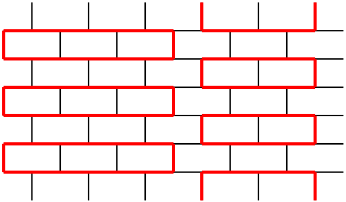
Fully-packed loops

Let G be bicubic and take $x \to \infty$



- State space is

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$$\phi_{G,n}(A) \propto n^{c(A)}, \qquad A \in \mathcal{F}(G)$$

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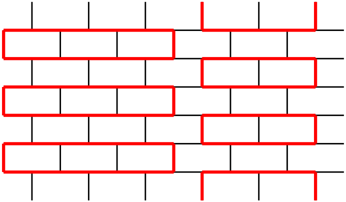

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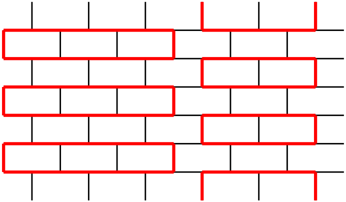

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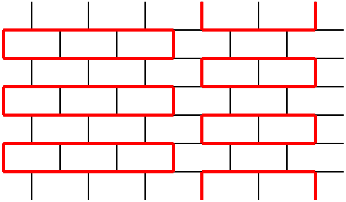

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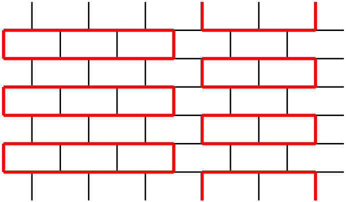

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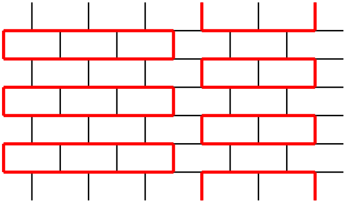

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Worm algorithm for fully-packed loops

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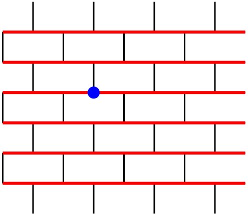

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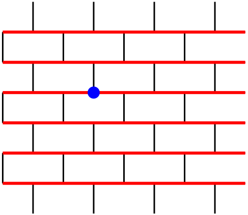

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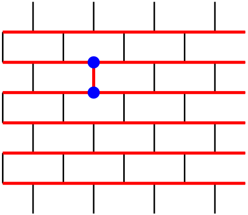

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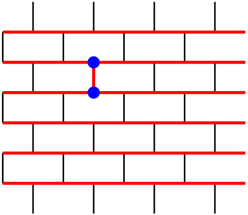

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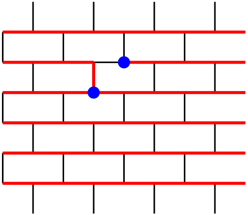

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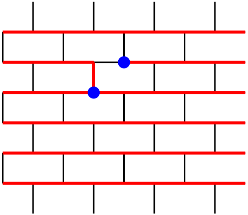

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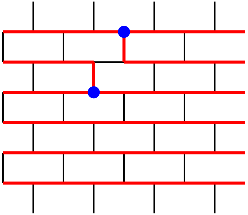

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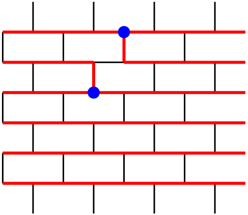

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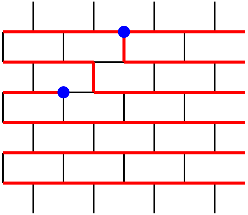

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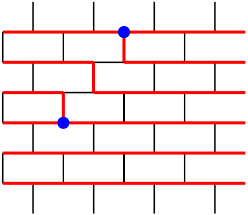

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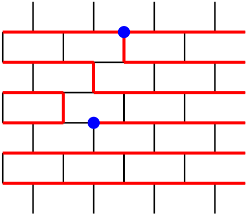

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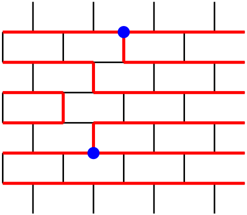

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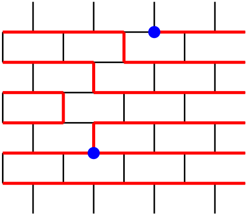

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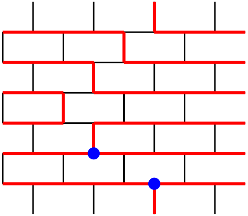

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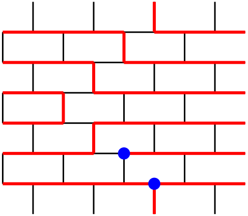

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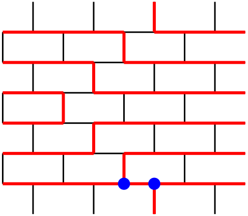

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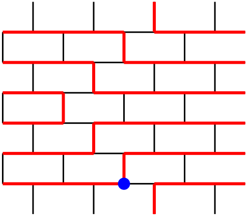

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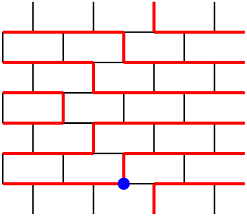

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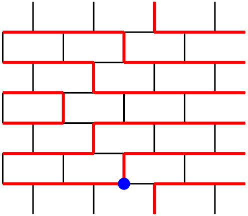

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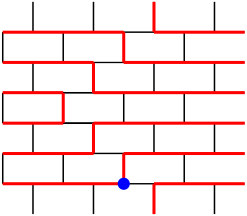

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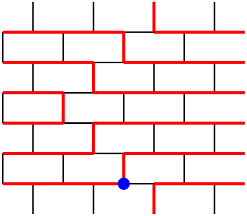

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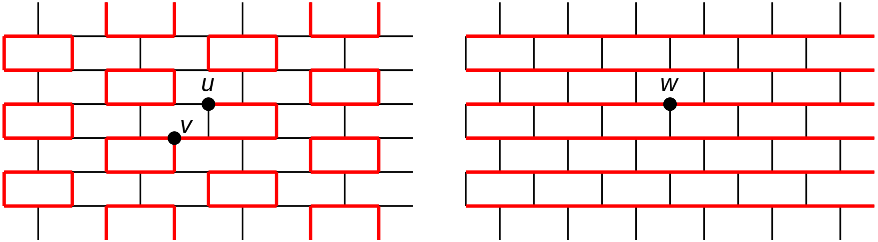

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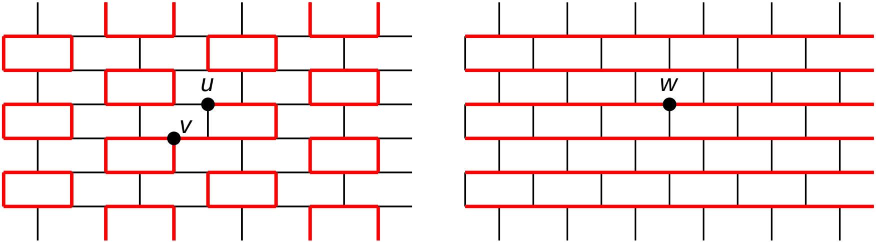

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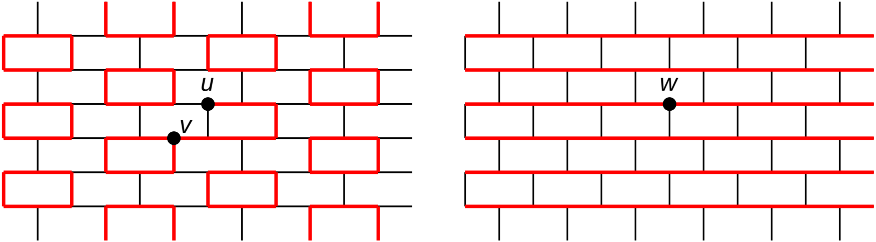

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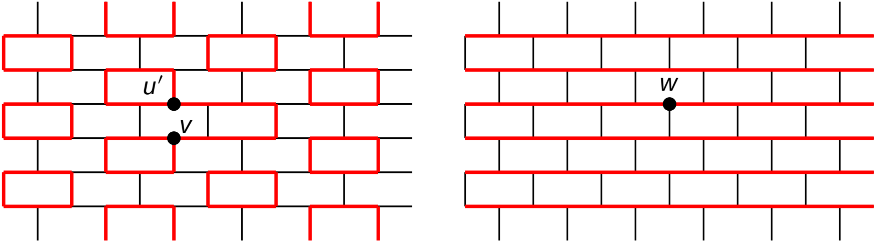

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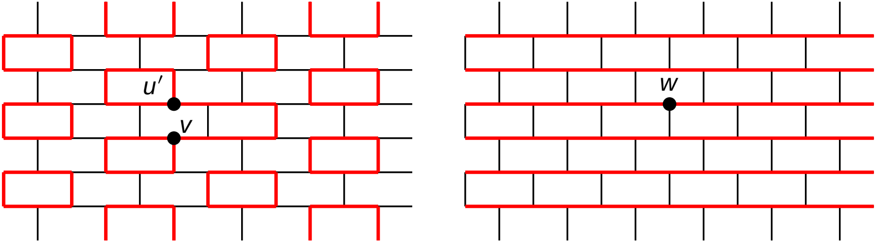

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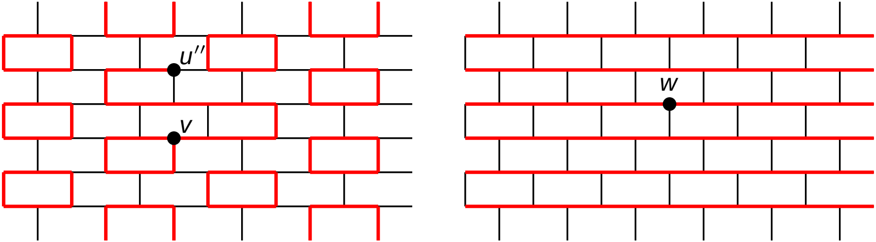

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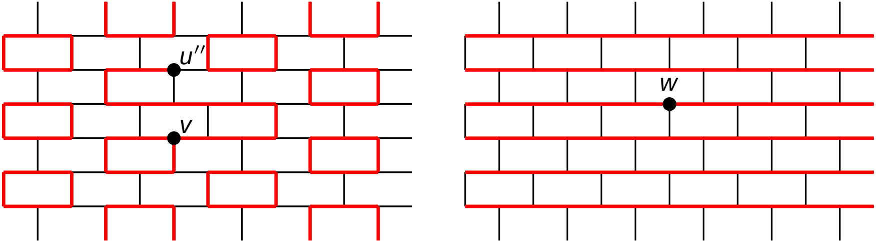

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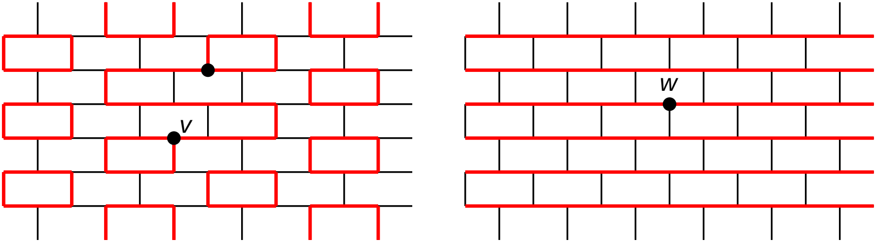

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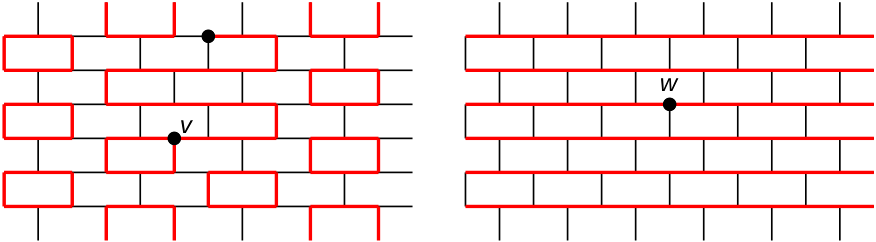

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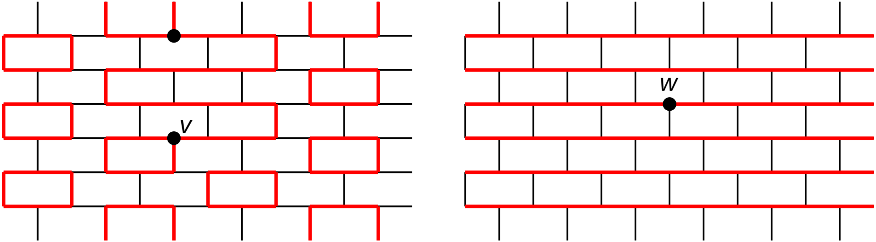

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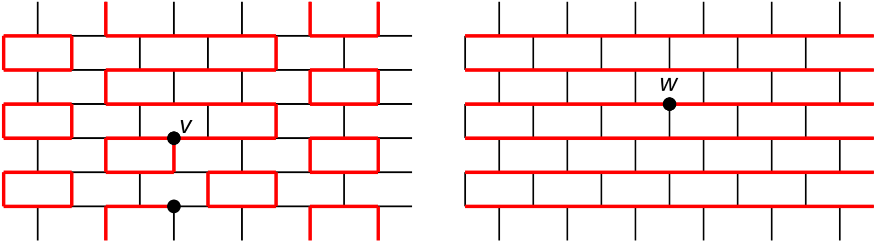

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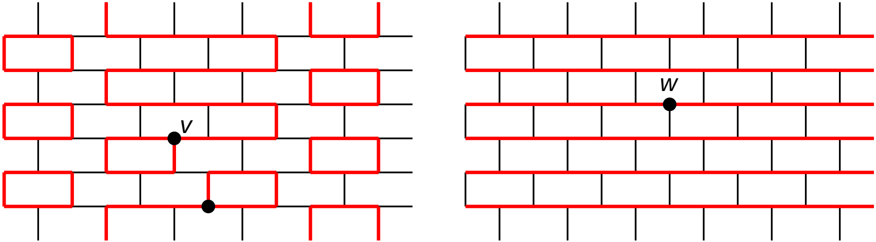

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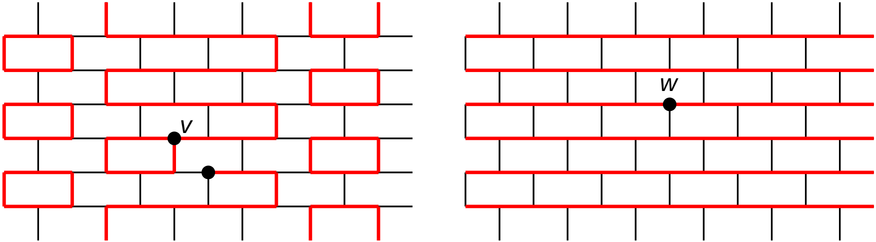

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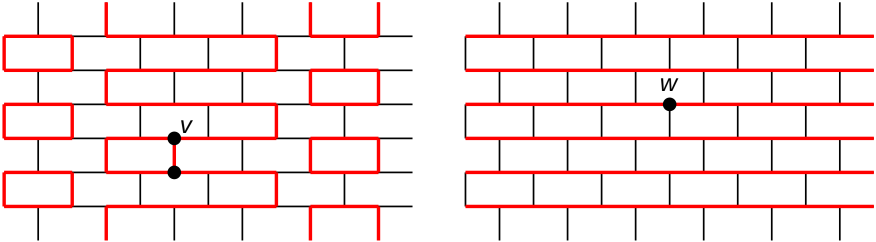

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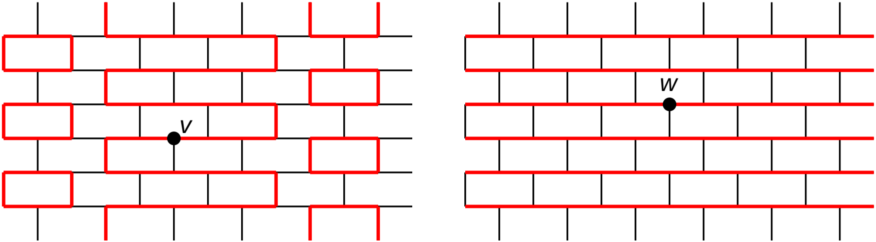

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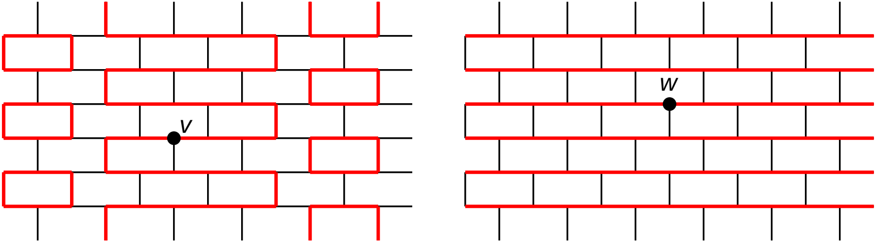

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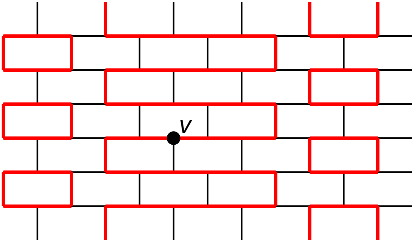

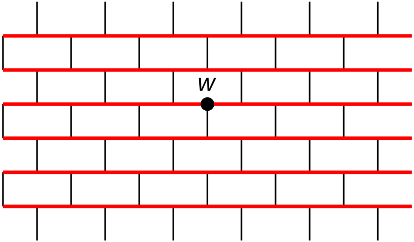

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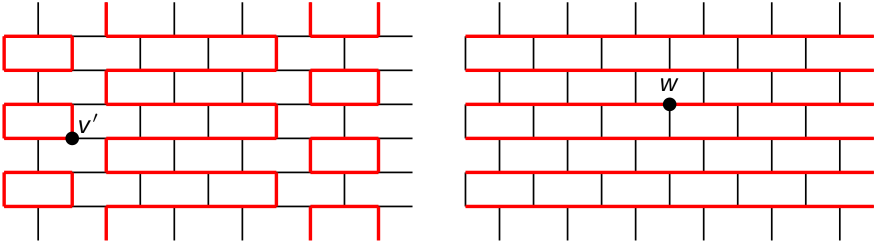

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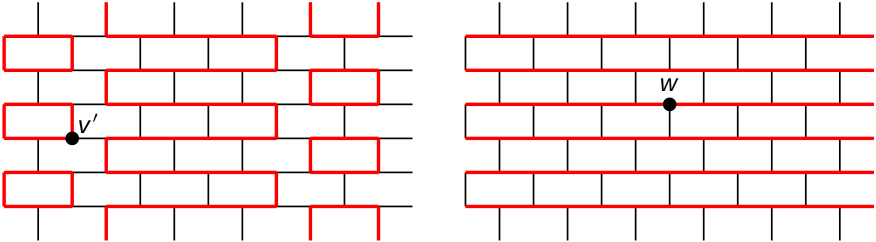

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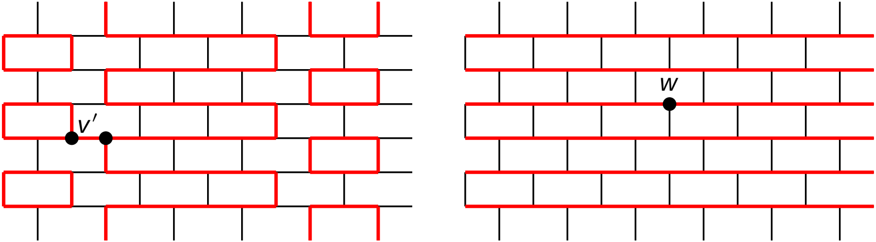

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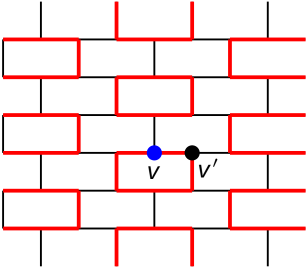

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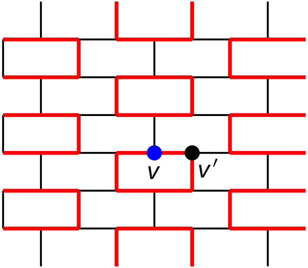

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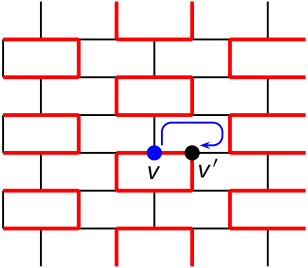

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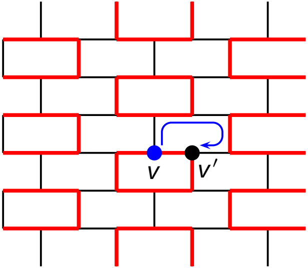

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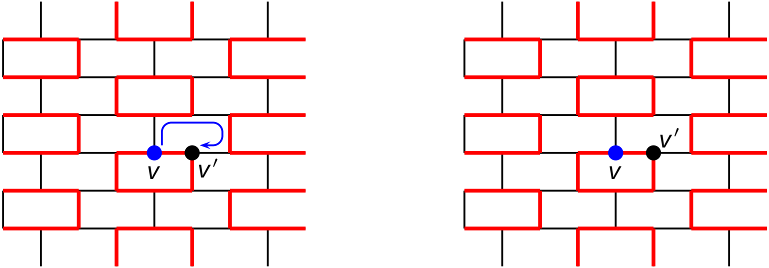

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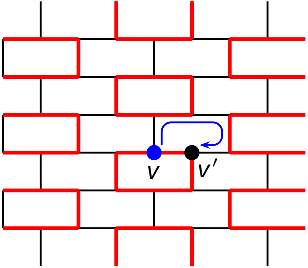

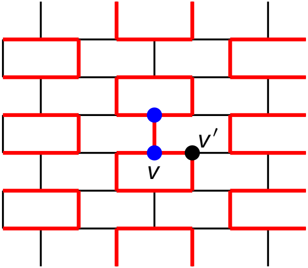

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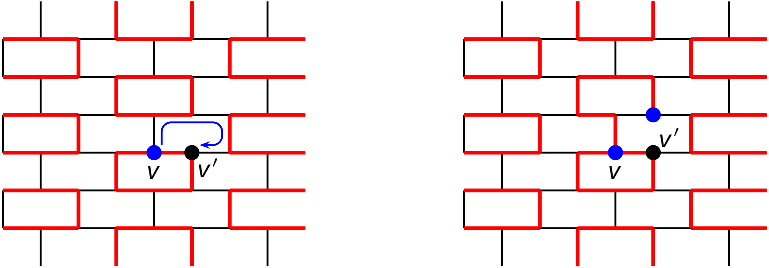

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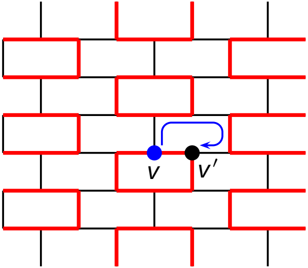

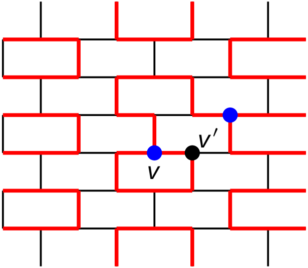

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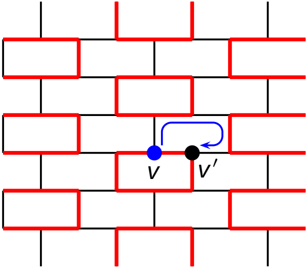

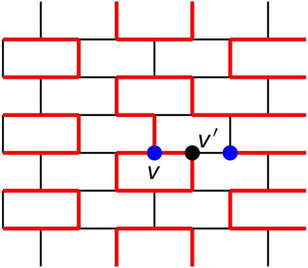

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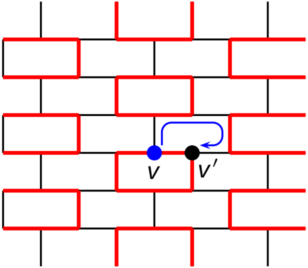

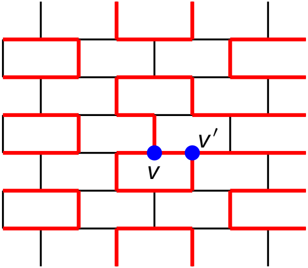

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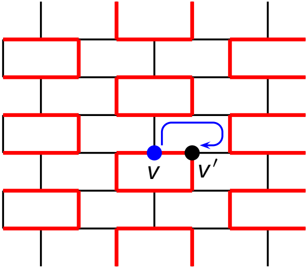

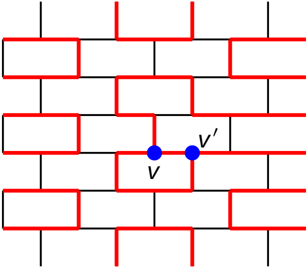

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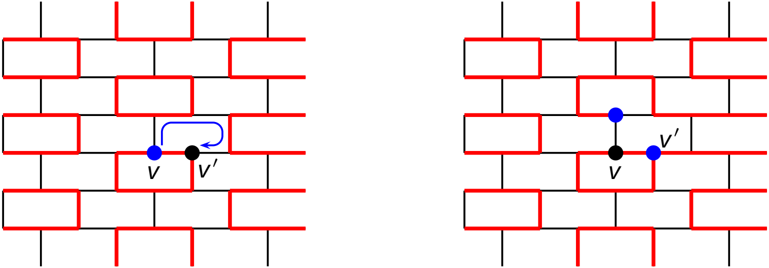

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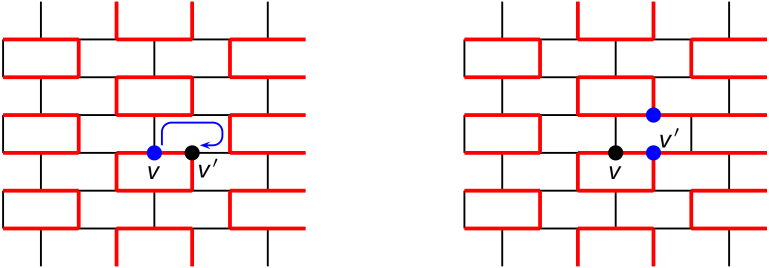

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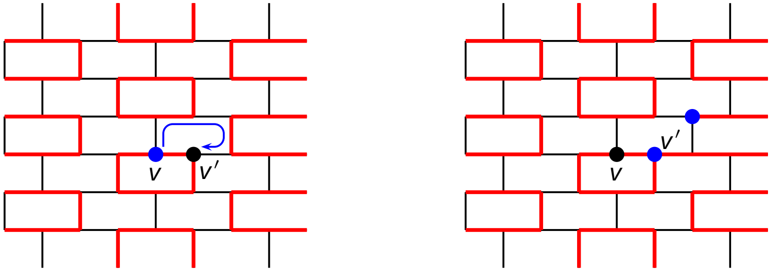

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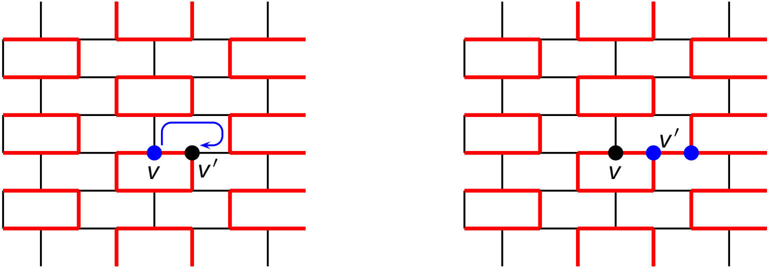

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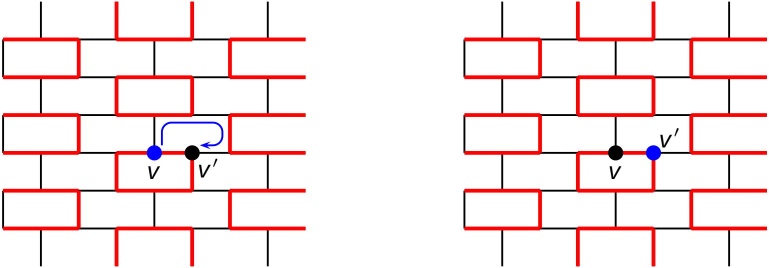

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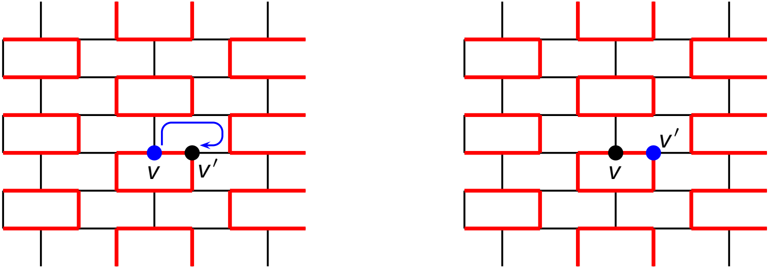

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- Then move second defect along $P_{v\,v'}$ so $(A, v, v) \leftrightarrow (A'', v', v')$
- But each edge is traversed (flipped) exactly twice so $A'' = A$

Colouring Lemma

Lemma

Let G be a finite bicubic graph. For every $A \in \mathcal{F}(G)$ and every $v \in V$, there is a path to each neighbor such that the edges alternate vacant, occupied, . . . , vacant

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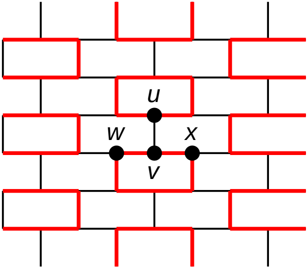

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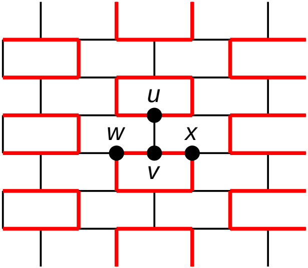

- Independently colour each cycle, alternating red, blue

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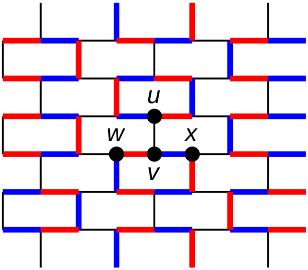

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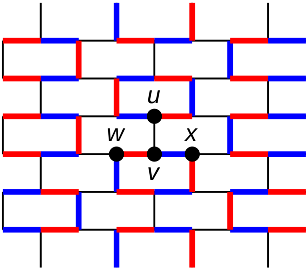

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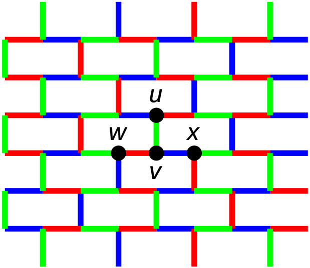

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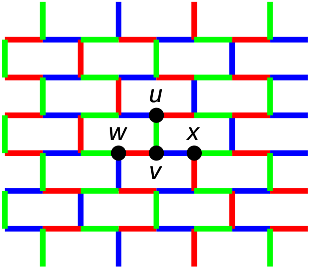

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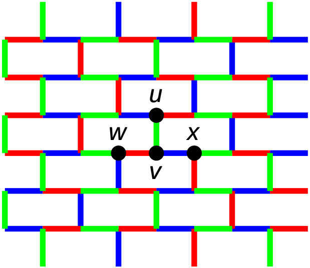

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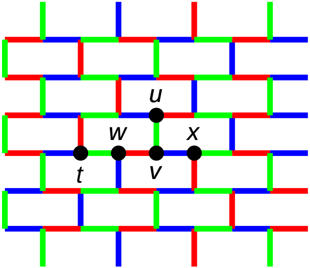

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- $A_{\text{red}} \cup A_{\text{green}} \in \mathcal{F}(G)$
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- So u, v, w all in same cycle
  $v\,u\,\ldots t\,w\,v \in A_{\text{red}} \cup A_{\text{green}}$

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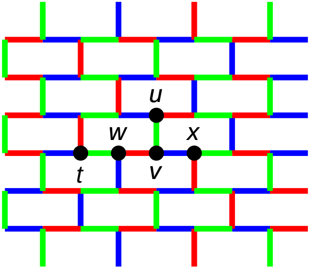

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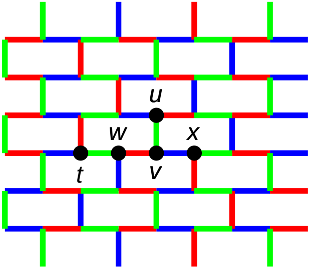

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- Cycle must be even
  - alternates green, red, ..., green, red
- $v\,u\,\ldots t\,w$ is the desired path

□

Potts models and Wang-Swendsen-Kotecký algorithm

- q-state Potts model on graph $G = (V, E)$
  - Spin configurations $\sigma \in \{1, 2, \ldots, q\}^V$ with $q \in \{2, 3, \ldots\}$
  - $H(\sigma) = -\beta \sum_{uv \in E} \delta(\sigma_u, \sigma_v)$
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  - $|\beta| = 1/T$

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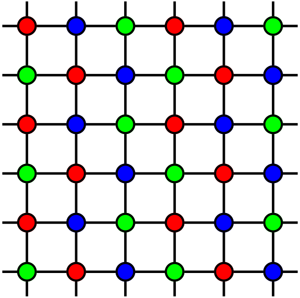
- WSK at $T = 0$ equivalent to “Kempe changes”
  - Each cluster is a Kempe chain

WSK algorithm



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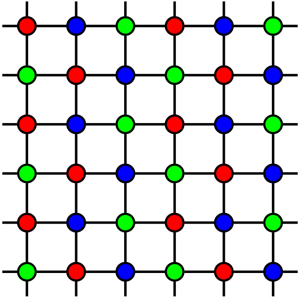

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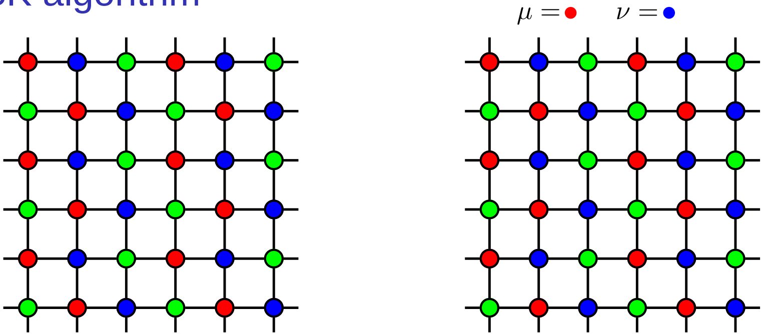

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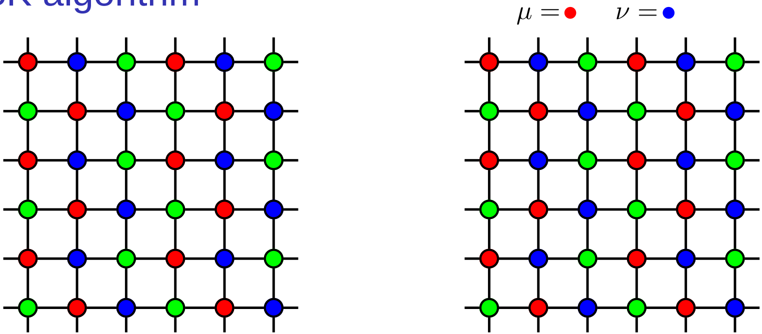

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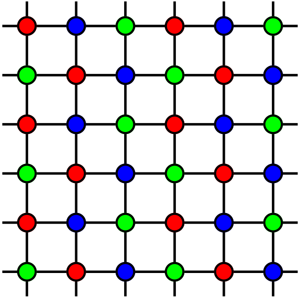

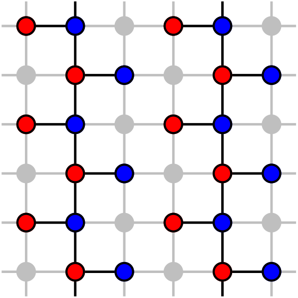

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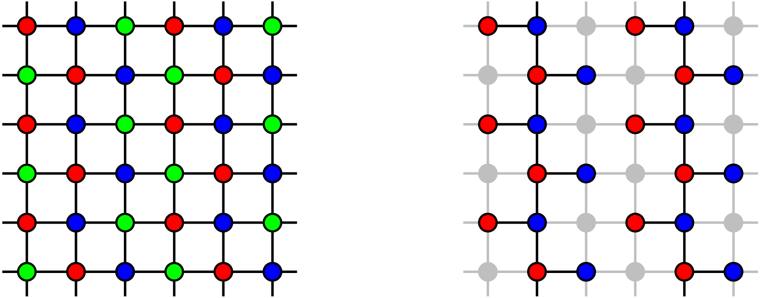

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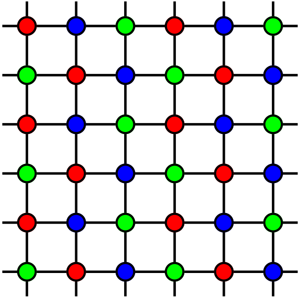
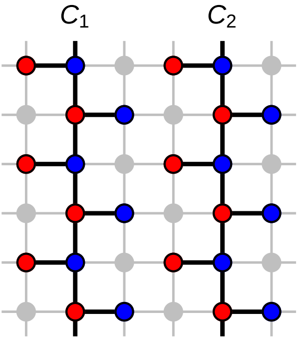
WSK algorithm





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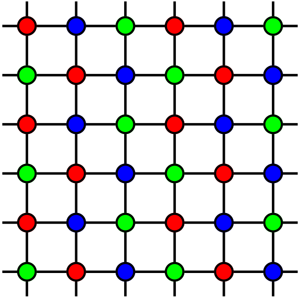

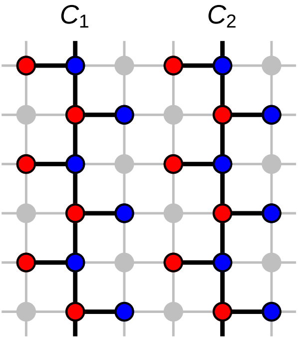

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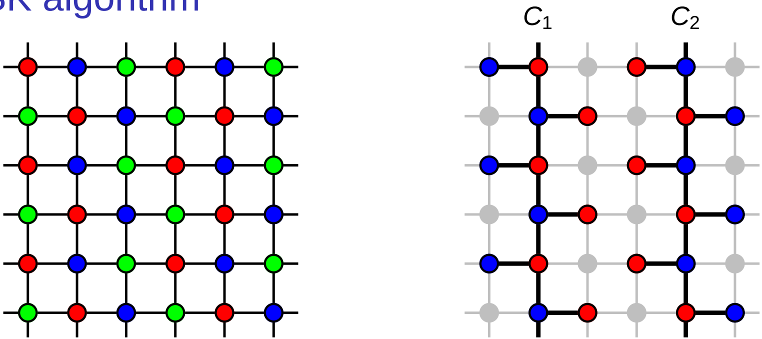

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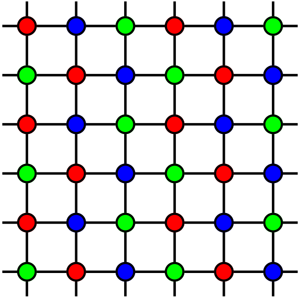

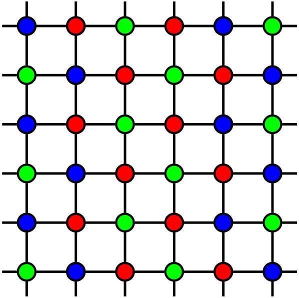

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Rigorous results for WSK algorithm

- Irreducible on all graphs when $T > 0$
- Irreducible on all graphs G when $T = 0$ and $q \geq \Delta(G) + 1$
- Irreducible on all bipartite graphs when $T = 0$
- Non-irreducible at $T = 0$:
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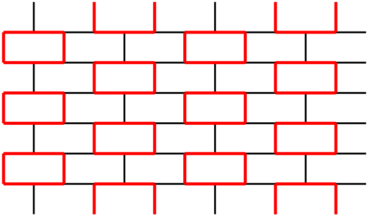
- Worm algorithm for honeycomb-lattice fully-packed loop model can be used to simulate both these models

Zero-temperature Potts antiferromagnets

Use $n = 2$ worm algorithm to simulate coloured loop configurations



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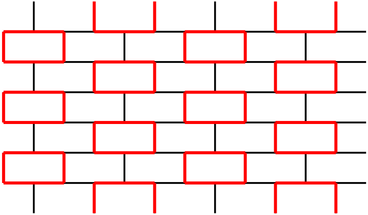

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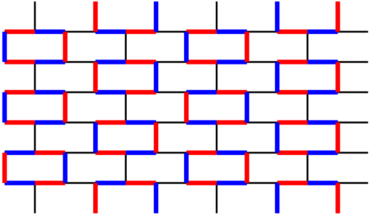
Zero-temperature Potts antiferromagnets

Use $n = 2$ worm algorithm to simulate coloured loop configurations



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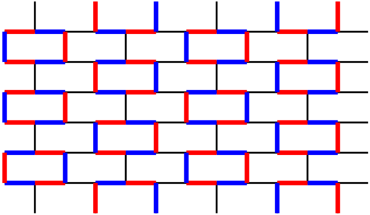

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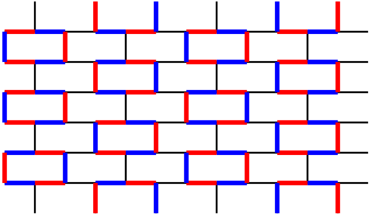

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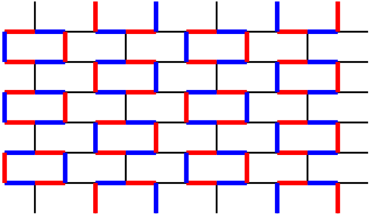

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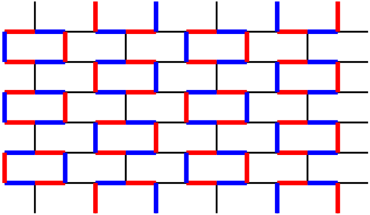

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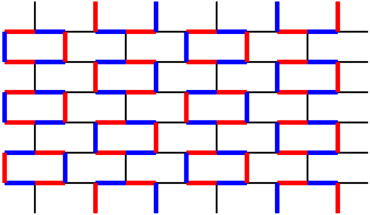

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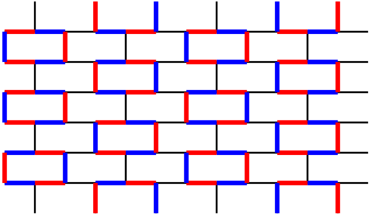

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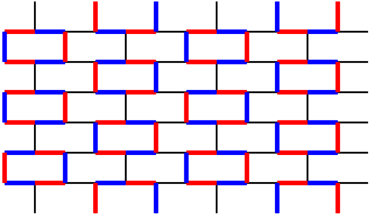

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Triangular-lattice Ising antiferromagnet

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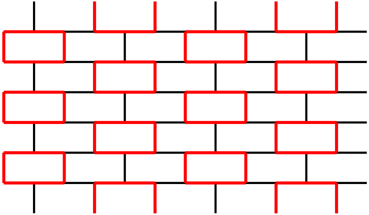

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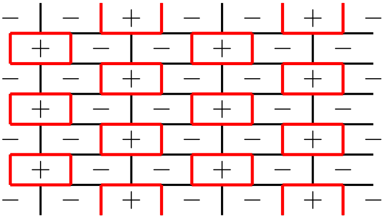

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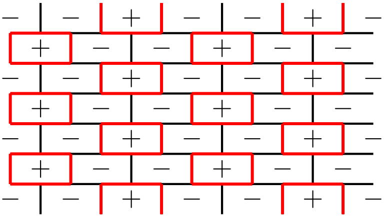

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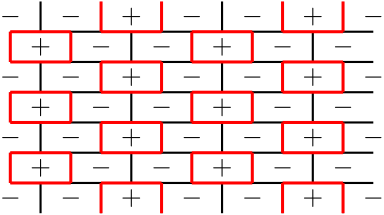

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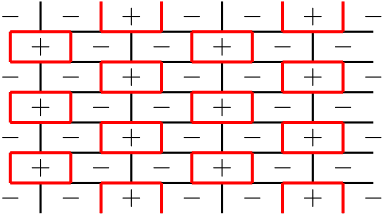

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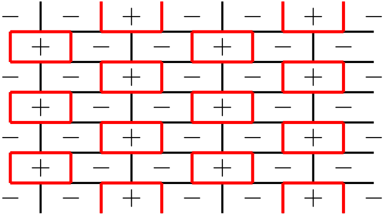

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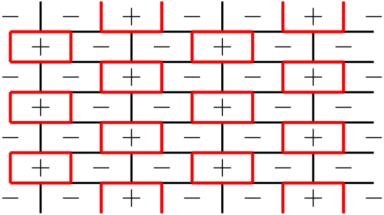

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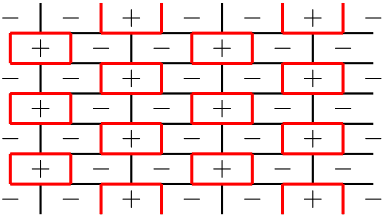

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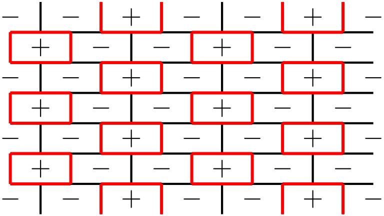

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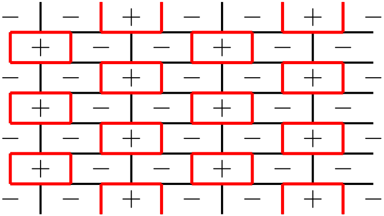

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- Tailor-made cluster algorithms non-irreducible at $T = 0$

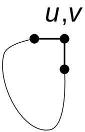
Summary

- Worm algorithms provide a simple way to simulate honeycomb-lattice loop models
  - Proven valid for all $n, x > 0$, including $x = +\infty$
- For $n = 1, 2$ also provide provably irreducible algorithms for certain critical antiferromagnetic models
  - Cluster algorithms fail for these models

Structure of the defect cluster

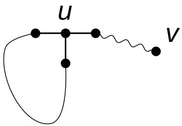
Partition $\mathcal{R}(G)$ according to structure of defect cluster

$$\mathcal{R} = \mathcal{E} \cup \mathcal{T} \cup \mathcal{D} \cup \Theta$$



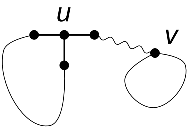
$(A, u, v) \in \mathcal{E}$

Cycle



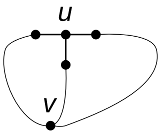
$(A, u, v) \in \mathcal{T}$

Tadpole



$(A, u, v) \in \mathcal{D}$

Dumbbell



$(A, u, v) \in \Theta$

Theta graph

Worm algorithm for fully-packed loop model

- Transition matrix:

$$P_n[(A,u,v) \to (A \triangle uu', u', v)] = P_n[(A,v,u) \to (A \triangle uu', v, u')]$$
$$= \begin{cases} 1/2 & (A,u,v) \in \mathcal{E}, \\ 1/2 & (A,u,v) \in \mathcal{T}, \\ 1/6 & (A,u,v) \in \Theta, \\ n/2(n+2) & (A,u,v) \in \mathcal{D} \text{ and } uu' \text{ is a bridge}, \\ 1/2(n+2) & (A,u,v) \in \mathcal{D} \text{ and } uu' \text{ is not a bridge}. \end{cases}$$

- Stationary distribution:

$$\pi_n(A,u,v) = \frac{n^{c(A)}}{Z_n} \begin{cases} 1/3 & (A,u,v) \in \mathcal{E}, \\ 1/3 & (A,u,v) \in \mathcal{T}, \\ (n+2)/3n & (A,u,v) \in \mathcal{D}, \\ 1/n & (A,u,v) \in \Theta. \end{cases}$$

Connectivity checking

$$P_{n,x}[(A,u,v) \to (A \triangle uu', u', v)] = P_{n,x}[(A,v,u) \to (A \triangle uu', v, u')]$$

$$= \frac{1}{2\,d(u)} \begin{cases} F(x\,n) & uu' \notin A \text{ and } u \leftrightarrow u' \text{ in } (V,A) \\ F(x) & uu' \notin A \text{ and } u \not\leftrightarrow u' \text{ in } (V,A) \\ F(1/n\,x) & uu' \in A \text{ and } u \leftrightarrow u' \text{ in } (V, A \setminus uu') \\ F(1/x) & uu' \in A \text{ and } u \not\leftrightarrow u' \text{ in } (V, A \setminus uu') \end{cases}$$

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- If $n>1$ the “colouring method” avoids the issue entirely

The colouring method

- Consider a finite graph $G = (V, E)$
- Let $K(A)$ denote the set of connected components of (V, A)
- Define a "generalized random-cluster model"

$$\mathbb{P}_W(A) \propto \prod_{C \in K(A)} W(C) \qquad A \subseteq E$$

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- Simulate $\mathbb{P}_W$ by introducing auxiliary vertex variables (colours)
- Like SW, choose bonds conditioned on colours & vice versa

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2. Choose a new bond configuration on G_α using any Markov chain for which W_α is stationary

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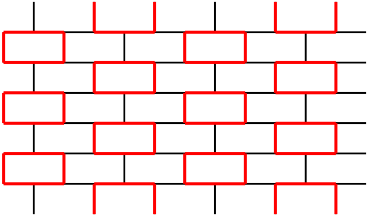
SW for antiferromagnetic Ising

SW for antiferromagnetic Ising model on finite graph $G = (V, E)$

$$\mathbb{P}(\sigma, n) \propto \prod_{ij \in E} [(1-p)\,\delta_{\omega_{ij},0} + p(1-\delta_{\sigma_i,\sigma_j})\delta_{\omega_{ij},1}]$$

Mapping 3-edge colorings to dual 4-vertex colorings



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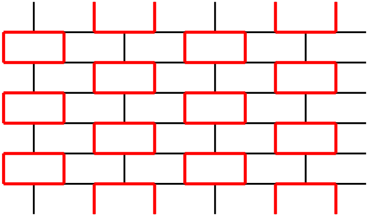

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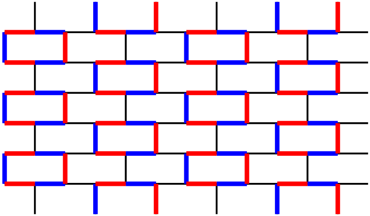

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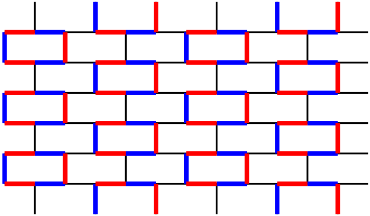

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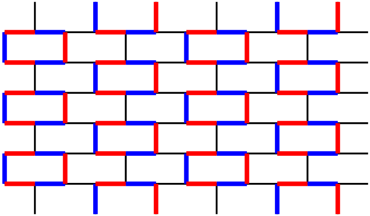

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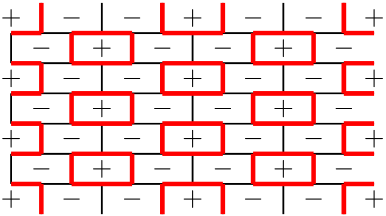

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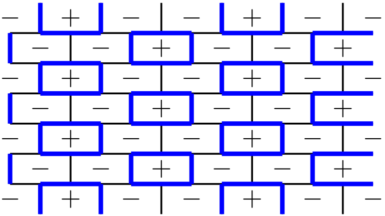

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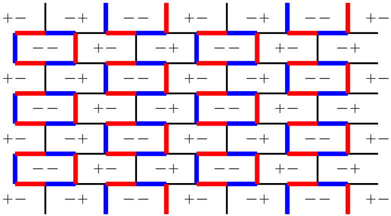

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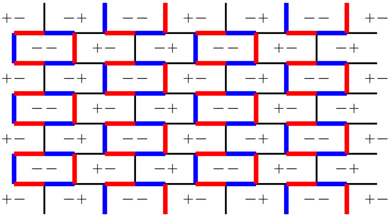

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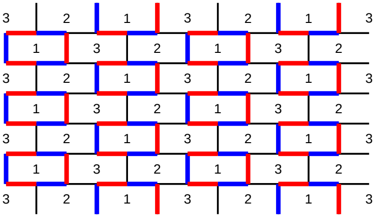

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- Stationary process – start “in equilibrium”

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- 1 “effectively independent” observation every $2\,\tau_{\text{int},X}$ steps

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Lemma

αP^t tends to π with rate bounded by $e^{-t/\tau_{\exp}}$

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  z_{exp}, and $z_{\mathrm{int},X}$ for each observable X.
- Different algorithms for the same model can have very different z
- E.g. $d = 2$ Ising model
  - Glauber (Metropolis) algorithm $z \approx 2$
  - Swendsen-Wang algorithm $z \approx 0.2$