Monte Carlo simulations of quantum systems with global updates

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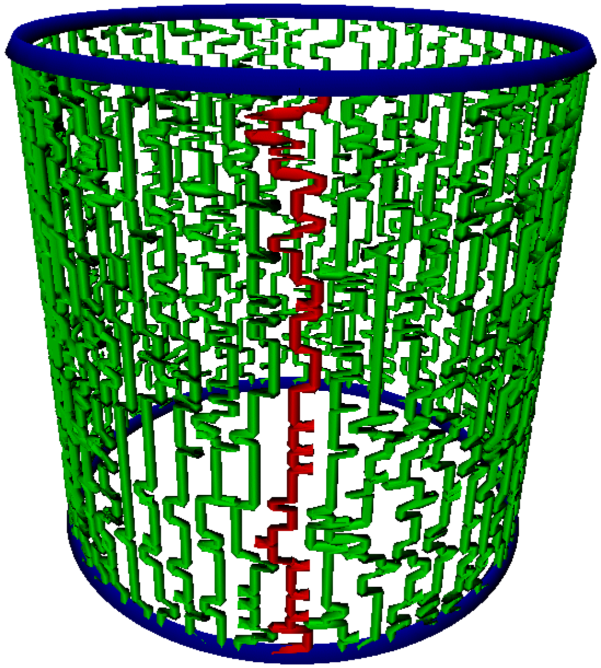
Quantum spin-systems II

Loop-algorithm and further developements



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$V(\mathcal{G}) \longrightarrow$ **weight of graph** $\mathcal{G}$**.**

$$\Delta(\boldsymbol{s}, \mathcal{G}) = \begin{cases} 1 & \text{if graph } \mathcal{G} \text{ compatible with } \boldsymbol{s} \\ 0 & \text{otherwise .} \end{cases}$$

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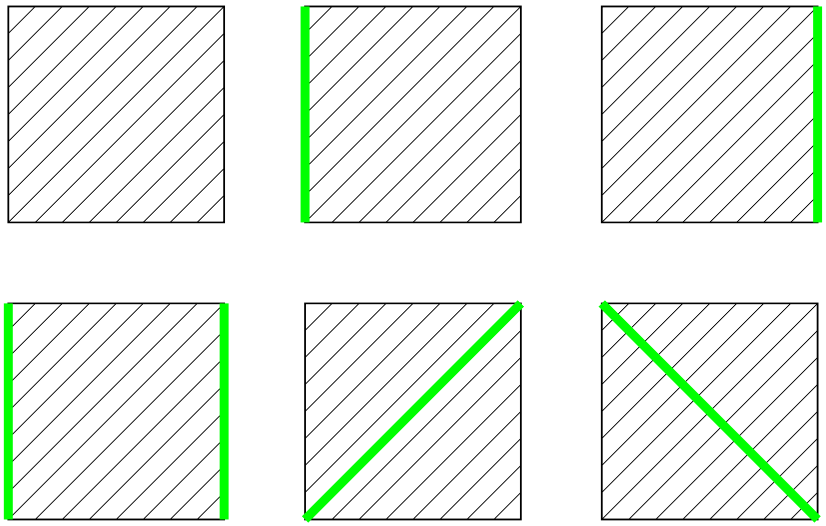
Probability of a graph given a configuration on a plaquette

$$p(g \mid u) = \frac{v(g)\Delta(u, g)}{w(u)}\,,$$

Graphs

Graphs

Consider all possible configurations of shaded plaquettes



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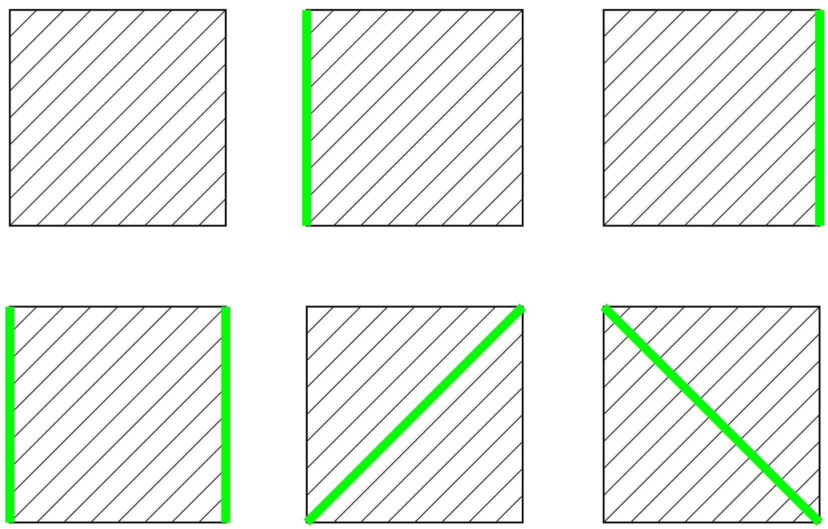

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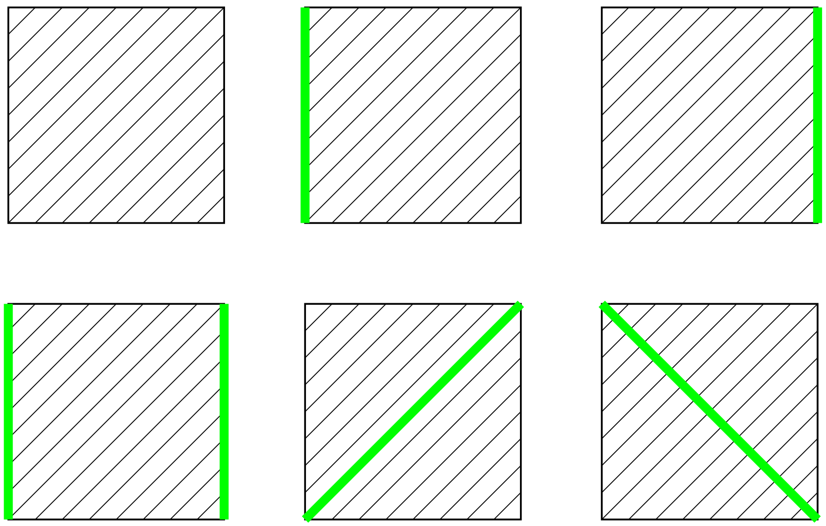

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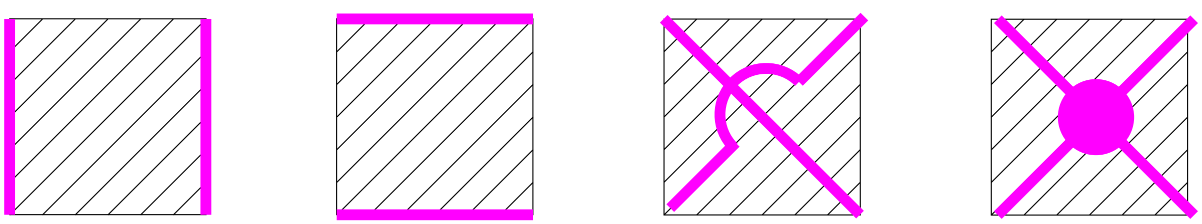
Possible graphs



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Compatibility table $\longrightarrow \Delta(u, g)$

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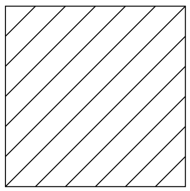
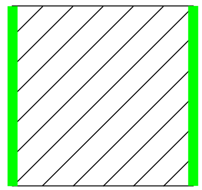
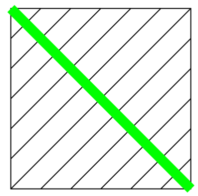
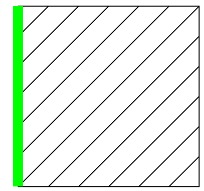
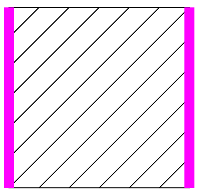
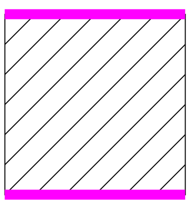
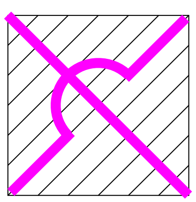
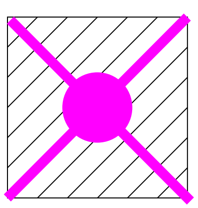
g \ u				
	1	1	0	1
	0	0	1	1
	1	1	1	0
	1	1	1	1

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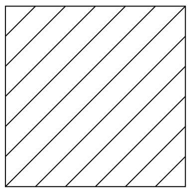
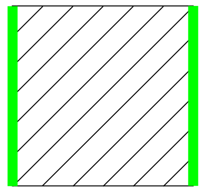
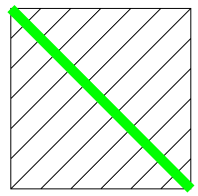
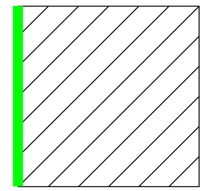
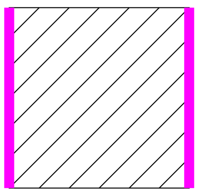
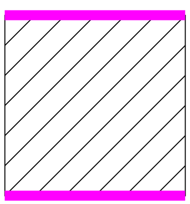
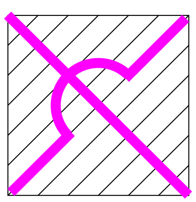
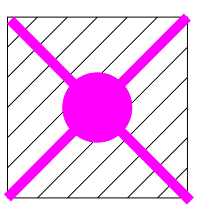
g \ u				
	1	1	0	1
	0	0	1	1
	1	1	1	0
	1	1	1	1

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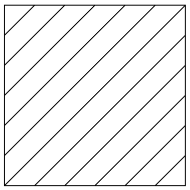
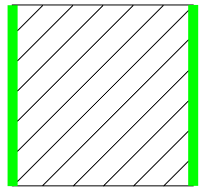
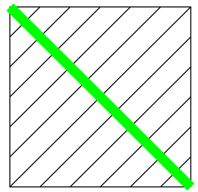
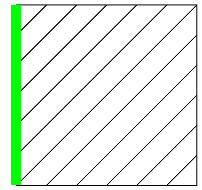
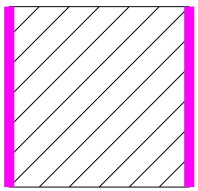
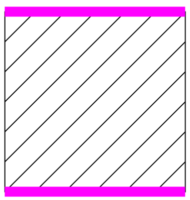
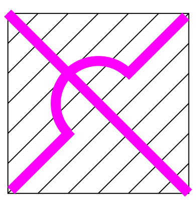
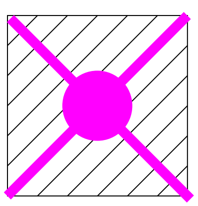
g \ u				
	1	1	0	1
	0	0	1	1
	1	1	1	0
	1	1	1	1

$$w(u) = \sum_g v(g)\Delta(u,g)$$

$$\Downarrow$$

$$\mathrm{e}^{-\Delta\tau J\Delta/4}$$
$$= v(\|) + v(\times) + v_1(\otimes)$$

$$\sinh(\Delta\tau J/2)\ \mathrm{e}^{\Delta\tau J\Delta/4}$$
$$= v(=) + v(\times) + v_2(\otimes)$$

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v(=) &= \frac{1}{2}\exp\left(-\frac{\Delta\tau J\Delta}{4}\right)\left\{\exp\left[\Delta\tau\left(\frac{J}{2}+\frac{J\Delta}{2}\right)\right]-1\right\} .
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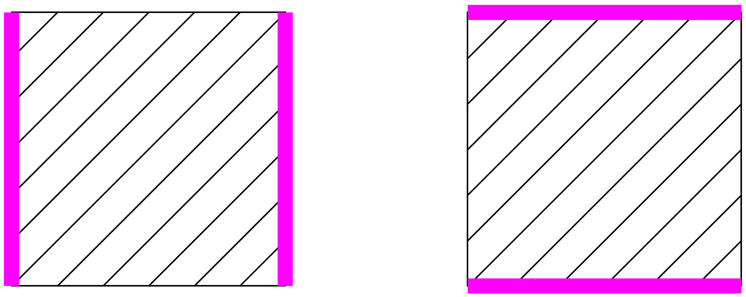
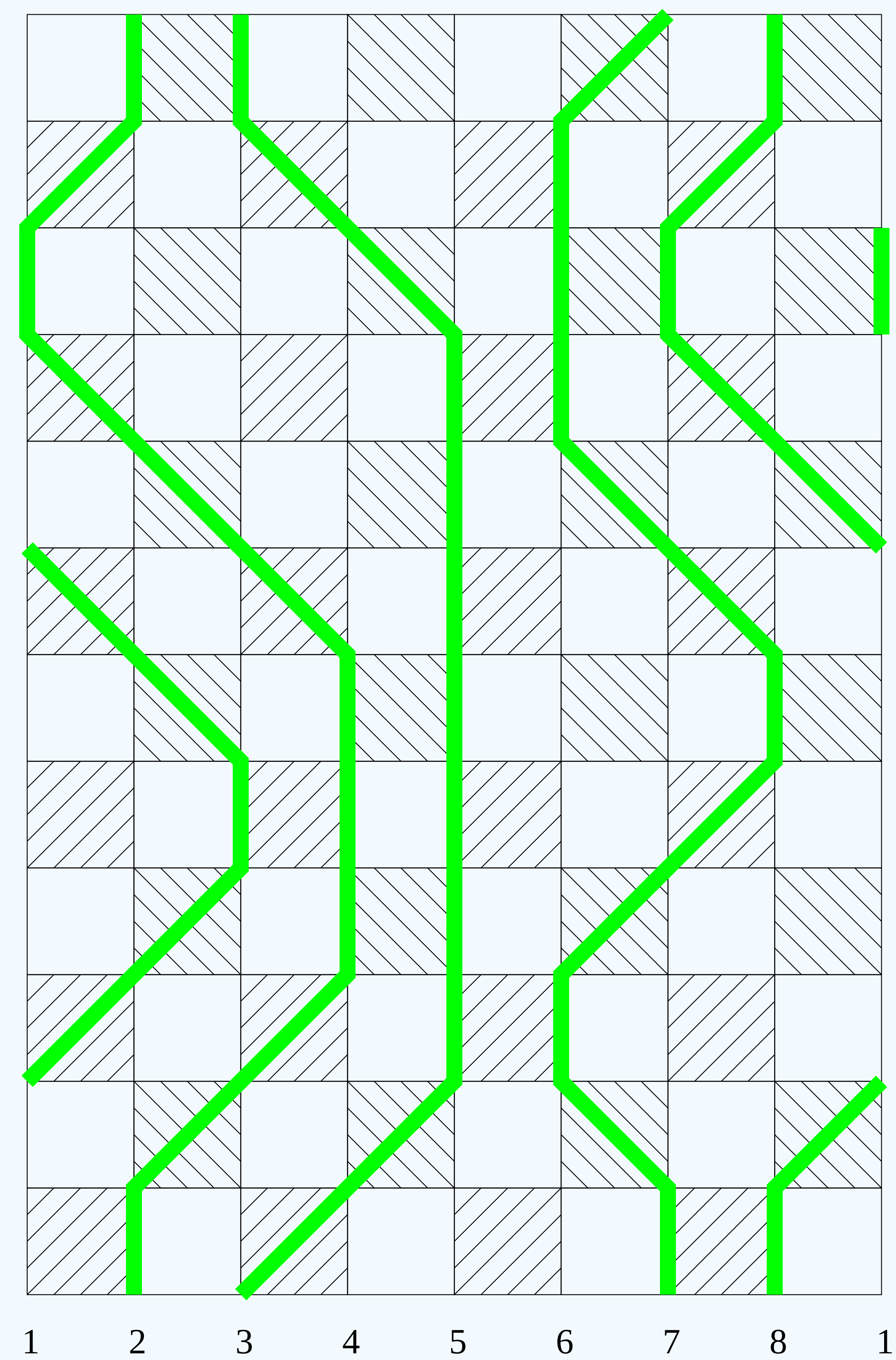
$\hookrightarrow$ **need only two graphs**



Example:
isotropic Heisenberg model

g \ u				
	1	1	0	1
	0	0	1	1



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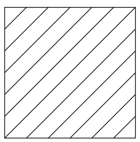
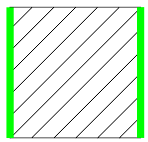
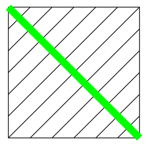
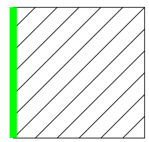
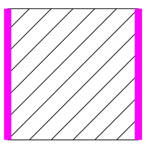
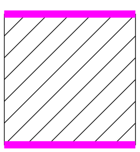
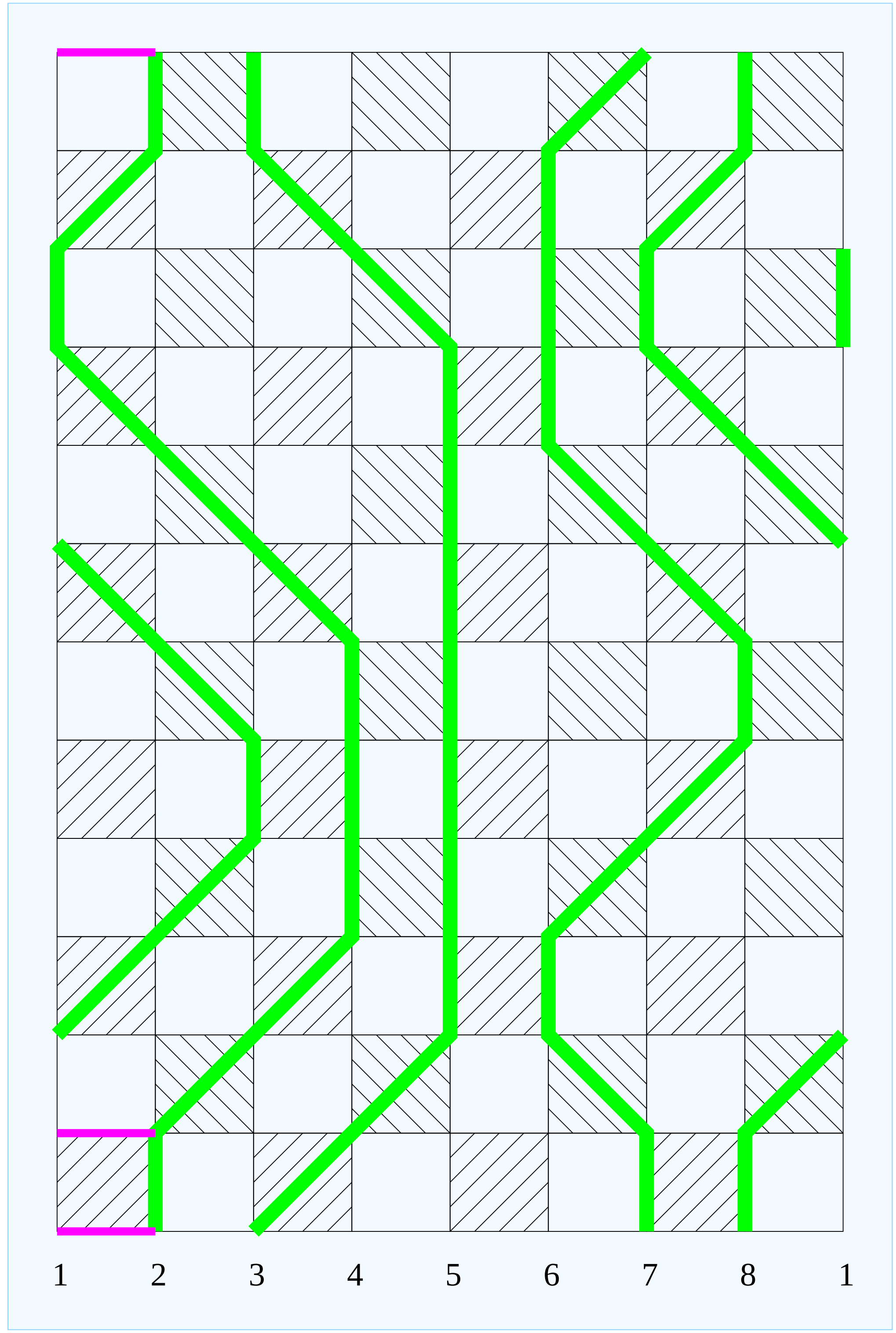
g \ u				
	1	1	0	1
	0	0	1	1



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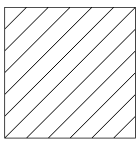
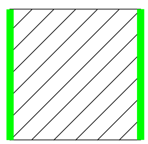
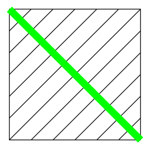
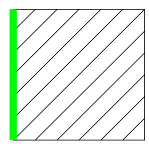
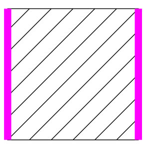
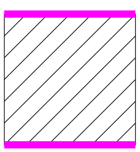
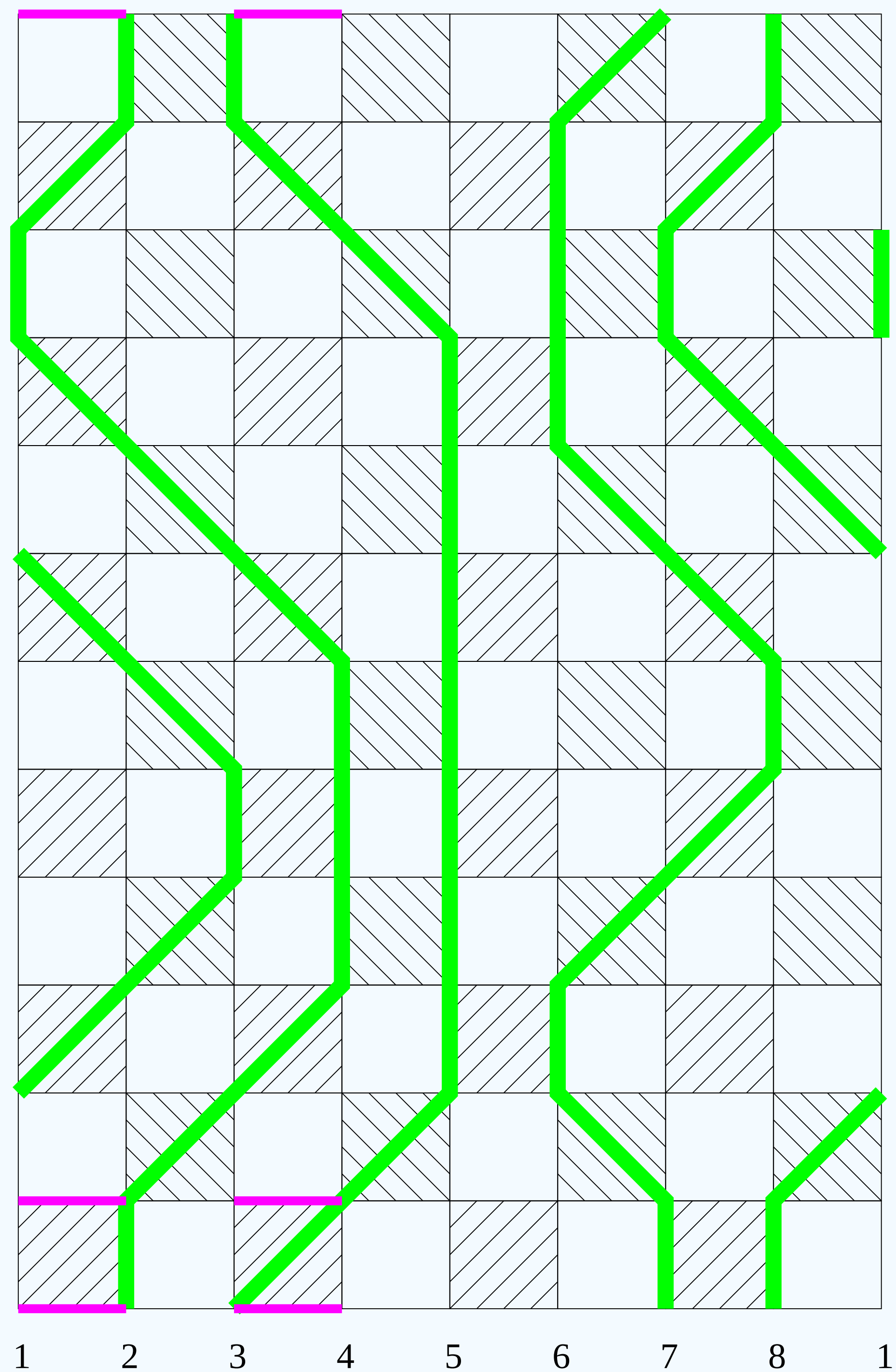
g \ u				
	1	1	0	1
	0	0	1	1



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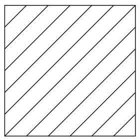
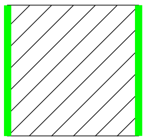
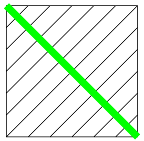
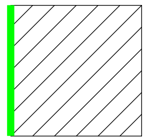
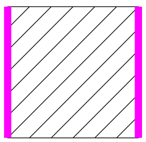
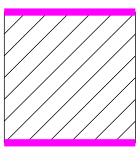
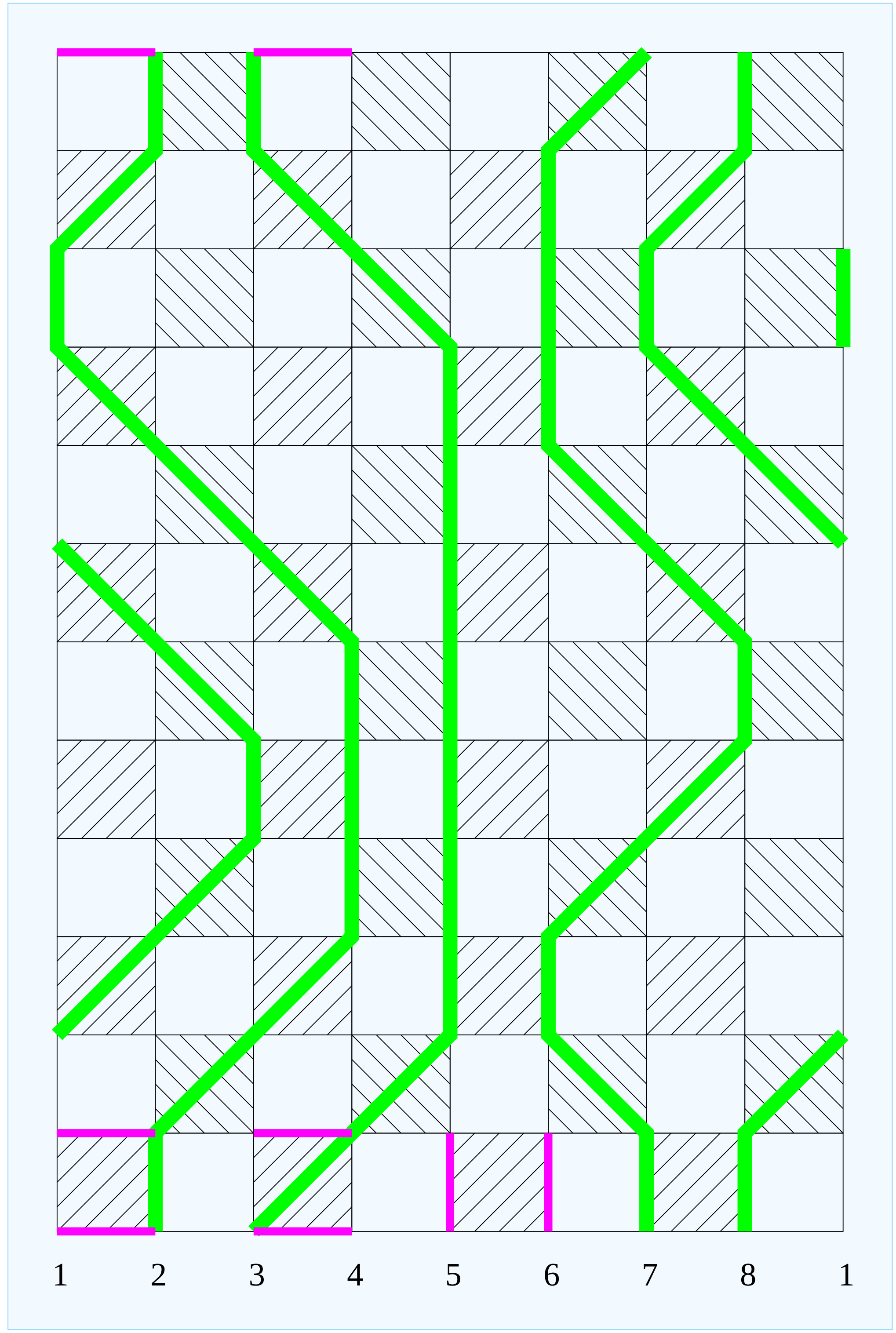
g \ u				
	1	1	0	1
	0	0	1	1



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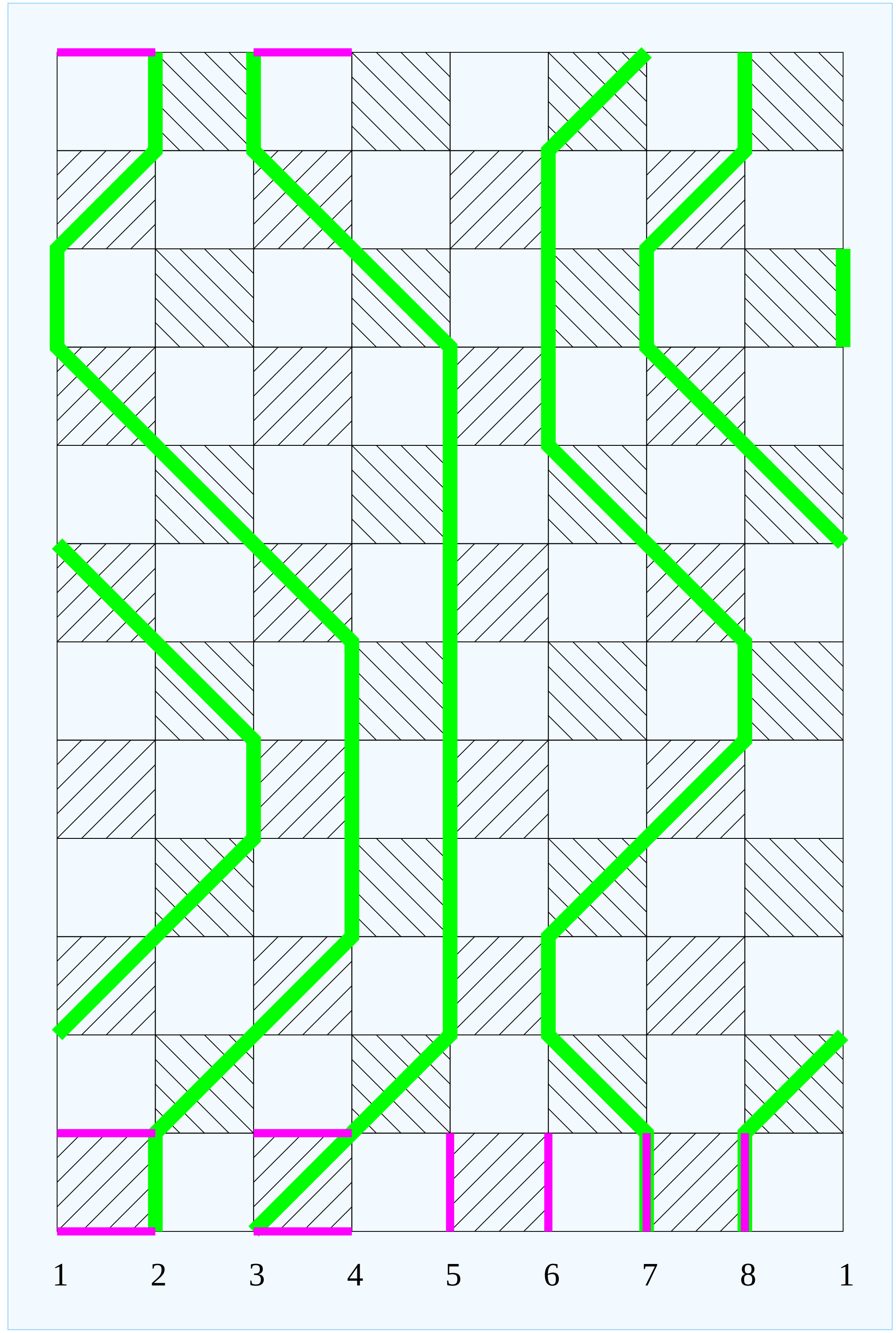

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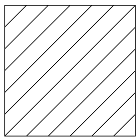
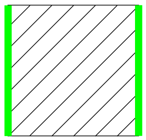
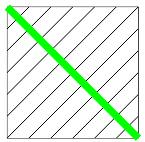
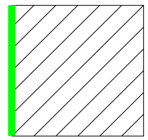
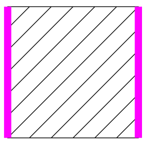
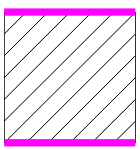
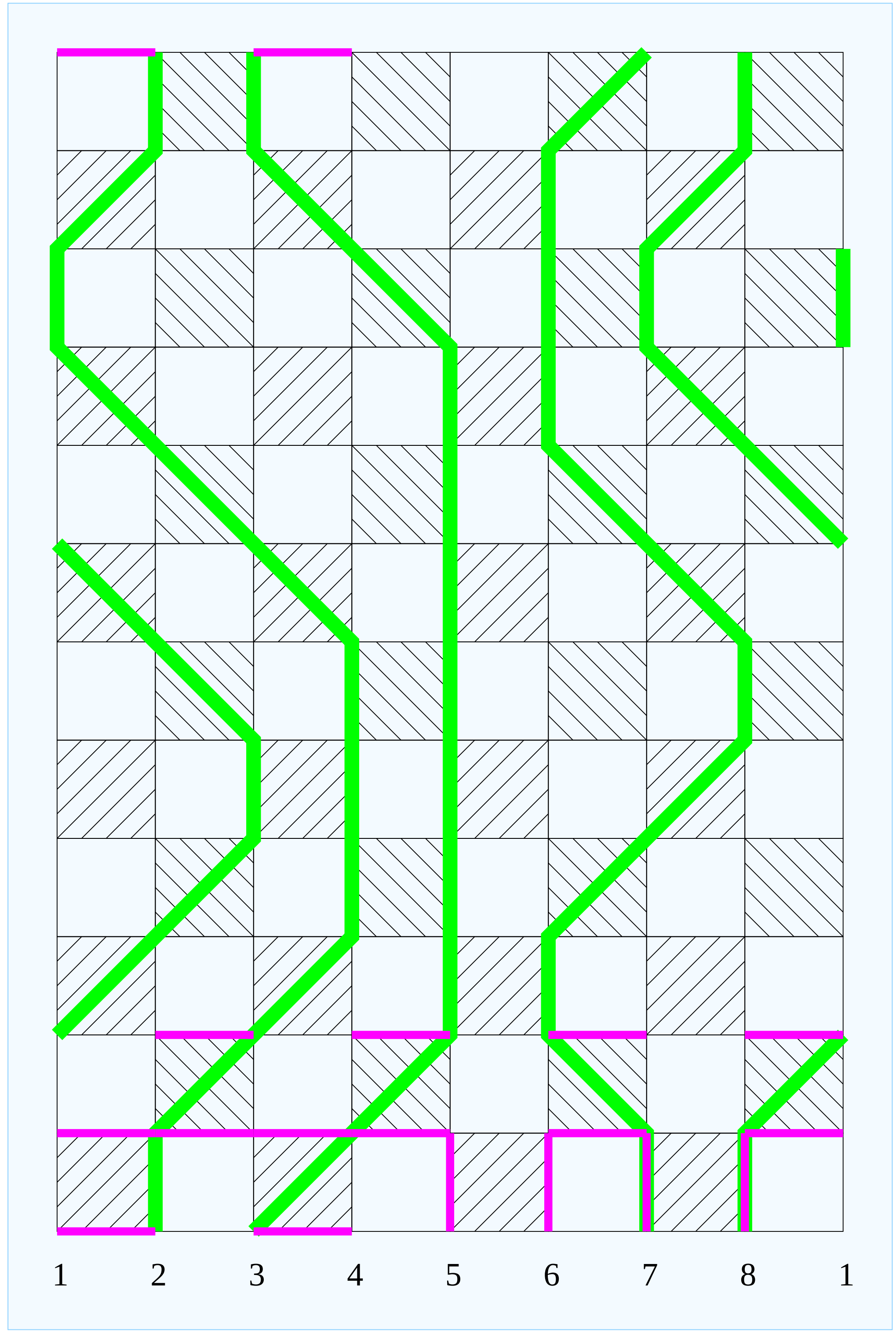
g \ u				
	1	1	0	1
	0	0	1	1



Example:

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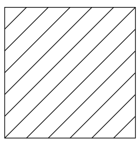
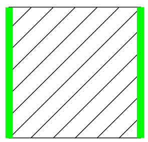
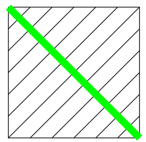
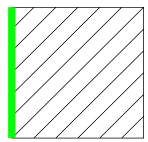
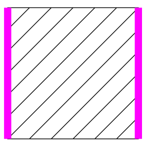
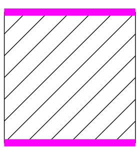
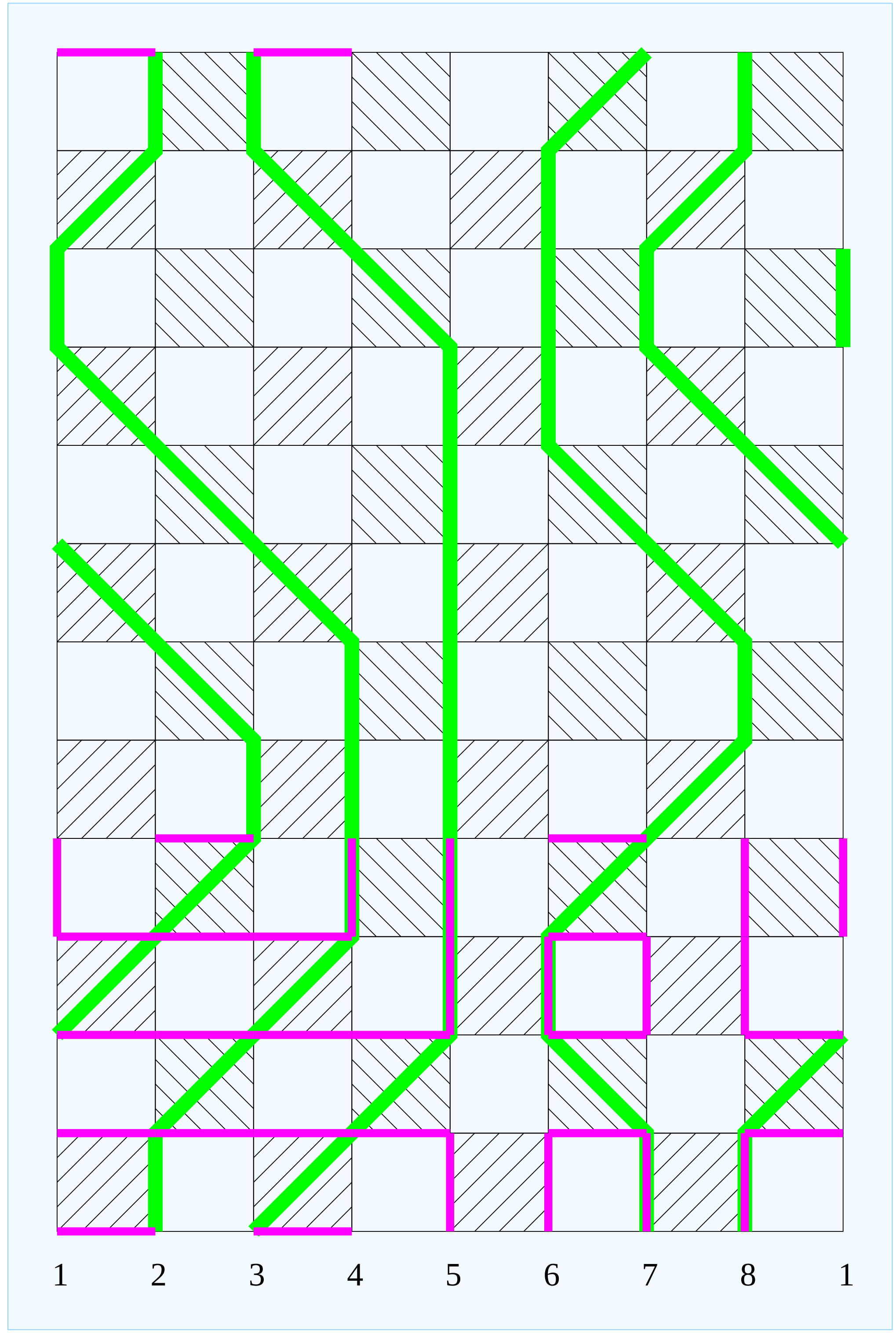
g \ u				
	1	1	0	1
	0	0	1	1



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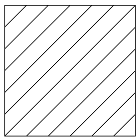
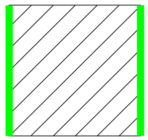
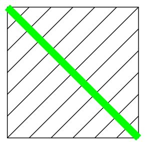
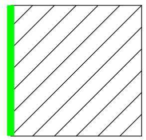
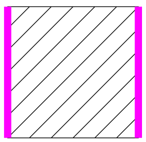
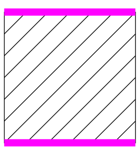
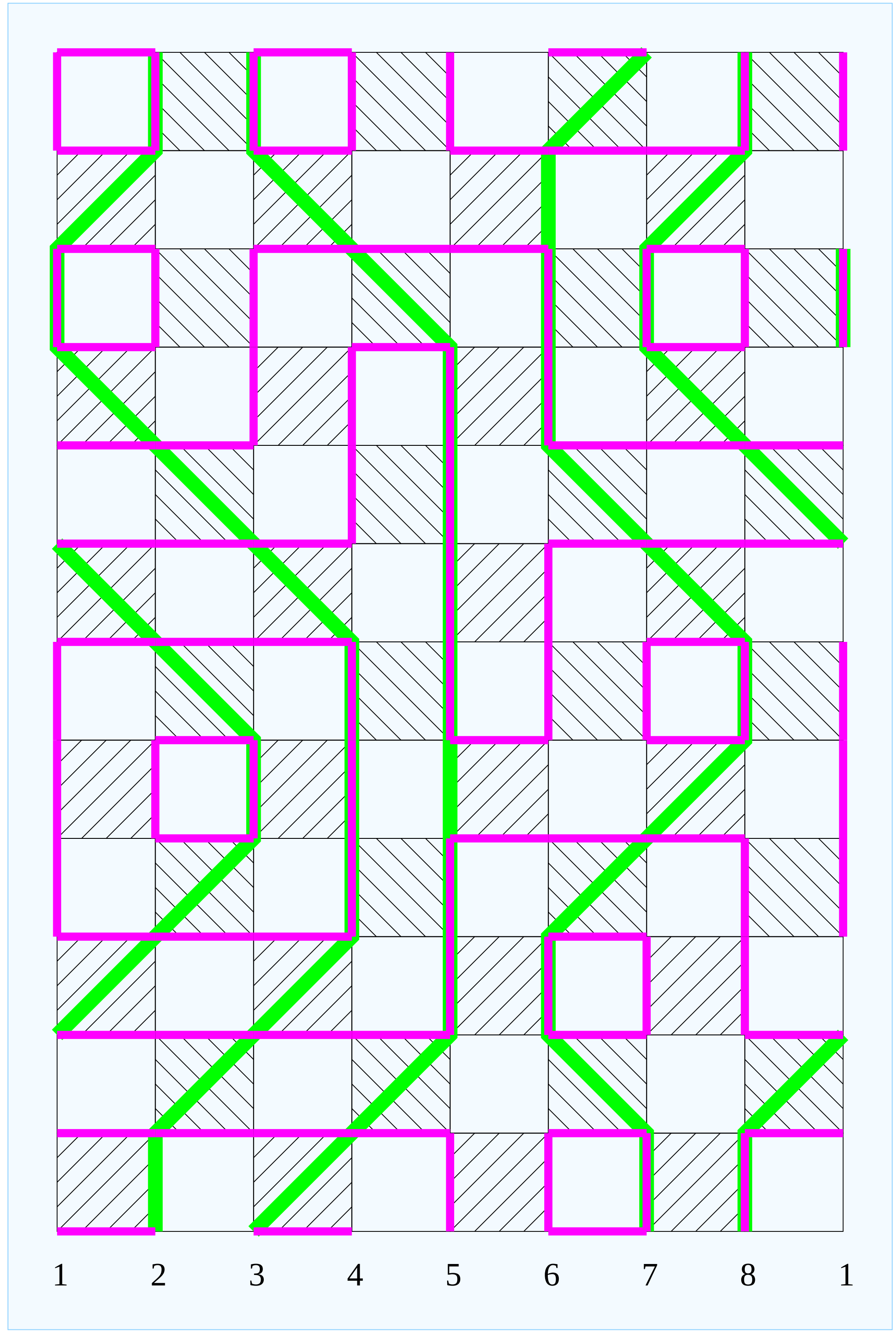
g \ u				
	1	1	0	1
	0	0	1	1



Update

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Configurations are changed by flipping all the states along the loop.

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Transition probability (heat-bath)

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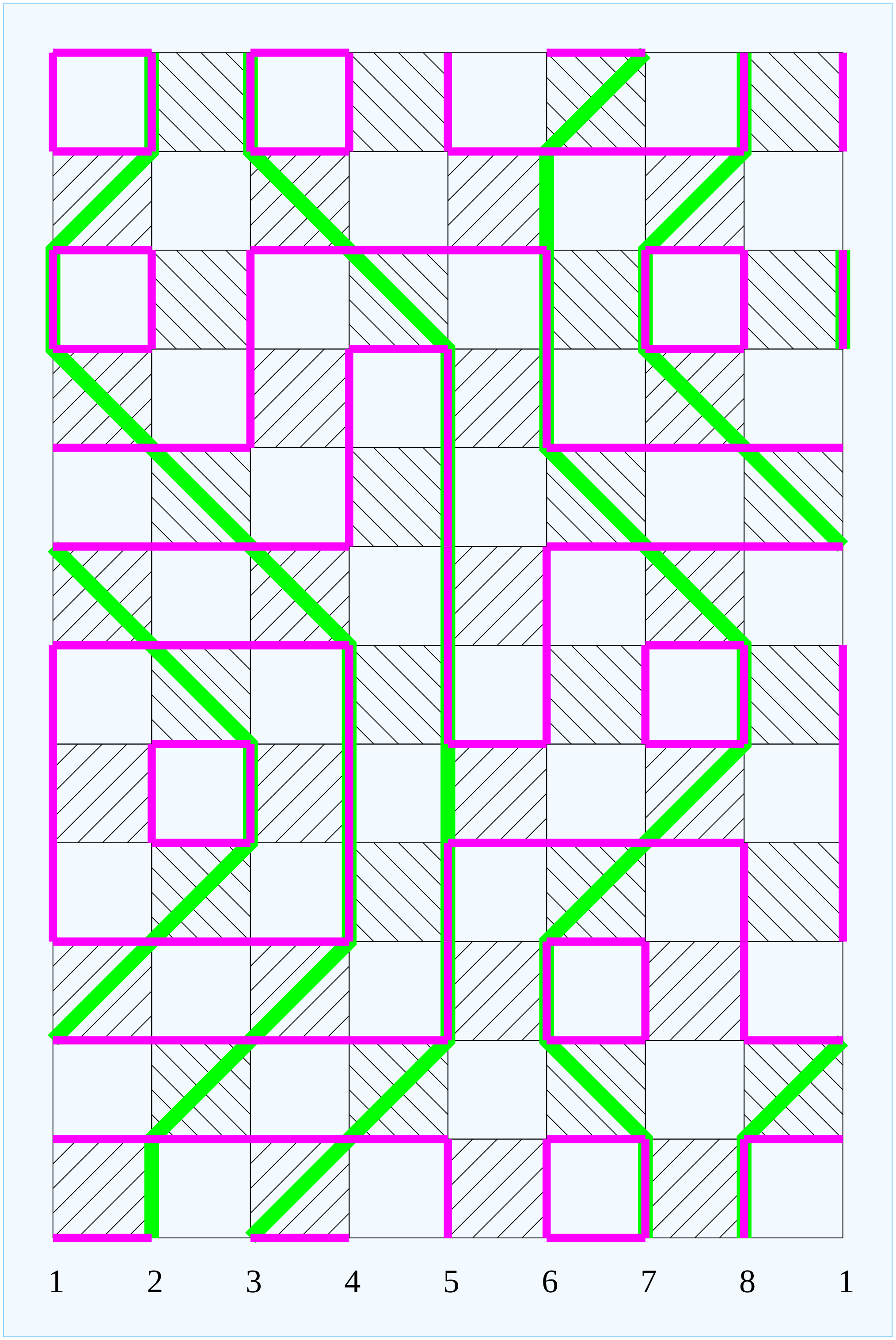
Update with loops

Isotropic Heisenberg model

Active loops

Flipped loops



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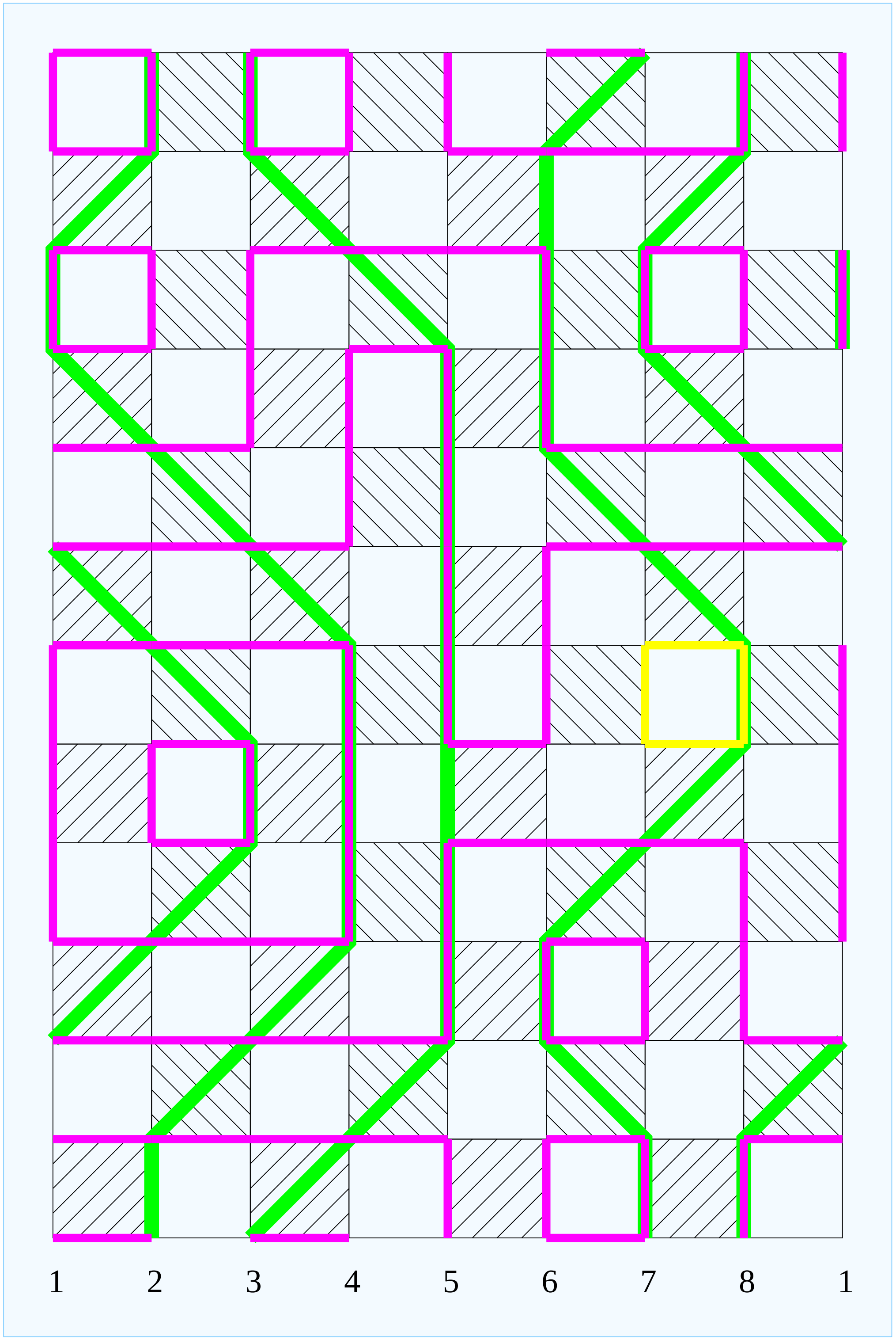

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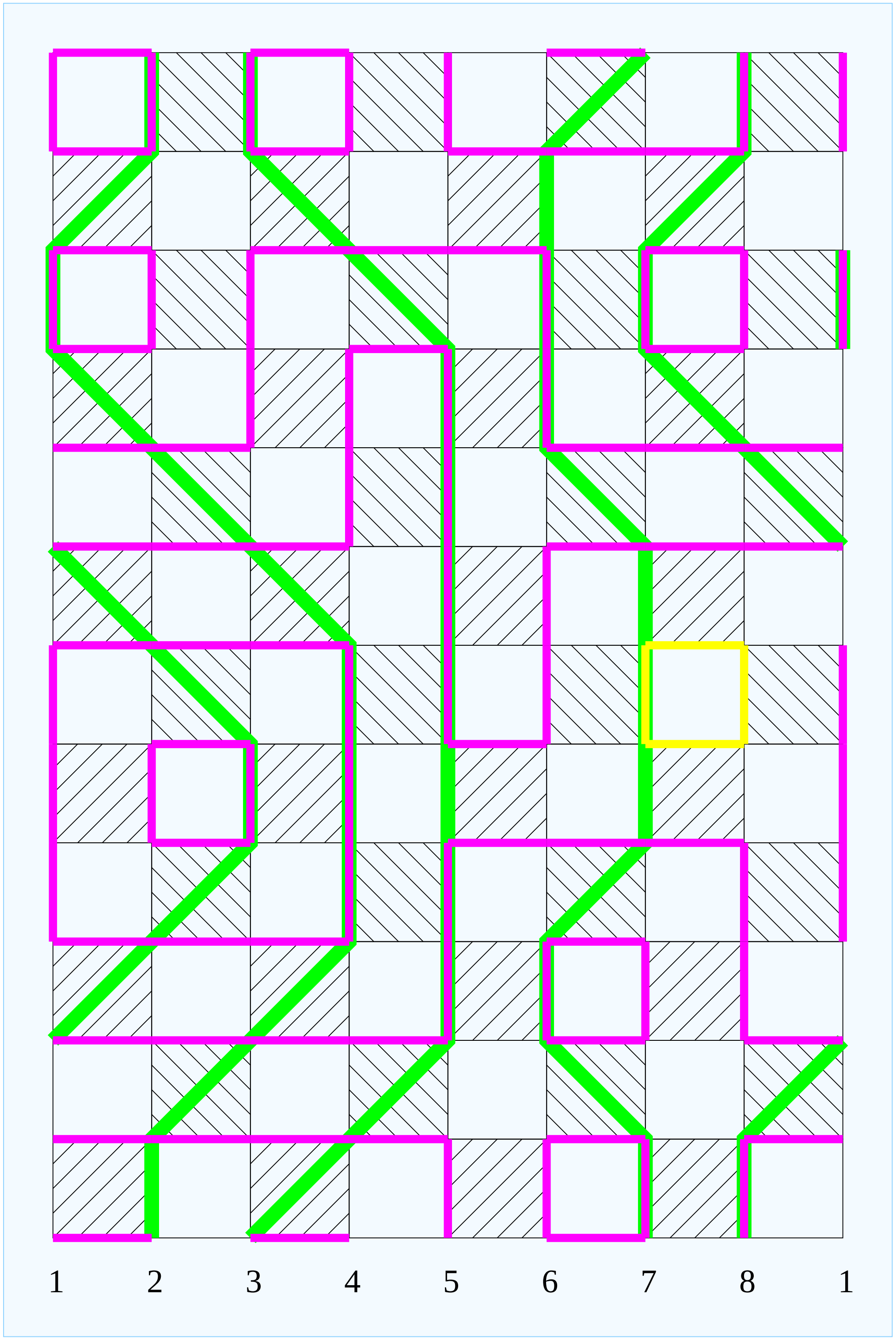

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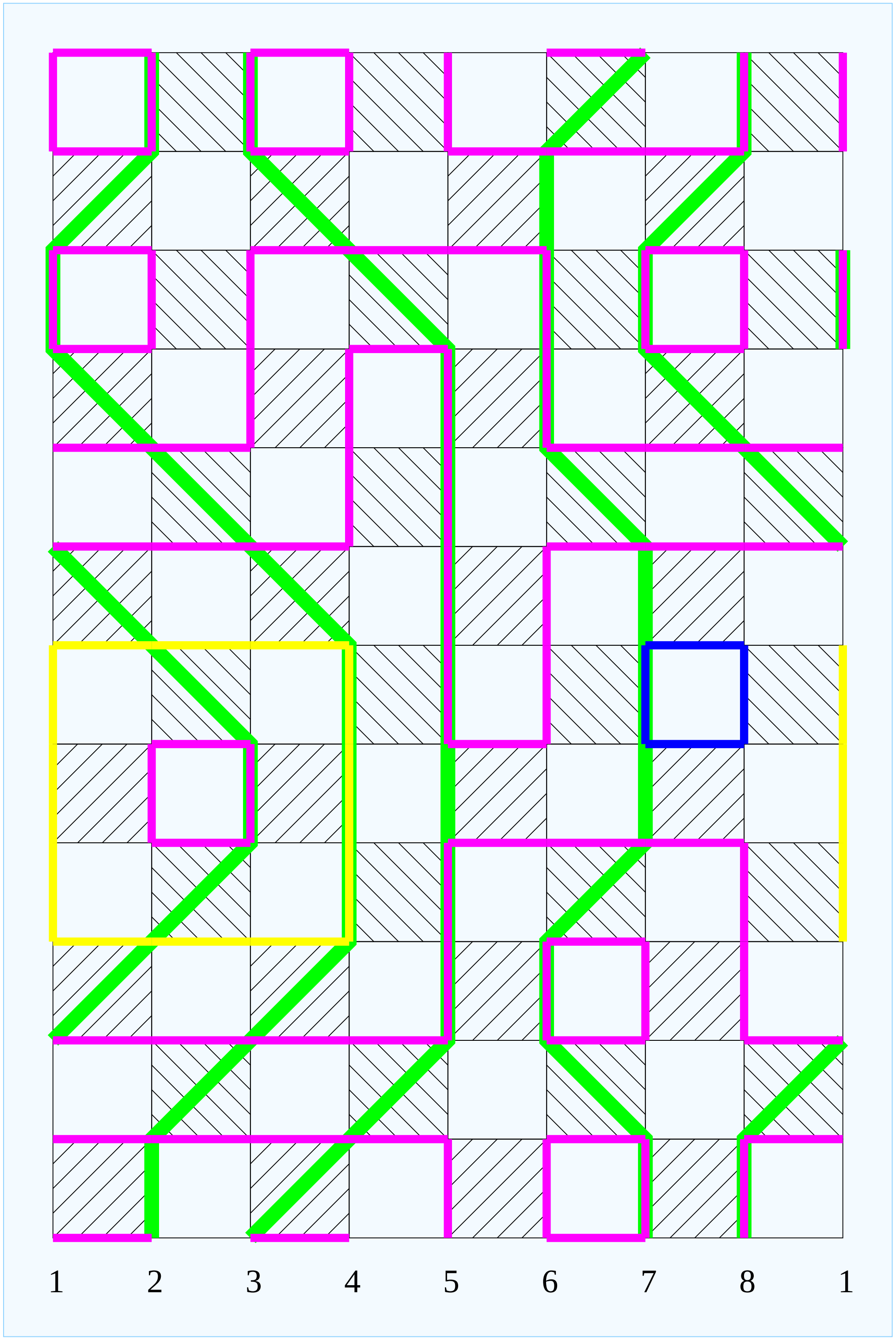

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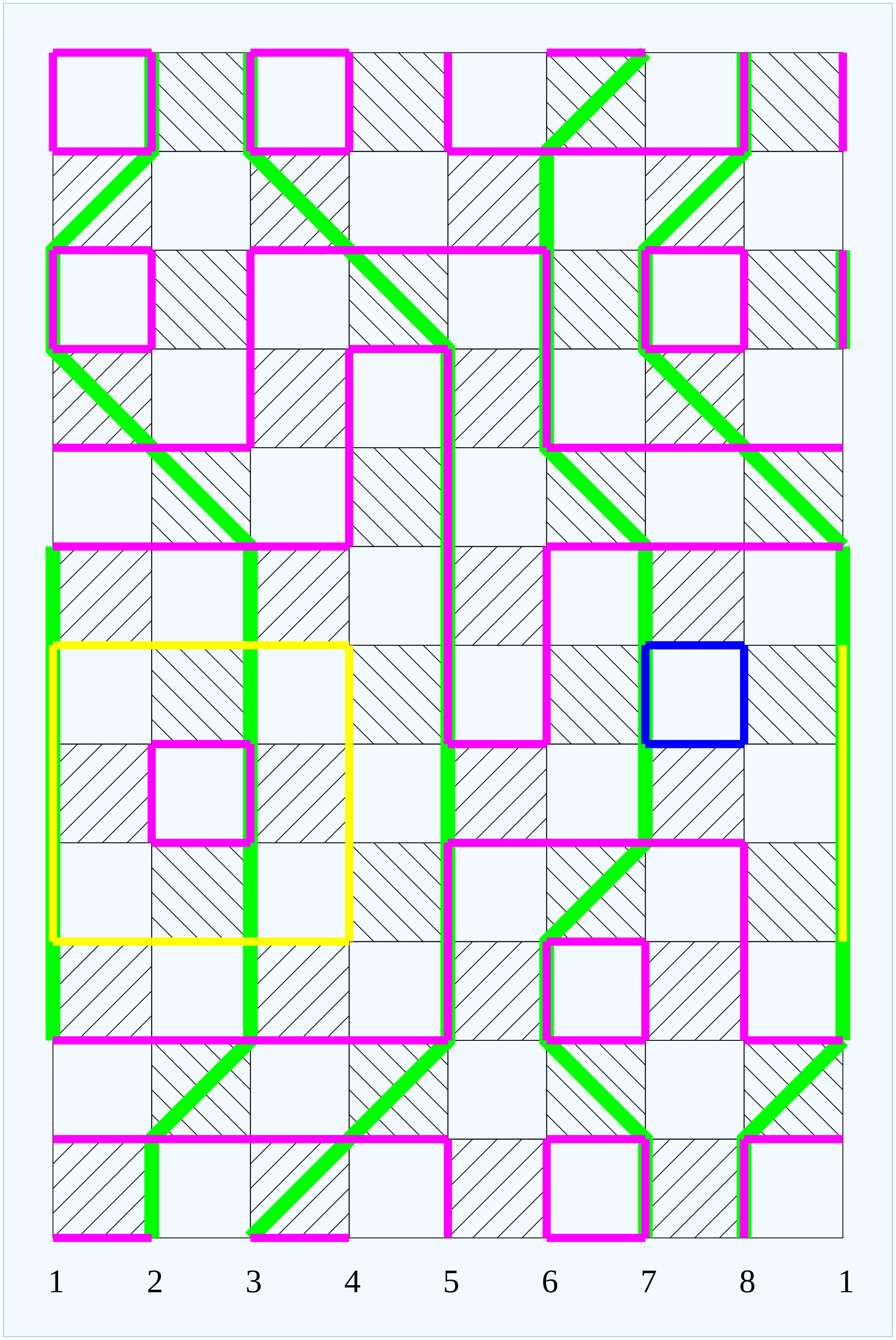

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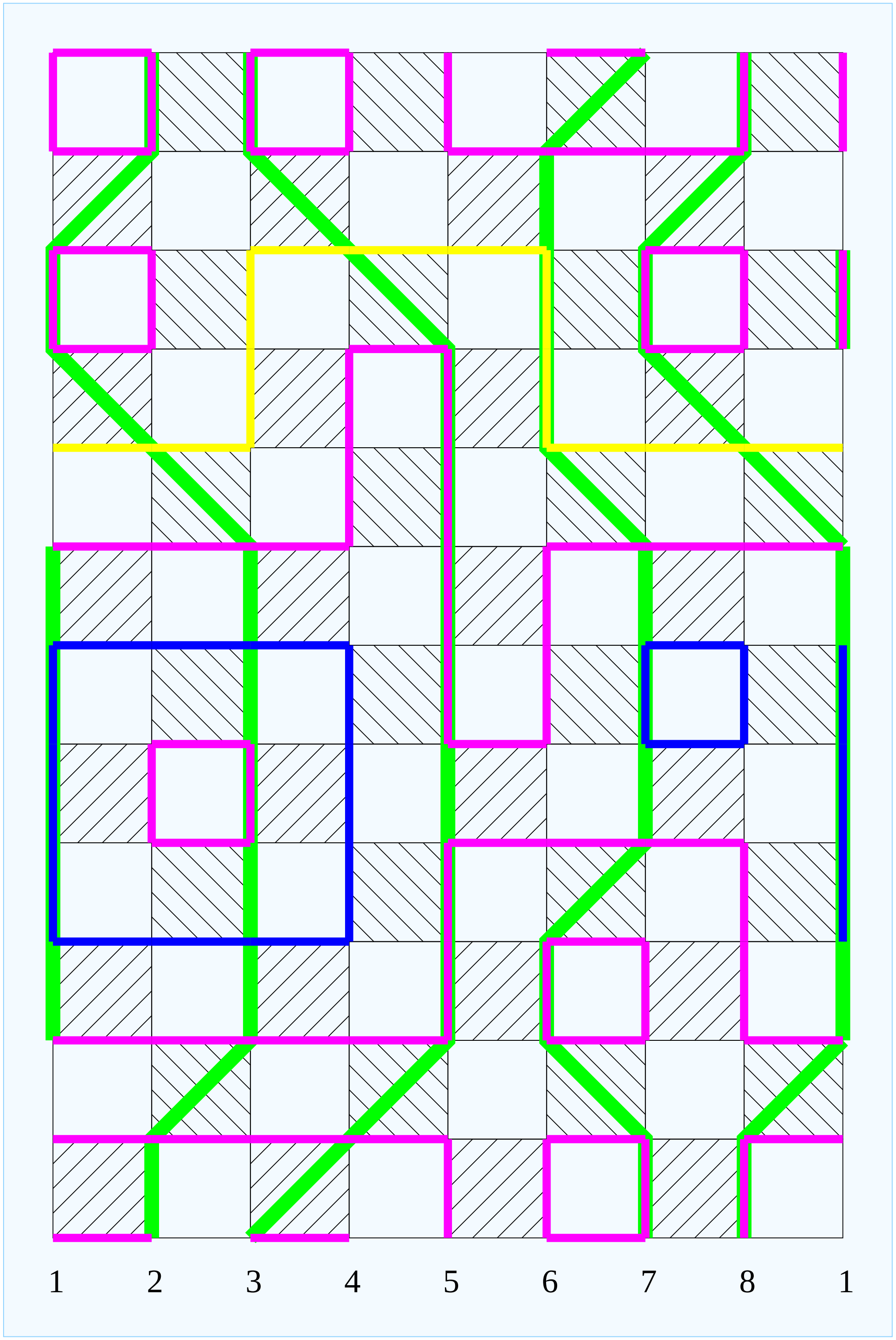

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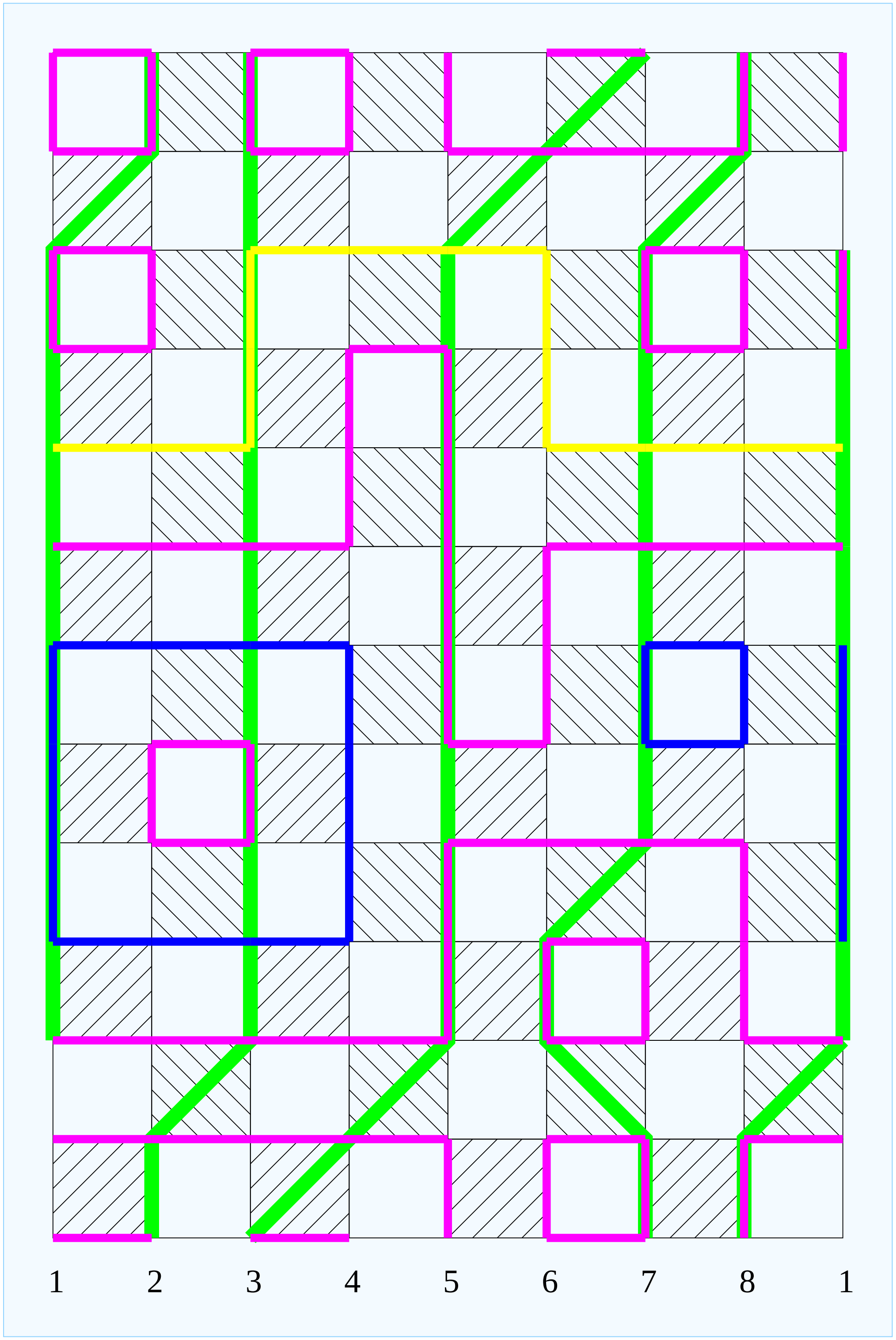

All S_T^z states accessible

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$\hookrightarrow$ Simulation in grand canonical ensemble

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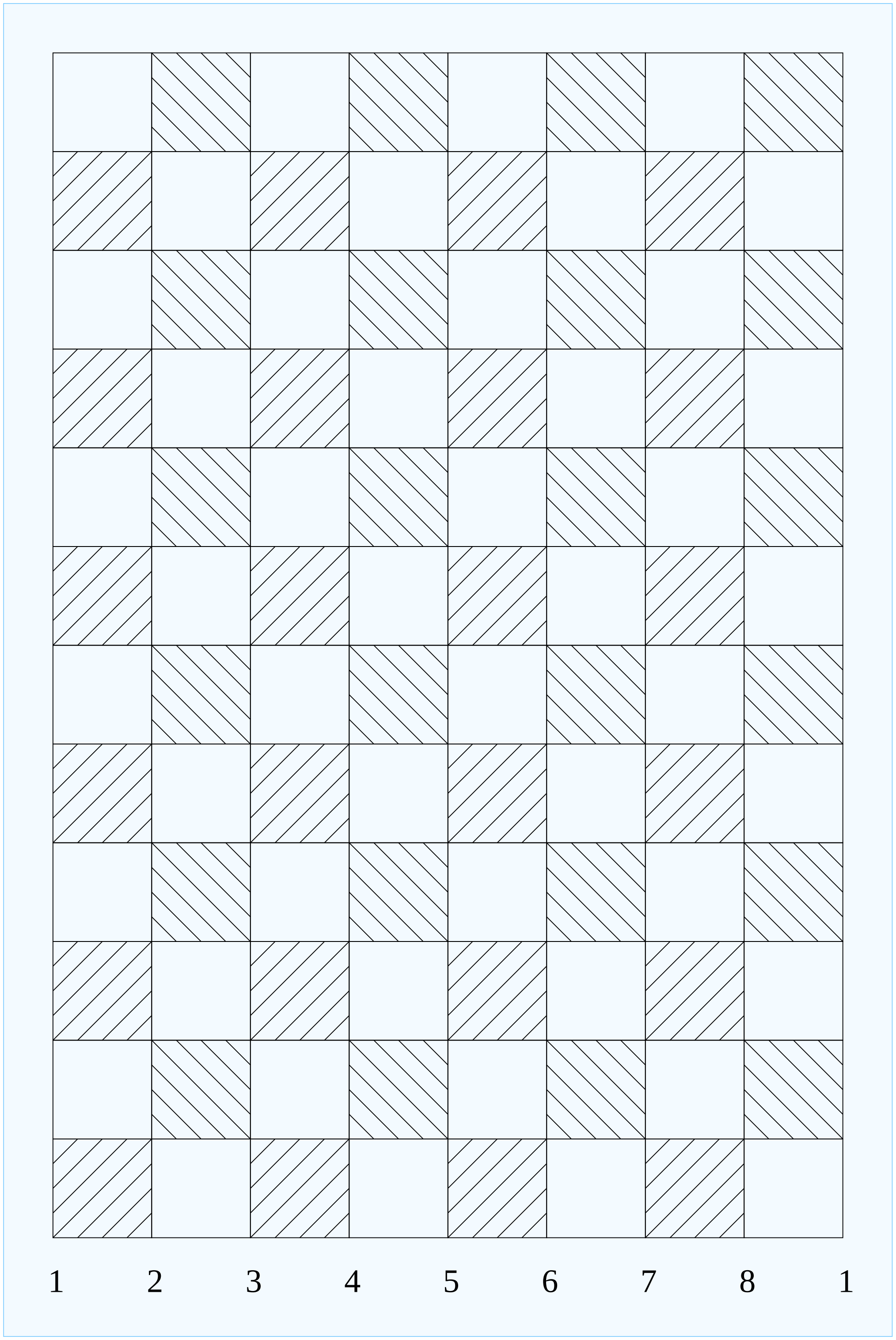
$\hookrightarrow$ **Simulation in grand canonical ensemble**

Loops

Active loops

World lines



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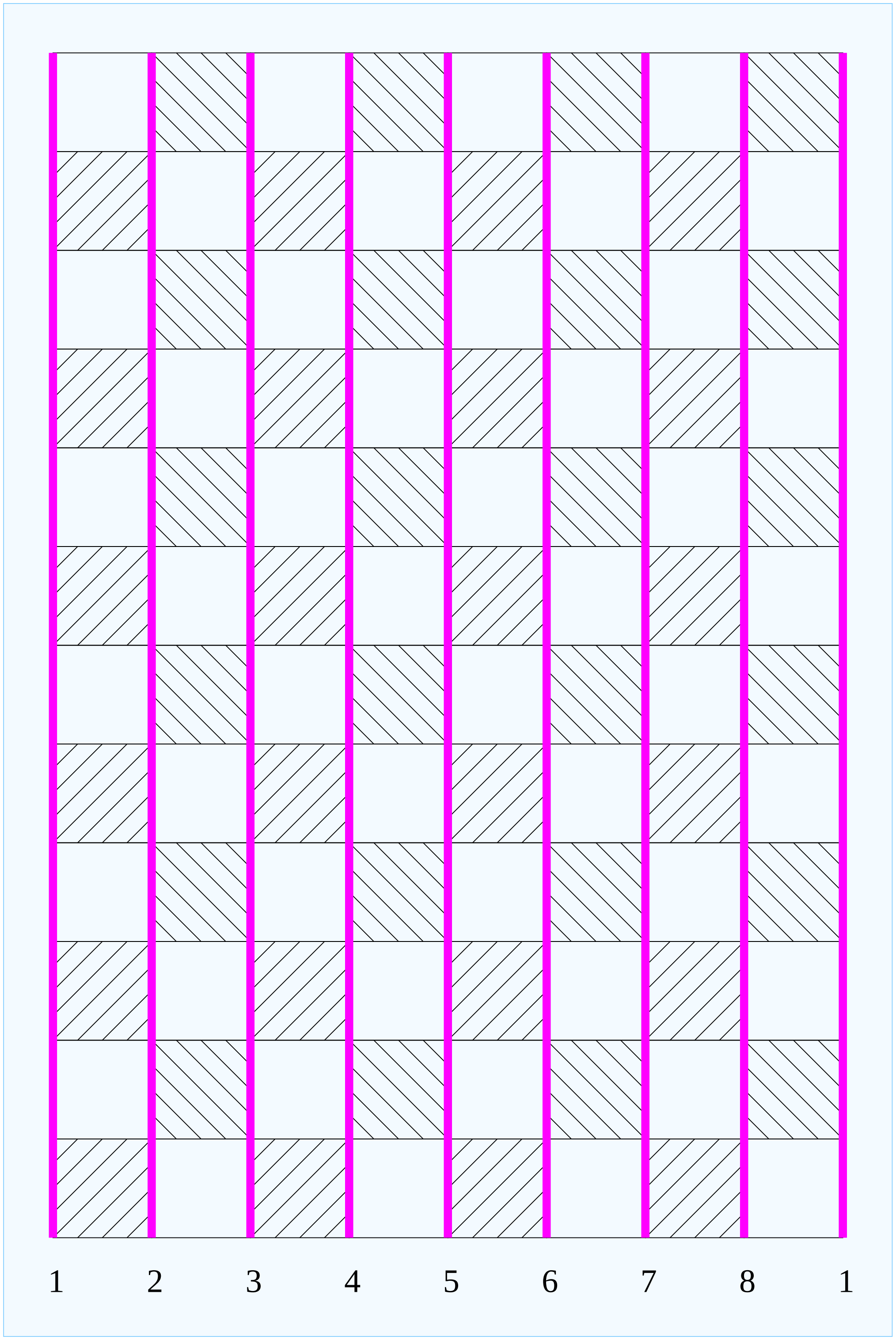

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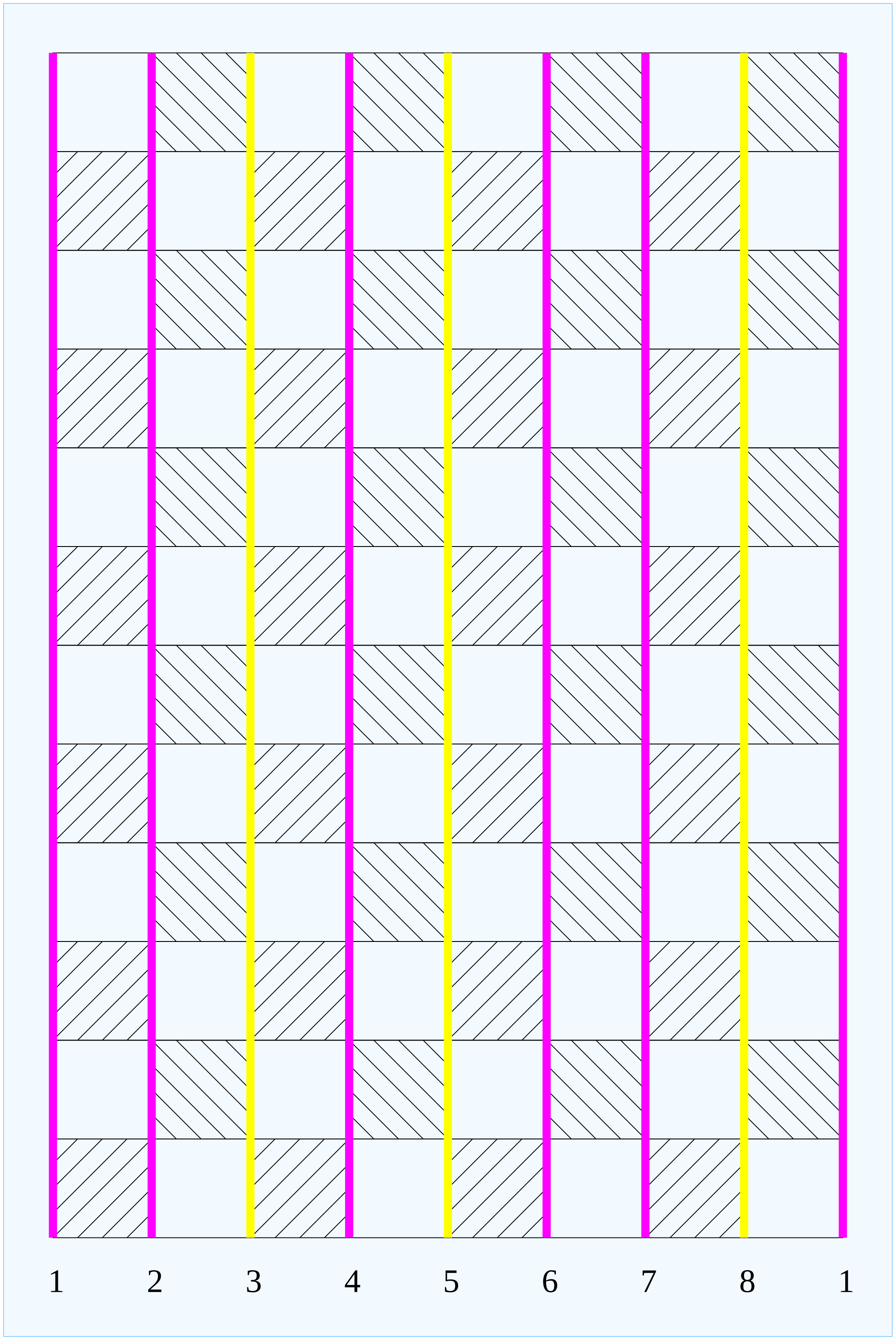

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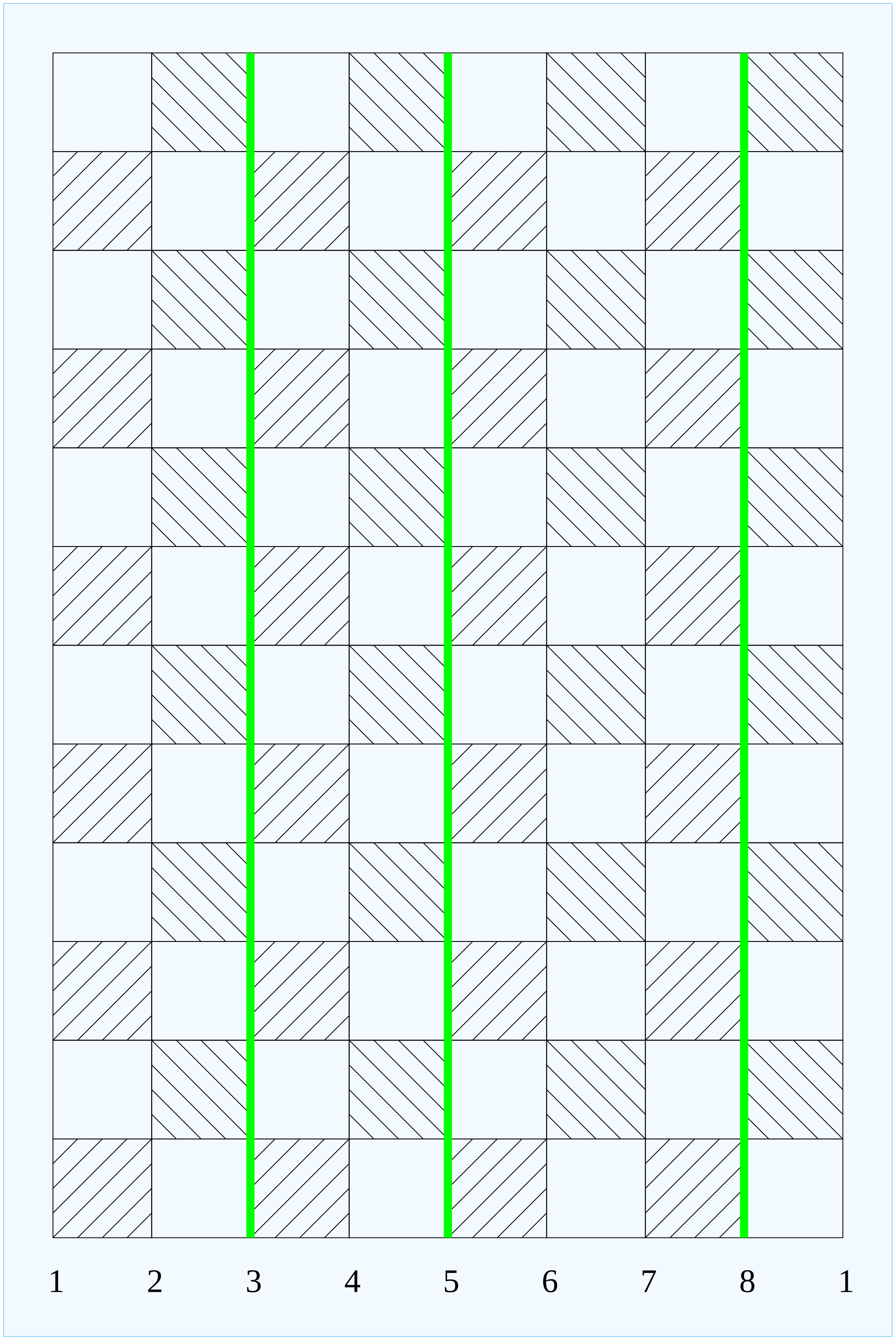

Change of winding numbers are possible

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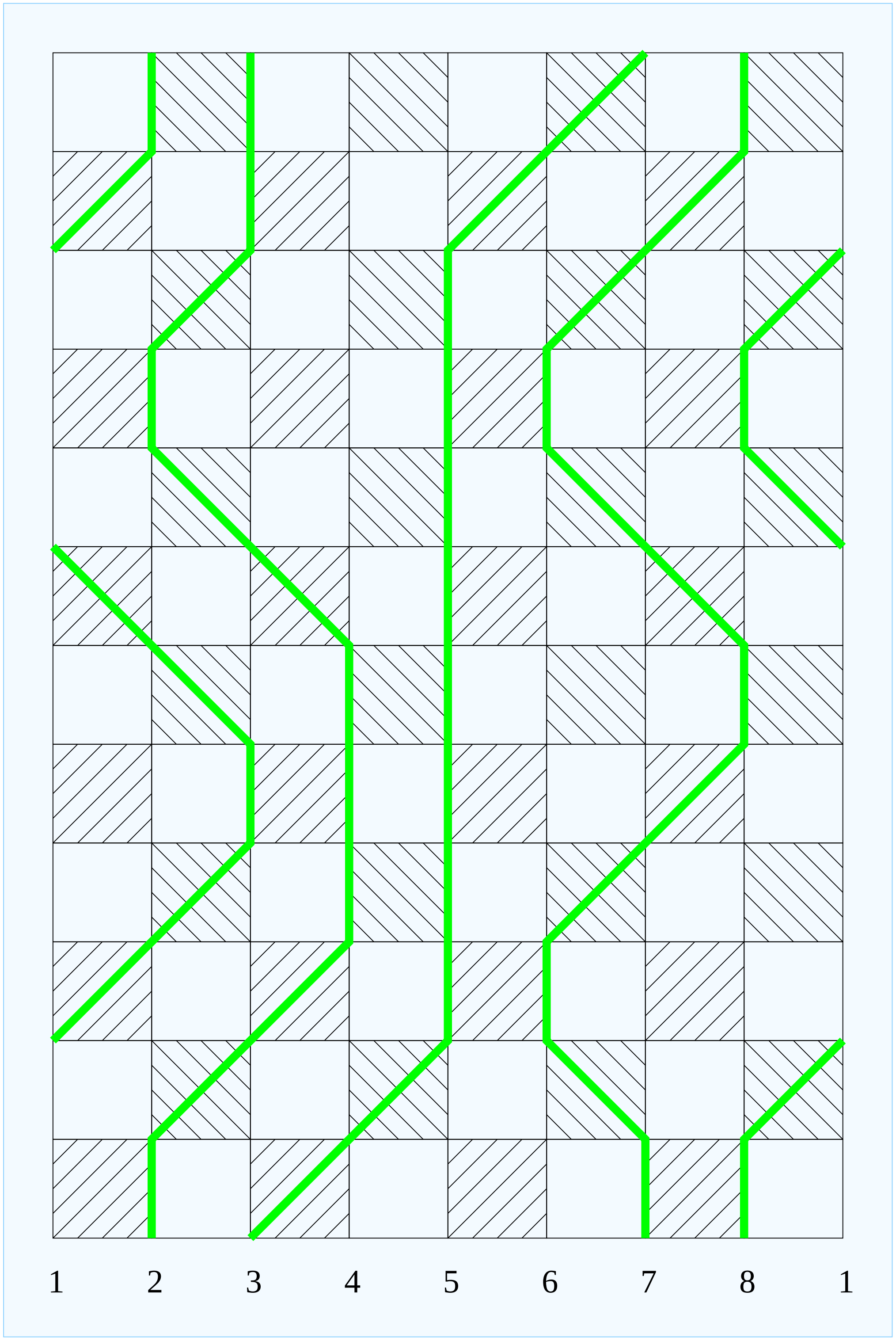
World lines

Active loops



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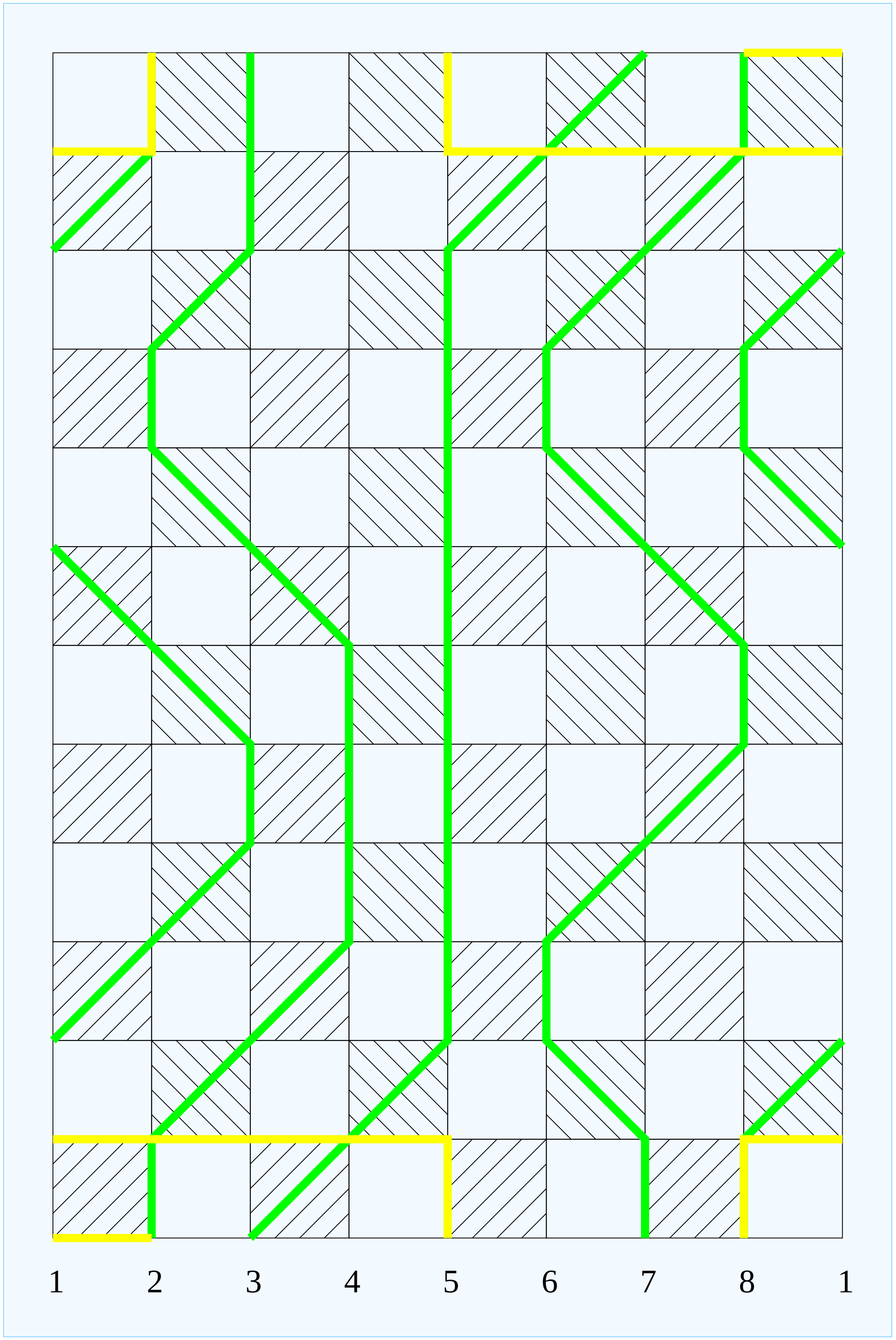
World lines (green line)

Active loops (yellow line)



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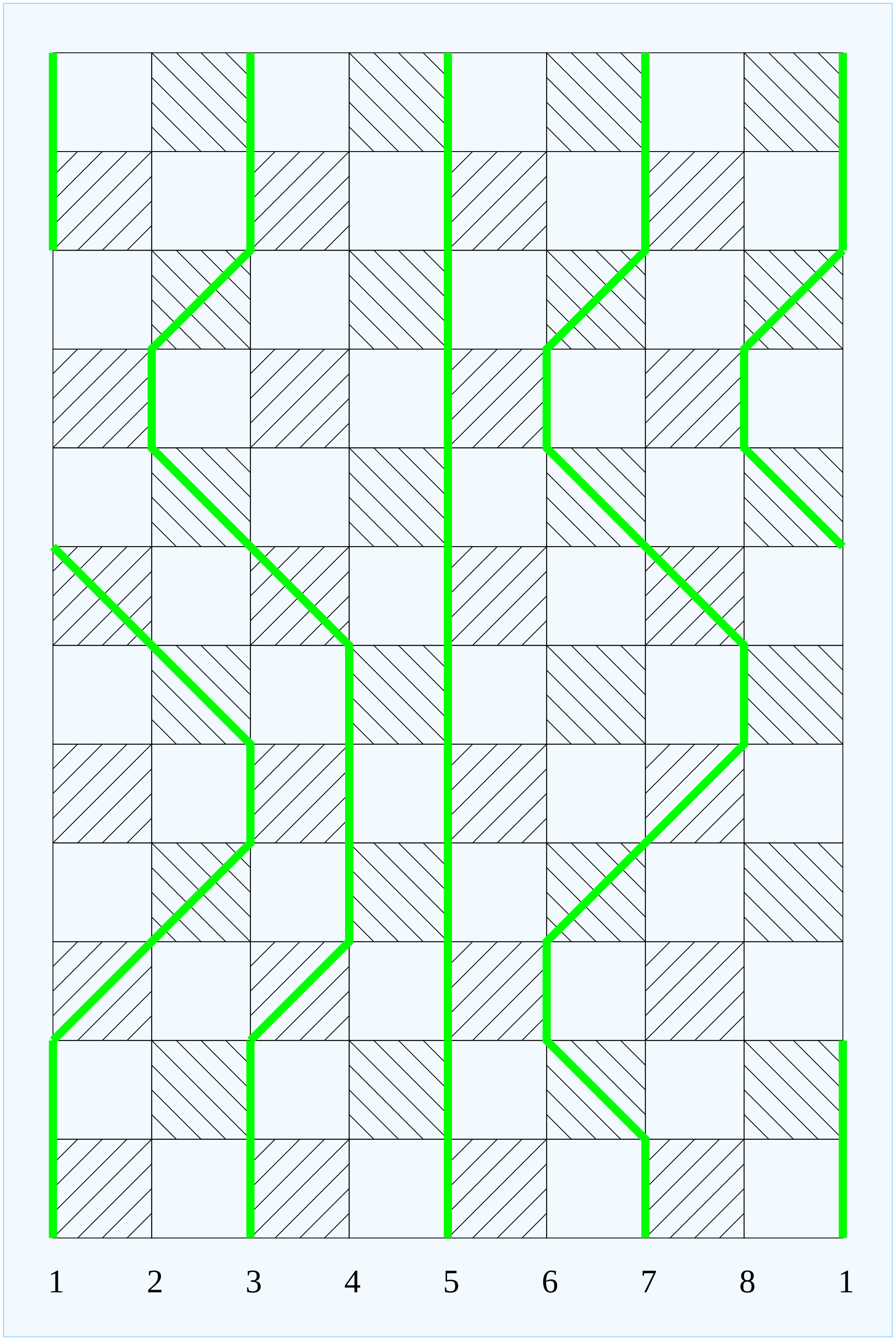
World lines

Active loops



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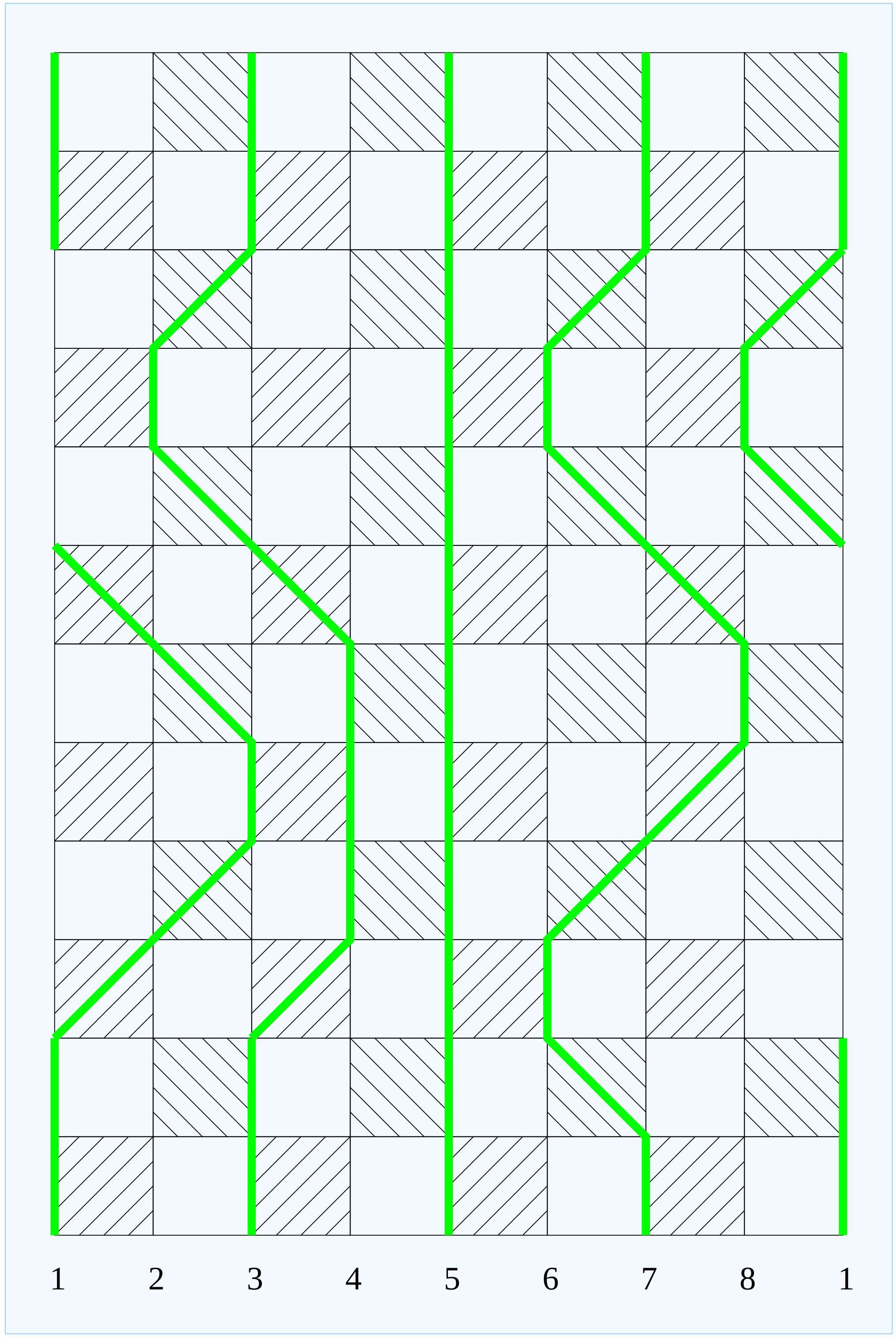
World lines

Active loops

Short autocorrelation times.



2.2 Improved estimators with the loop-algorithm

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Estimator for the expectation value

$$< \mathcal{O} > \quad = \quad \frac{\sum_{\boldsymbol{s}} W\left(\boldsymbol{s}\right)\, \mathcal{O}\left(\boldsymbol{s}\right)}{\sum_{\boldsymbol{s}} W\left(\boldsymbol{s}\right)}$$

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$< \mathcal{O} >$ **is an expectation value in the ensemble of graphs.**

Consider $\mathcal{O} = 4S_i^z S_j^z$, where i and j are points in space-time.

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$$4S_i^z S_j^z \left(\mathcal{G} = \text{loop}\right) \quad = \quad \begin{cases} \sigma_i \sigma_j & \text{in the same cluster} \\ 0 & \text{otherwise} \end{cases}$$

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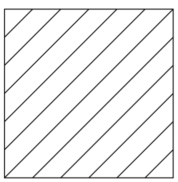
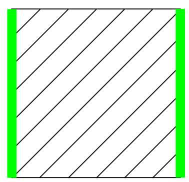
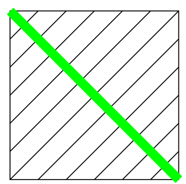
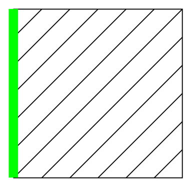
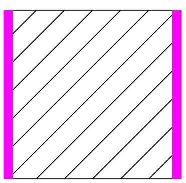
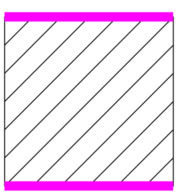
g \ u				
	1	1	0	1
	0	0	1	1

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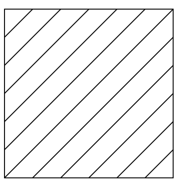
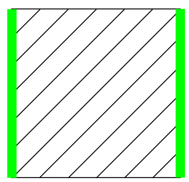
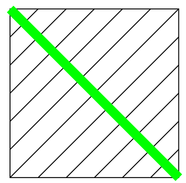
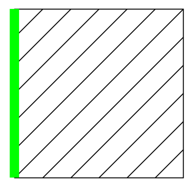
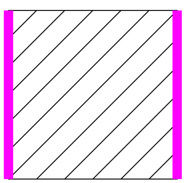
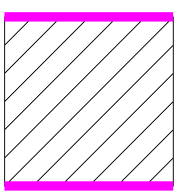
g \ u				
	1	1	0	1
	0	0	1	1

vertical lines join sites with equal spins

horizontal lines join sites with alternating spins

For staggered susceptibility

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Improved estimators reduce fluctuations

2.3 Off-diagonal operators

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$\hookrightarrow$ **Change to a basis where $\mathcal{O}$ is diagonal**

As in the case of diagonal operators,

$$4S_i^x S_j^x\left(\mathcal{G} = \text{loop}\right) \;=\; \begin{cases} \sigma_i\sigma_j & \text{in the same cluster} \\ 0 & \text{otherwise} \end{cases}$$

2.4 Continuous imaginary time

B.B. Beard and U.J. Wiese, Phys. Rev. Lett. **77**, 5130 (1996)

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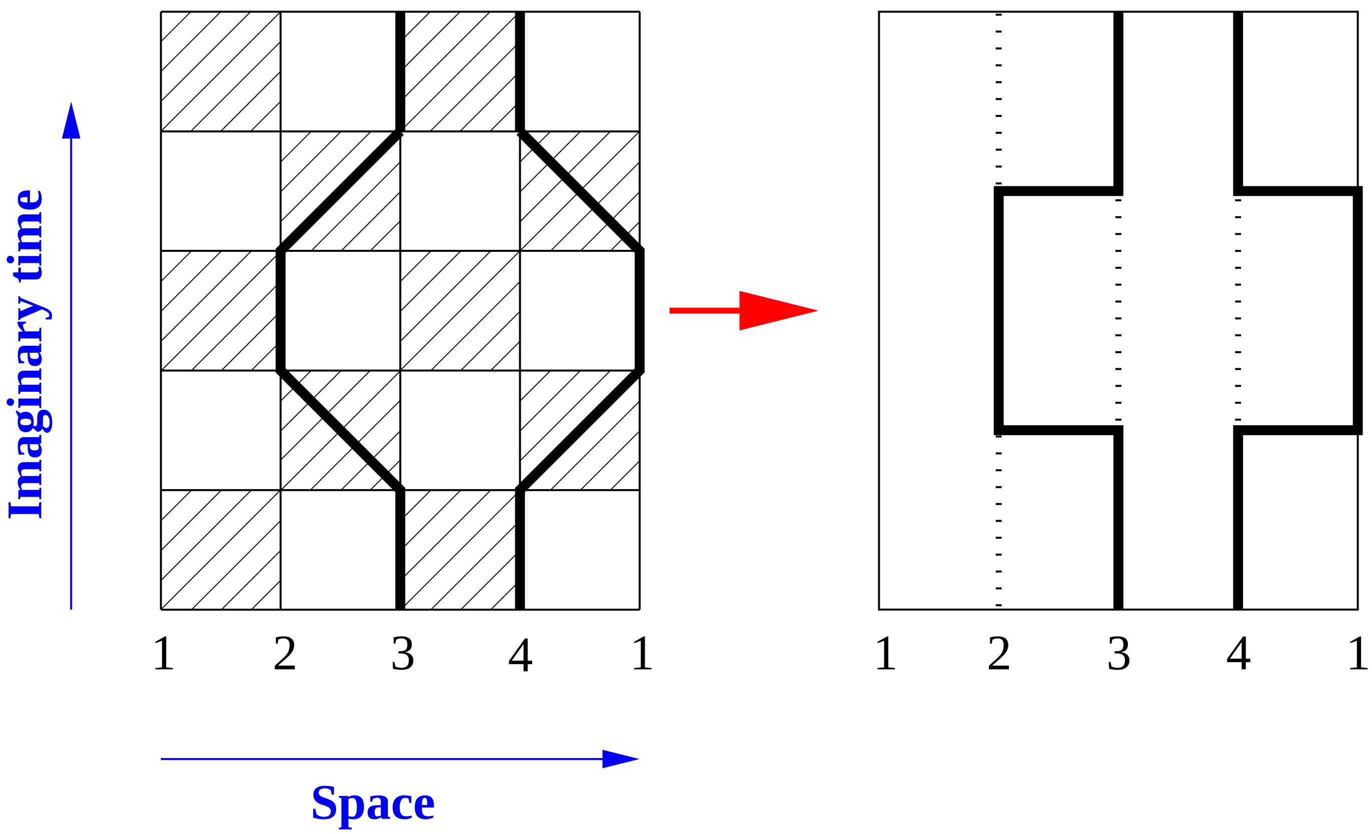

Recall graph probabilities

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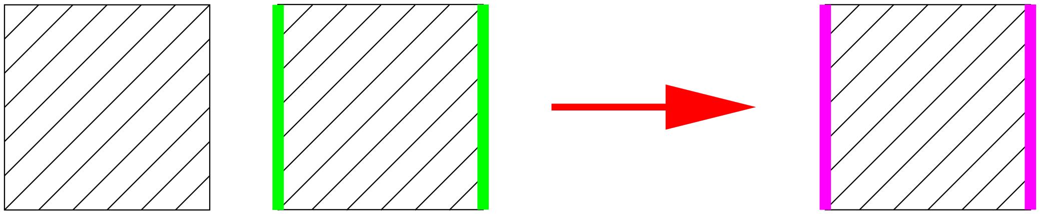

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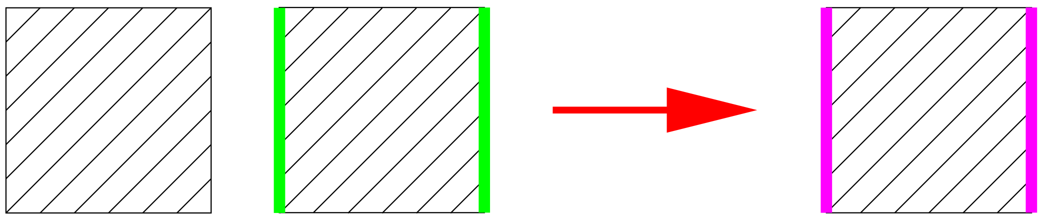

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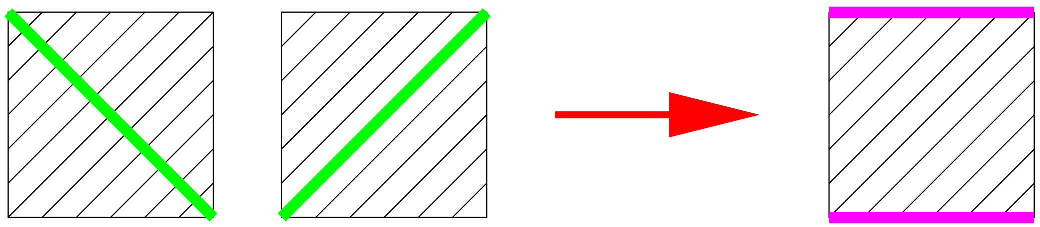

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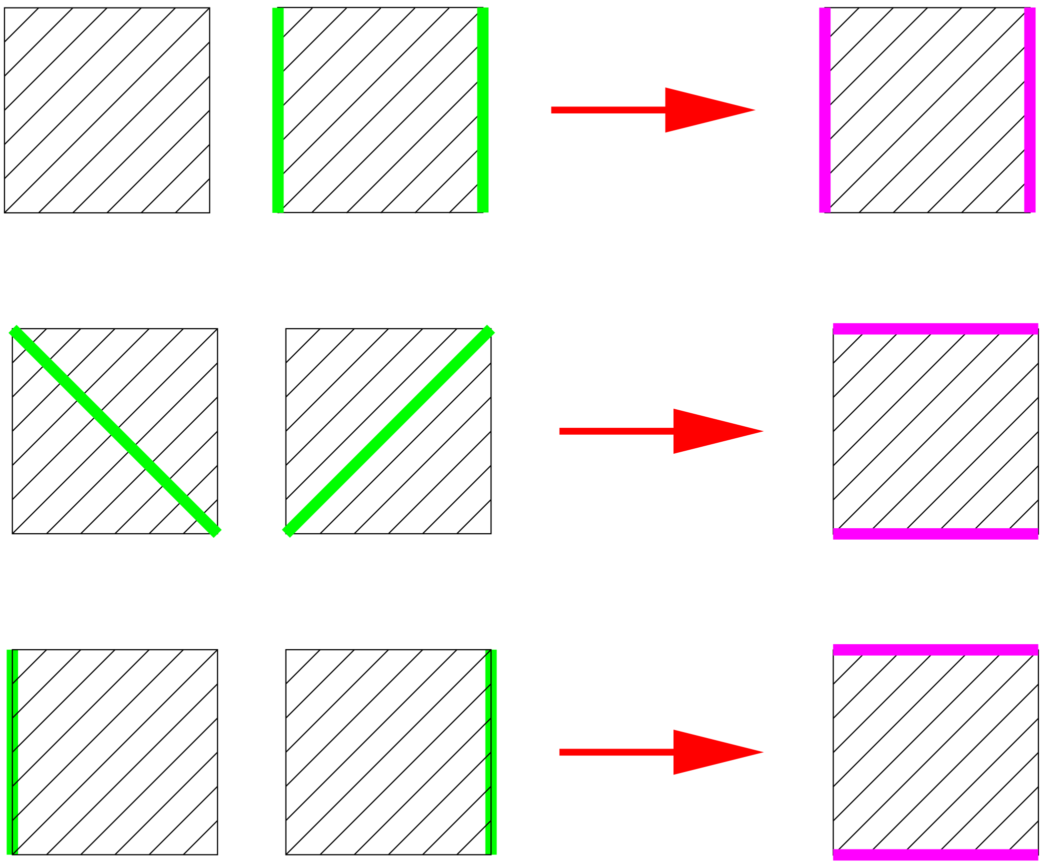

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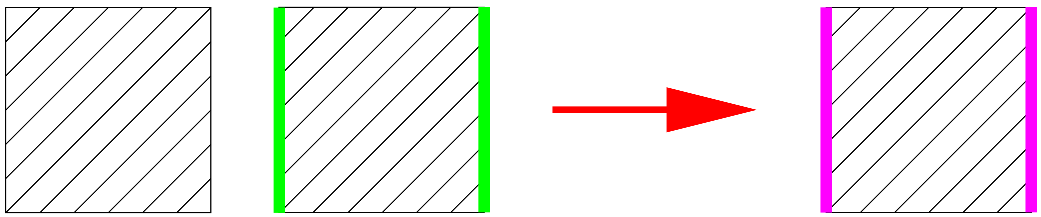
$$p(=) = 1$$

$$p(=) = \tanh\left(\Delta\tau\, J/2\right)$$

Recall graph probabilities



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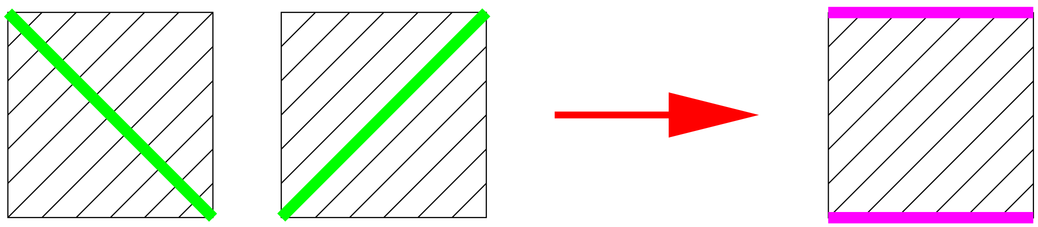

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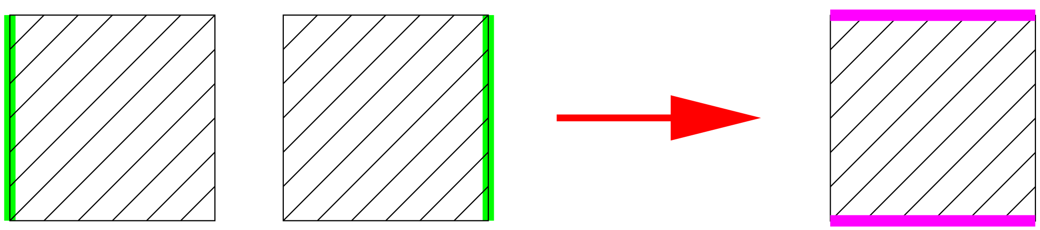

$$p(=) = \tanh\left(\Delta\tau\, J/2\right)$$

Continuum limit $\longrightarrow$ **probability density per unit time**

$$\frac{p(=)}{\Delta\tau} \quad \longrightarrow \quad \frac{J}{2}$$

Rules for a loop

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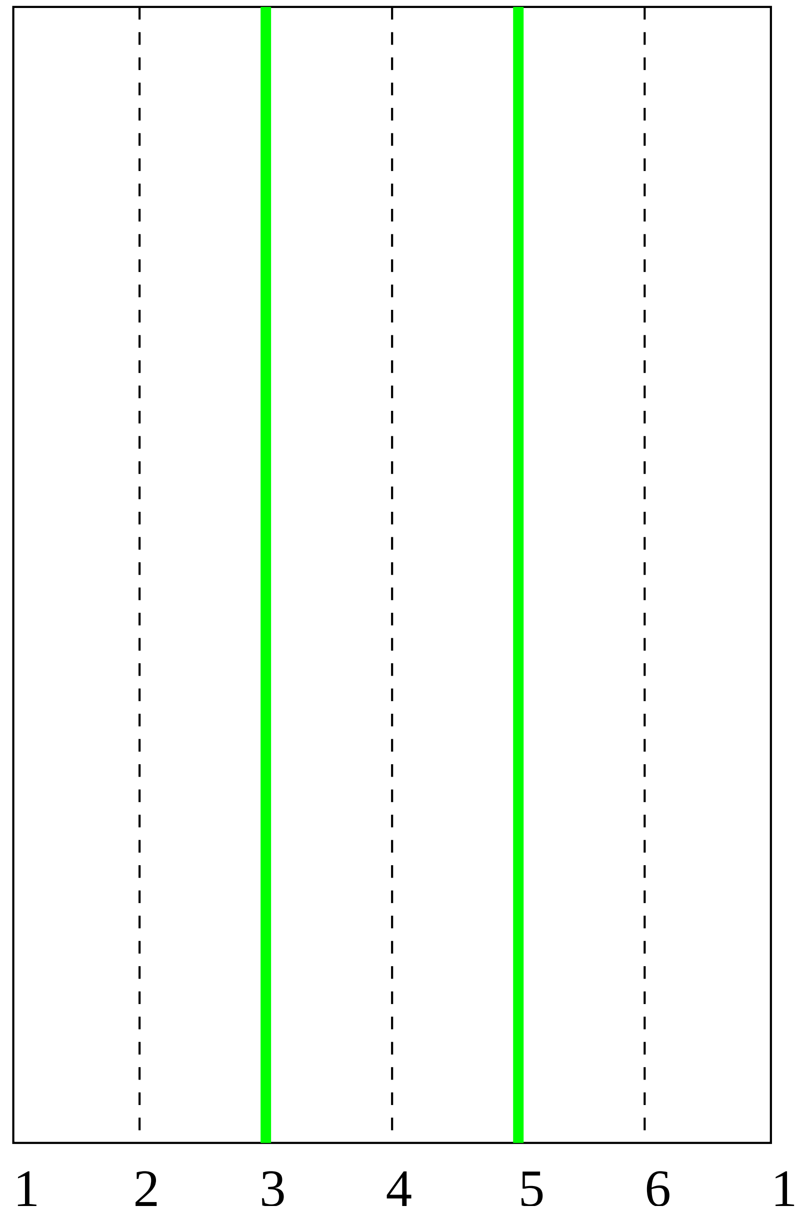
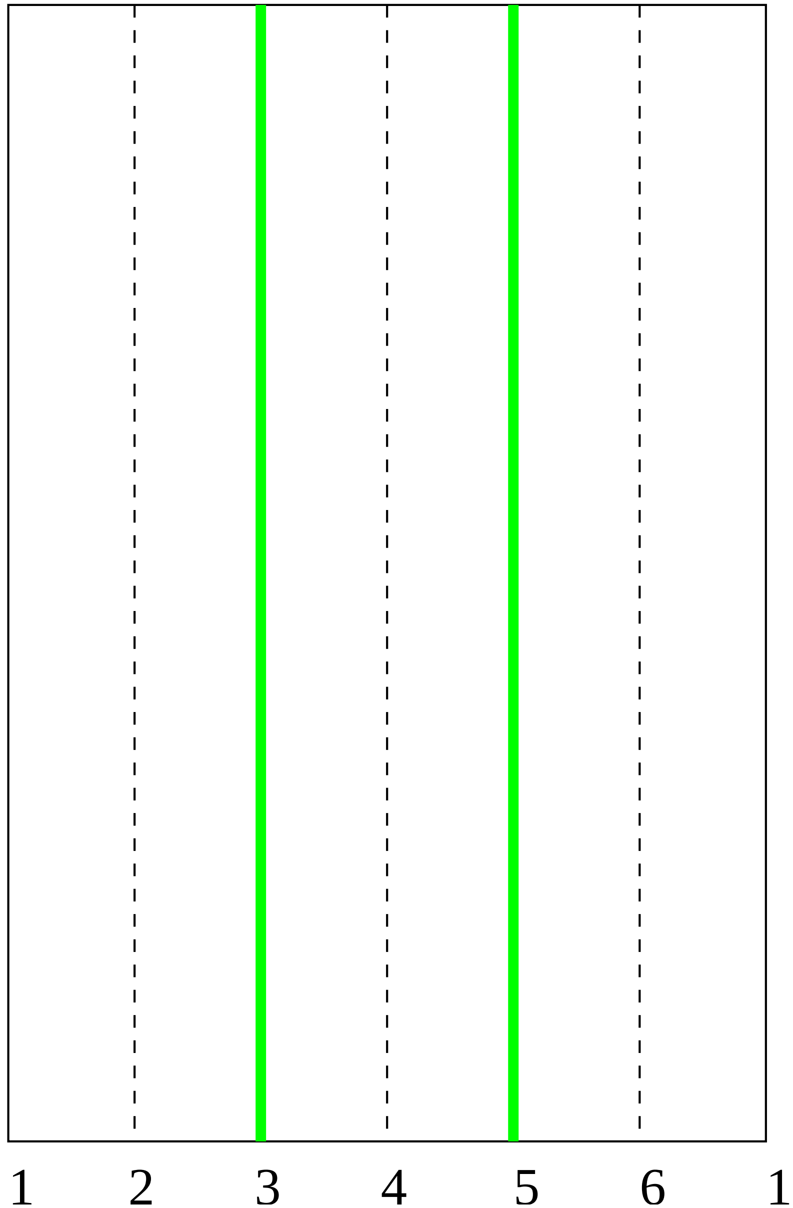


Rules for a loop

Start at some point of the lattice



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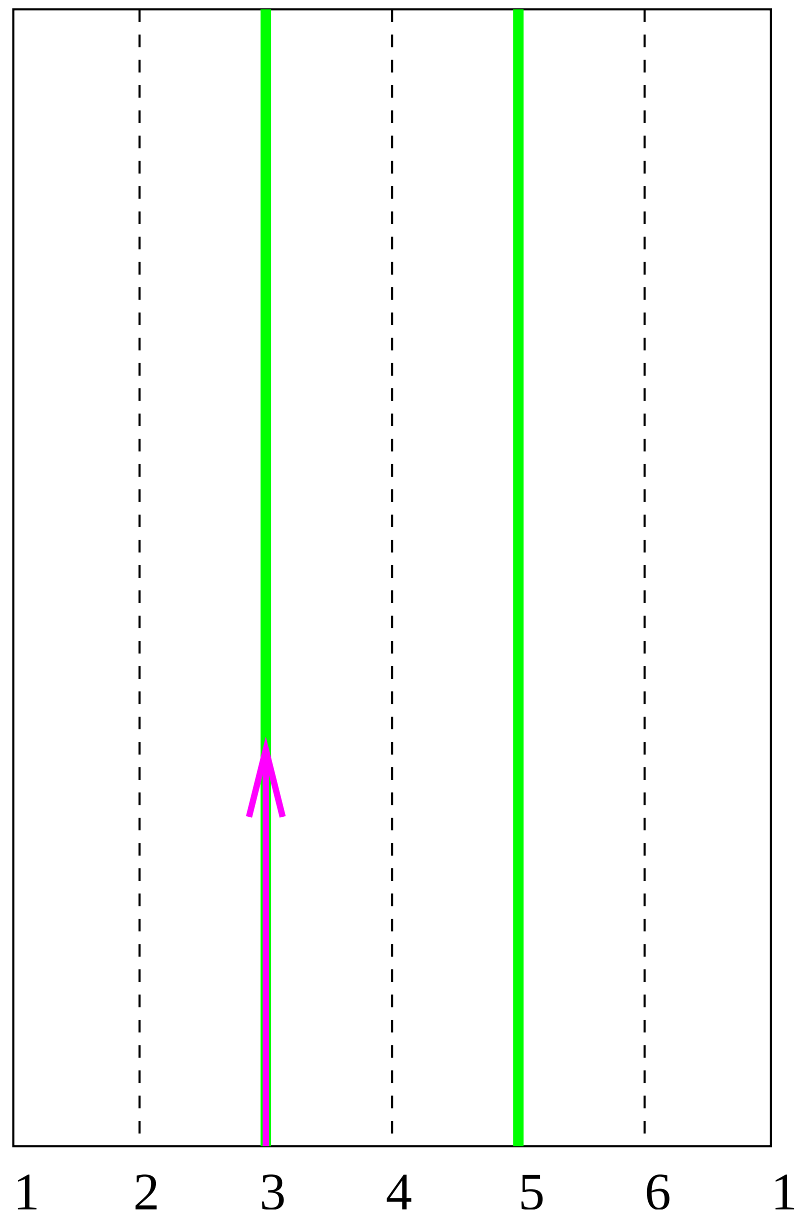

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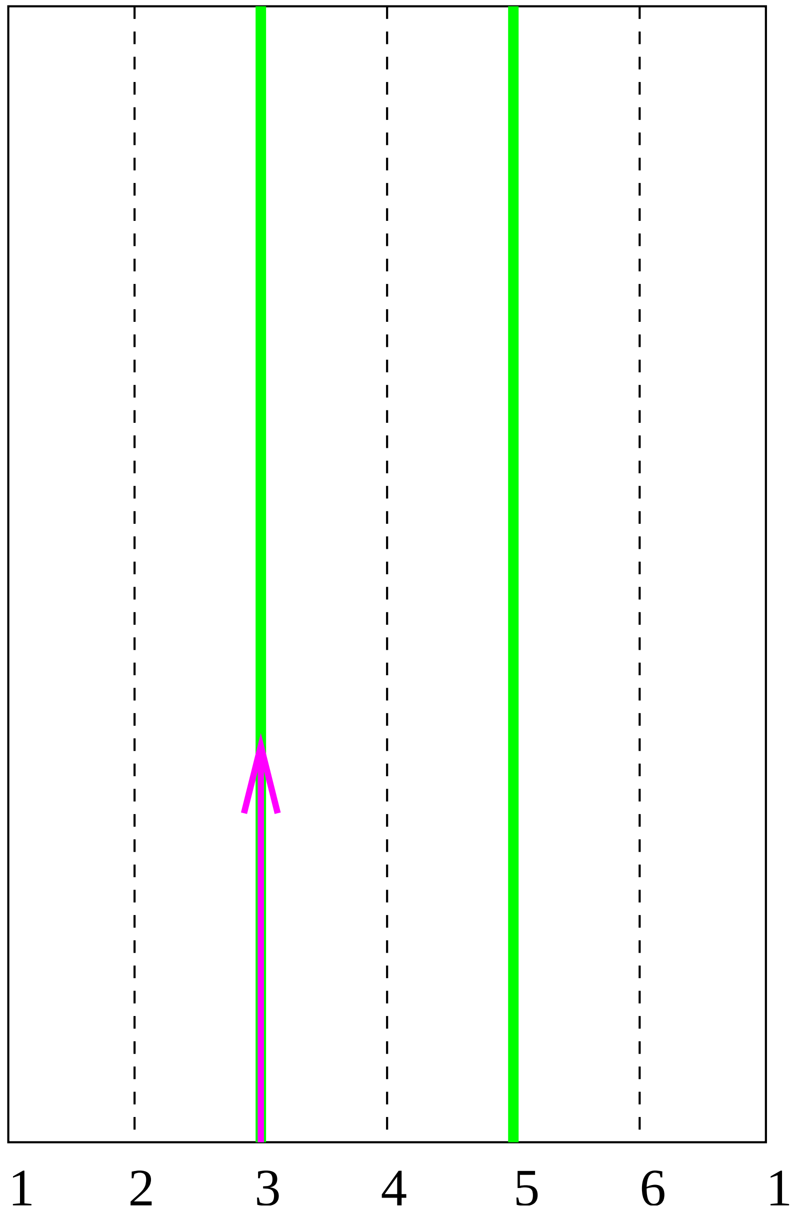
Start at some point of the lattice

Put an horizontal line with probability density $\rho(=) = J/2$



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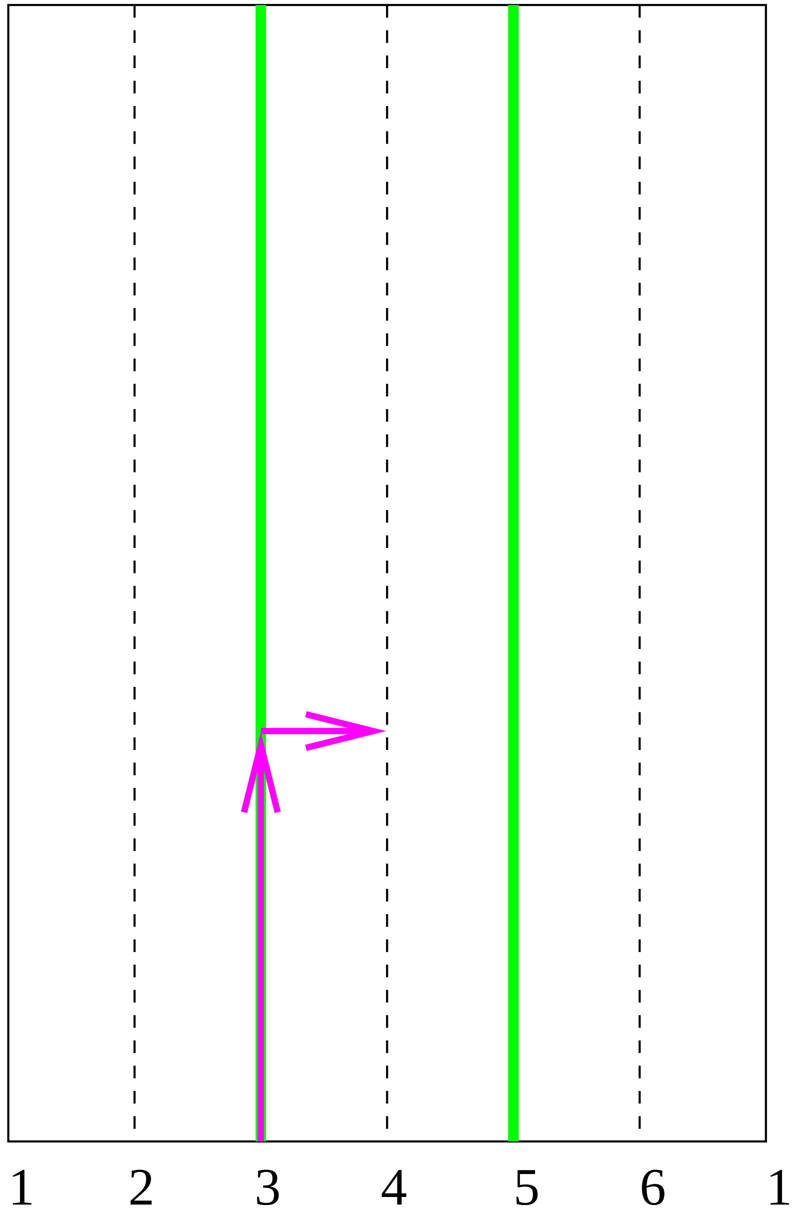

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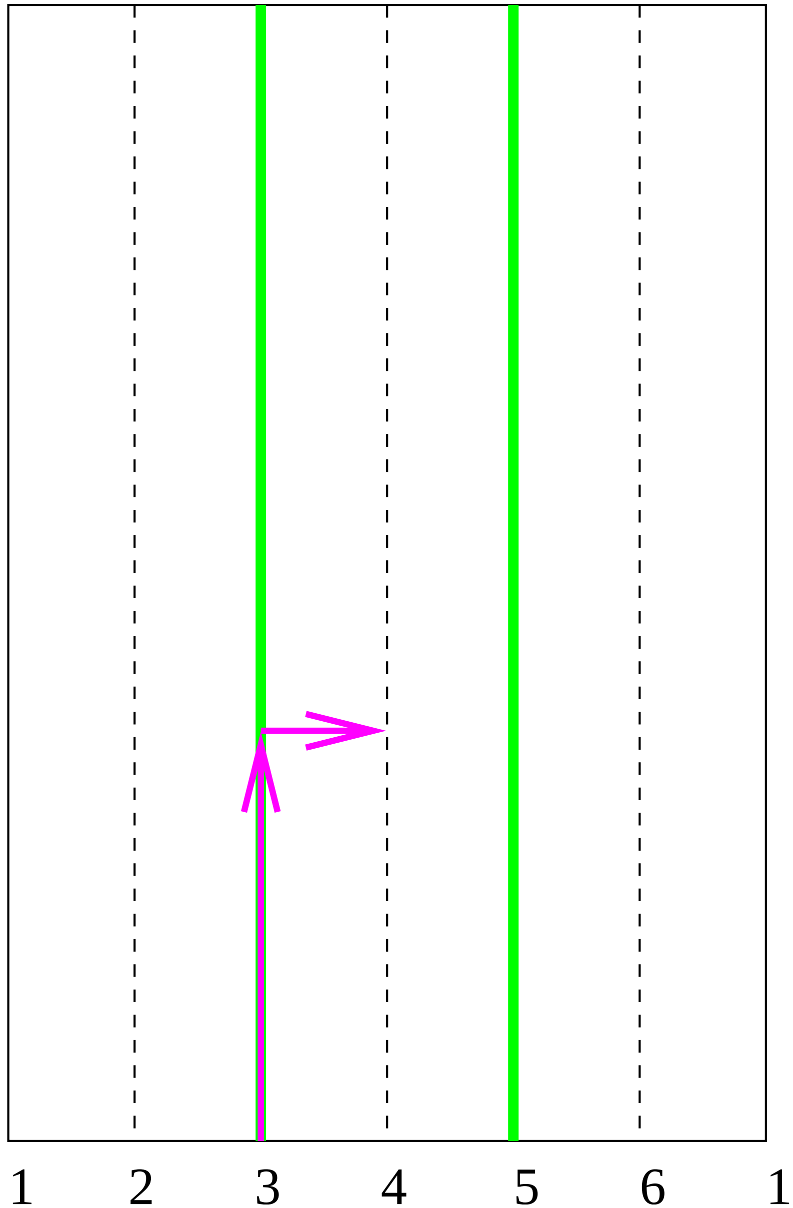
Reverse direction



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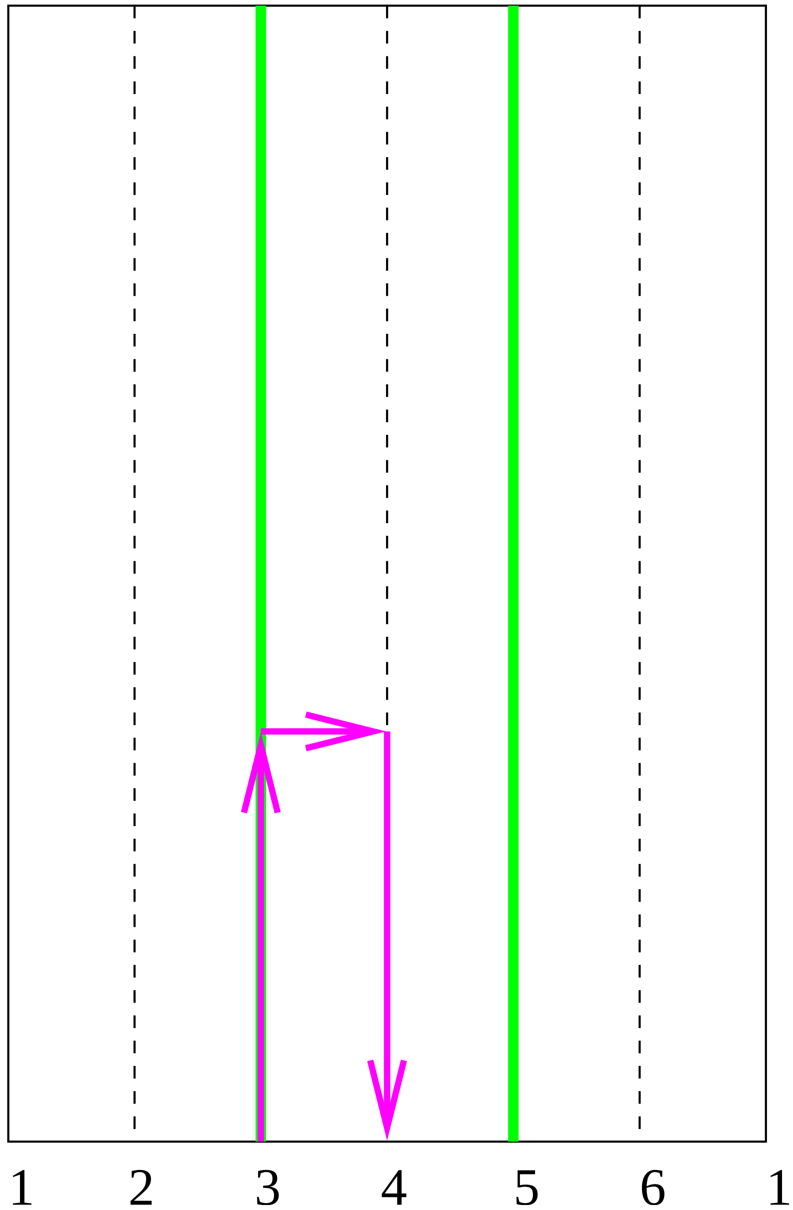

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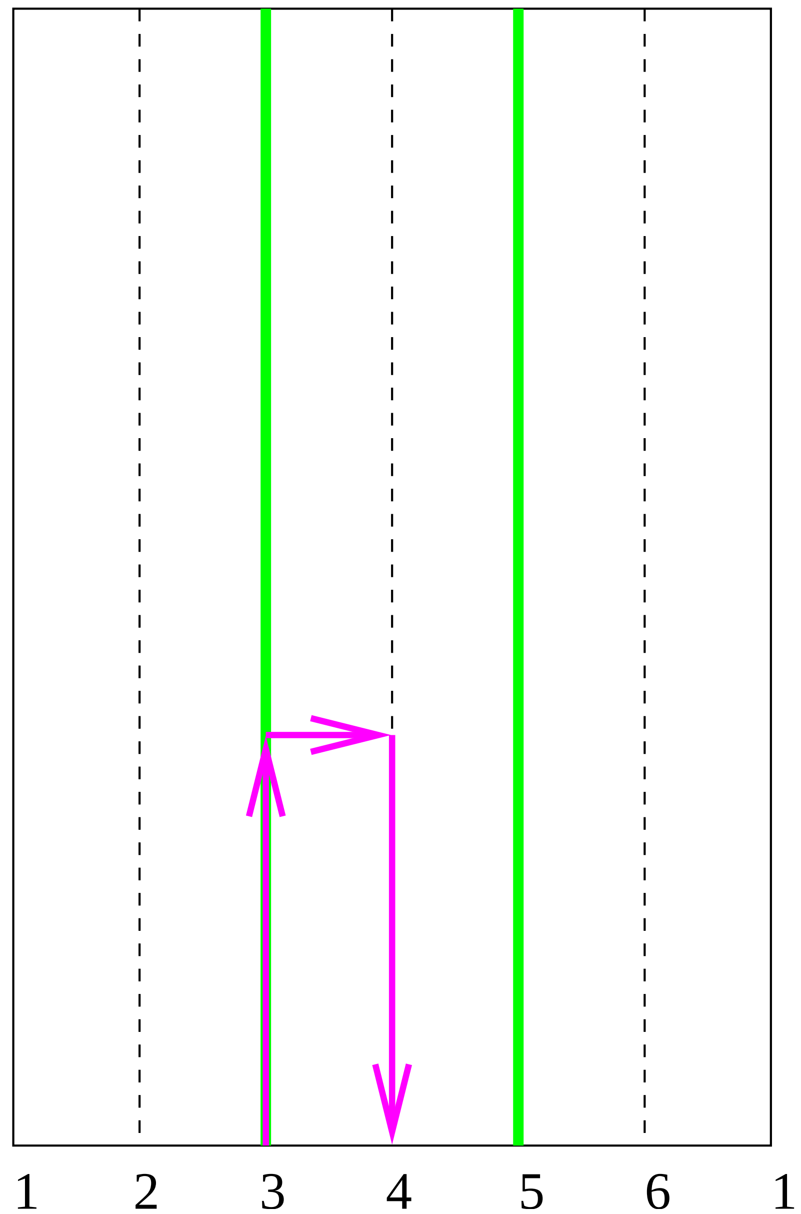
Repeat until loop closes



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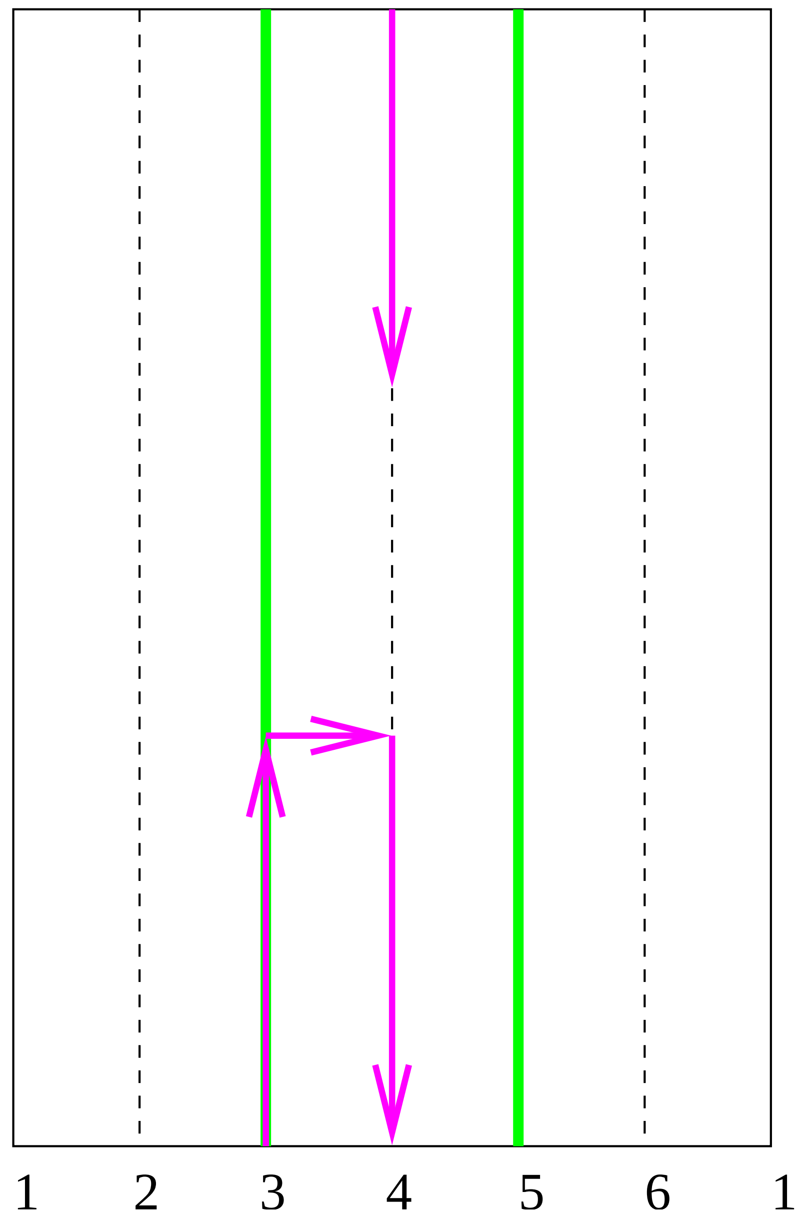

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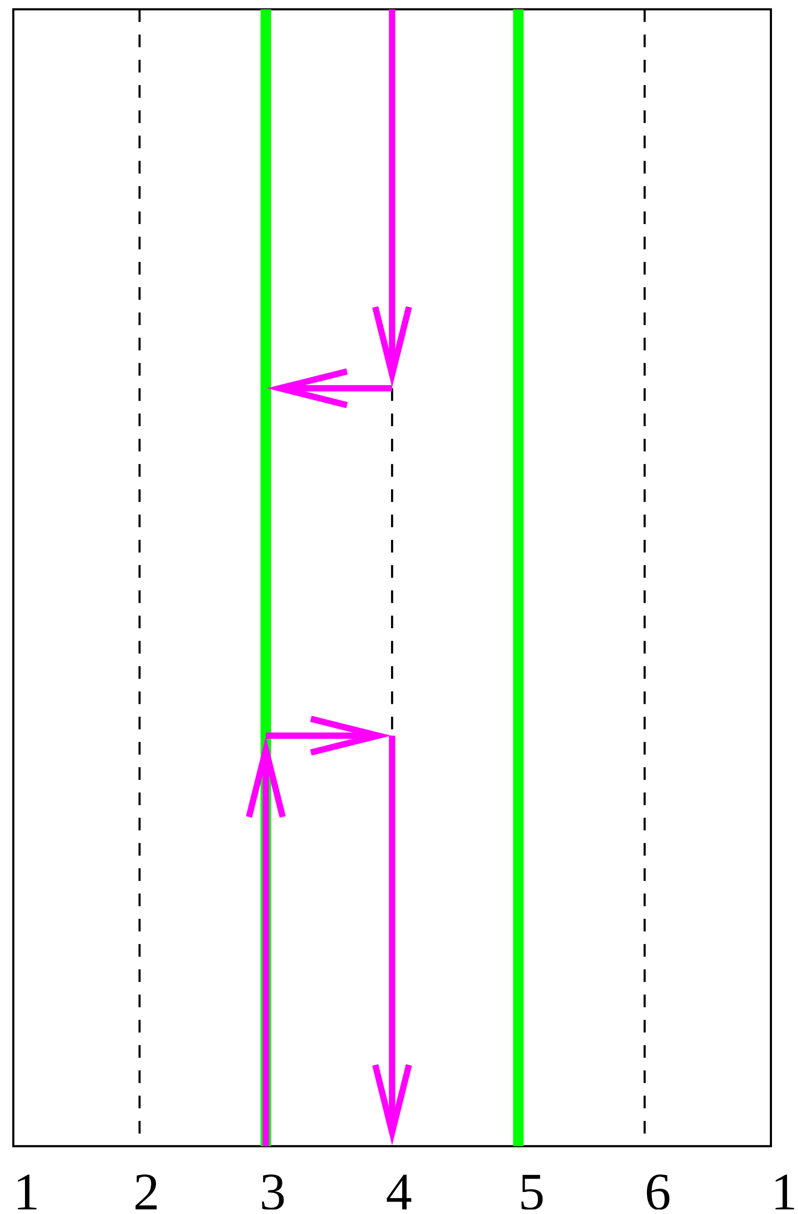

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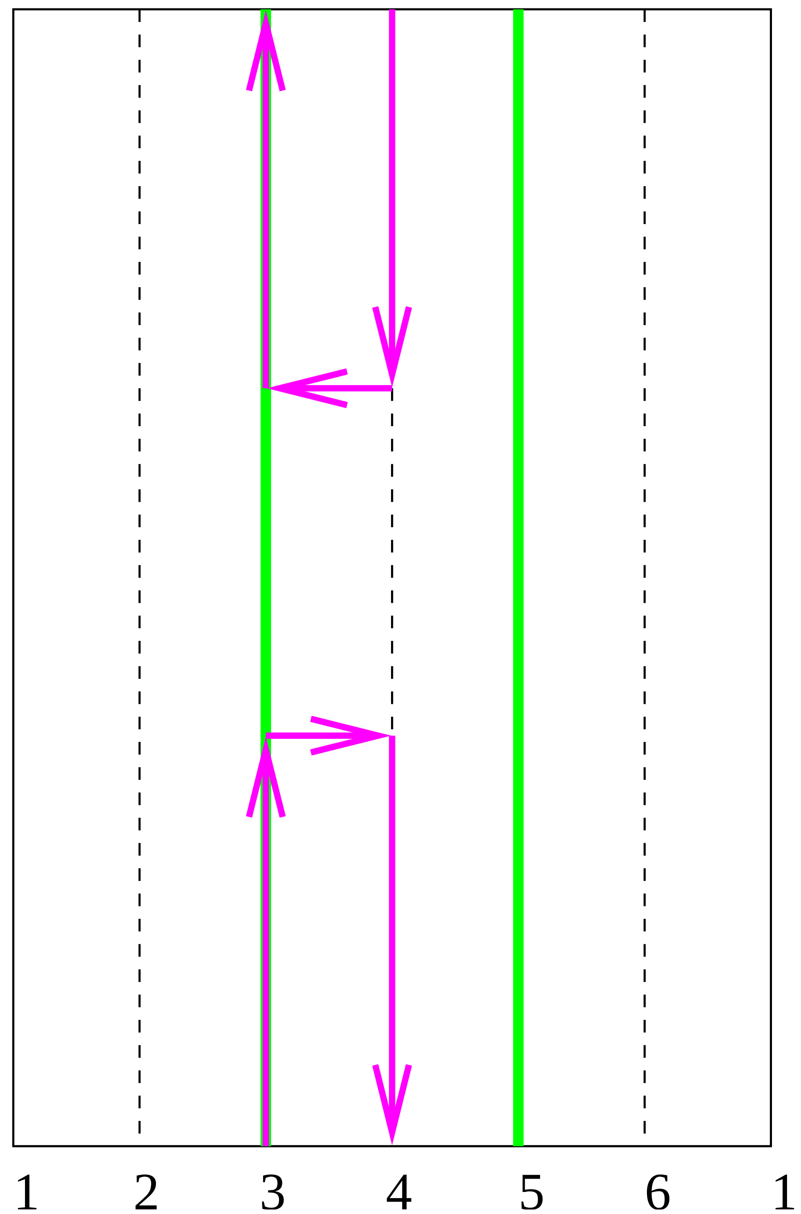

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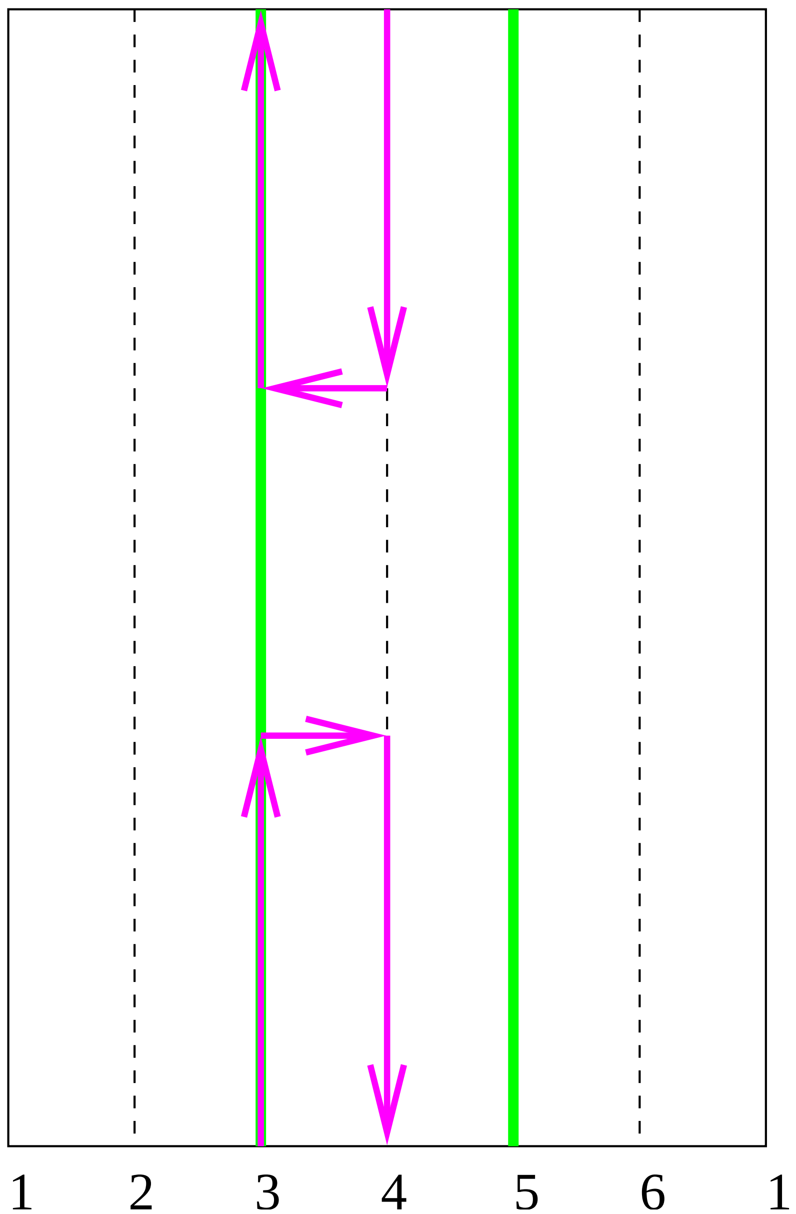
Flip the loop



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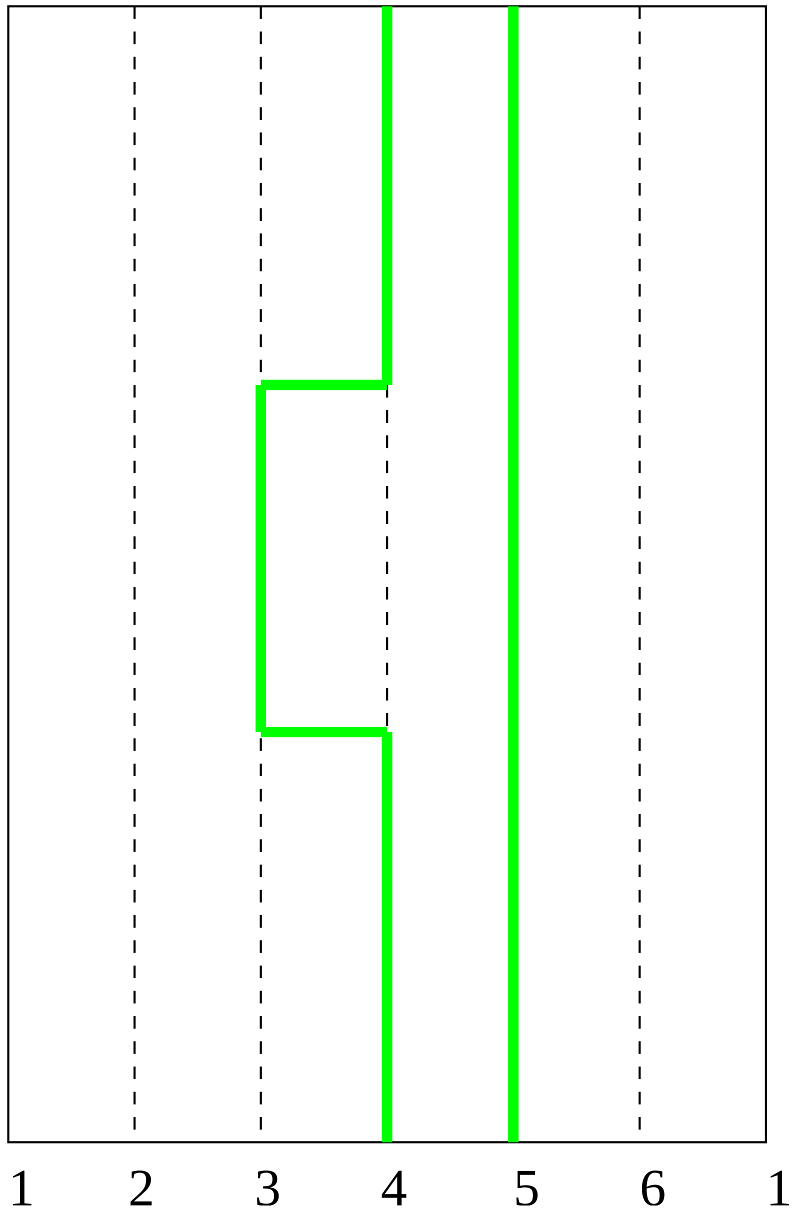

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- **Stochastic series expansion**
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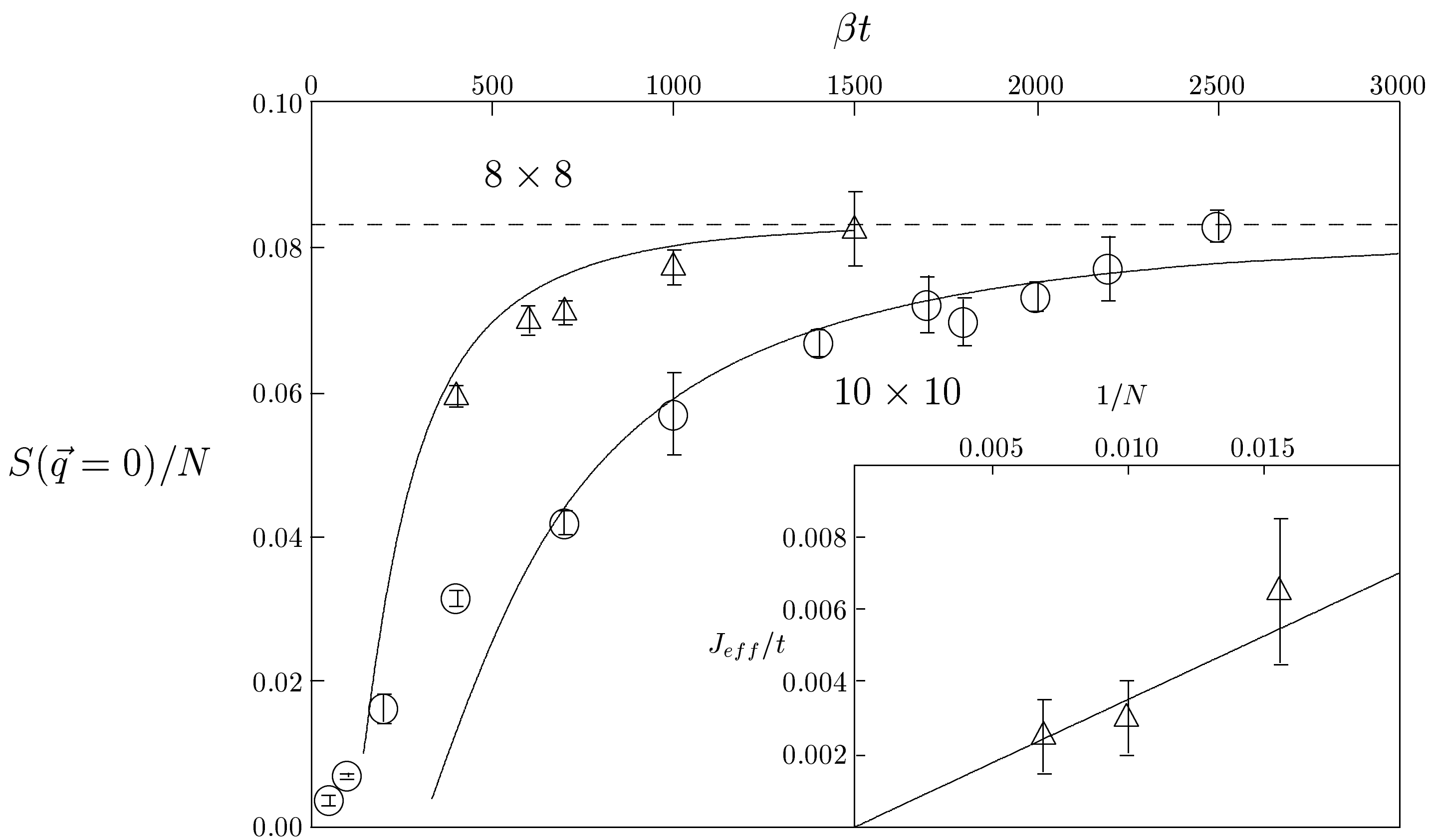
Loop-algorithm for the t-J model

Two dimensional t-model (J=0) with one hole

Nagaoka's ferromagnetism



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