Monte Carlo simulations of quantum systems with global updates

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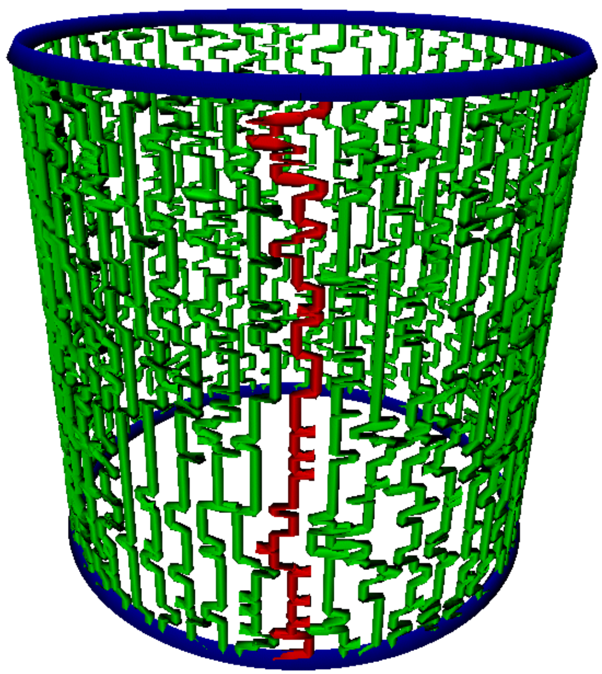
Quantum spin-systems I

World-lines and the loop-algorithm



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$$(1) \longrightarrow -t \sum_i \left(c_i^\dagger c_{i+1} + h.c \right) + V \sum_i \left(n_i - \frac{1}{2} \right) \left(n_{i+1} - \frac{1}{2} \right)$$

with $t = J/2$ **and** $V = J\Delta \Longrightarrow$ **isotropic HAF** $\longrightarrow V = 2t$.

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$\hookrightarrow$ **quantum Monte Carlo simulations**

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Partition function

$$\begin{aligned} Z &= \mathrm{Tr}\, \mathrm{e}^{-\beta H} = \mathrm{Tr} \prod_{\ell=1}^{L} \mathrm{e}^{-\Delta\tau H} \\ &= \sum_{\{i_\ell\}} < i_1 | \mathrm{e}^{-\Delta\tau H} | i_L >< i_L | \mathrm{e}^{-\Delta\tau H} | i_{L-1} > \cdots < i_2 | \mathrm{e}^{-\Delta\tau H} | i_1 > , \end{aligned}$$

where $\Delta\tau = \beta/L$, and $\{|i_\ell >\}$ complete sets of states at each time slice.

Trotter-Suzuki decomposition $\longrightarrow$ $H = H_1 + H_2$.

$$\mathrm{e}^{-\Delta\tau H} = \mathrm{e}^{-\Delta\tau H_1}\mathrm{e}^{-\Delta\tau H_2} + \mathcal{O}\left[(\Delta\tau)^2\right] \ .$$

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Choose

$$H_{1\,(2)} = \sum_{i\,\mathrm{odd}\,(\mathrm{even})} H_{i,i+1} \, ,$$

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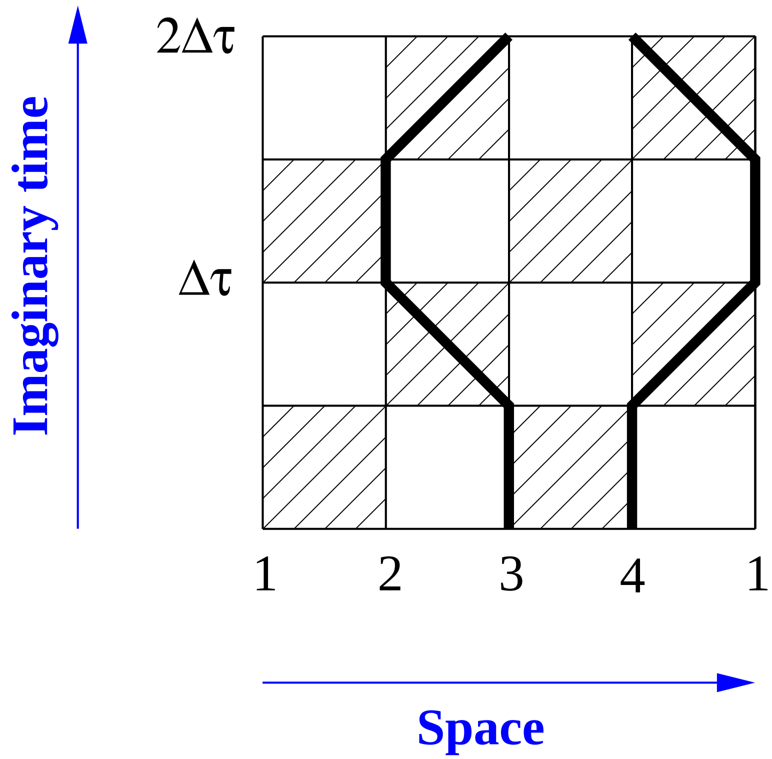
$\hookrightarrow$ **the matrix elements are reduced to a product of two-site matrix elements:**

$$\begin{aligned} &< i_\ell \mid \mathrm{e}^{-\Delta\tau H} \mid i_{\ell+1} > \\ &= \ < i_{2\ell} \mid \mathrm{e}^{-\Delta\tau H_1} \mid i_{2\ell-1} >< i_{2\ell-1} \mid \mathrm{e}^{-\Delta\tau H_2} \mid i_{2\ell-2} > + \mathcal{O}\left[(\Delta\tau)^2\right] \\ &= \ \prod_{i\,\mathrm{odd}} < i_{2\ell} \mid \mathrm{e}^{-\Delta\tau H_{i,i+1}} \mid i_{2\ell-1} > \\ &\qquad \times \prod_{i\,\mathrm{even}} < i_{2\ell-1} \mid \mathrm{e}^{-\Delta\tau H_{i,i+1}} \mid i_{2\ell-2} > + \mathcal{O}\left[(\Delta\tau)^2\right] \ . \end{aligned}$$

World-lines in a checkerboard in space-time (imaginary time)



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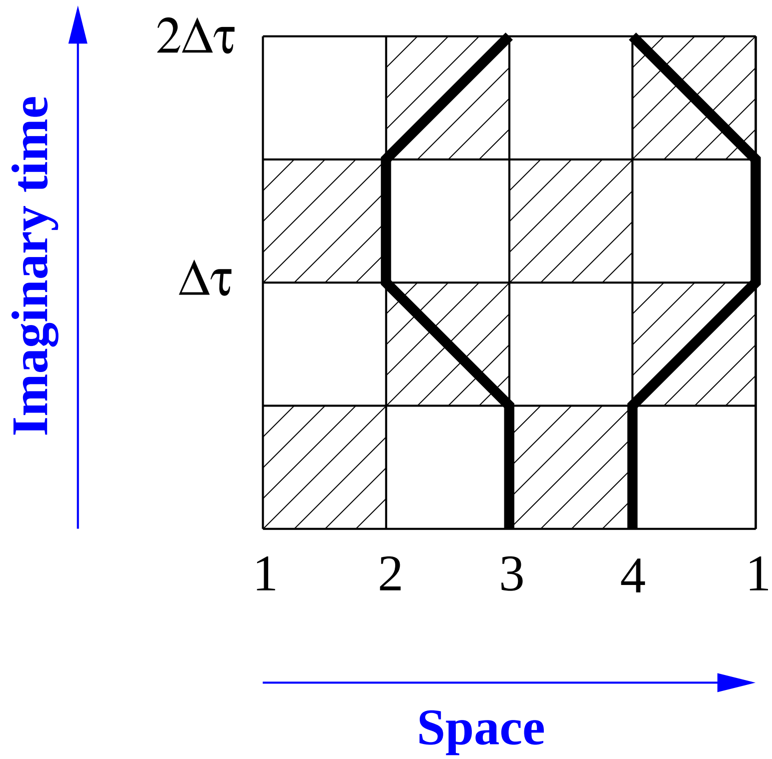

Matrix elements

$$
\begin{aligned}
<\uparrow\uparrow|\,\mathrm{e}^{-\Delta\tau H_{i,i+1}}\,|\uparrow\uparrow> &= <\downarrow\downarrow|\cdots|\downarrow\downarrow> = \mathrm{e}^{-\Delta\tau J\Delta/4} \\
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<\uparrow\downarrow|\,\mathrm{e}^{-\Delta\tau H_{i,i+1}}\,|\downarrow\uparrow> &= <\downarrow\uparrow|\cdots|\uparrow\downarrow> = -\mathrm{e}^{+\Delta\tau J\Delta/4}\sinh\Delta\tau J/2\ .
\end{aligned}
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Canonical transformation (only on bipartite lattices)

$$\begin{aligned} S_i^x &\rightarrow (-1)^i\, S_i^x \\ S_i^y &\rightarrow (-1)^i\, S_i^y \\ S_i^z &\rightarrow S_i^z\ , \end{aligned}$$

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Hamiltonian

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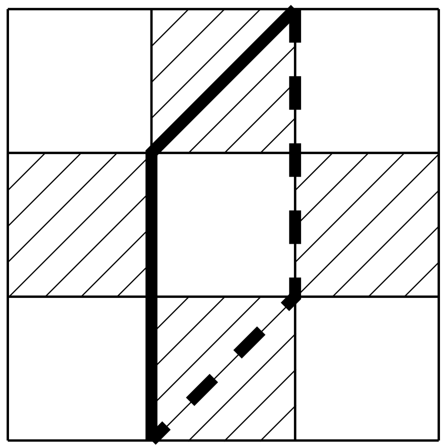
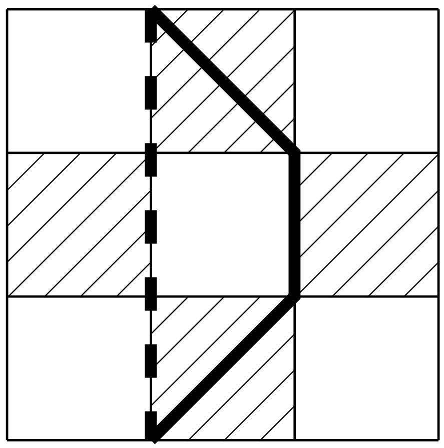
Minus-sign problem on frustrated lattices

Local moves





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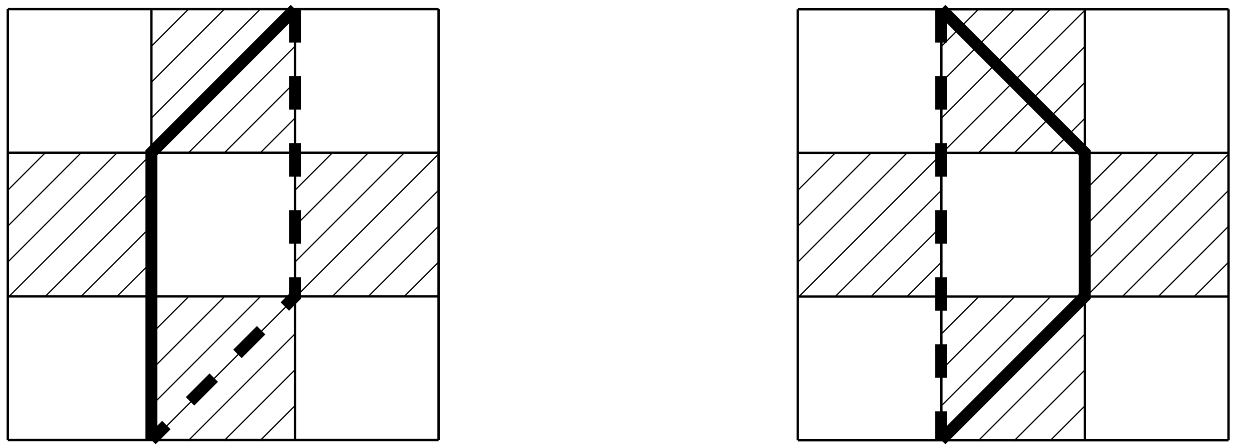


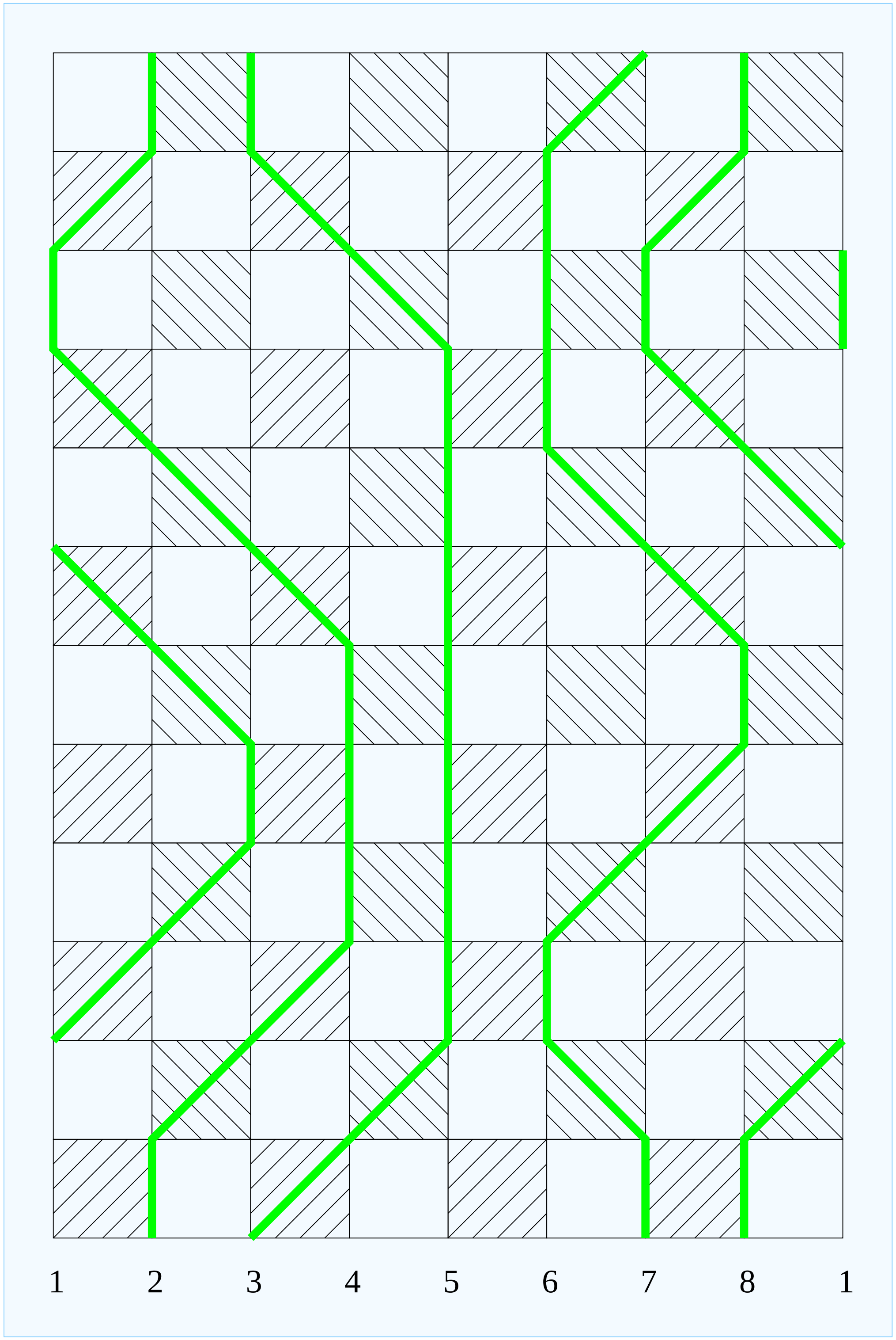
Update

$$R = \frac{W_{\text{new}}}{W_{\text{old}}} = [\tanh \Delta\tau J/2]^{su} \left[\cosh \Delta\tau J/2 \mathrm{e}^{\Delta\tau J\Delta/2}\right]^{sv}$$

with

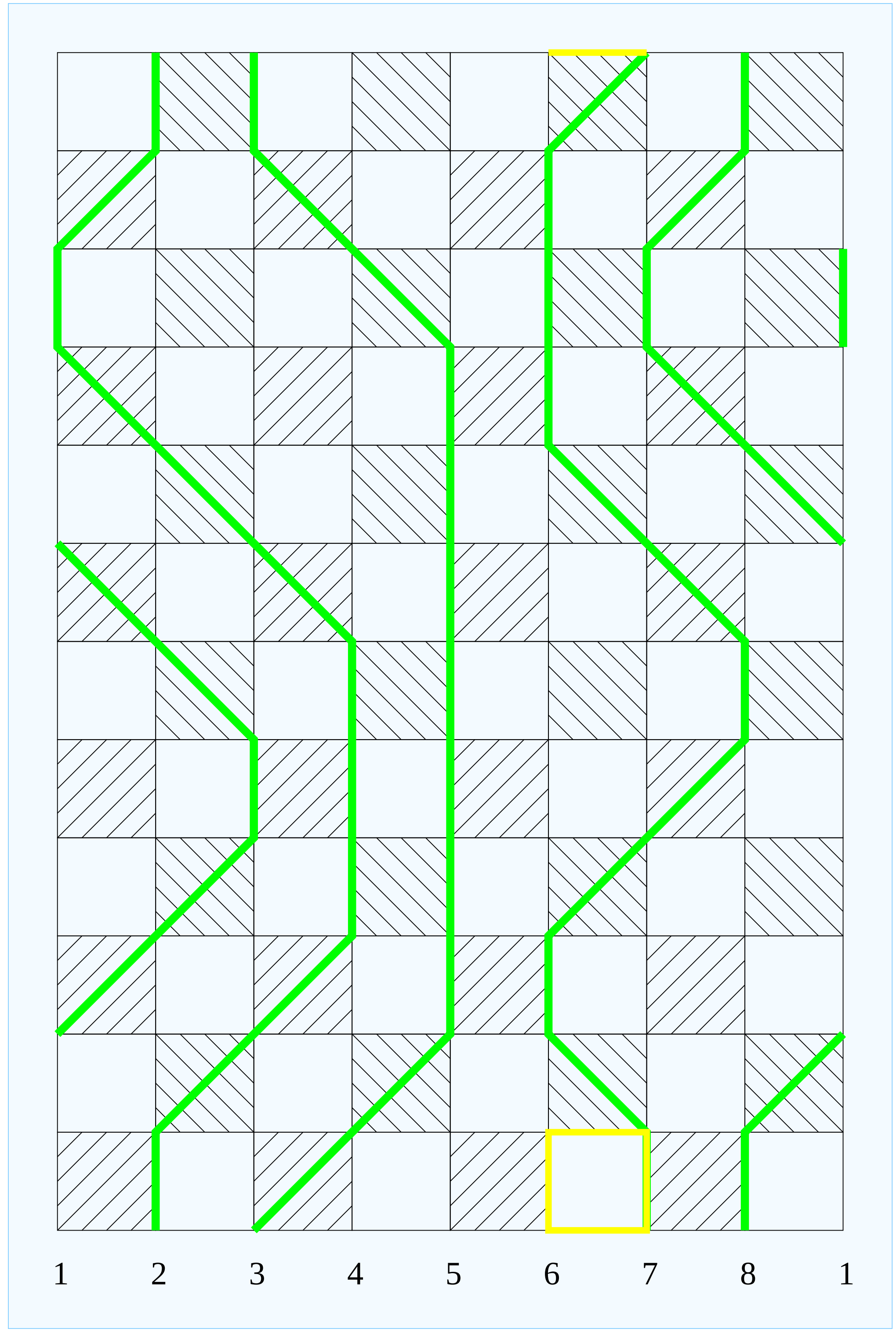
$$\begin{aligned} s &\equiv n(i,j) + n(i,j+1) - n(i+1,j) - n(i+1,j+1)\ , \\ u &= 1 - n(i+1,j-1) - n(i+1,j+2), \\ v &= n(i-1,j) - n(i+2,j)\ . \end{aligned}$$

Simulation



Simulation

active plaquette



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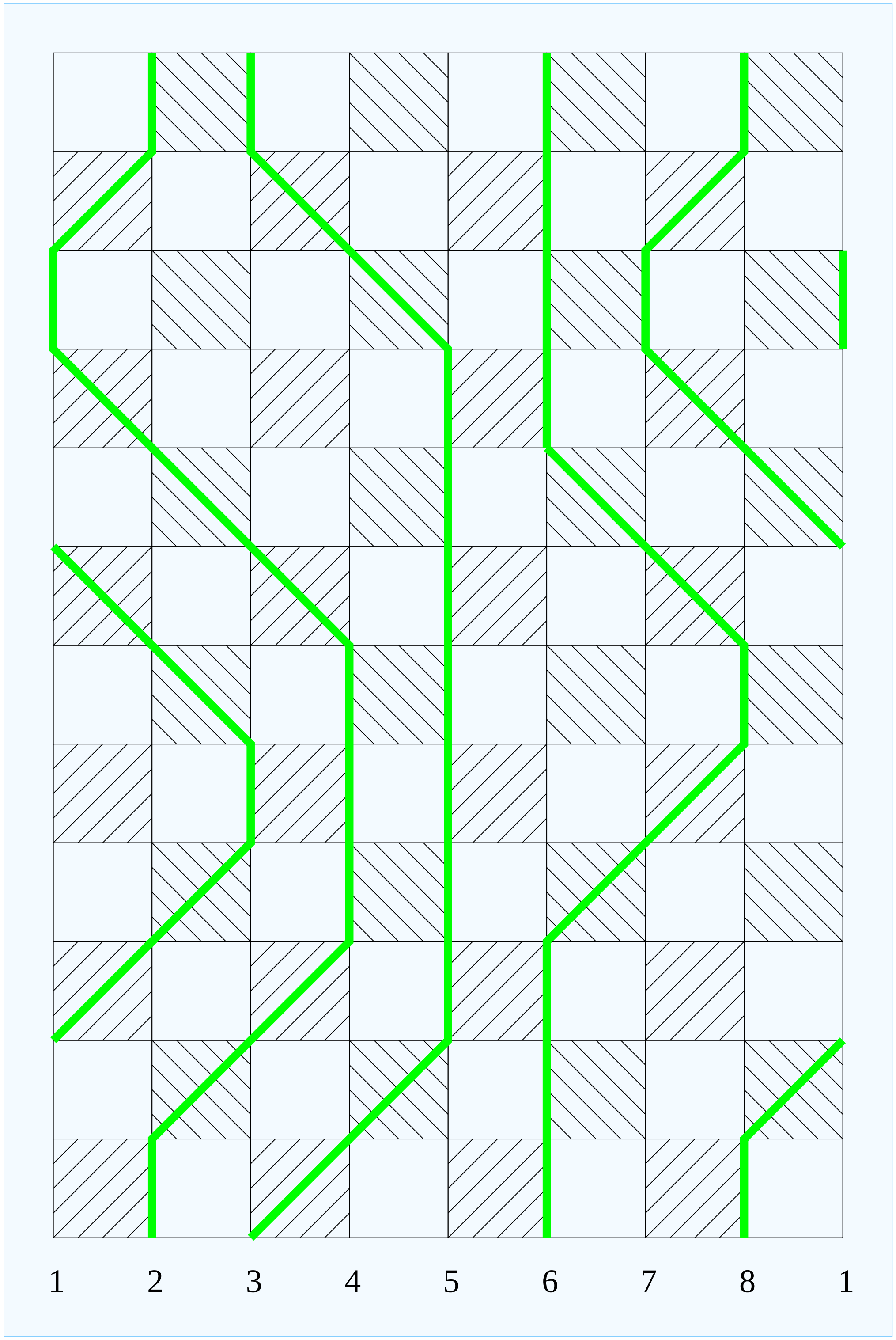

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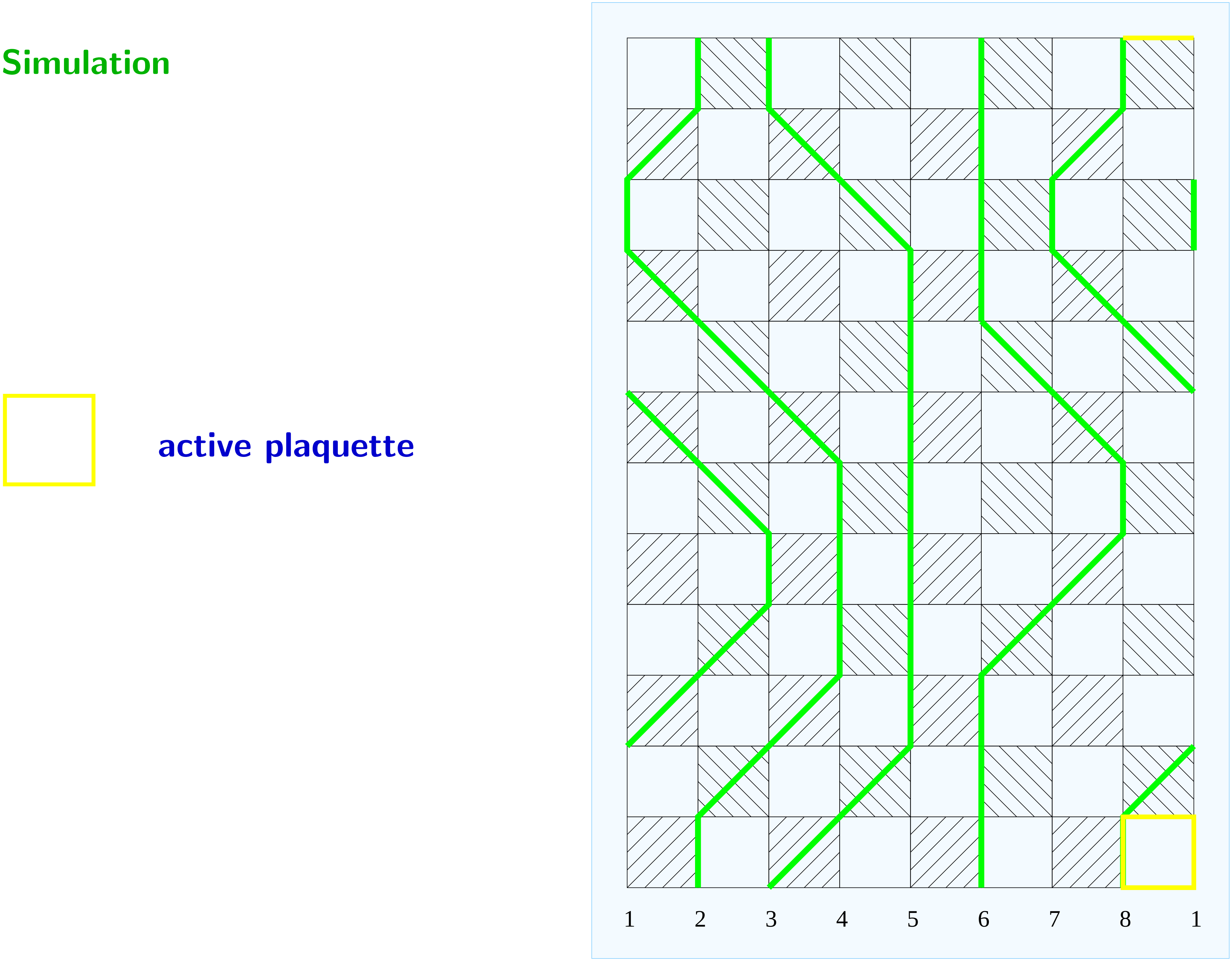

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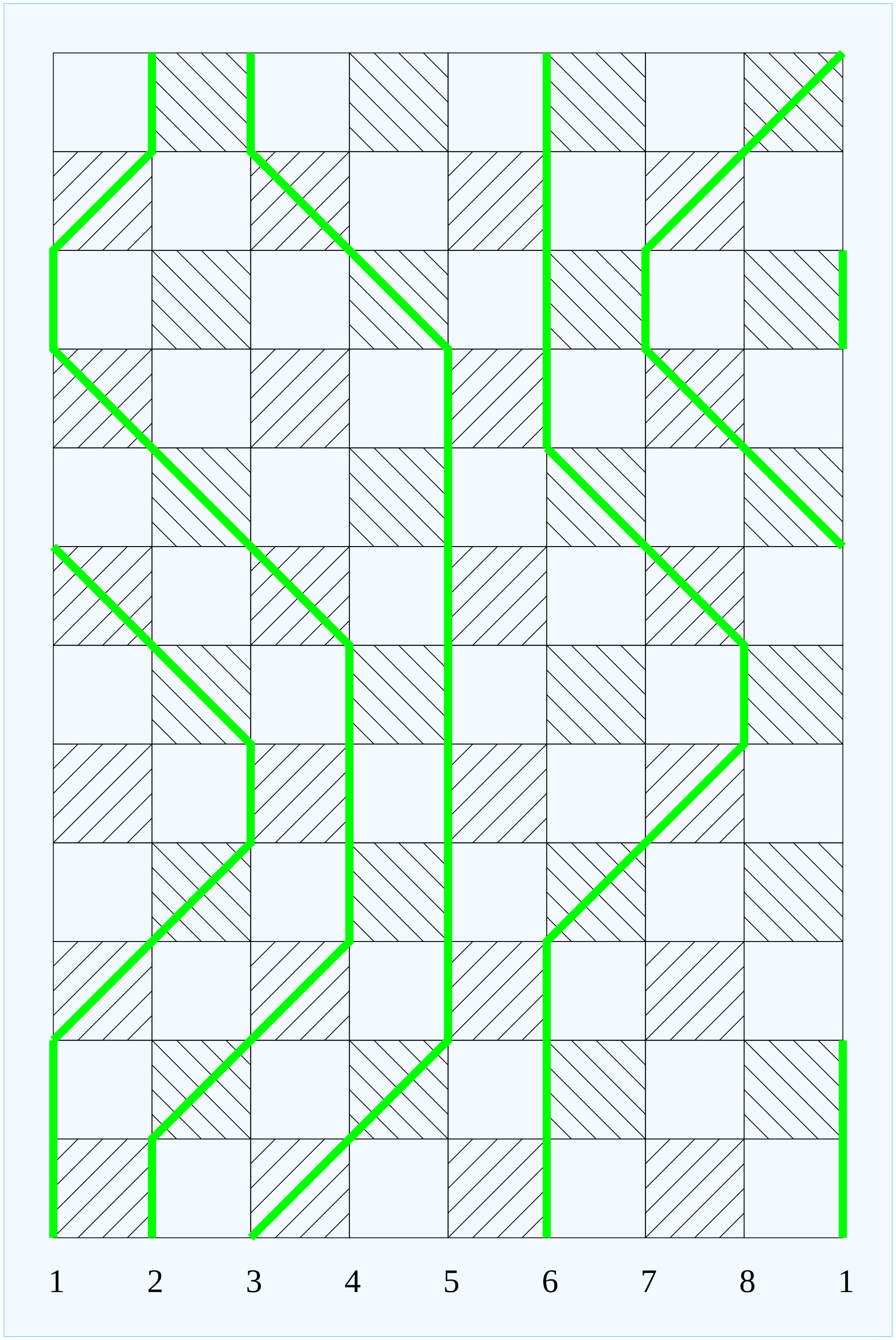

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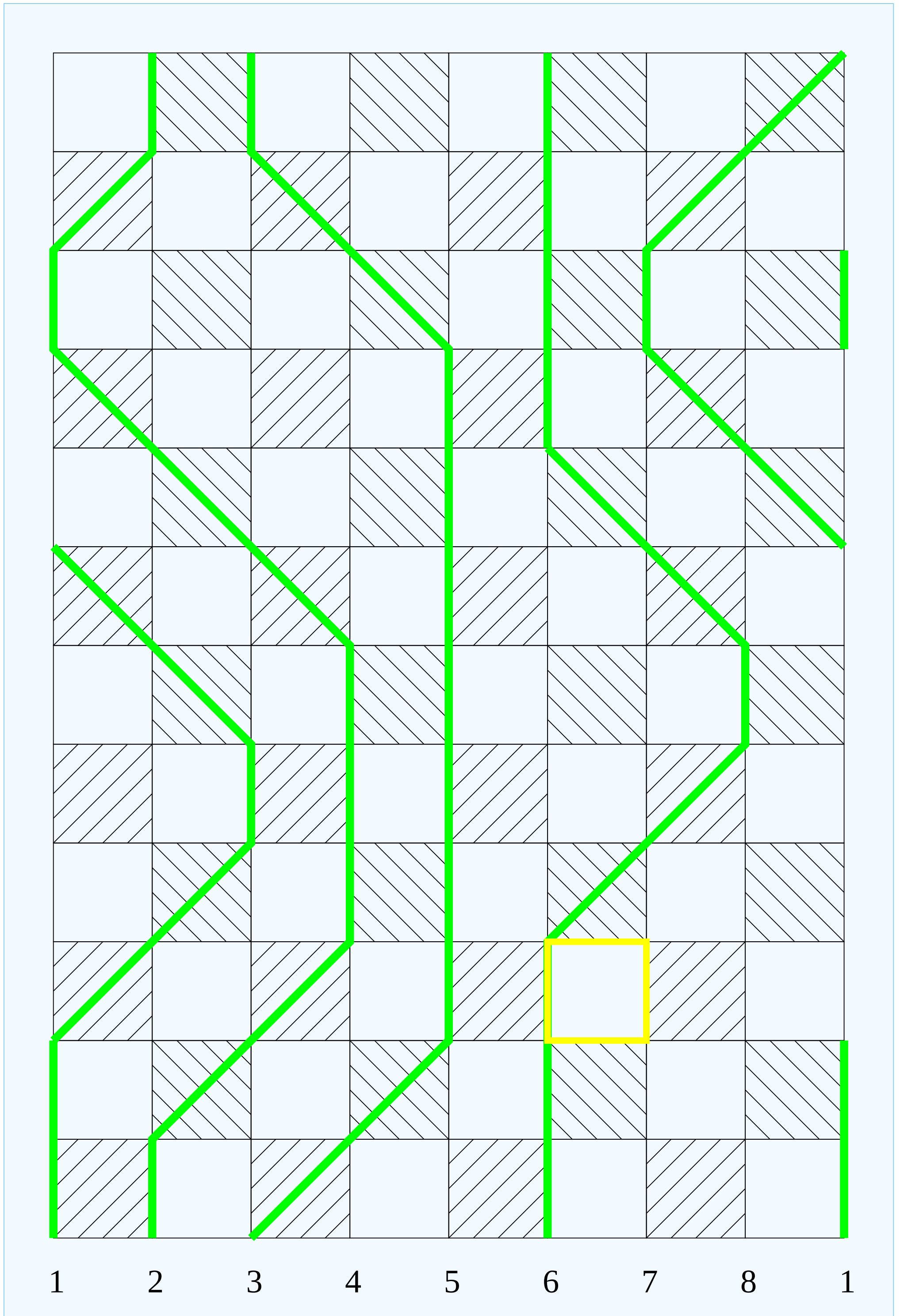

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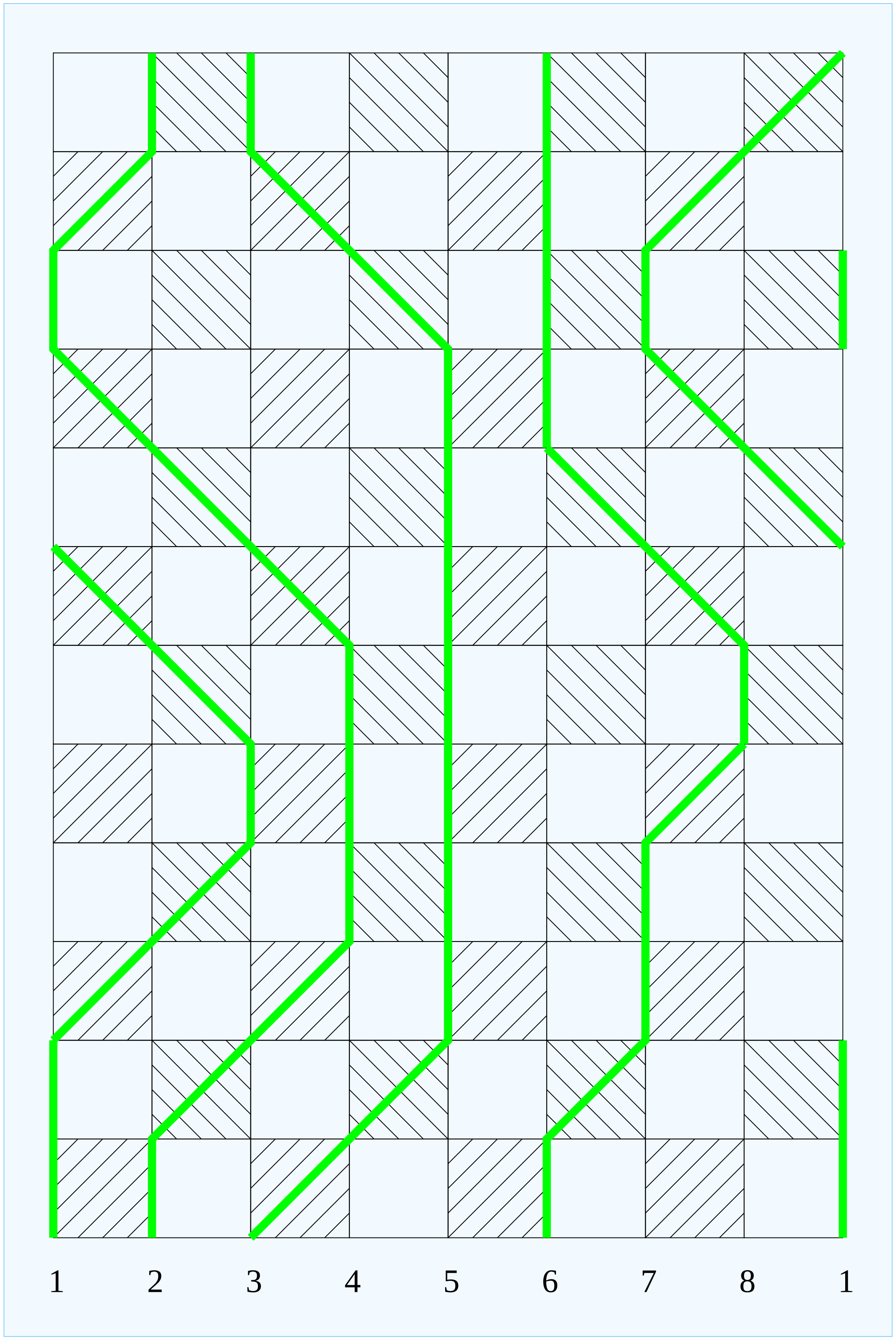

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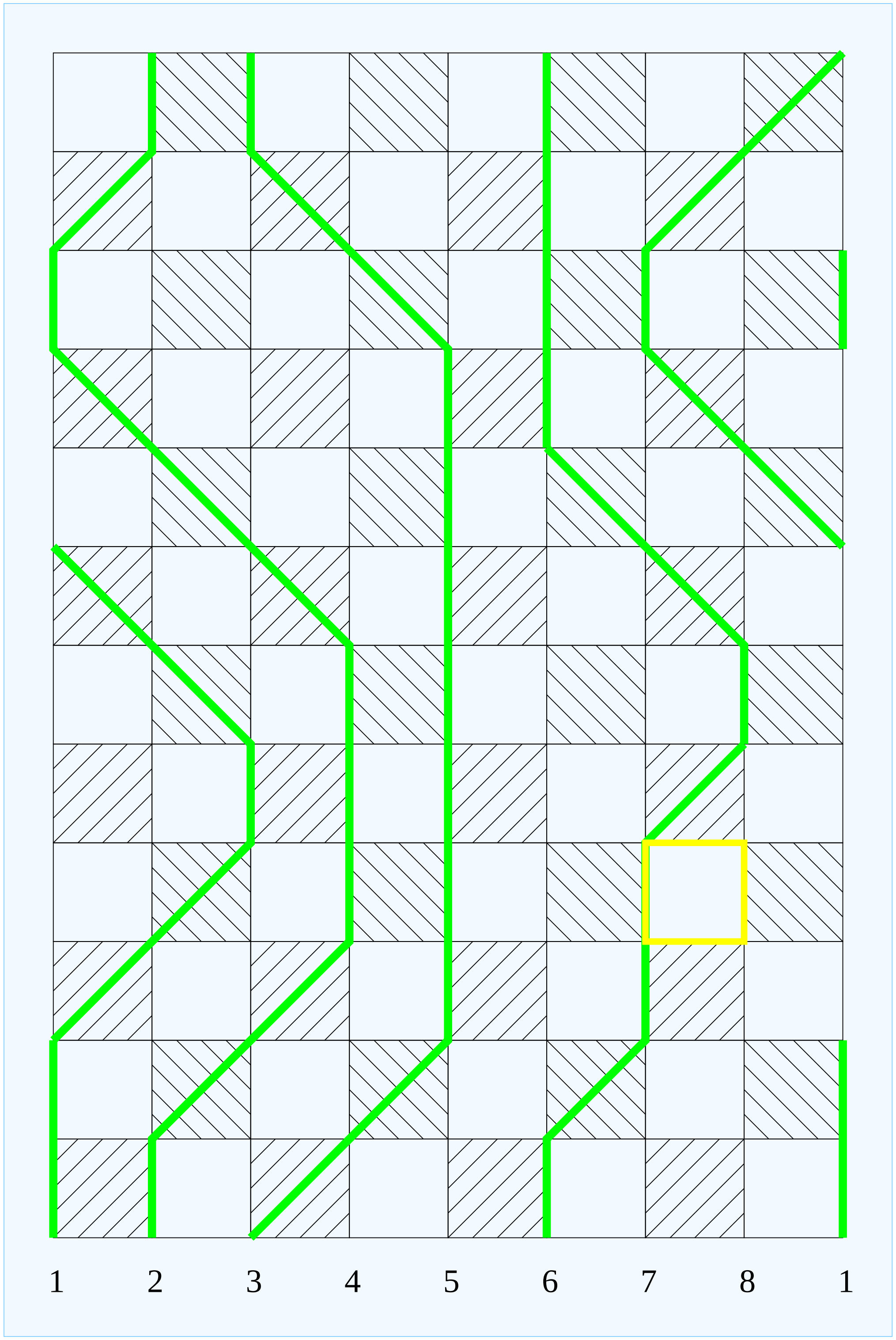

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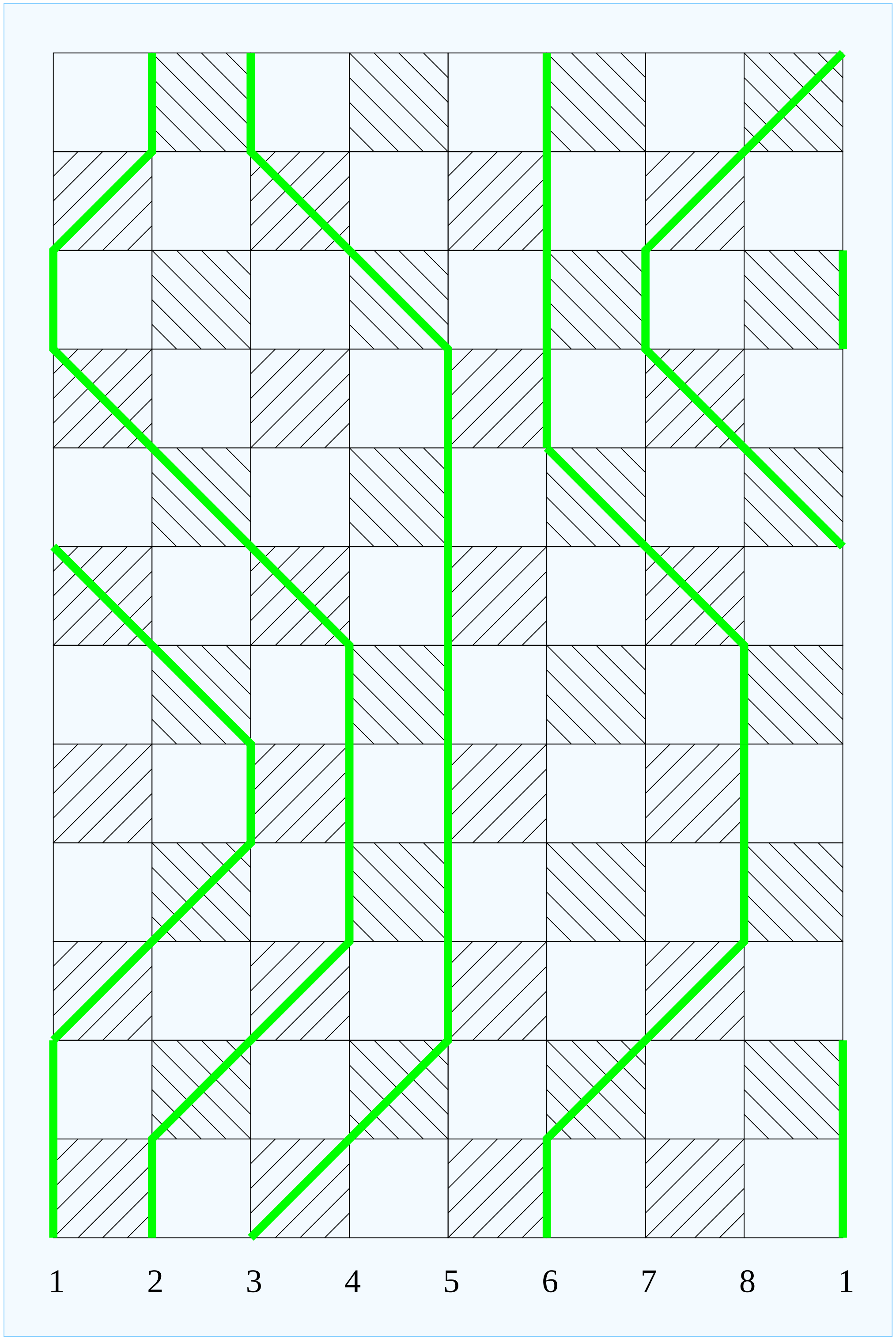

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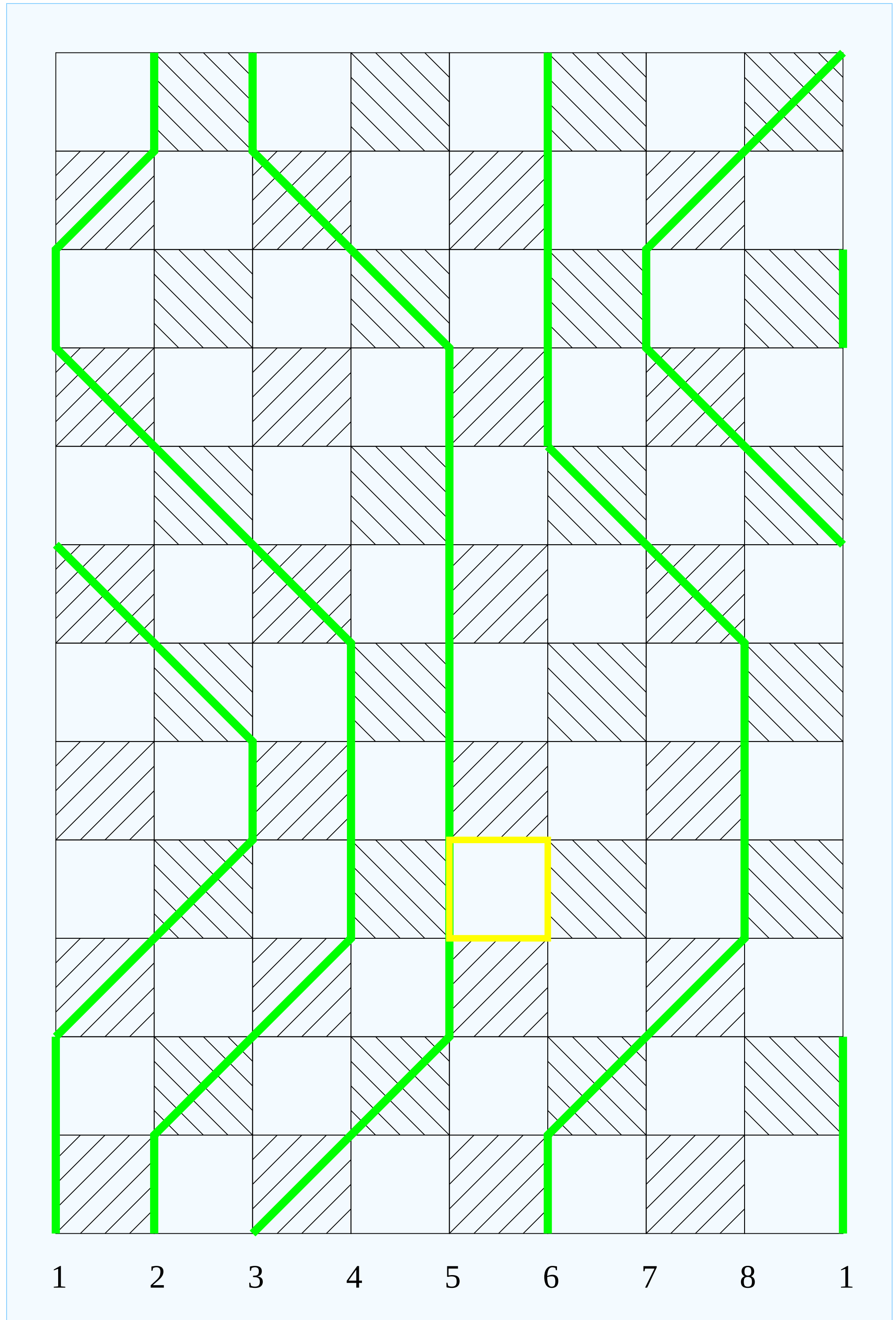

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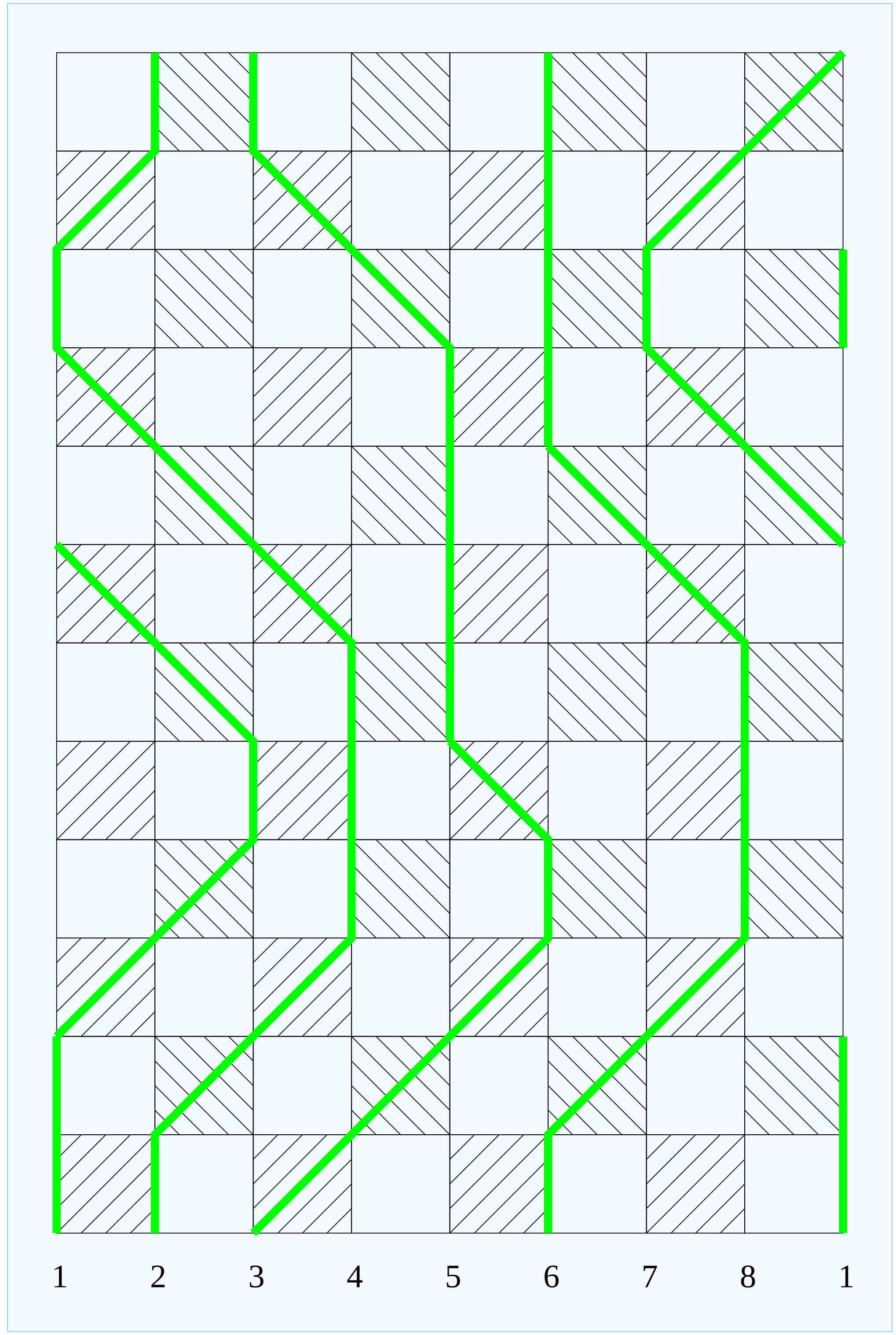

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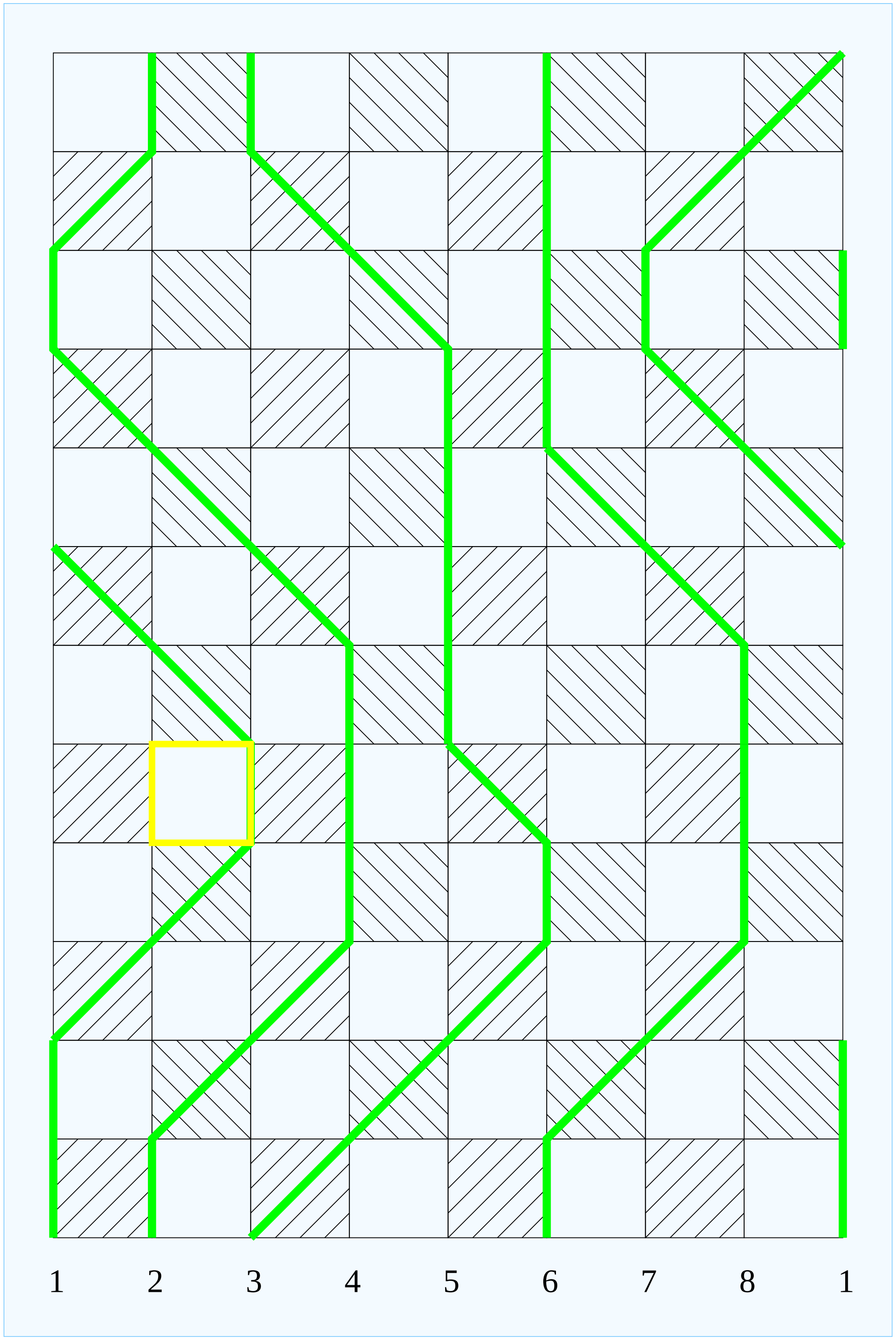

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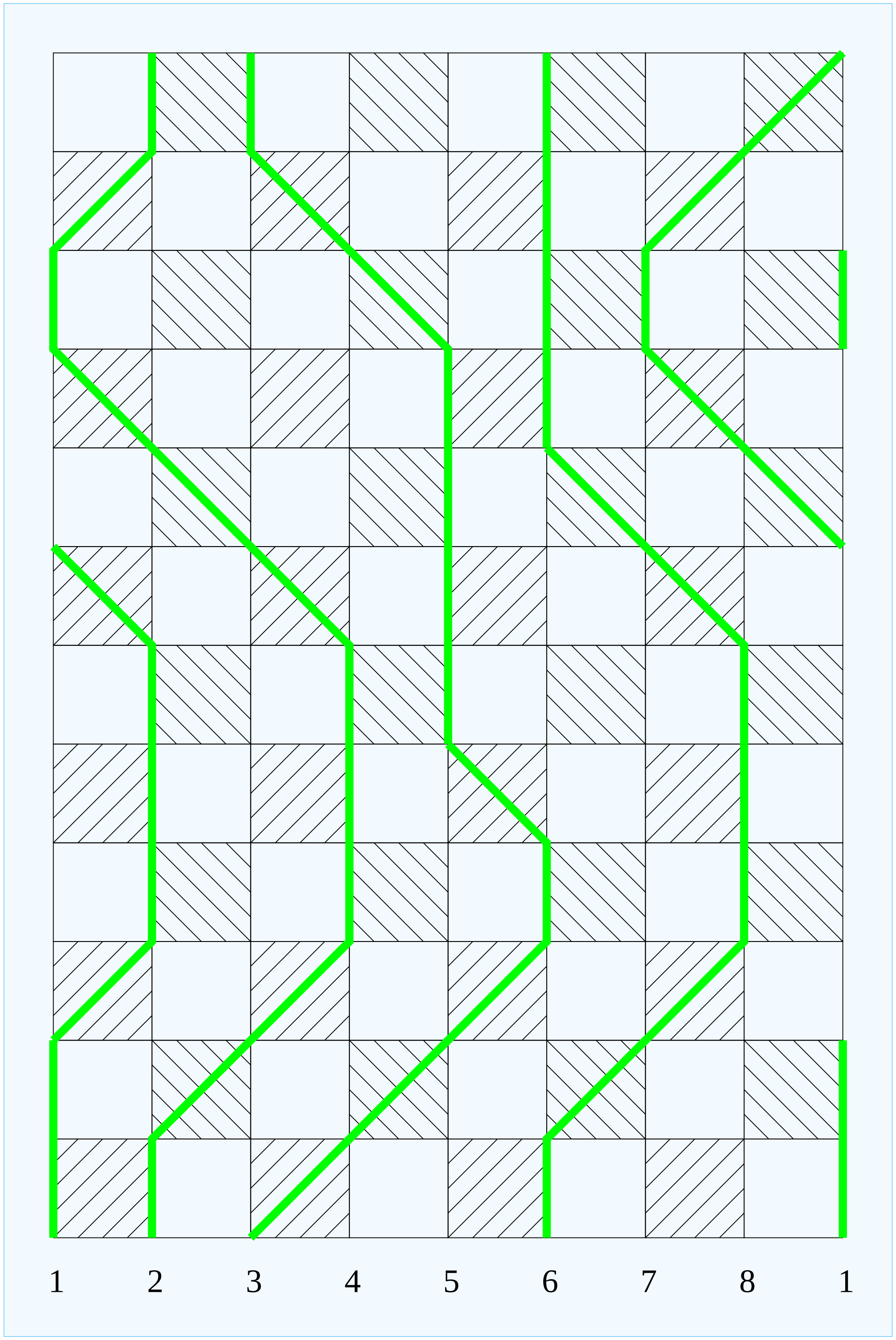

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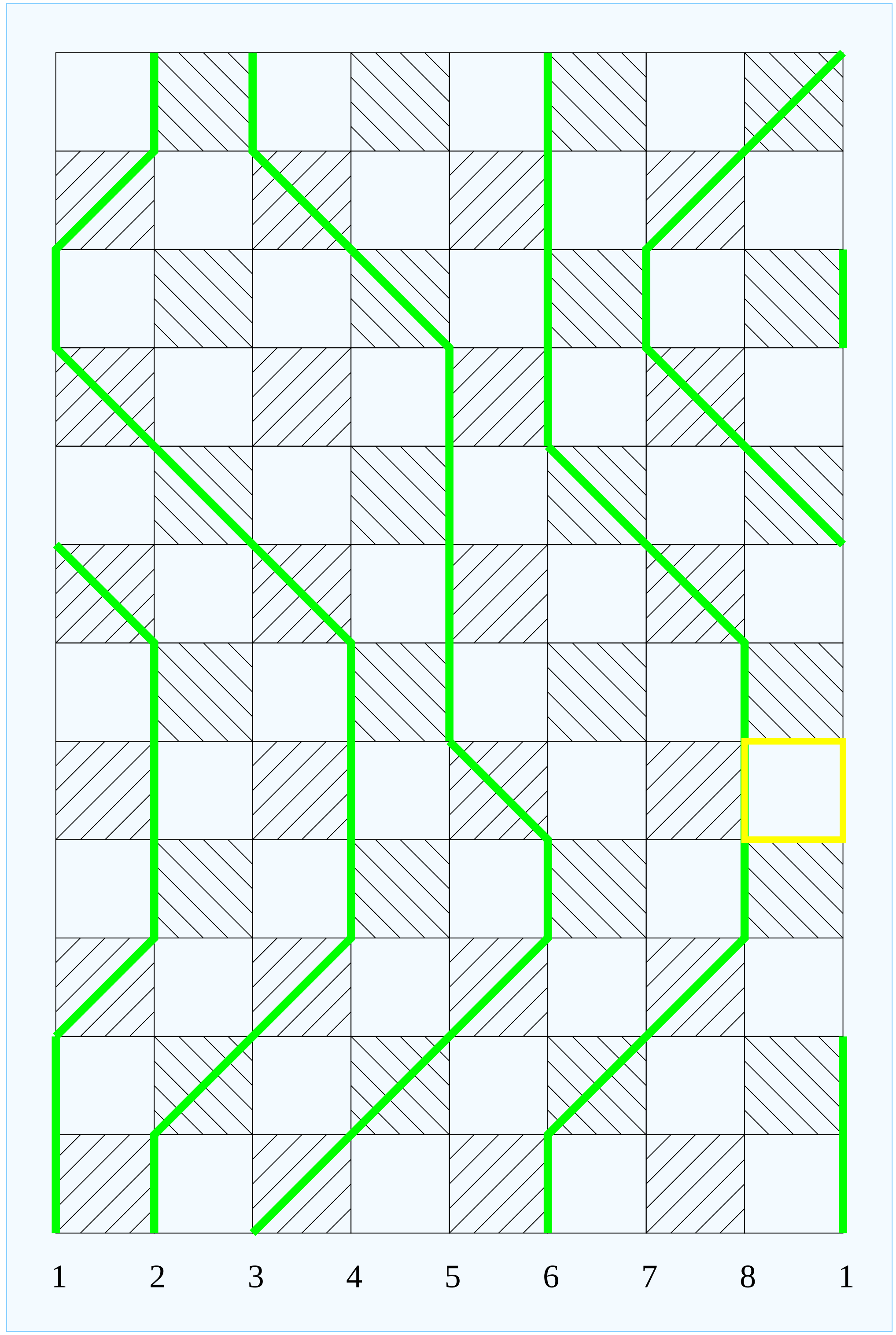

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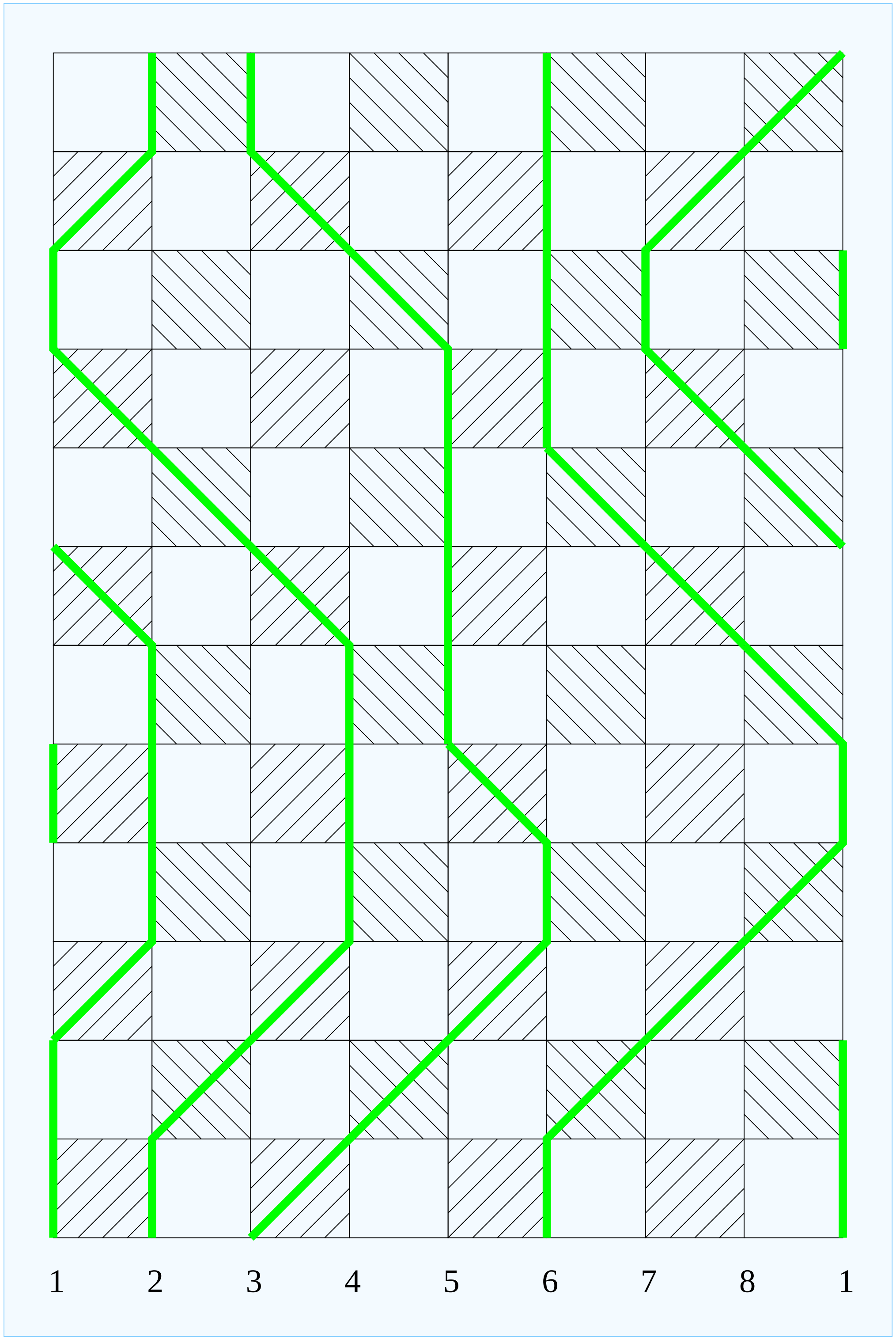

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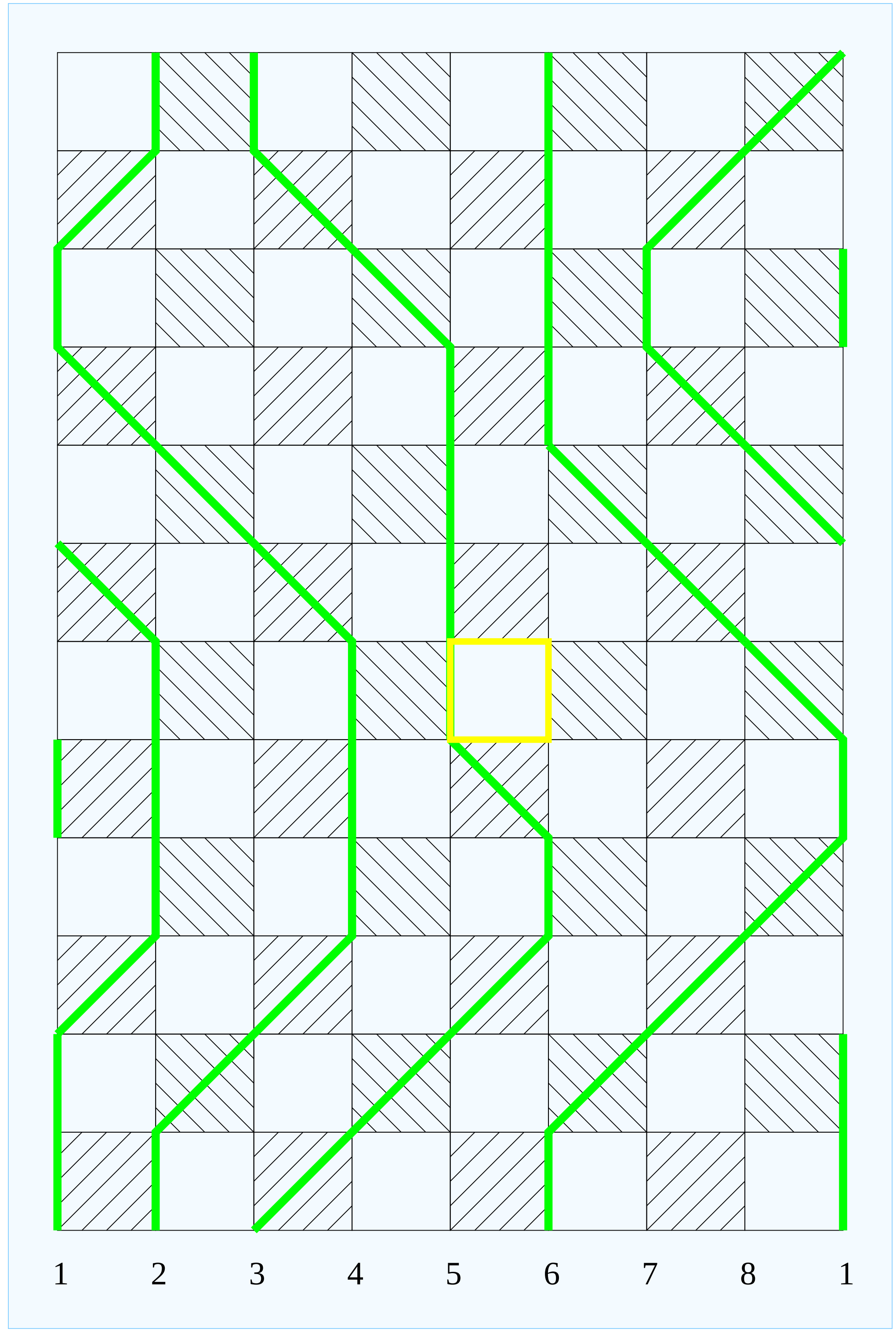

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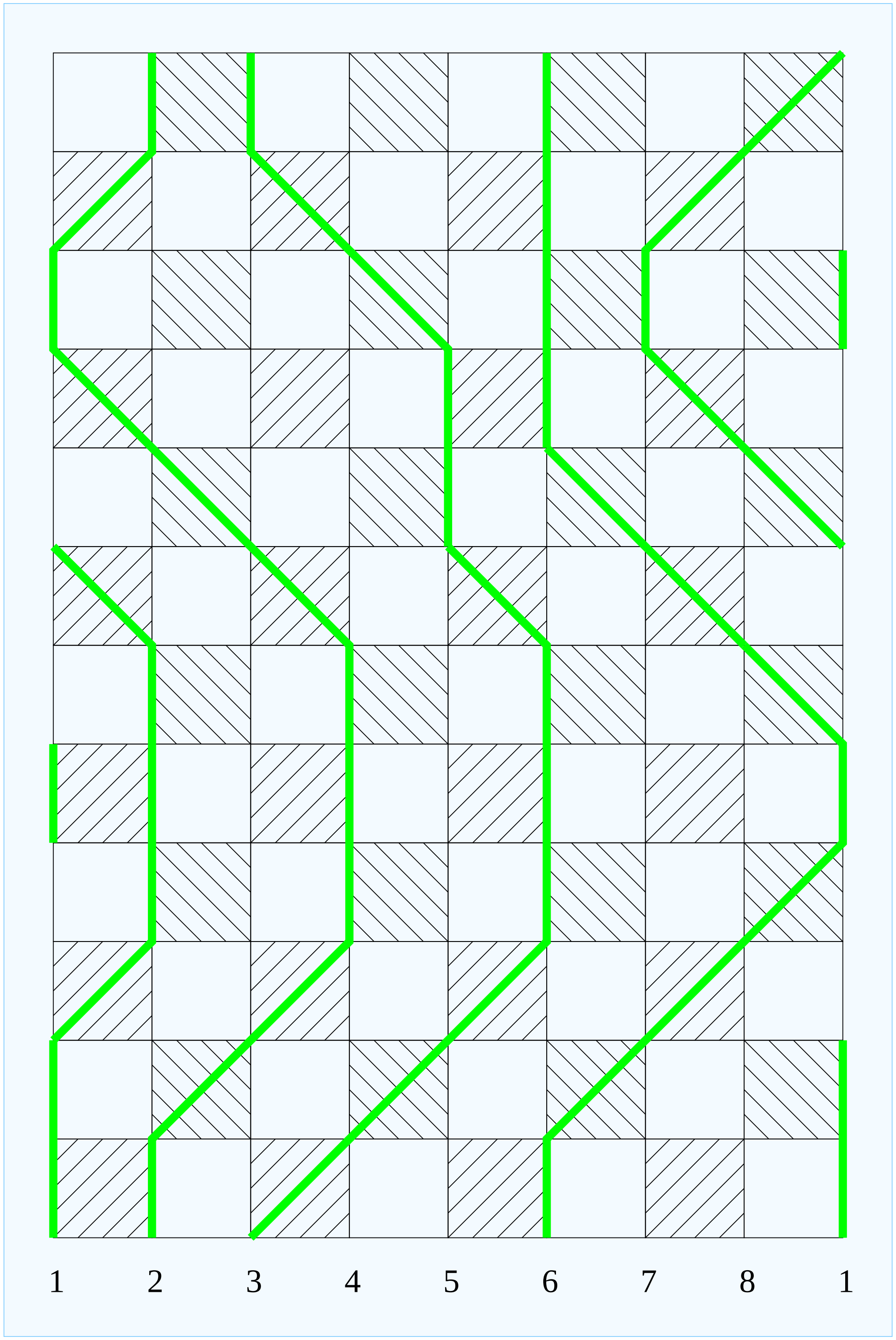

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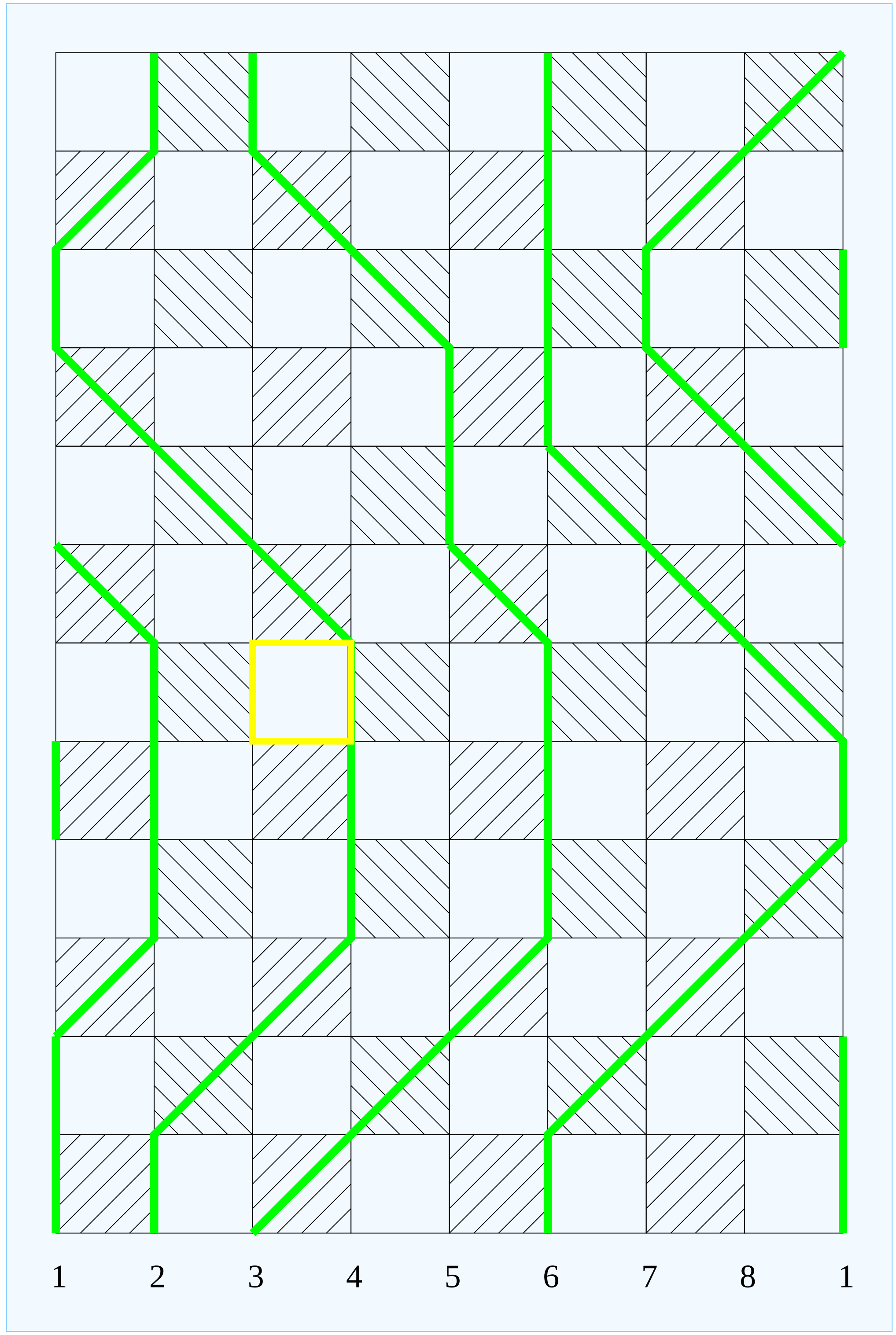

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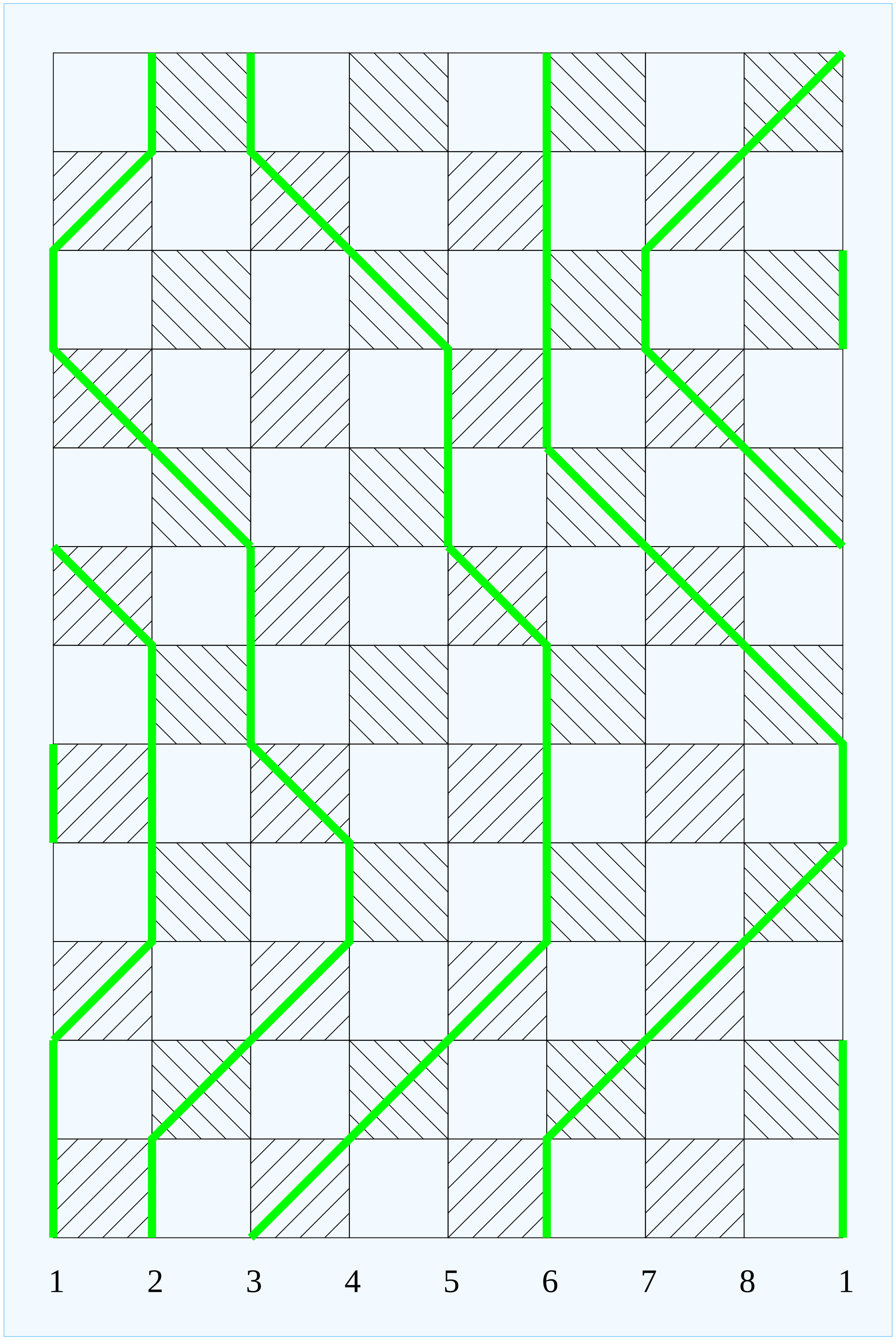

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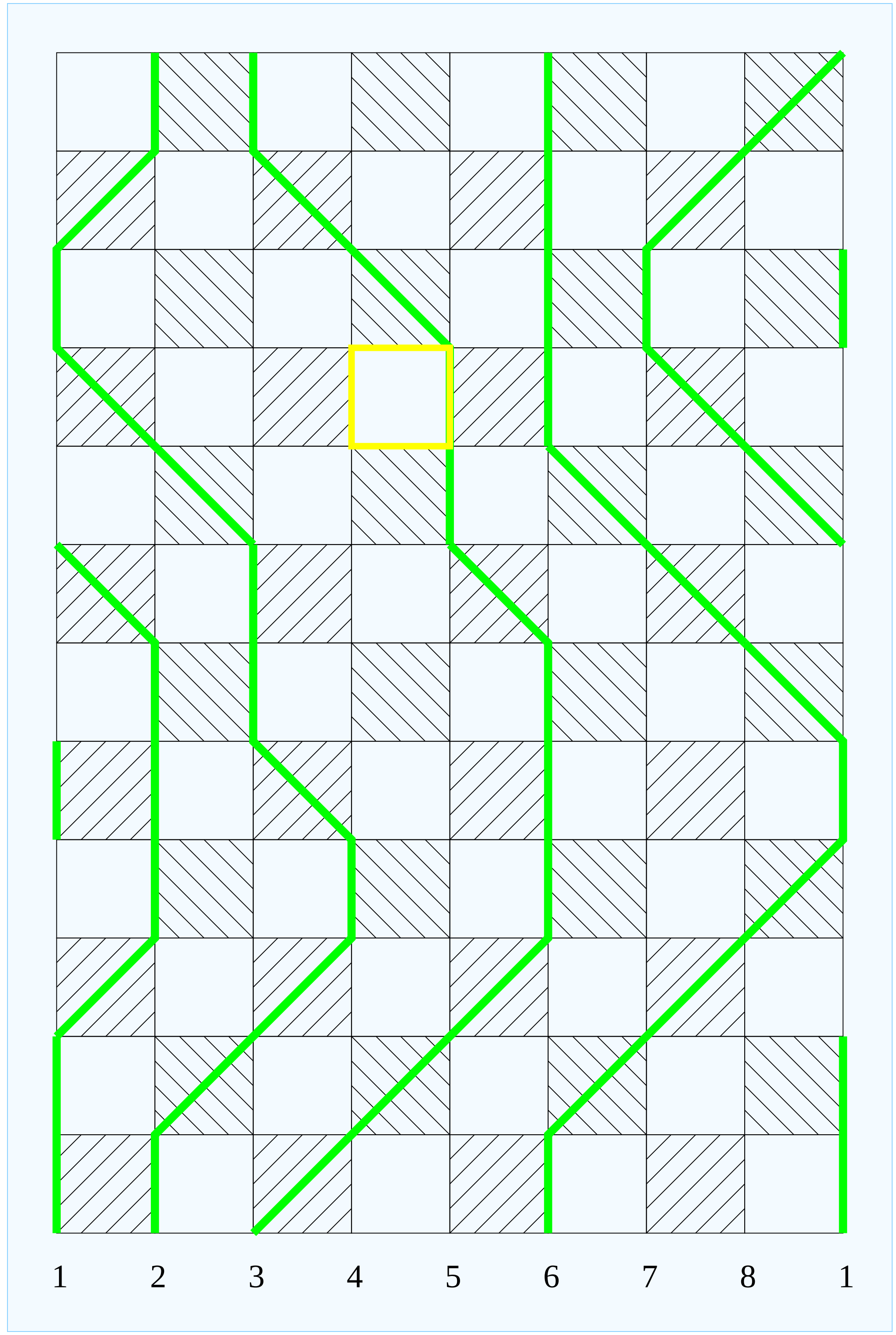

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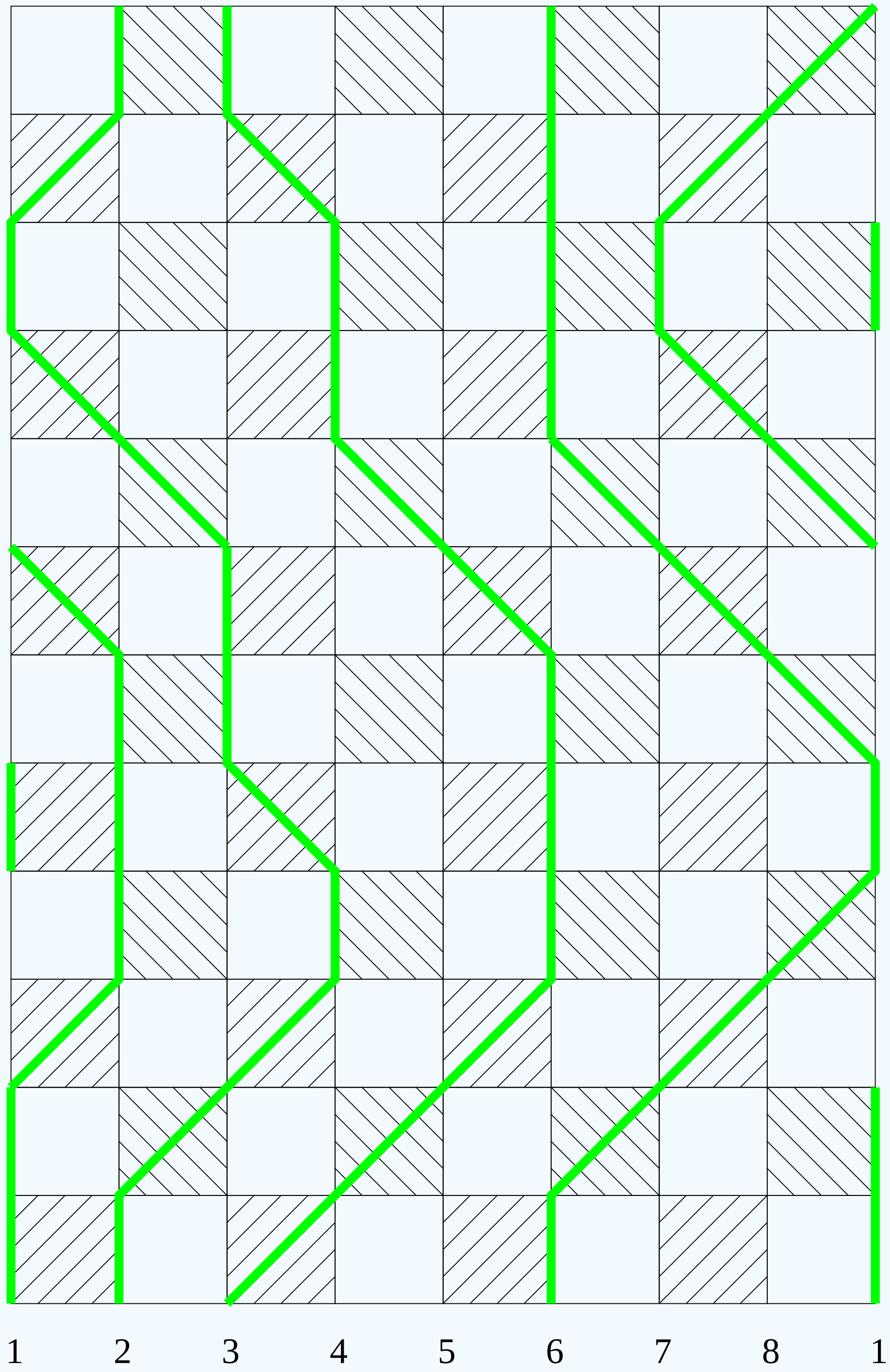

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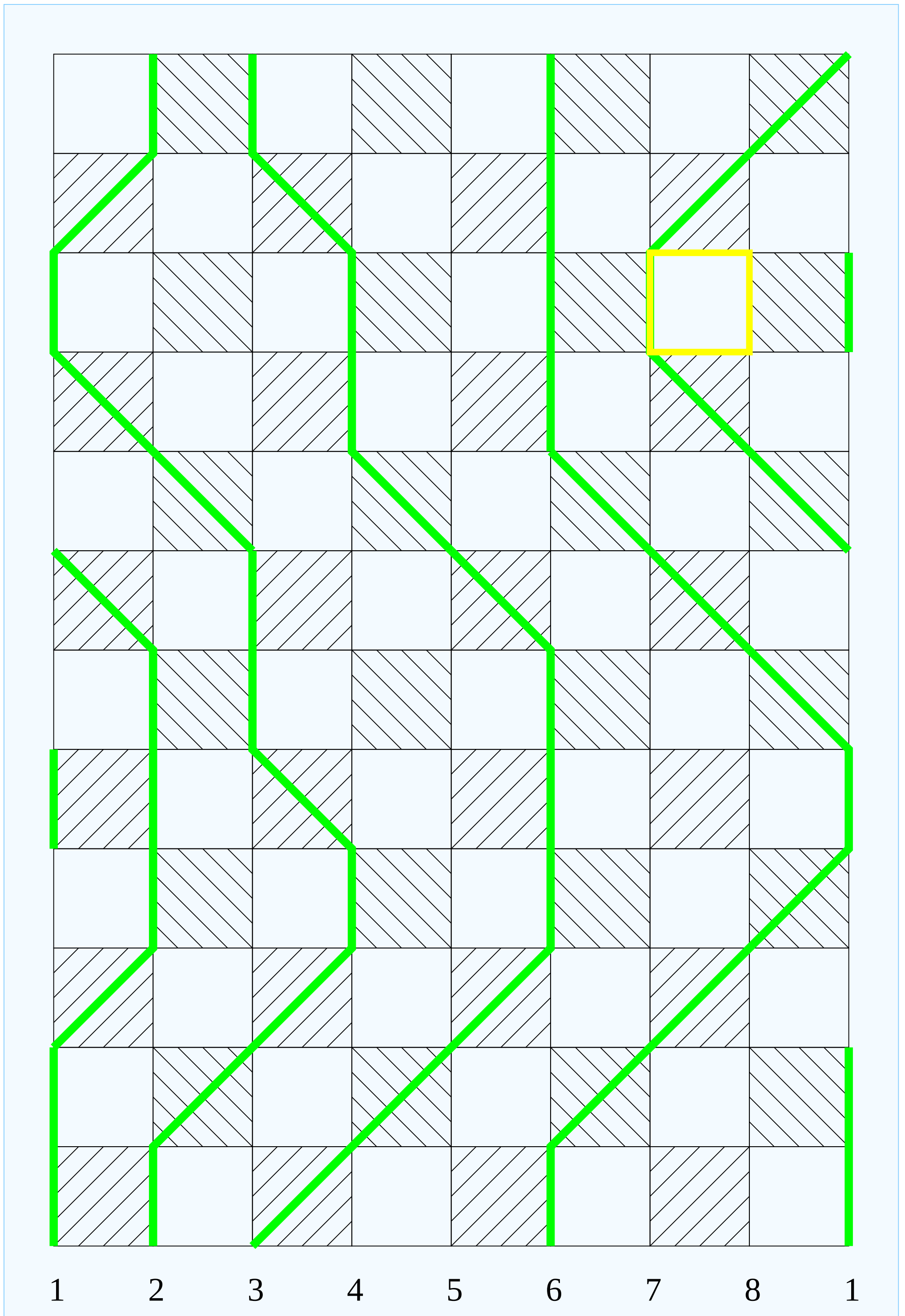

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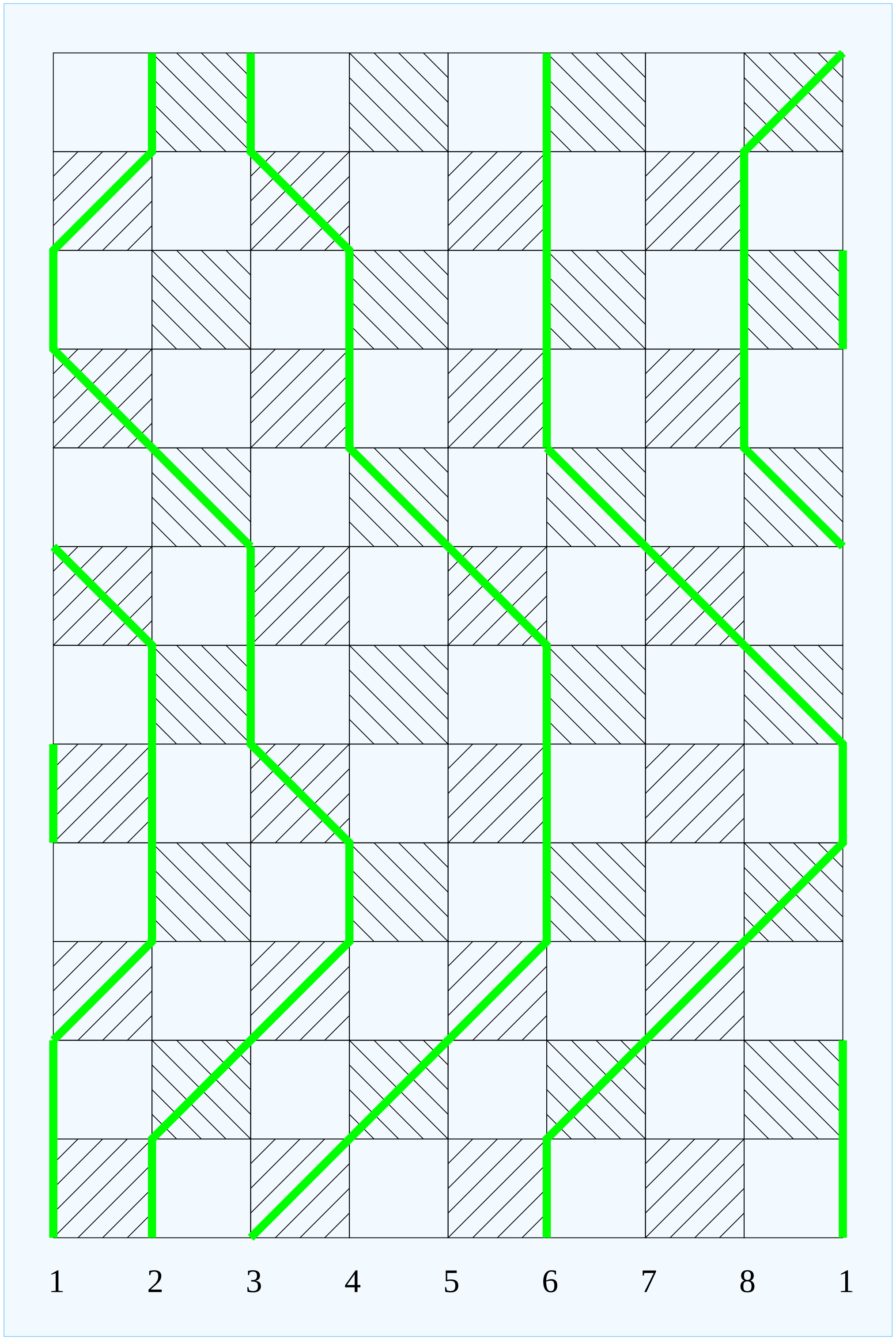

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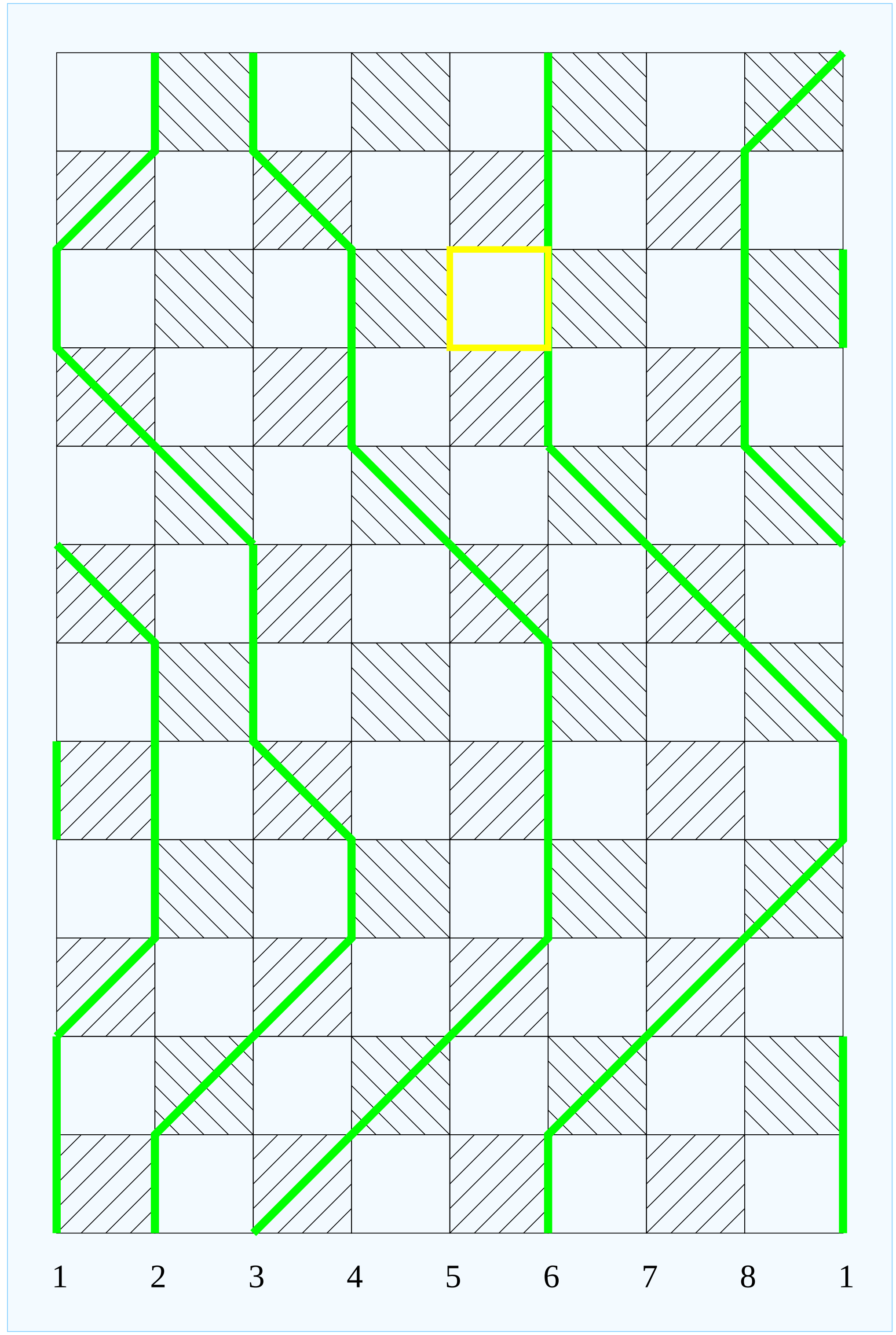

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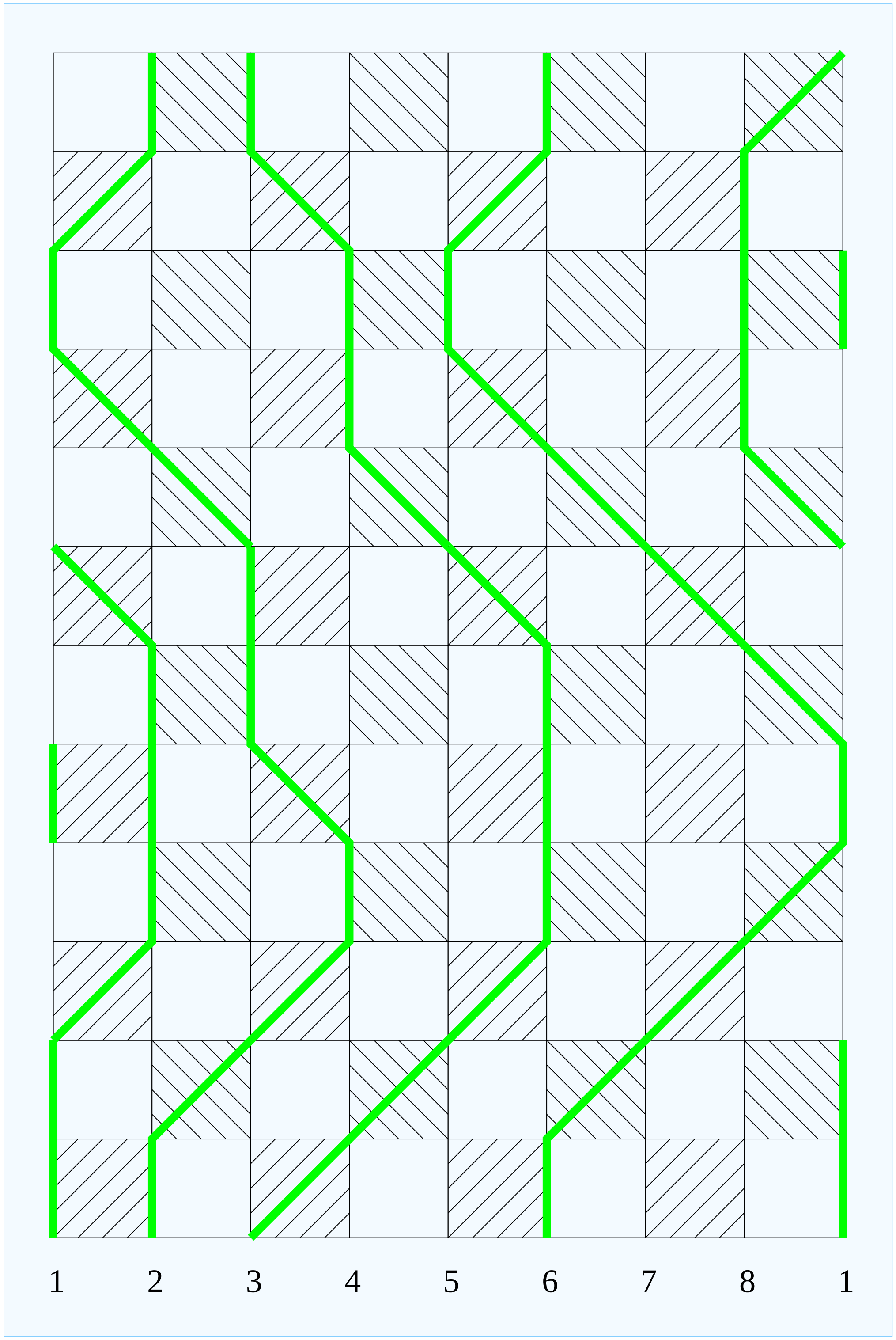

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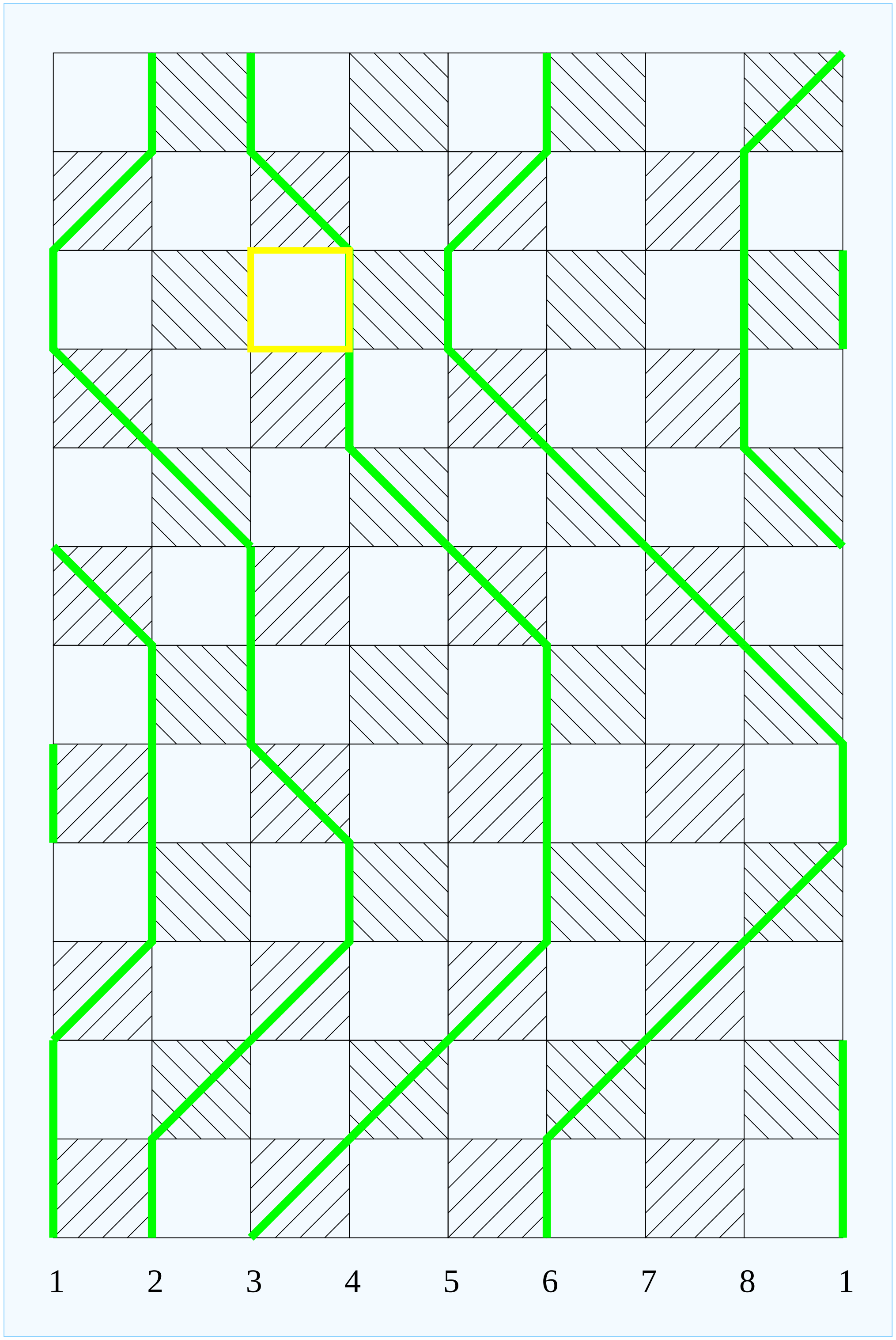

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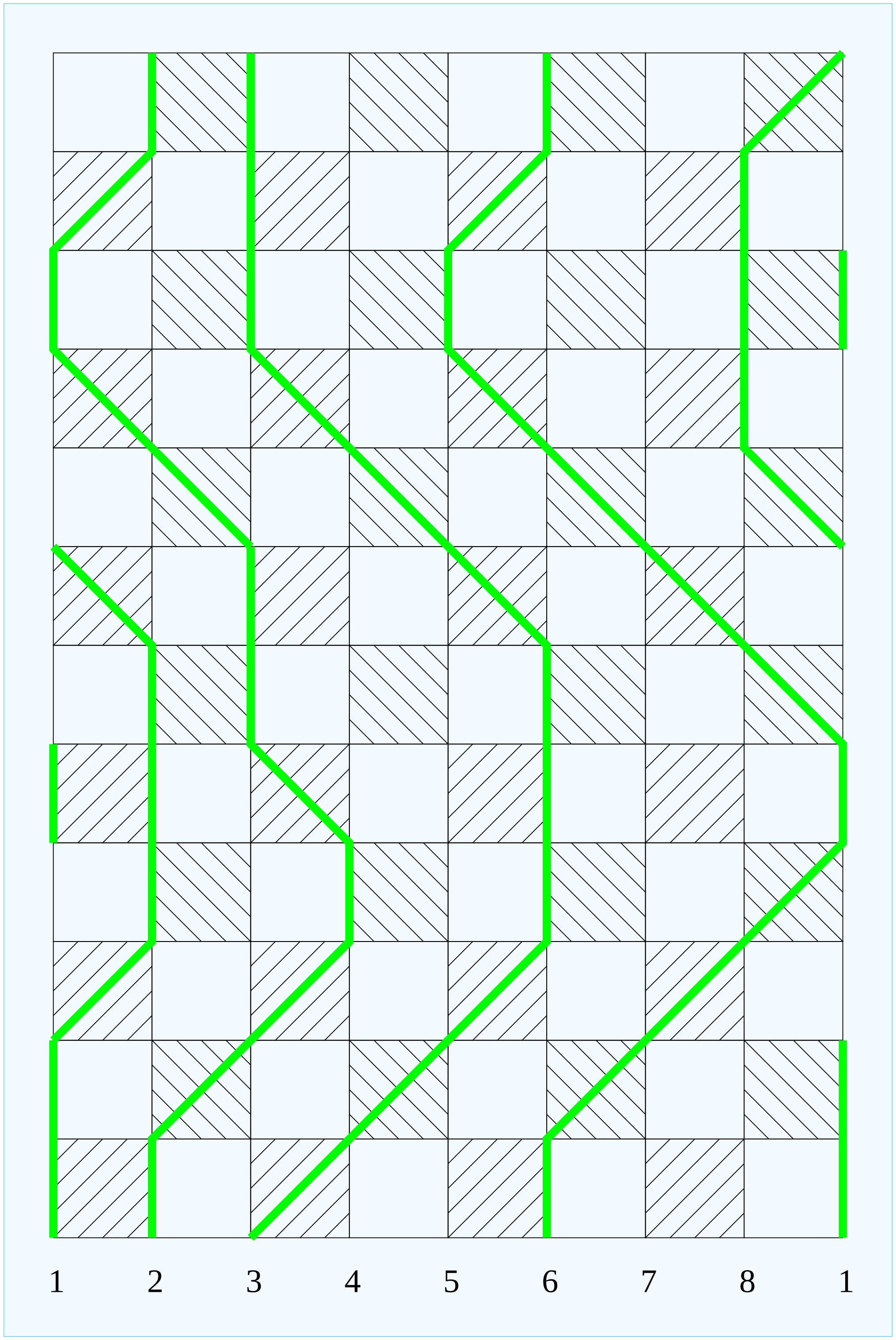

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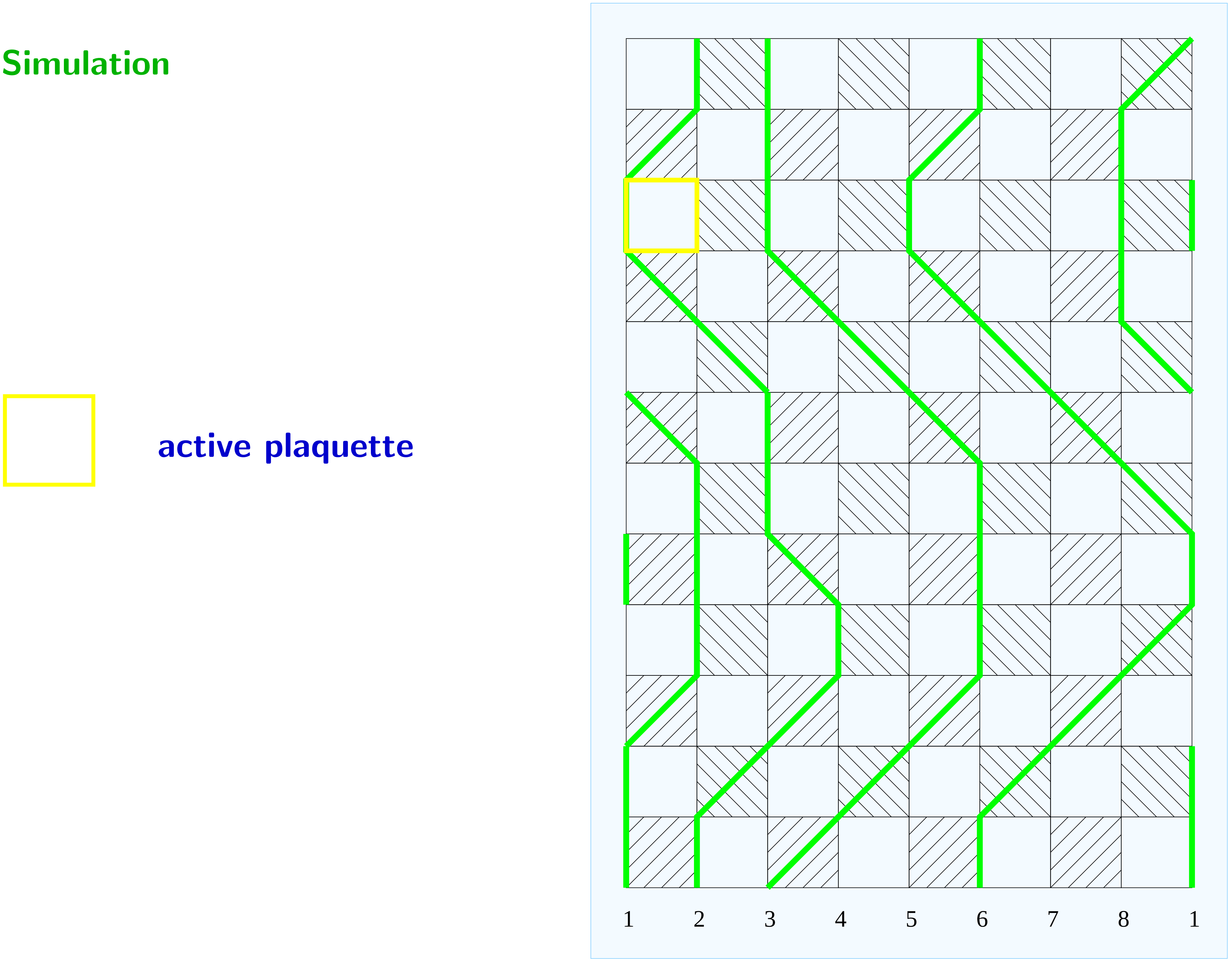

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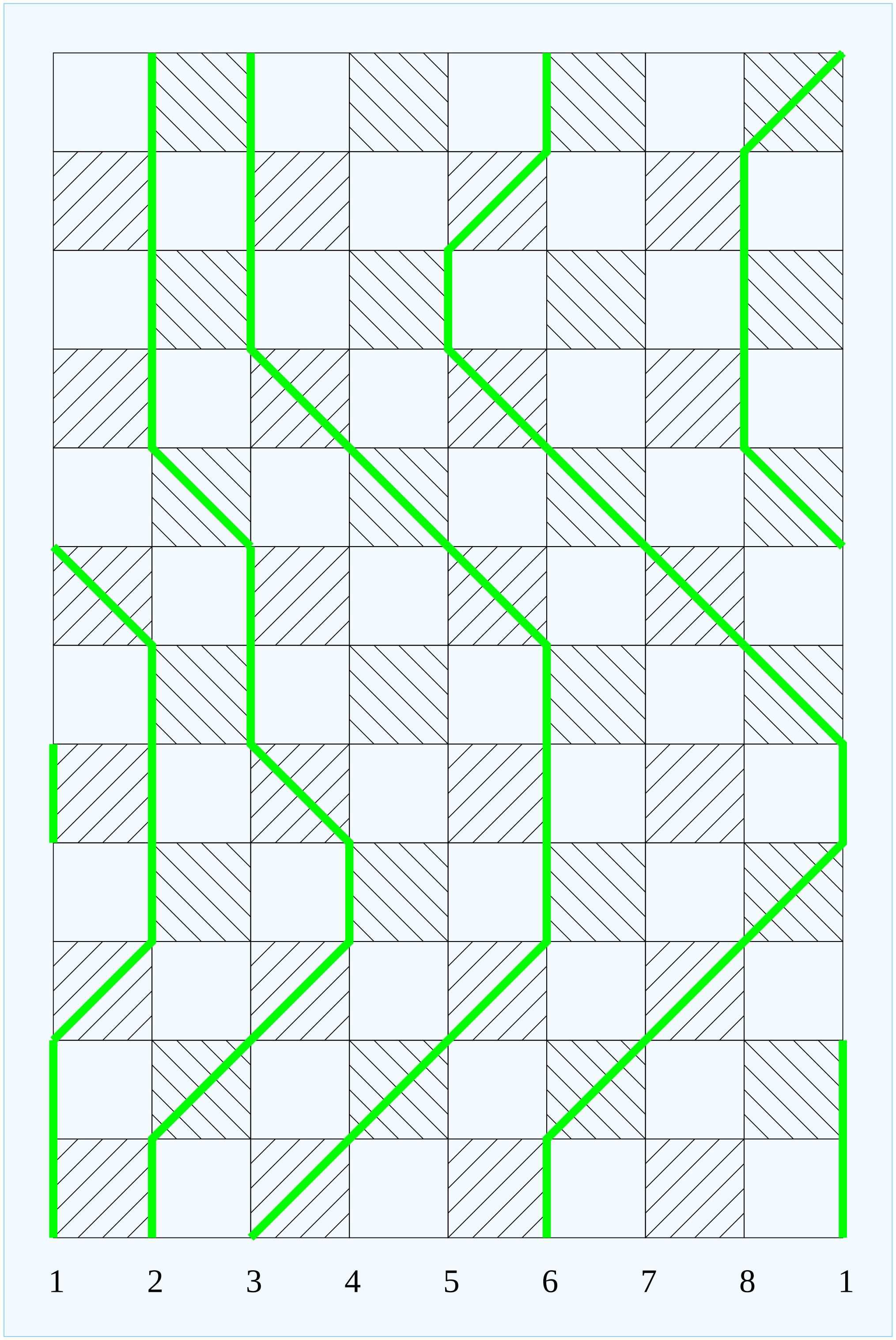

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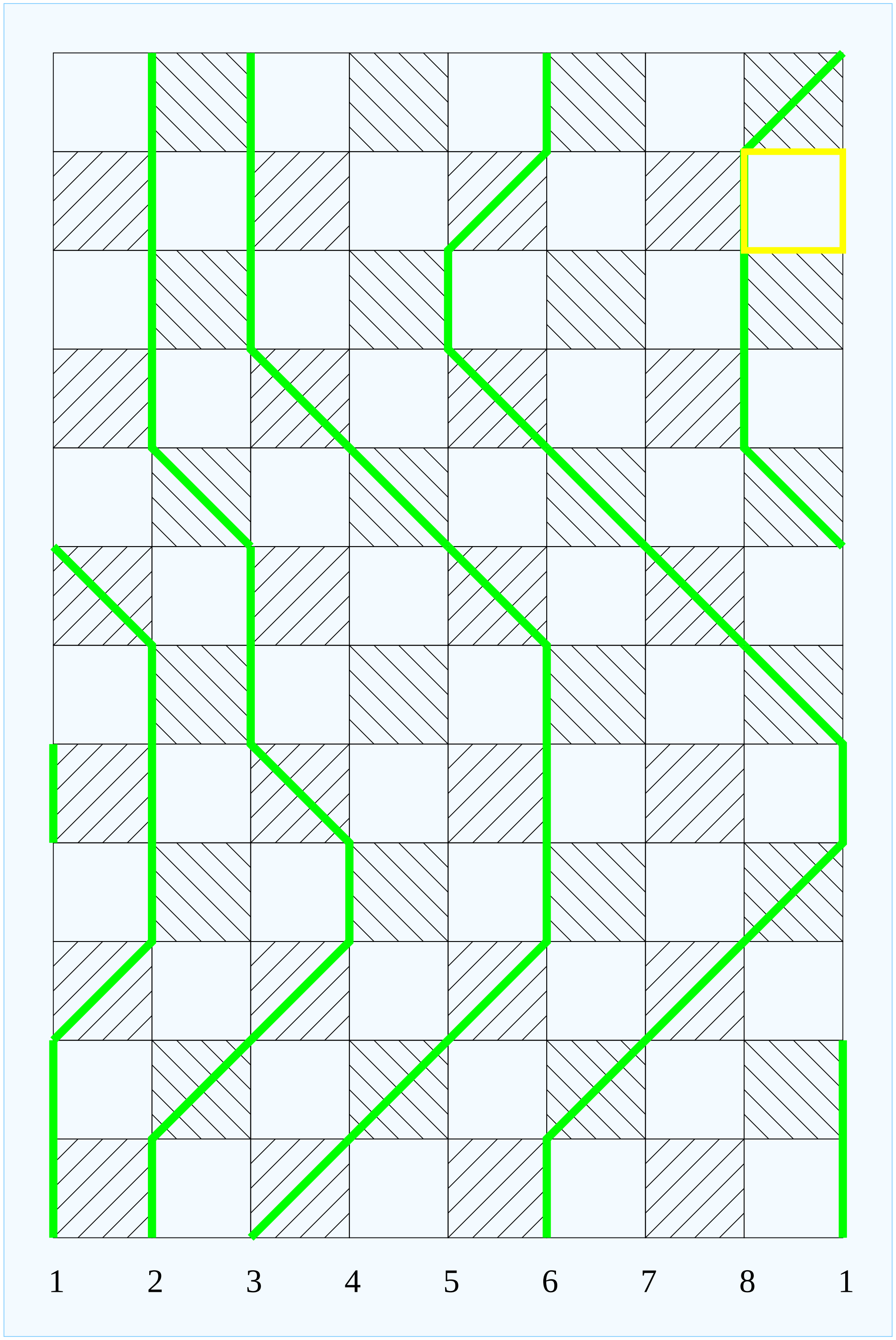

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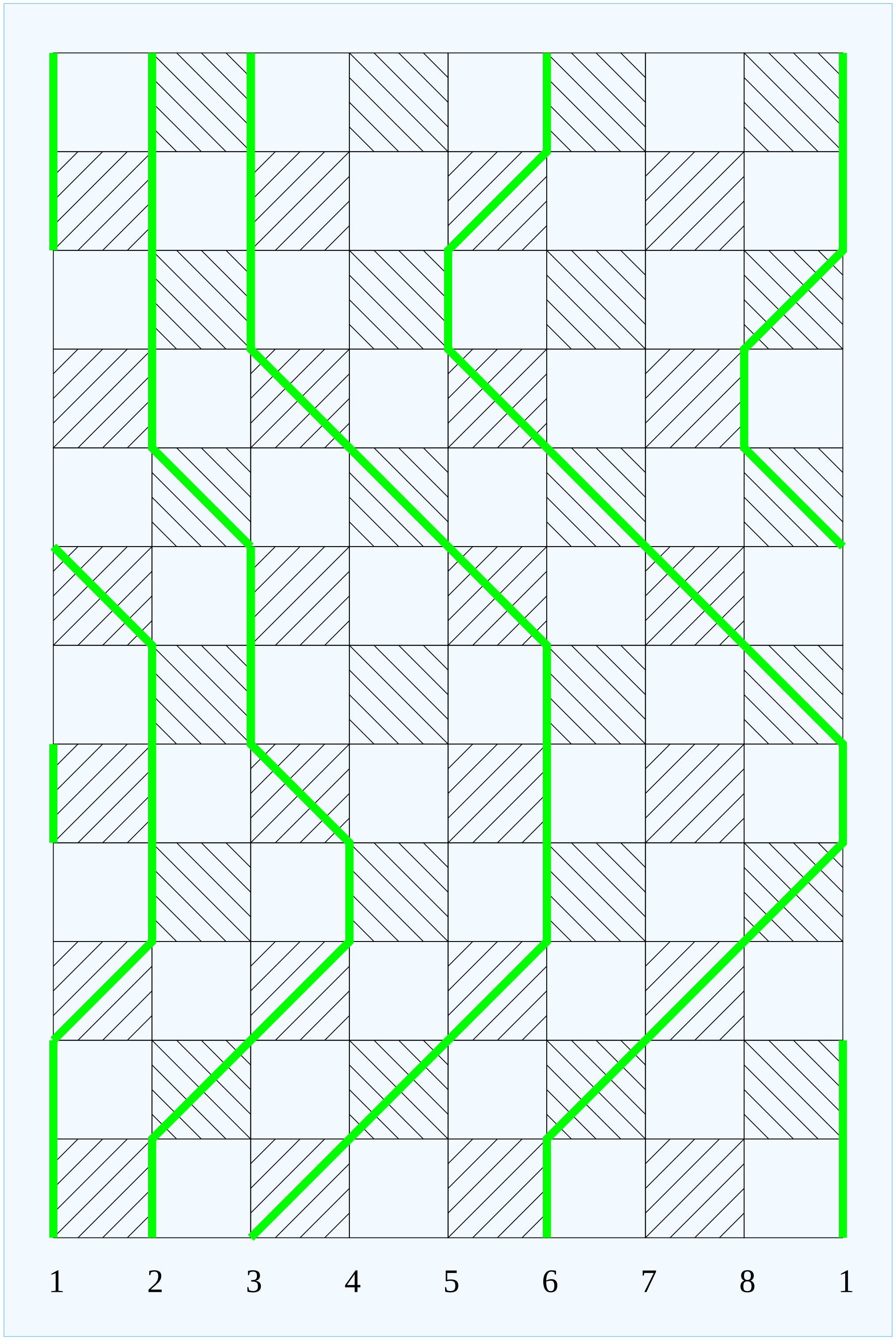

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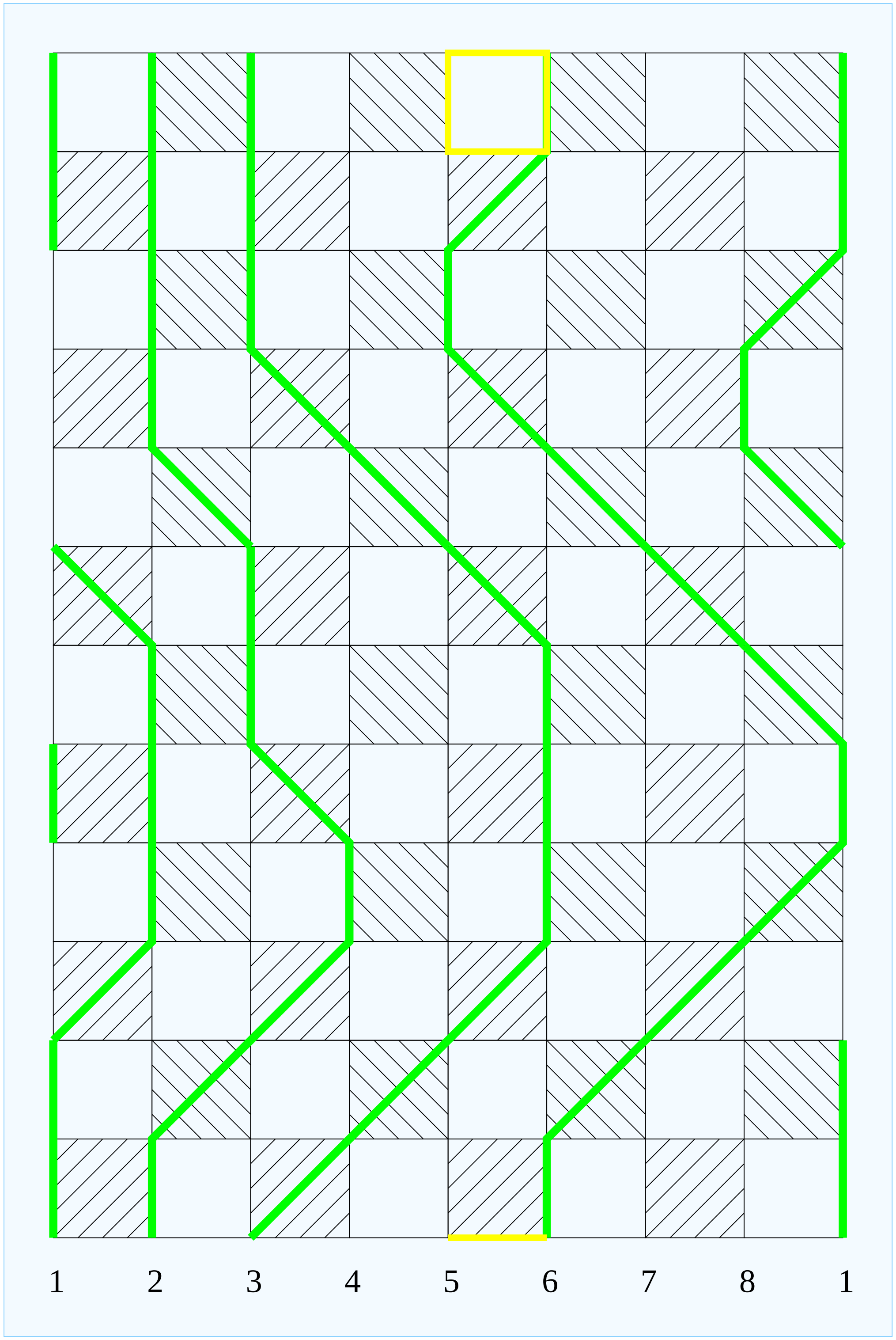

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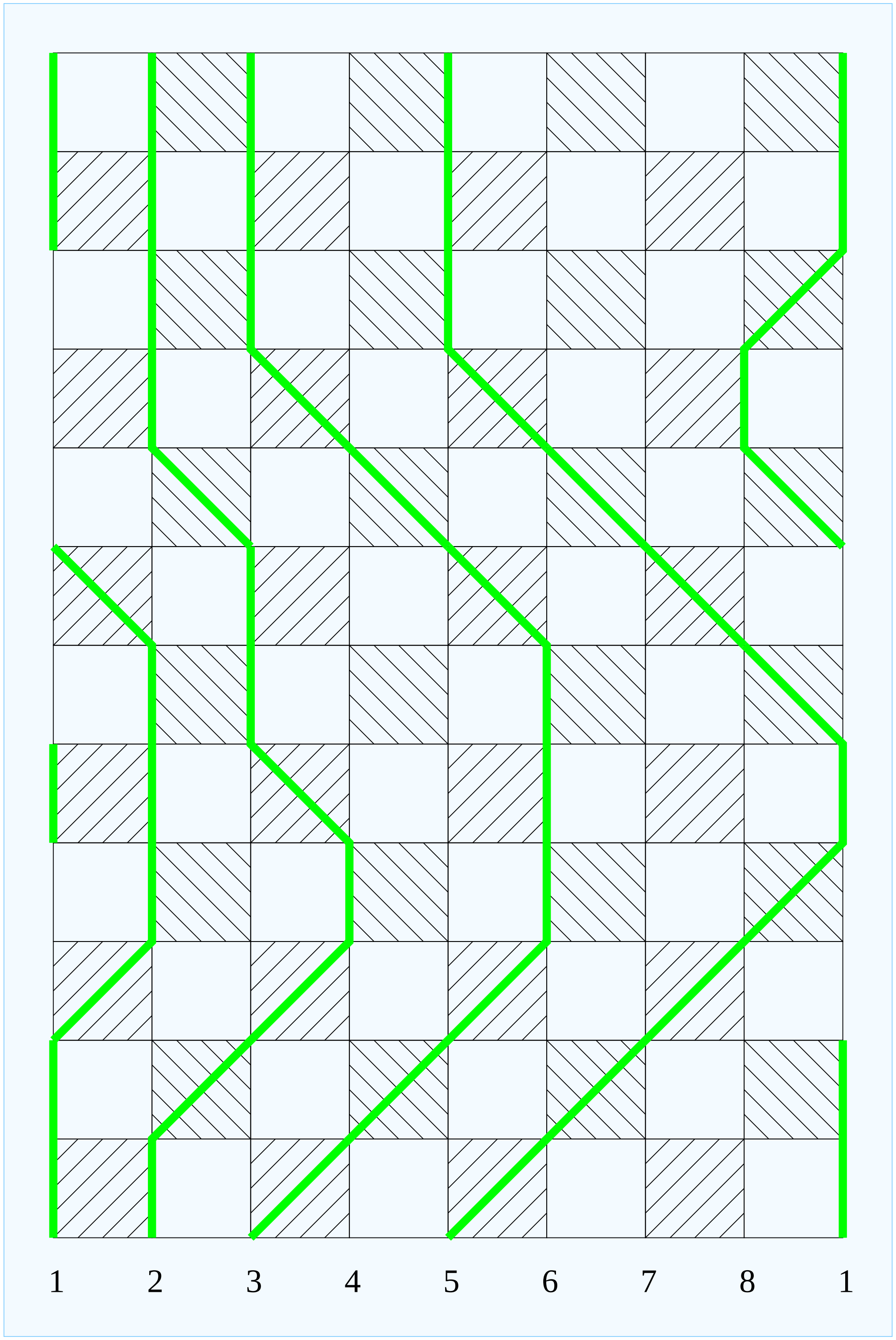

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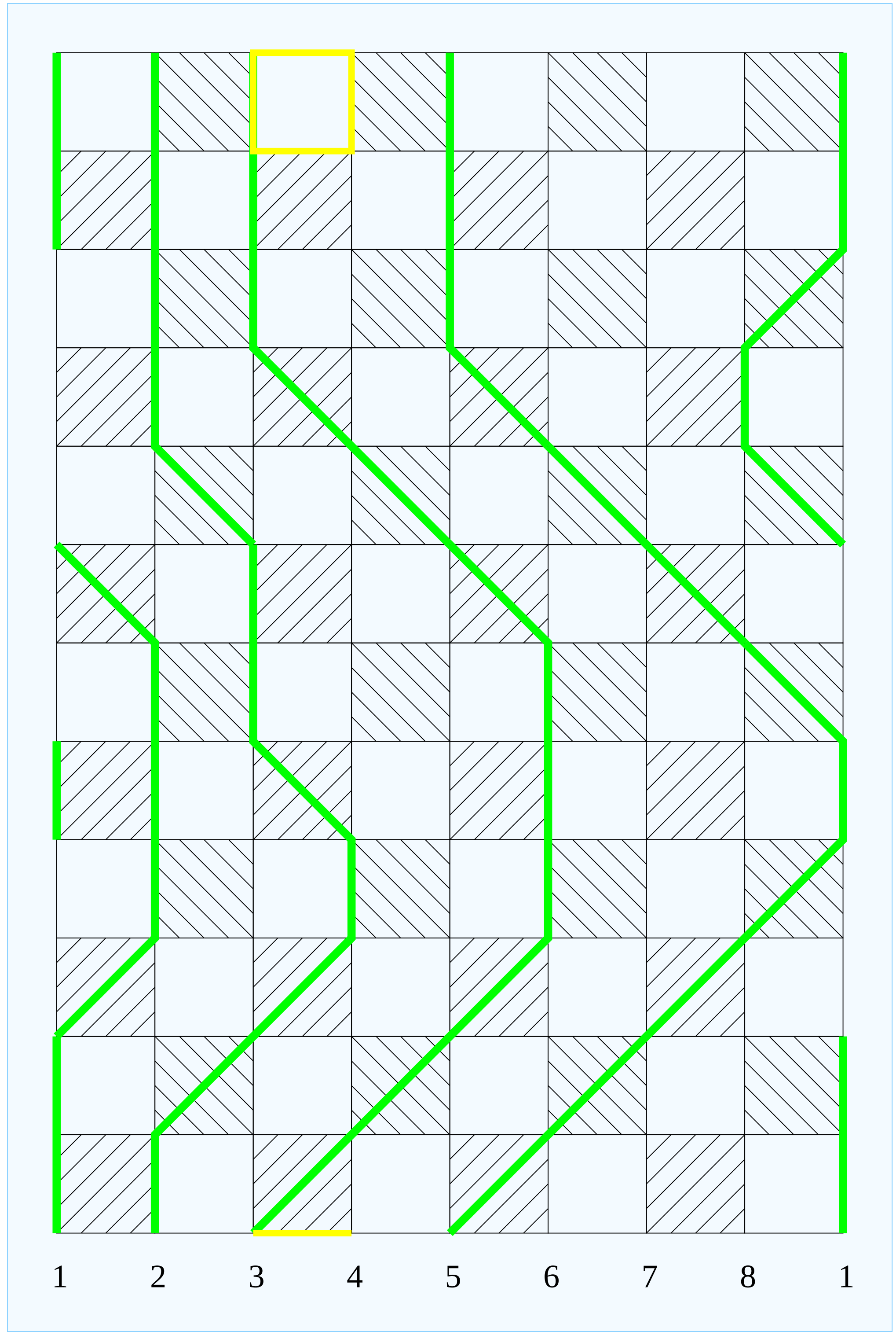

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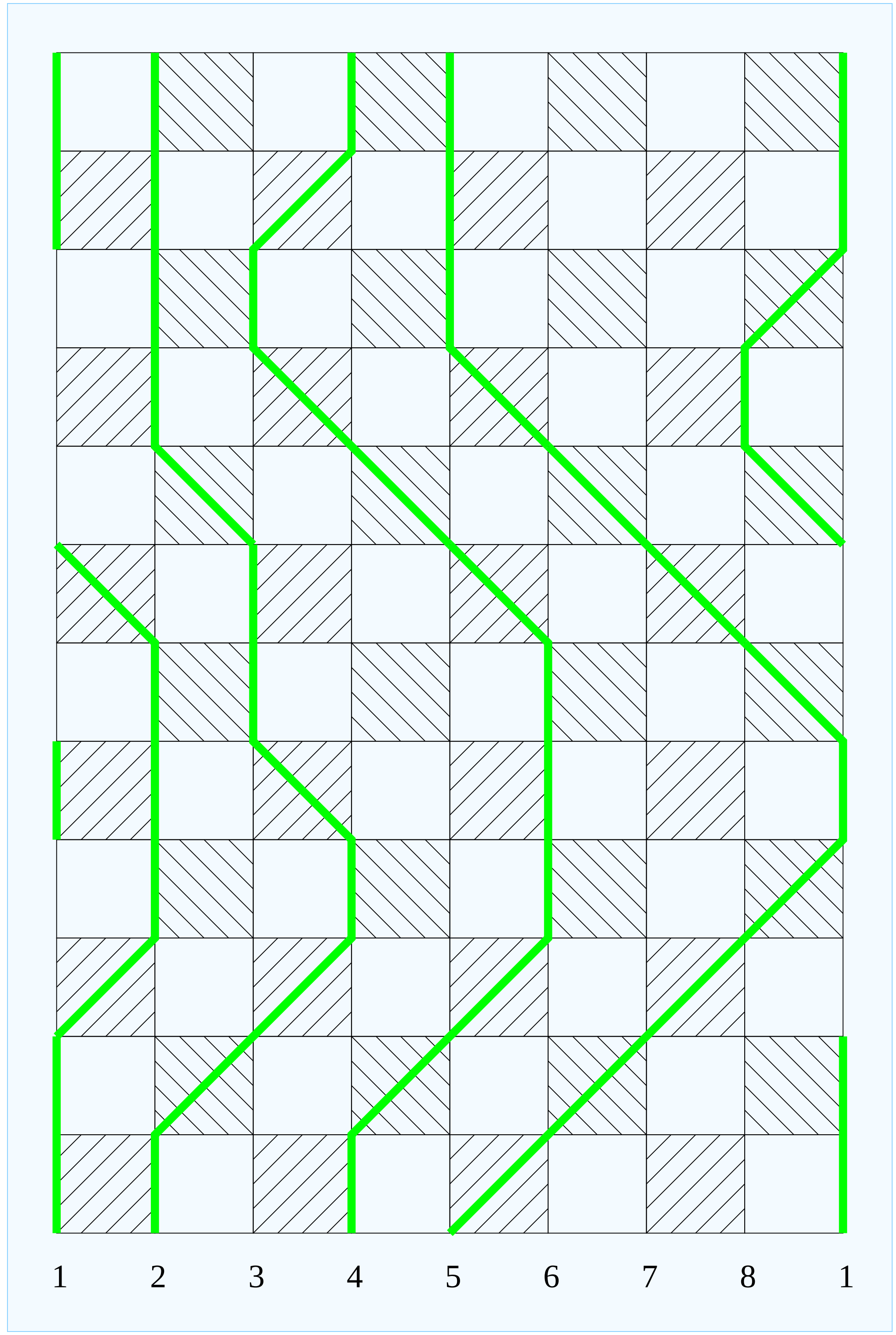

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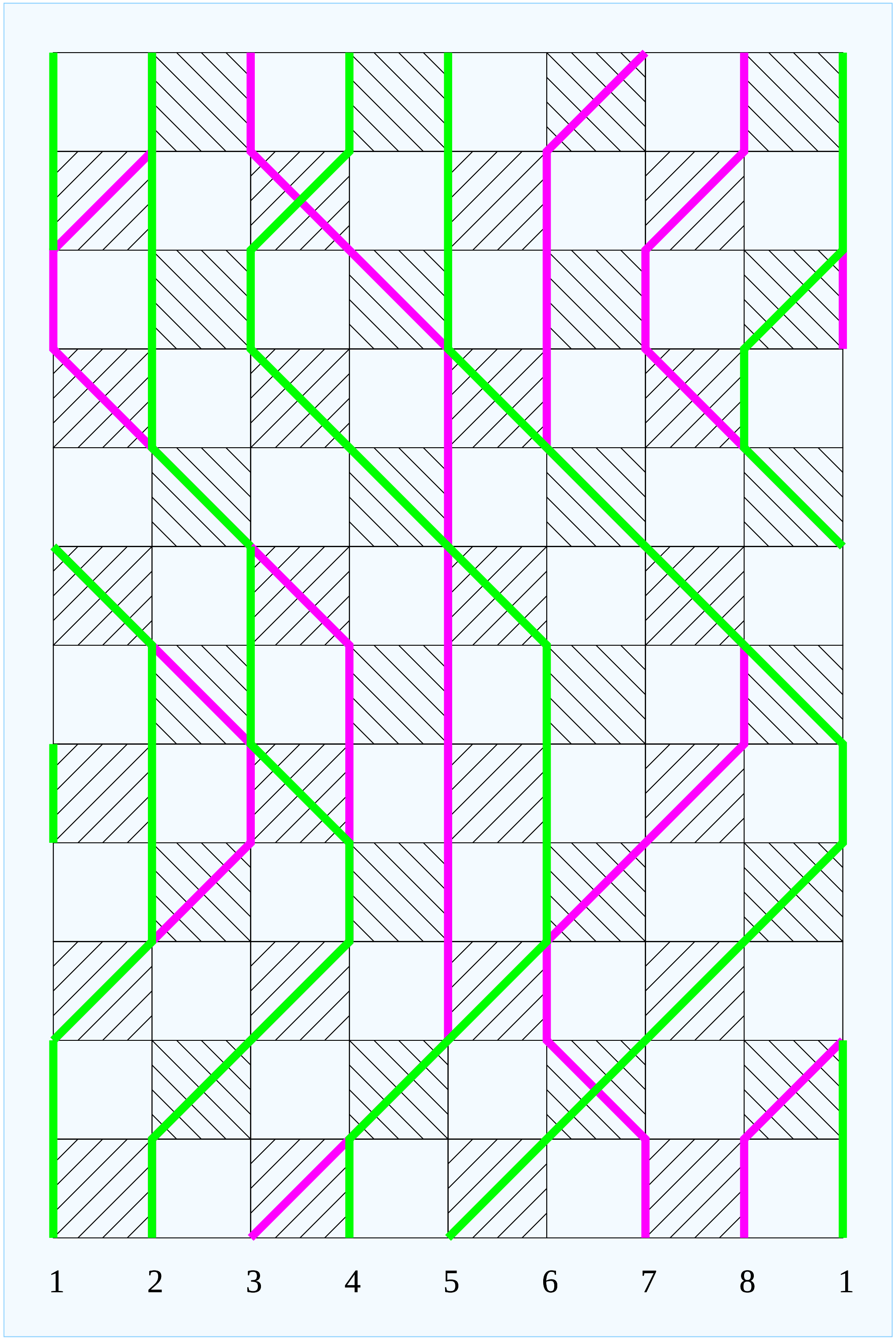
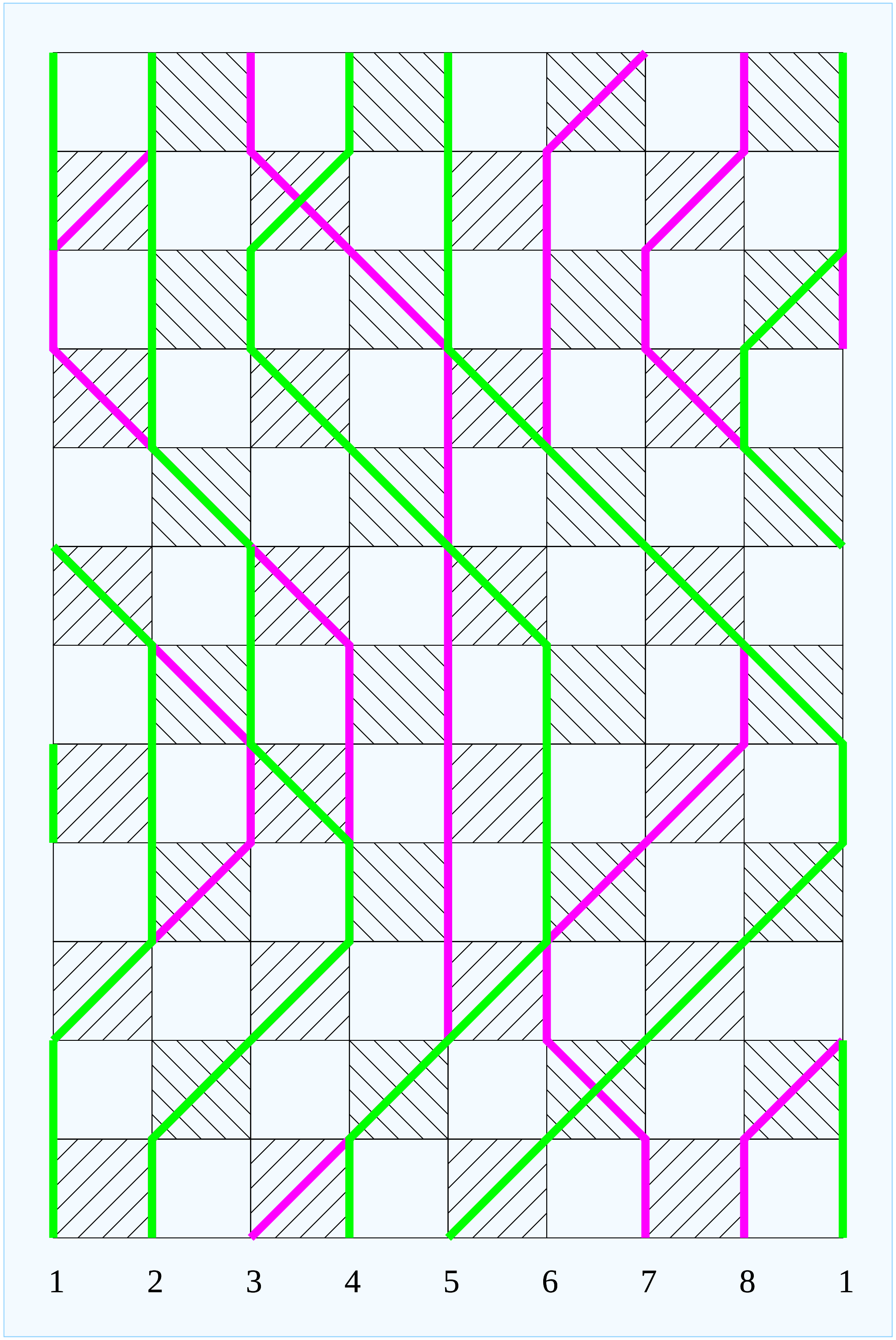


initial configuration

final configuration

Simulation

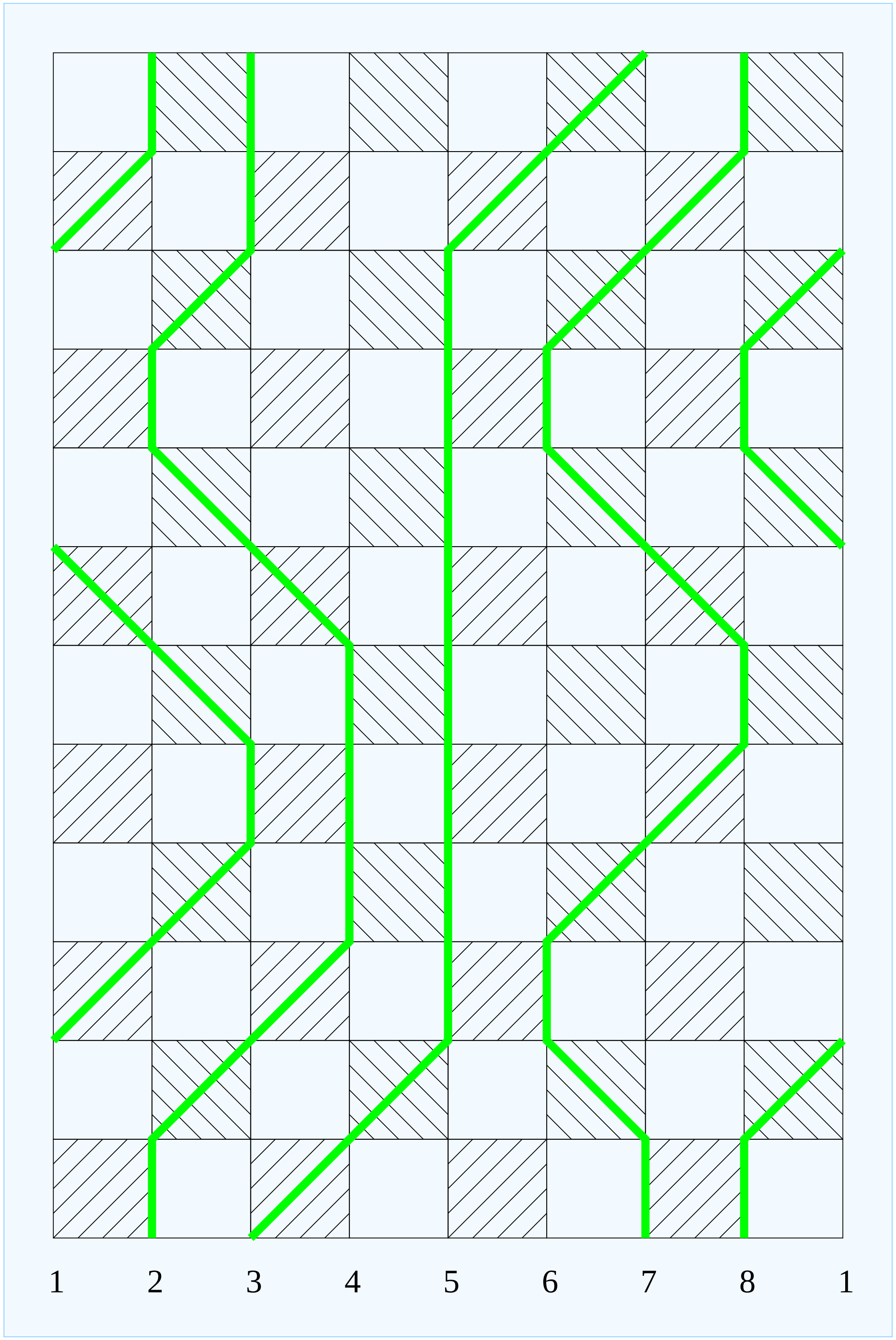


initial configuration

final configuration

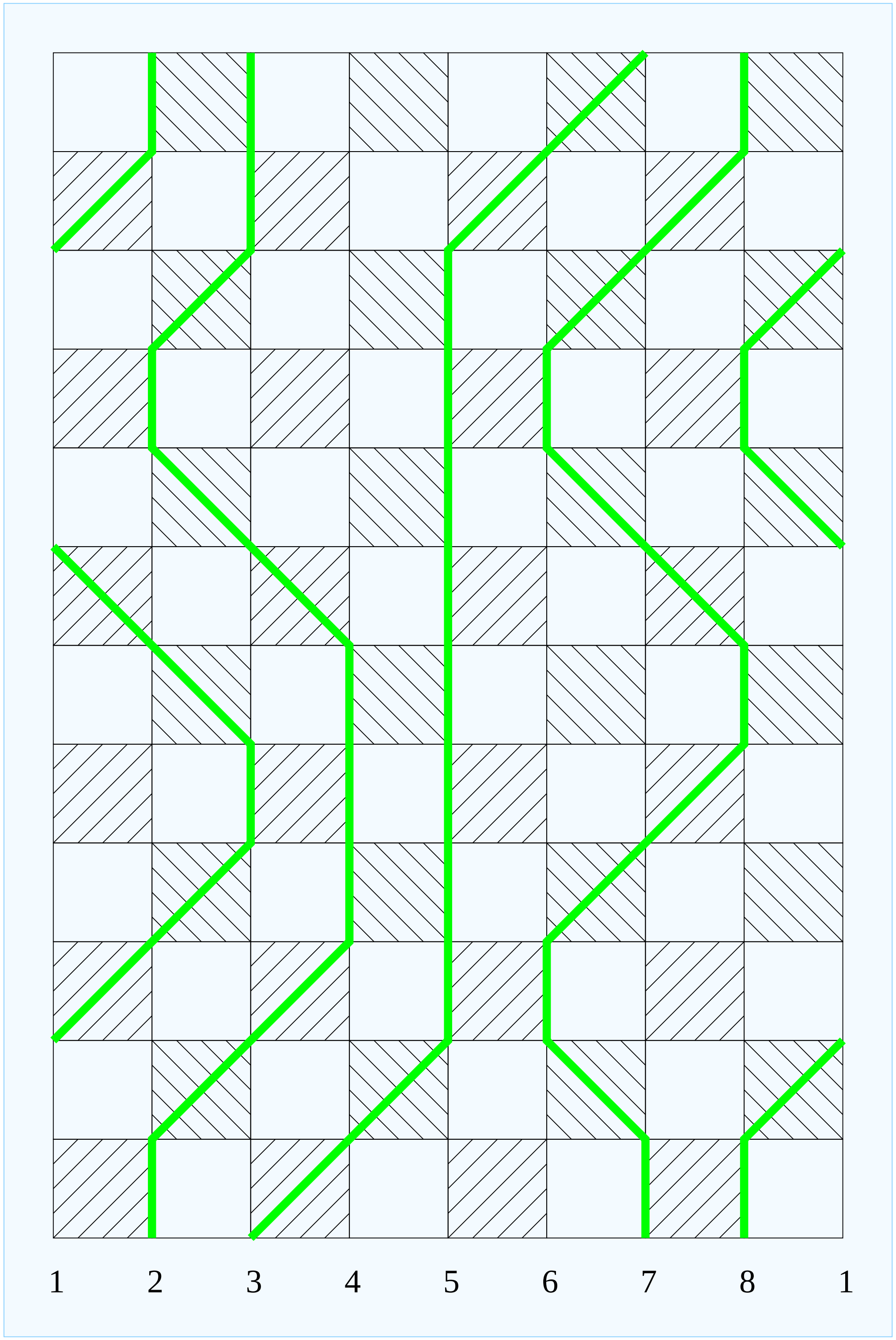
Local moves are inefficient for an ergodic sampling

Winding numbers



Winding numbers

Identical particles



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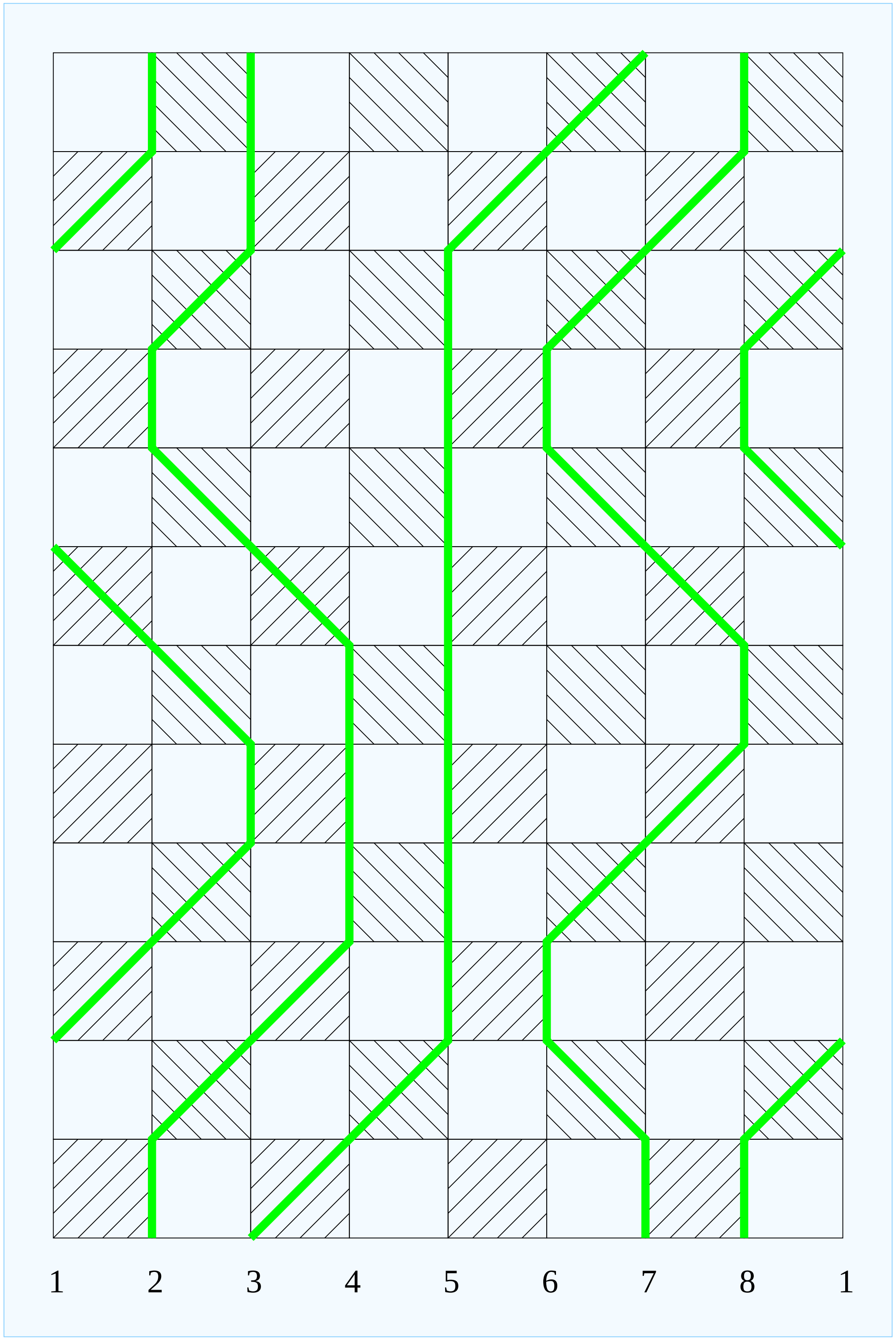
↓

Allow for all possible permutations



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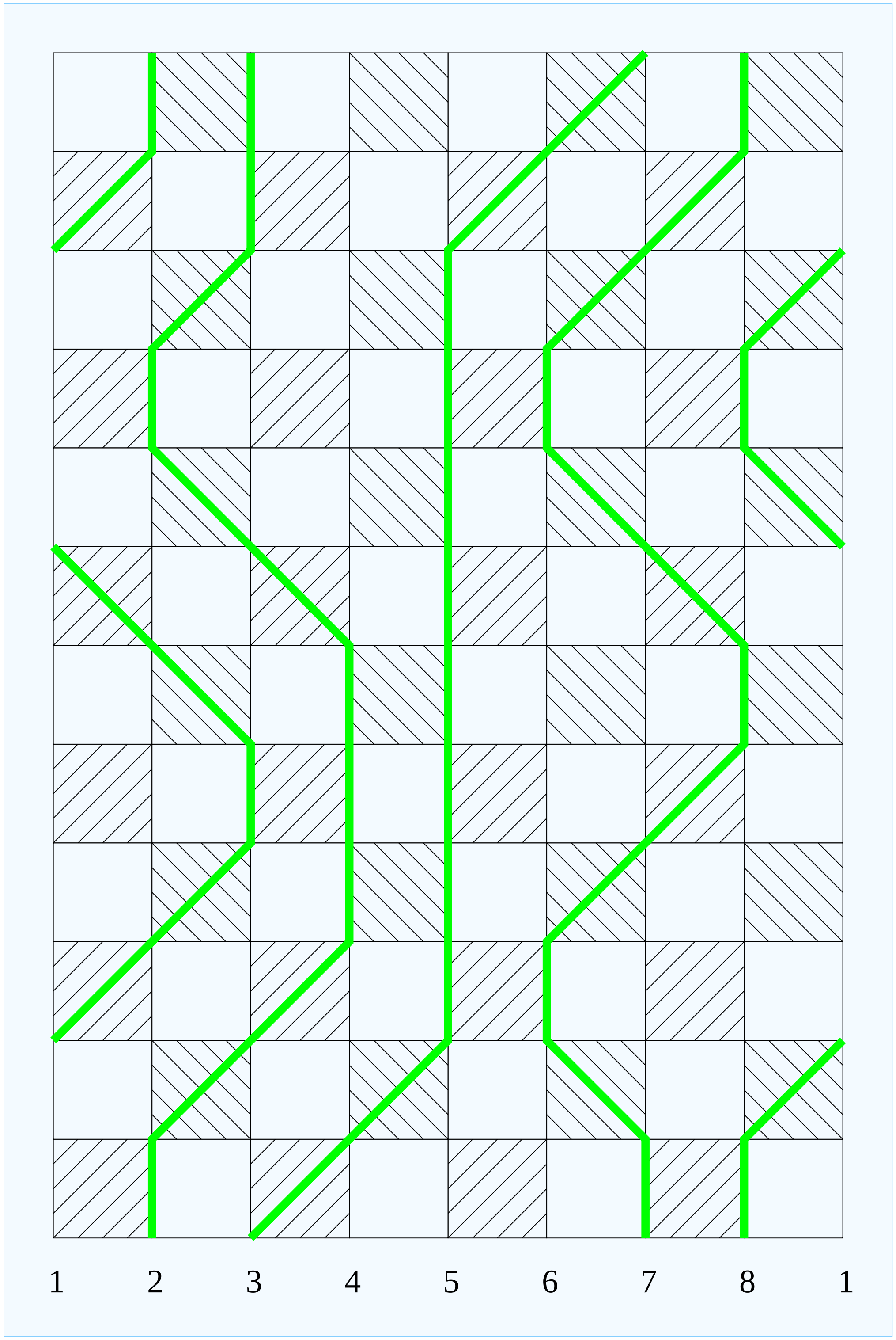
Winding numbers $\neq 0$



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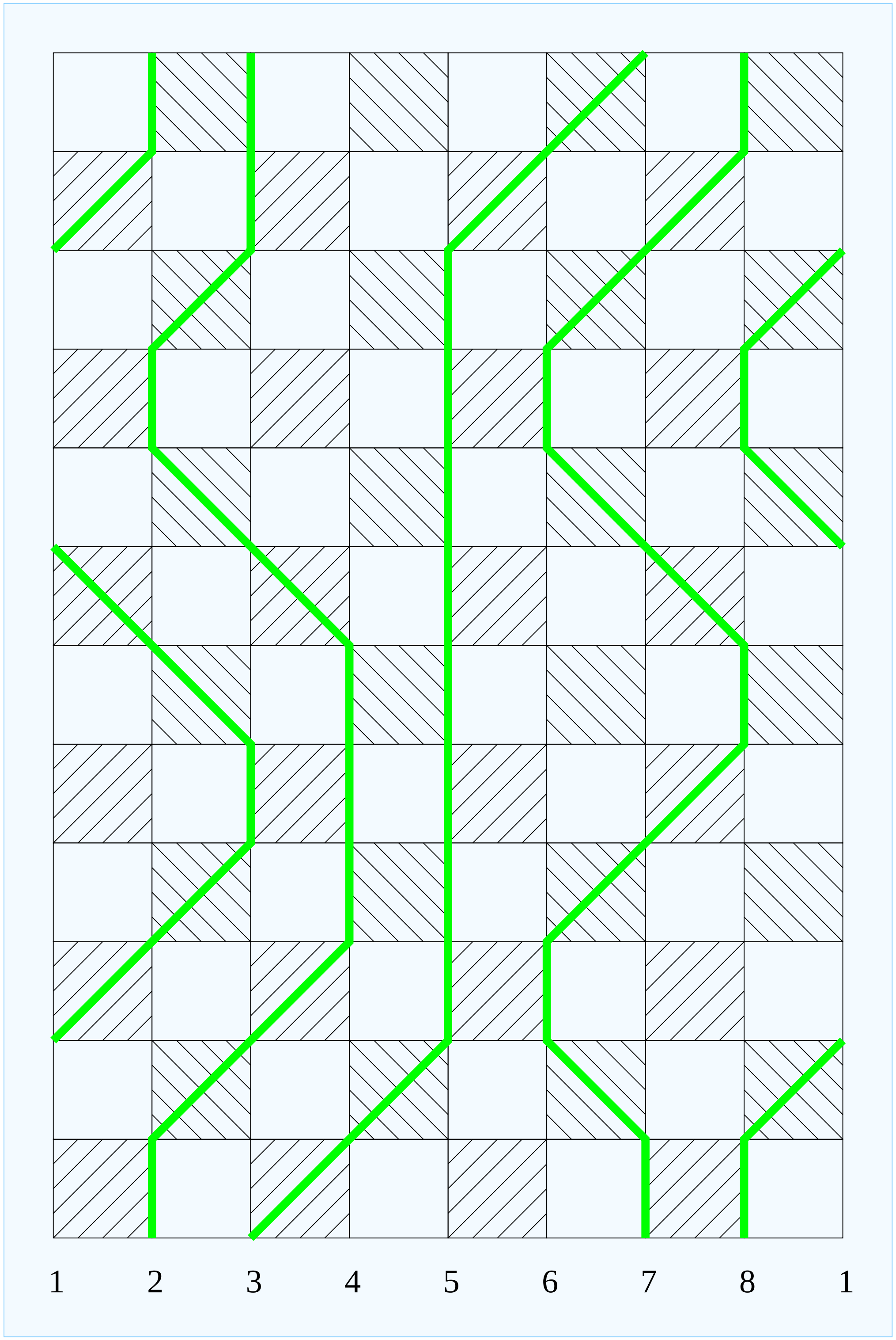
Local moves are not ergodic



Measurements

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Observables diagonal in occupation numbers

$$< \mathcal{O} >= \lim_{M\to\infty} \frac{1}{N\,2L\,M} \sum_{k=1}^{M} \sum_{j=1}^{2L} \sum_{i=1}^{N} \mathcal{O}(n_i^k(j)) \ ,$$

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Energy

$$\begin{aligned} < H > &= \frac{1}{Z}\mathrm{Tr}\ (H_1 + H_2) \left[\mathrm{e}^{-\Delta\tau H_1} \mathrm{e}^{-\Delta\tau H_2} \right]^L \\ &= \sum_{\{i_1 \cdots i_{2L}\}} P(i_1, \ldots, i_{2L}) \left\{ \frac{< i_1 \mid \mathcal{O}_1 \mathrm{e}^{-\Delta\tau H_1} \mid i_2 >}{< i_1 \mid \mathrm{e}^{-\Delta\tau H_1} \mid i_2 >} \right. \\ &\qquad \left. + \frac{< i_{2L} \mid \mathrm{e}^{-\Delta\tau H_2} \mathcal{O}_2 \mid i_1 >}{< i_{2L} \mid \mathrm{e}^{-\Delta\tau H_2} \mid i_1 >} \right\} , \end{aligned}$$

where

$$P(i_1, \ldots, i_{2L}) \equiv \frac{1}{Z} < i_1 \mid \mathrm{e}^{-\Delta\tau H_1} \mid i_2 > \cdots < i_{2L} \mid \mathrm{e}^{-\Delta\tau H_2} \mid i_1 >$$

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$$G_{ij} =< c_i(\tau) c_j^\dagger(0) > \,, \quad \longleftrightarrow \quad < S_i^+ S_j^- >$$

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Insert additional states

$$G_{ij} = \frac{\sum < i_1 \mid c_j^\dagger c_i \mid i'_1 >< i'_1 \mid \mathrm{e}^{-\Delta\tau H_1} \mid i_2 > \cdots}{\sum < i_1 \mid i'_1 >< i'_1 \mid \mathrm{e}^{-\Delta\tau H_1} \mid i_2 > \cdots} \equiv \frac{<< i_1 \mid c_j^\dagger c_i \mid i'_1 >>_{\tilde{P}}}{<< i_1 \mid i'_1 >>_{\tilde{P}}} \,,$$

where the new probability distribution is given by

$$\tilde{P} \equiv \frac{< i'_1 \mid \mathrm{e}^{-\Delta\tau H_1} \mid i_2 > \cdots < i_{2L} \mid \mathrm{e}^{-\Delta\tau H_2} \mid i_1 >}{\sum < i'_1 \mid \mathrm{e}^{-\Delta\tau H_1} \mid i_2 > \cdots < i_{2L} \mid \mathrm{e}^{-\Delta\tau H_2} \mid i_1 >} \,.$$

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  N. Kawashima, J. E. Gubernatis, and H. G. Evertz, Phys. Rev. B **50**, 136 (1994).

1.3 The loop-algorithm

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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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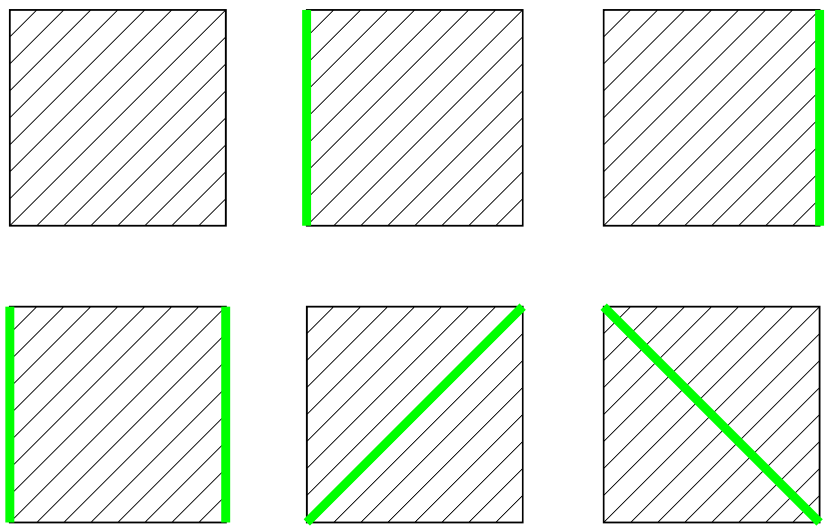
Probability of a graph given a configuration on a plaquette

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

Graphs

Graphs

Consider all possible configurations of shaded plaquettes



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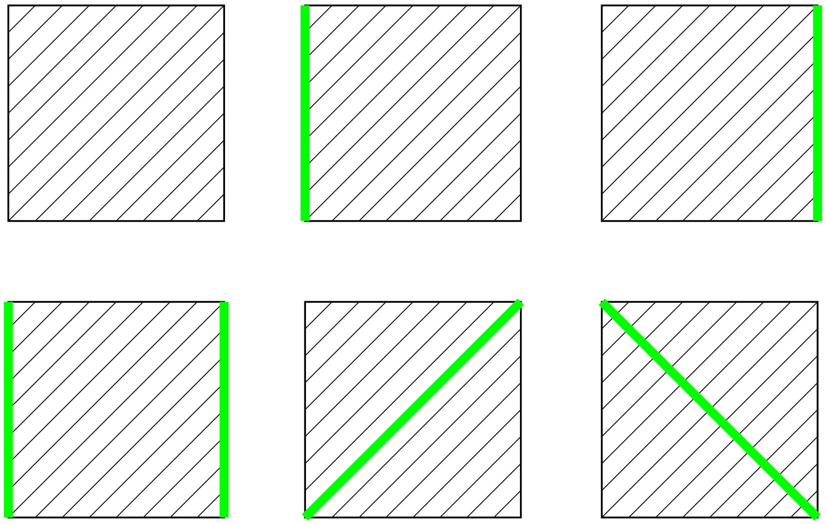

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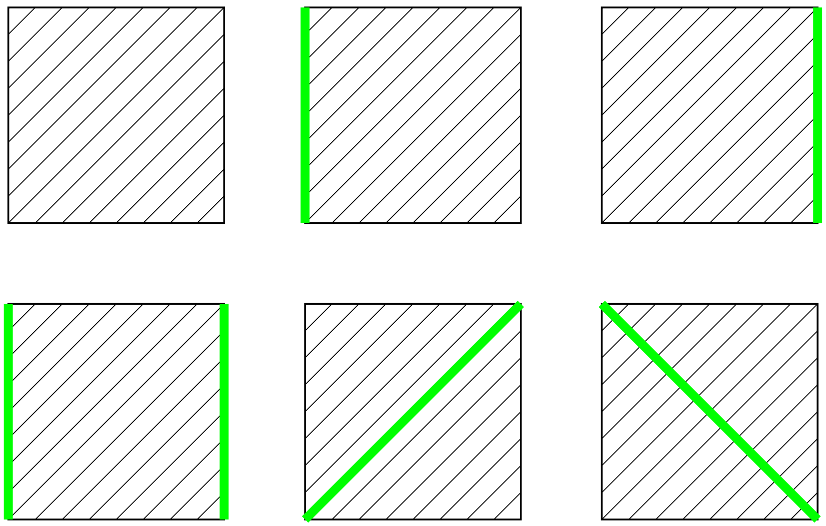

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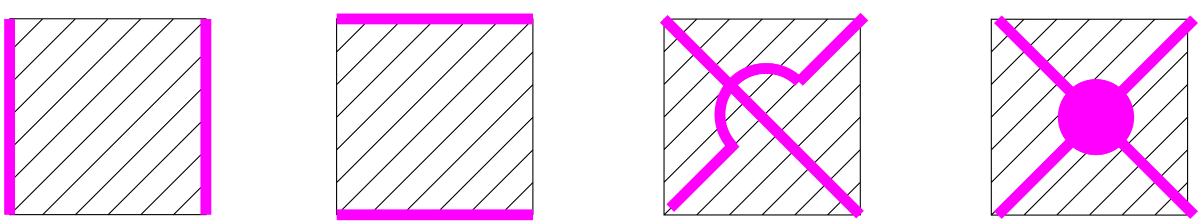
Possible graphs



$\upsilon\,(||)$ $\upsilon\,(=)$ $\upsilon\,(X)$ $\upsilon\,(\otimes)$

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

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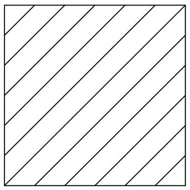
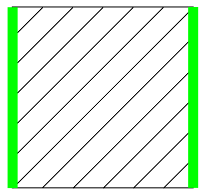
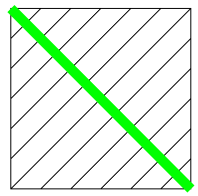
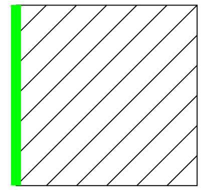
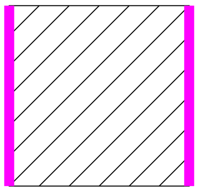
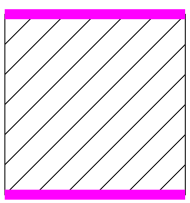
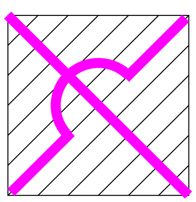
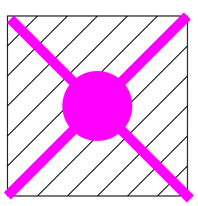
g \ u				
	1	1	0	1
	0	0	1	1
	1	1	1	0
	1	1	1	1

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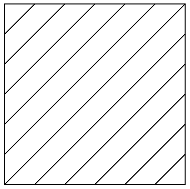
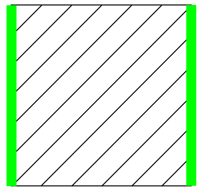
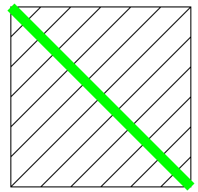
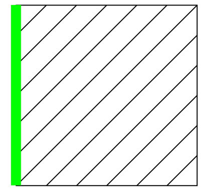
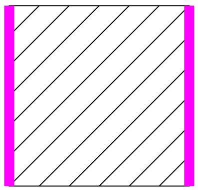
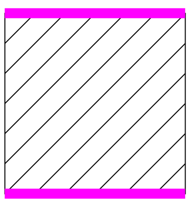
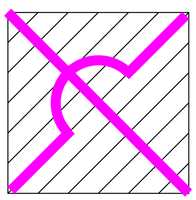
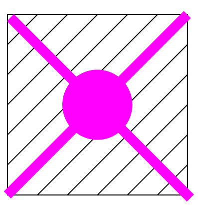
g \ u				
	1	1	0	1
	0	0	1	1
	1	1	1	0
	1	1	1	1

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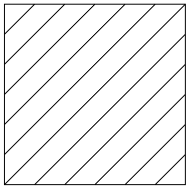
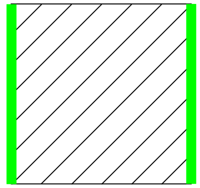
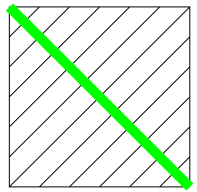
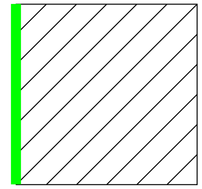
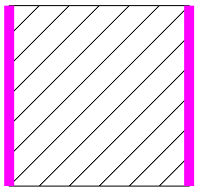
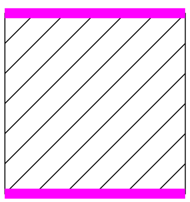
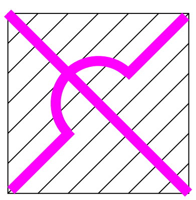
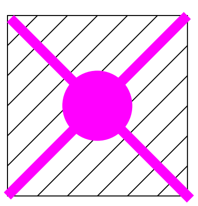
$g \backslash u$				
	1	1	0	1
	0	0	1	1
	1	1	1	0
	1	1	1	1

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

$$\downarrow$$

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

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

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Solution

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$$
\begin{aligned}
\hookrightarrow v(\times) &= \frac{1}{2}\exp\left(-\frac{\Delta\tau J\Delta}{4}\right)\left\{1 - \exp\left[-\Delta\tau\left(\frac{J}{2} - \frac{J\Delta}{2}\right)\right]\right\}\ , \\
v(\|) &= \frac{1}{2}\exp\left(-\frac{\Delta\tau J\Delta}{4}\right)\left\{1 + \exp\left[-\Delta\tau\left(\frac{J}{2} - \frac{J\Delta}{2}\right)\right]\right\}\ , \\
v(=) &= \frac{1}{2}\exp\left(-\frac{\Delta\tau J\Delta}{4}\right)\left\{\exp\left[\Delta\tau\left(\frac{J}{2} + \frac{J\Delta}{2}\right)\right] - 1\right\}\ .
\end{aligned}
$$

Solution

Set $v_i\,(\otimes) = 0$

$$
\begin{aligned}
\hookrightarrow v(\times) &= \frac{1}{2}\exp\left(-\frac{\Delta\tau J\Delta}{4}\right)\left\{1-\exp\left[-\Delta\tau\left(\frac{J}{2}-\frac{J\Delta}{2}\right)\right]\right\}\,,\\
v(\|) &= \frac{1}{2}\exp\left(-\frac{\Delta\tau J\Delta}{4}\right)\left\{1+\exp\left[-\Delta\tau\left(\frac{J}{2}-\frac{J\Delta}{2}\right)\right]\right\}\,,\\
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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For the isotropic Heisenberg model $v(\times) = 0$**.**

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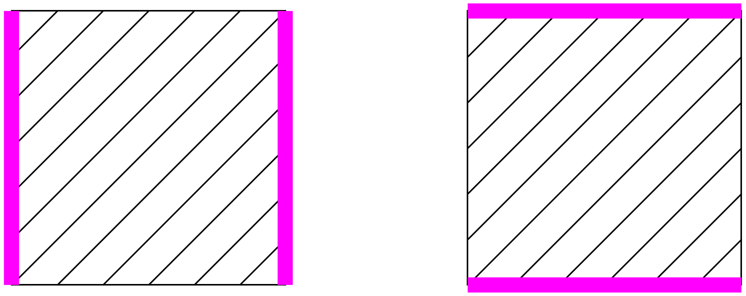
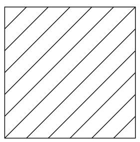
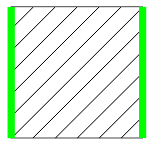
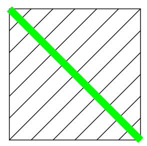
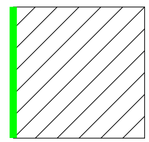
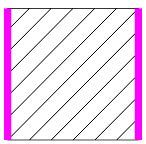
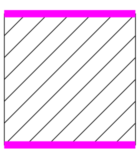
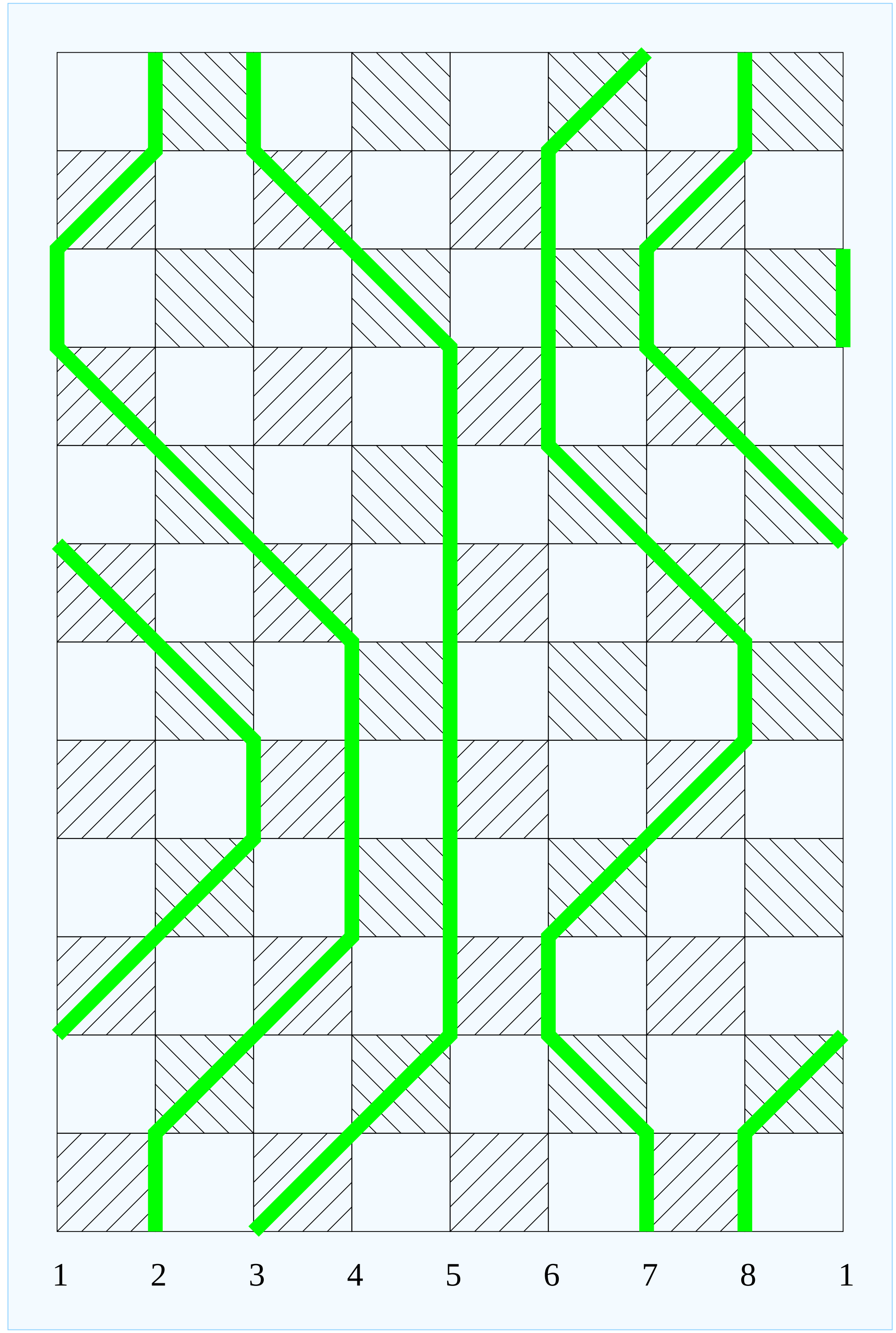
$\hookrightarrow$ **need only two graphs**



Example:
isotropic Heisenberg model

g \ u				
	1	1	0	1
	0	0	1	1



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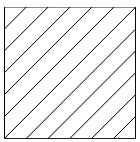
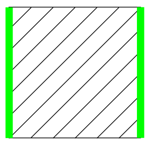
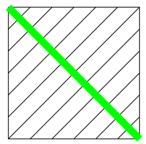
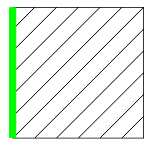
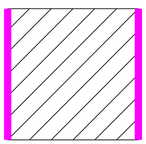
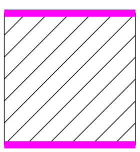
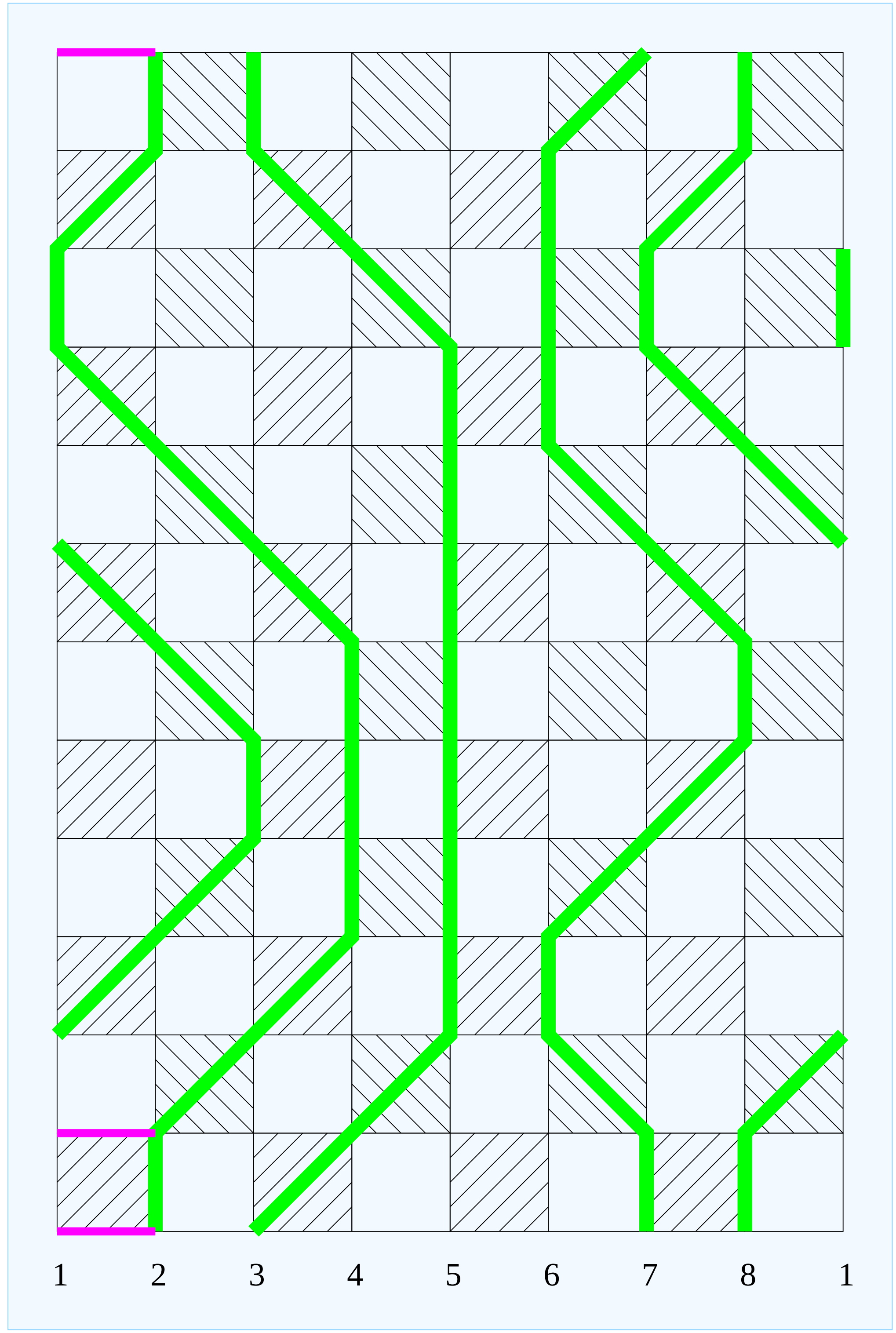
g \ u				
	1	1	0	1
	0	0	1	1



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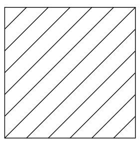
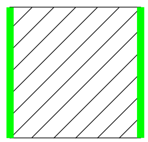
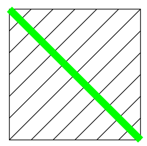
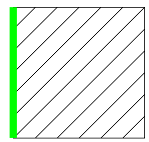
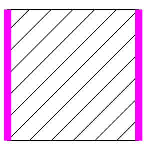
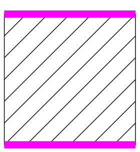
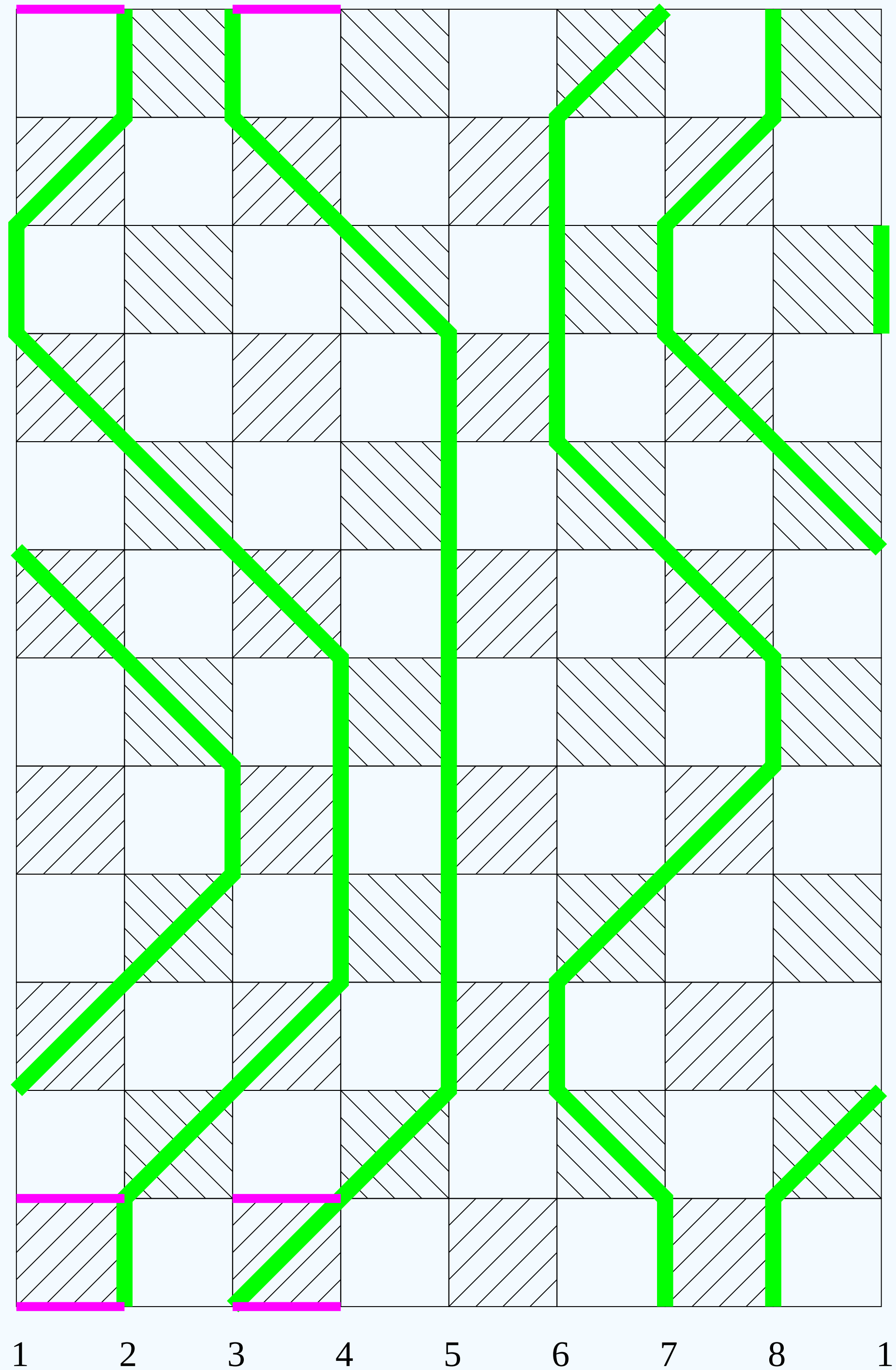
g \ u				
	1	1	0	1
	0	0	1	1



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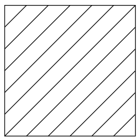
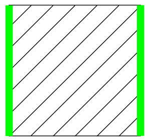
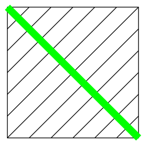
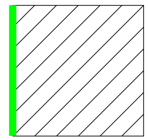
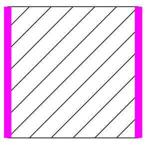
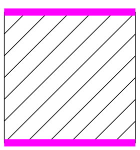
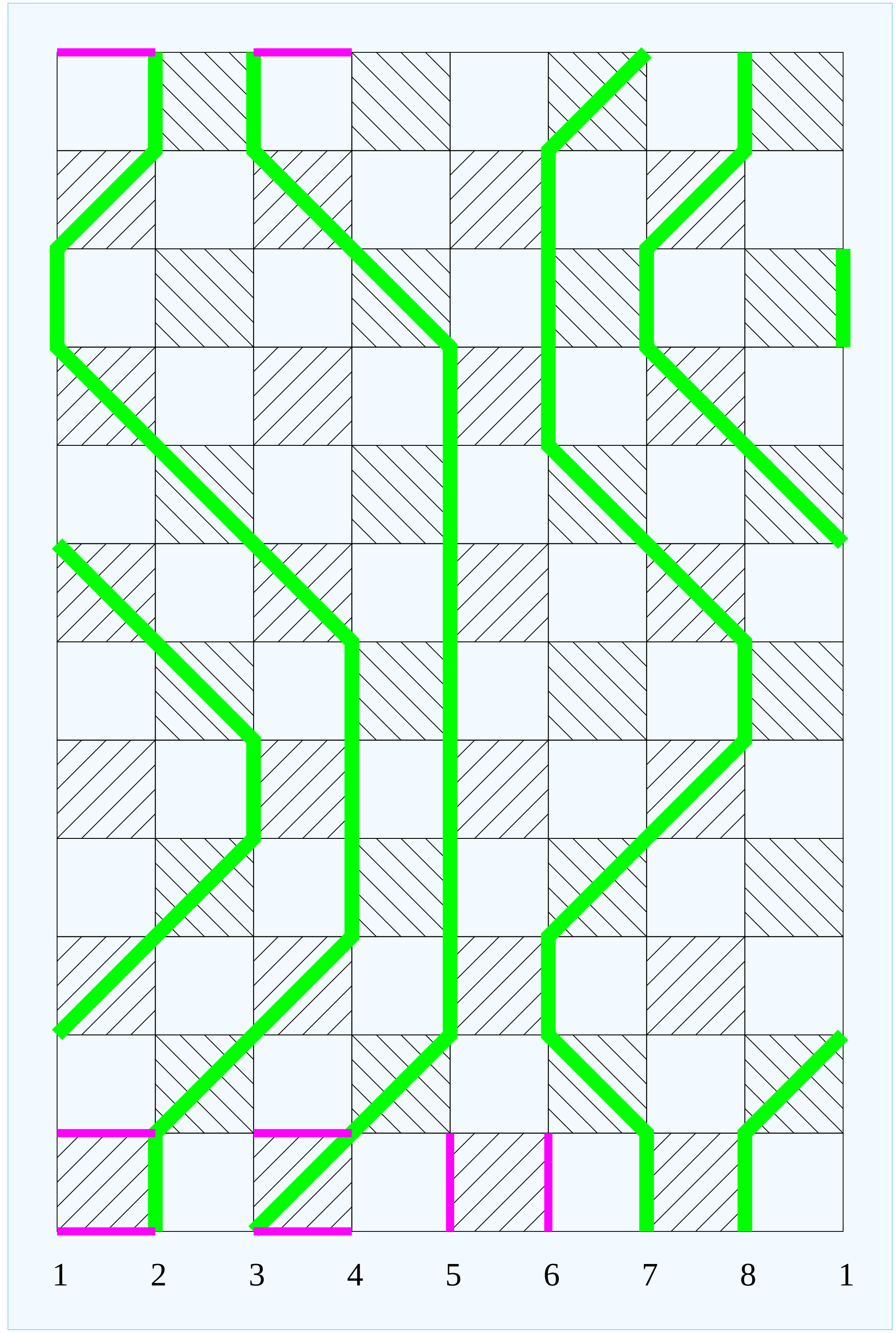
isotropic Heisenberg model

g \ u				
	1	1	0	1
	0	0	1	1



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isotropic Heisenberg model

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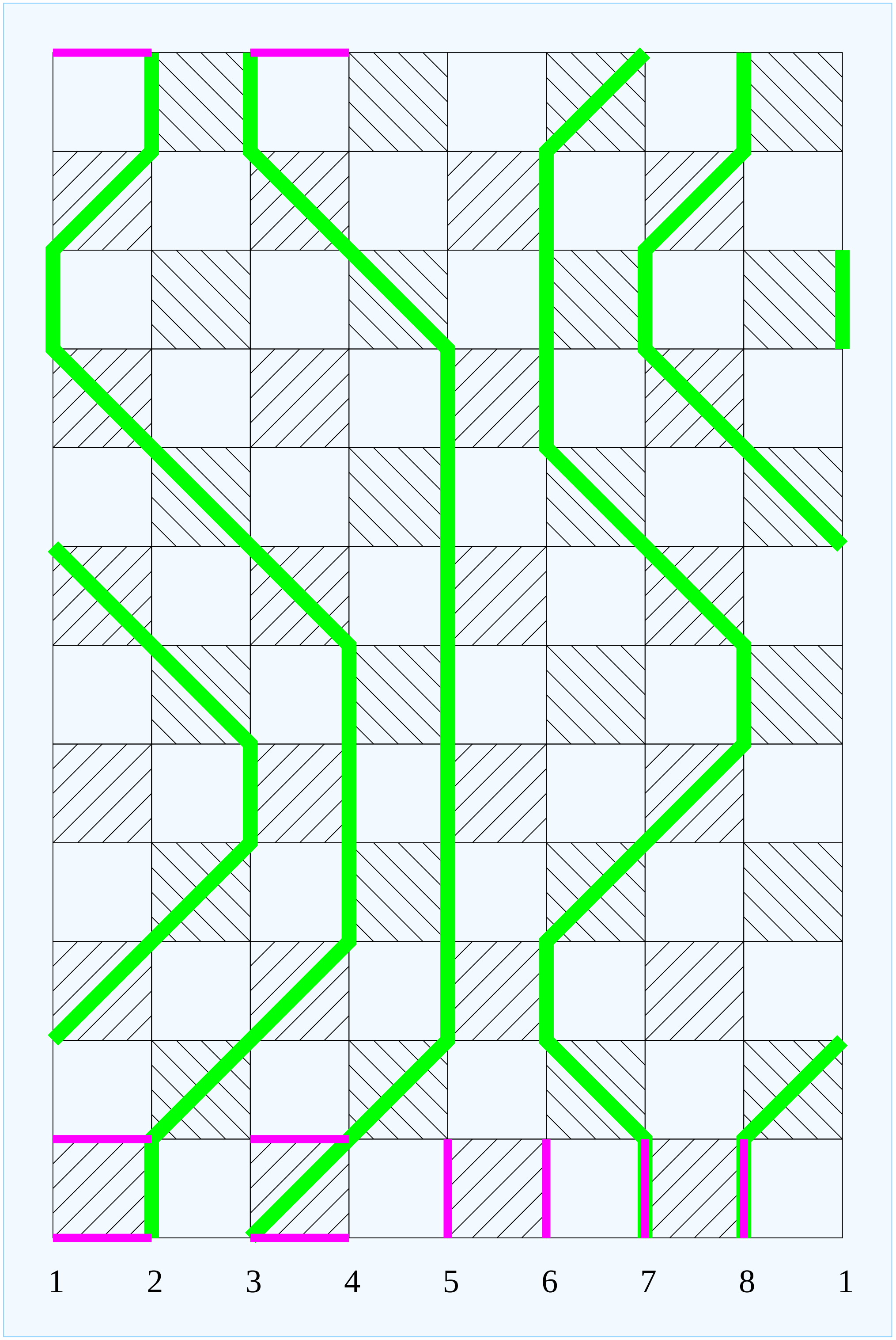

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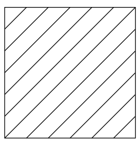
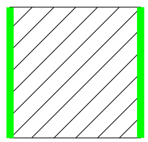
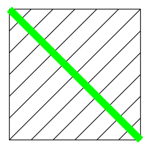
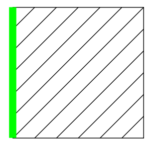
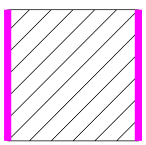
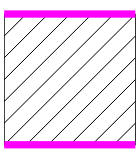
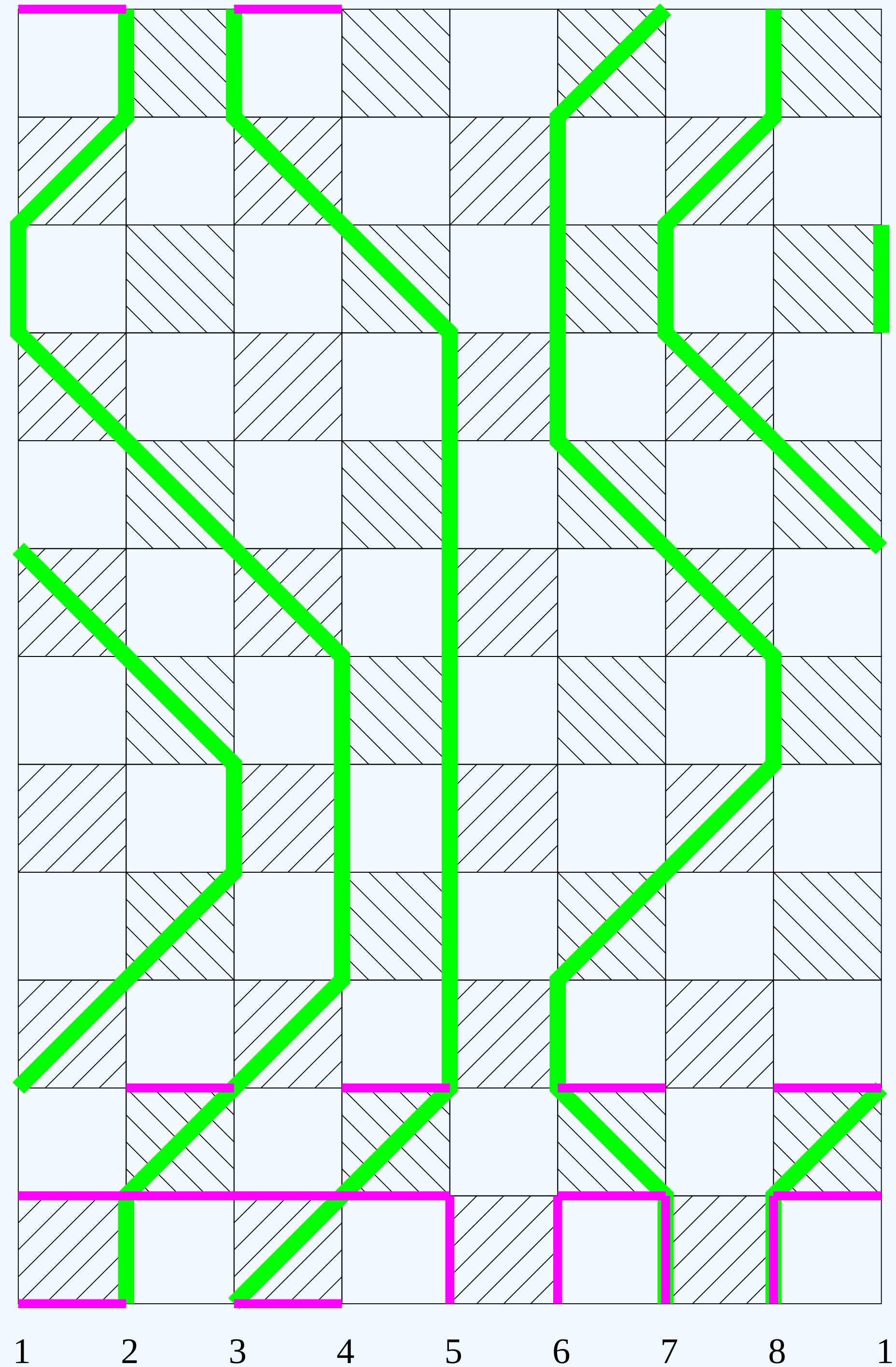
g \ u				
	1	1	0	1
	0	0	1	1



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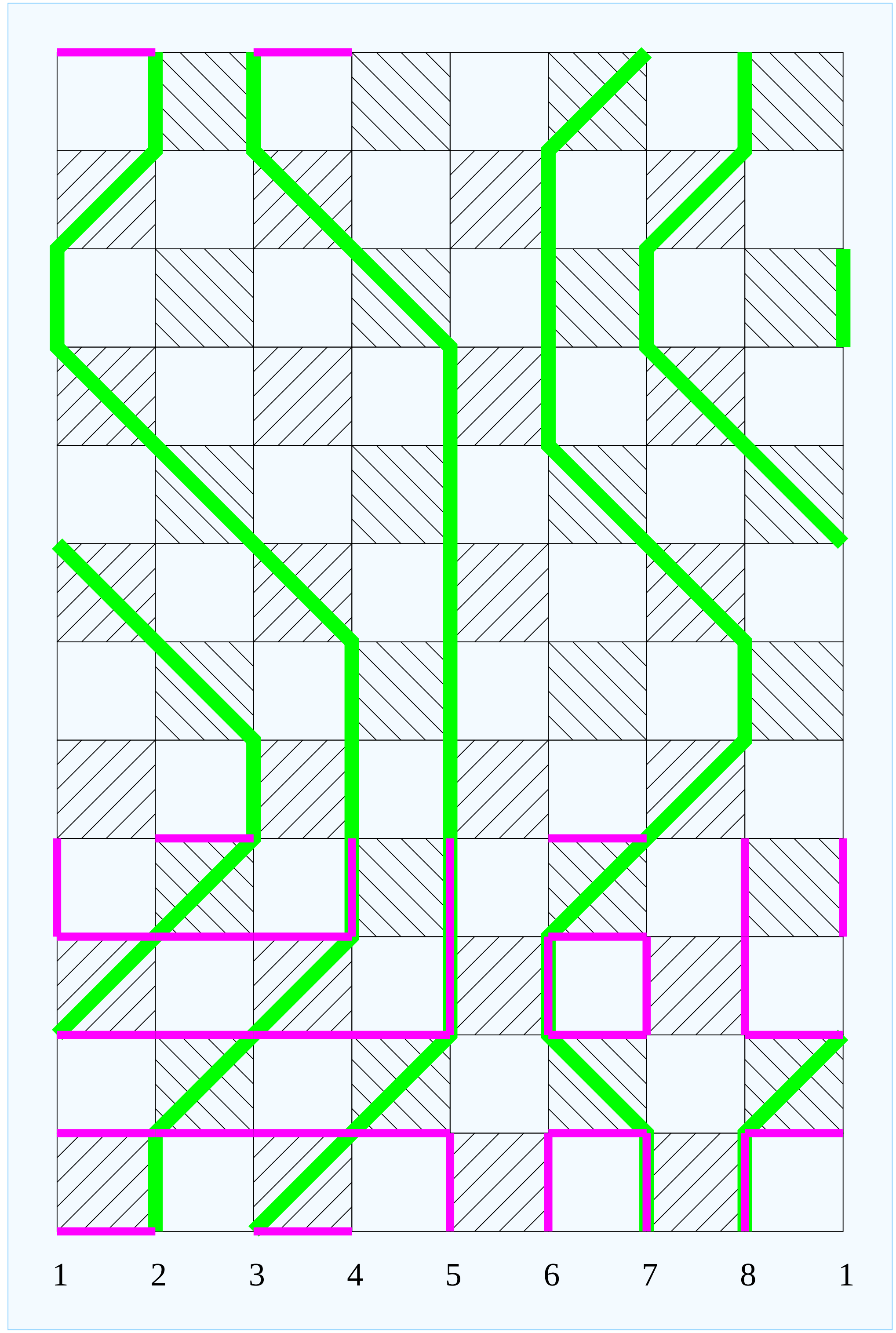

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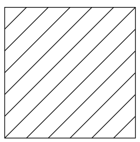
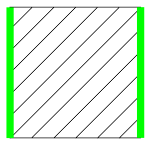
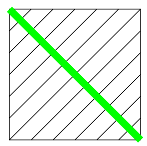
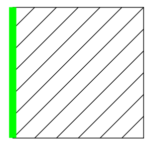
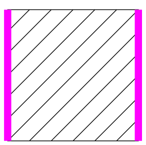
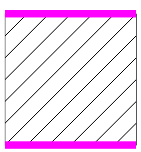
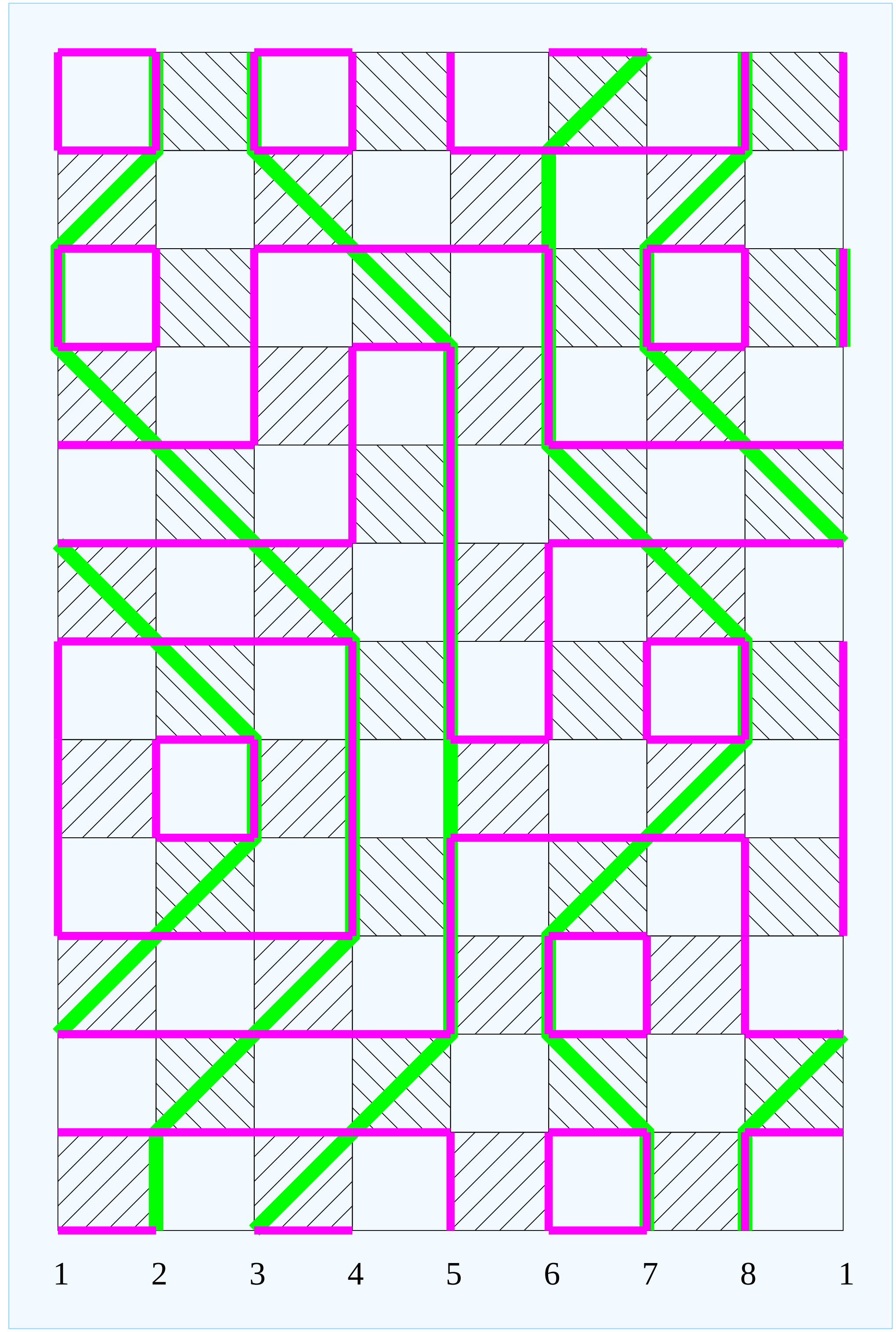
g \ u				
	1	1	0	1
	0	0	1	1



Update

Update

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

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$\hookrightarrow$ **both configurations belong to the same graph.**

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Detailed balance

$$W(\boldsymbol{s},\mathcal{G}) \, p(\boldsymbol{s} \to \boldsymbol{s}',\mathcal{G}) = W(\boldsymbol{s}',\mathcal{G}) \, p(\boldsymbol{s}' \to \boldsymbol{s},\mathcal{G}) \; .$$

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Transition probability (heat-bath)

$$p(\boldsymbol{s} \to \boldsymbol{s}',\mathcal{G}) = \frac{W(\boldsymbol{s}',\mathcal{G})}{W(\boldsymbol{s},\mathcal{G}) + W(\boldsymbol{s}',\mathcal{G})} \ ,$$

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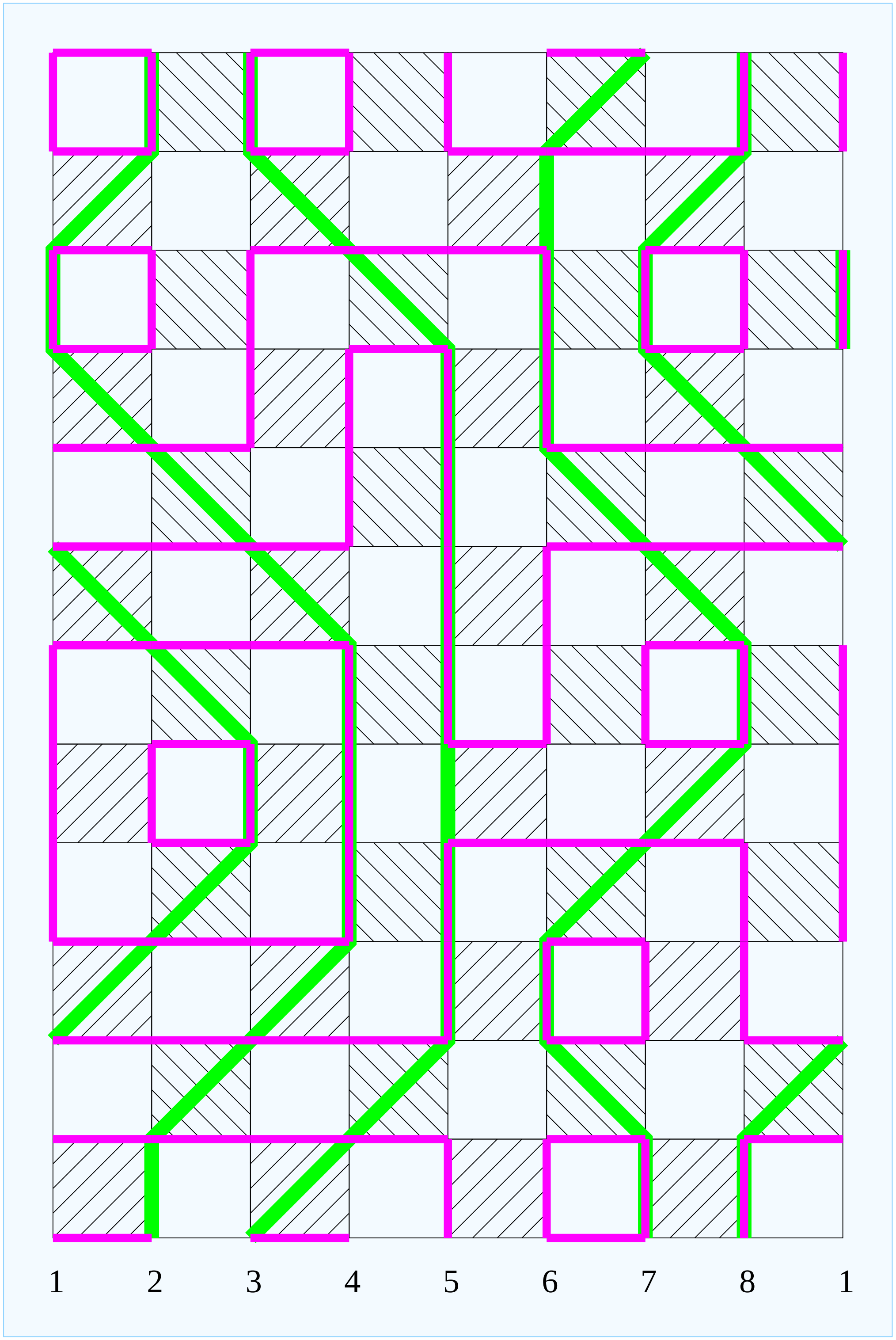
Update with loops

Isotropic Heisenberg model

Active loops

Flipped loops



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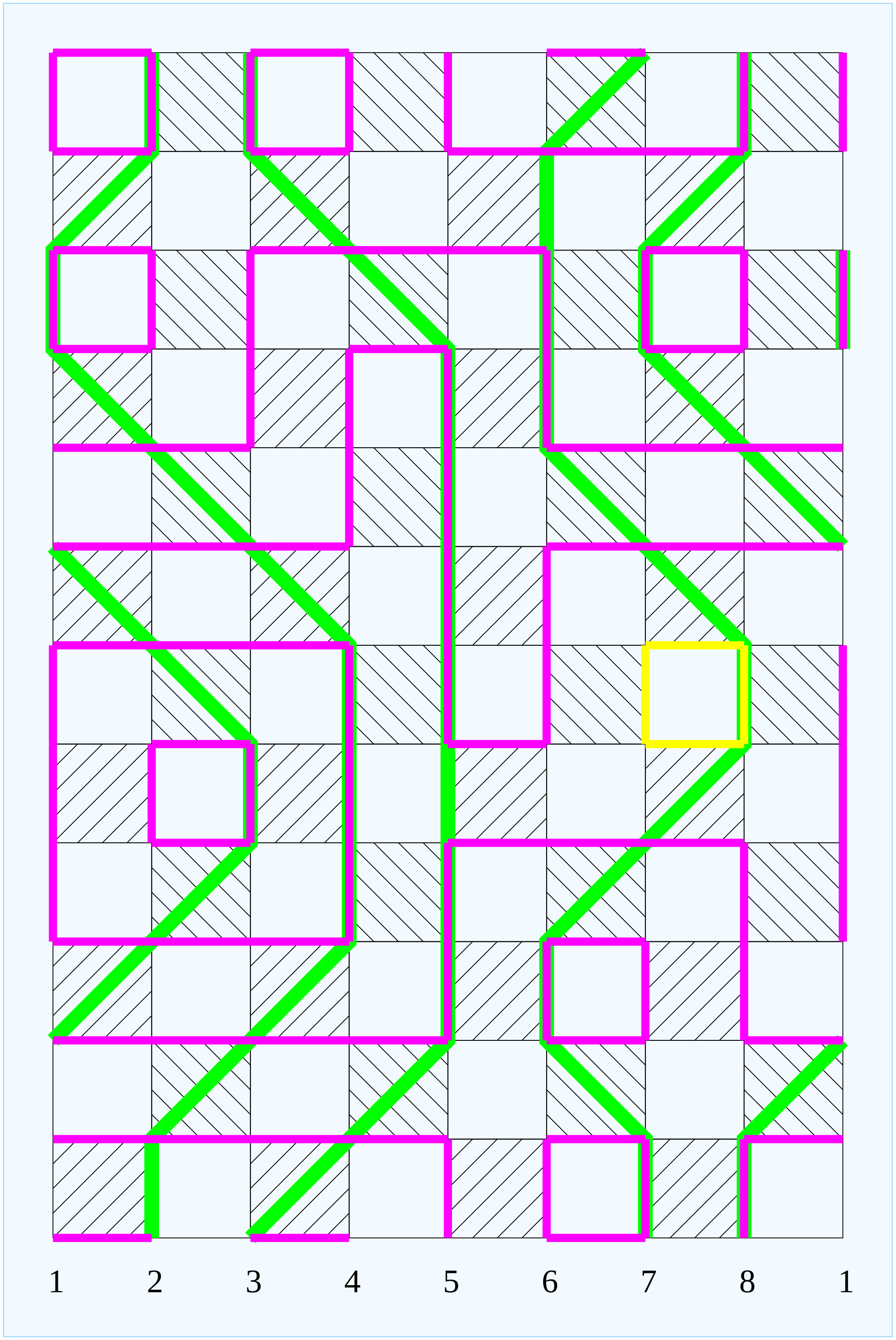

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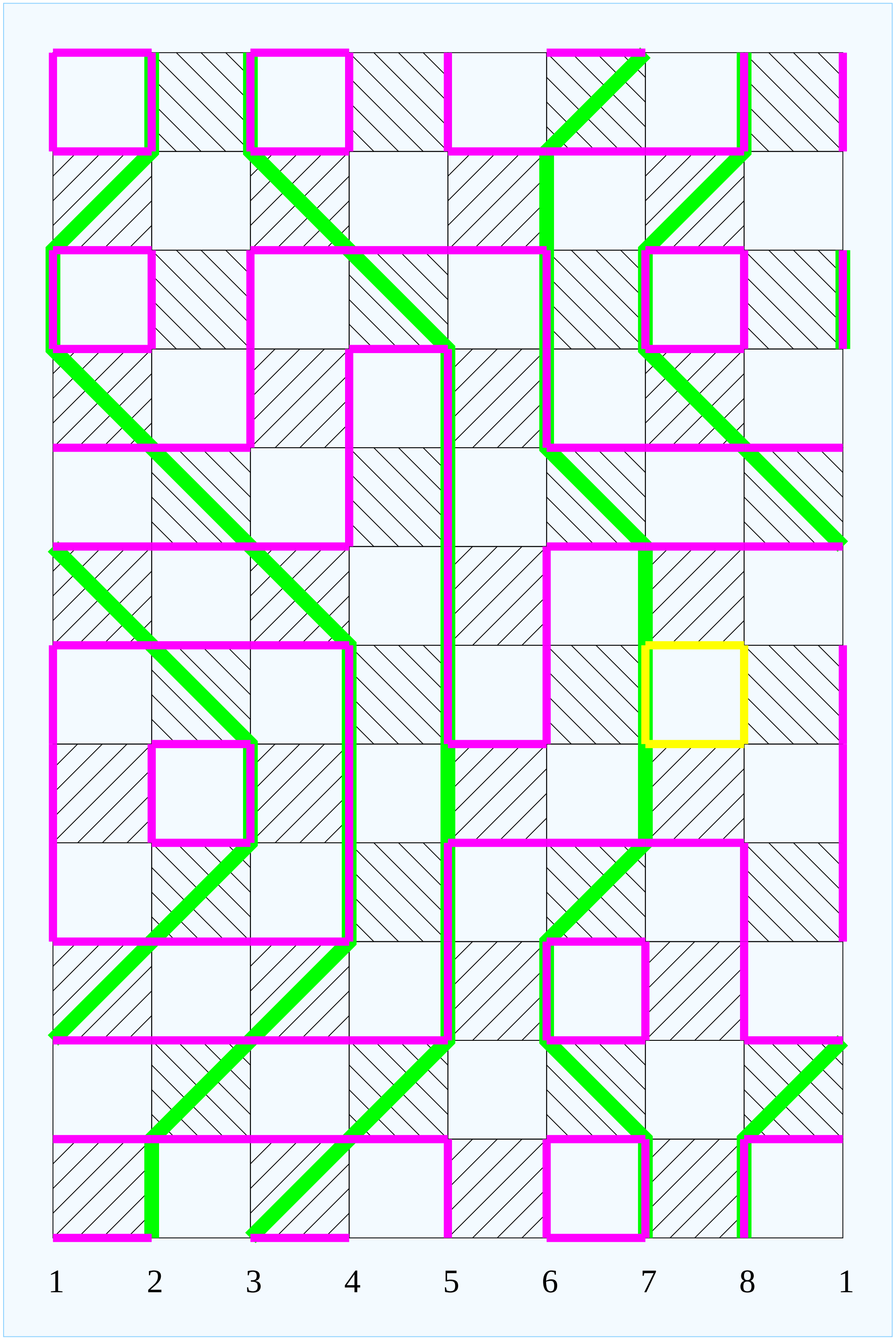

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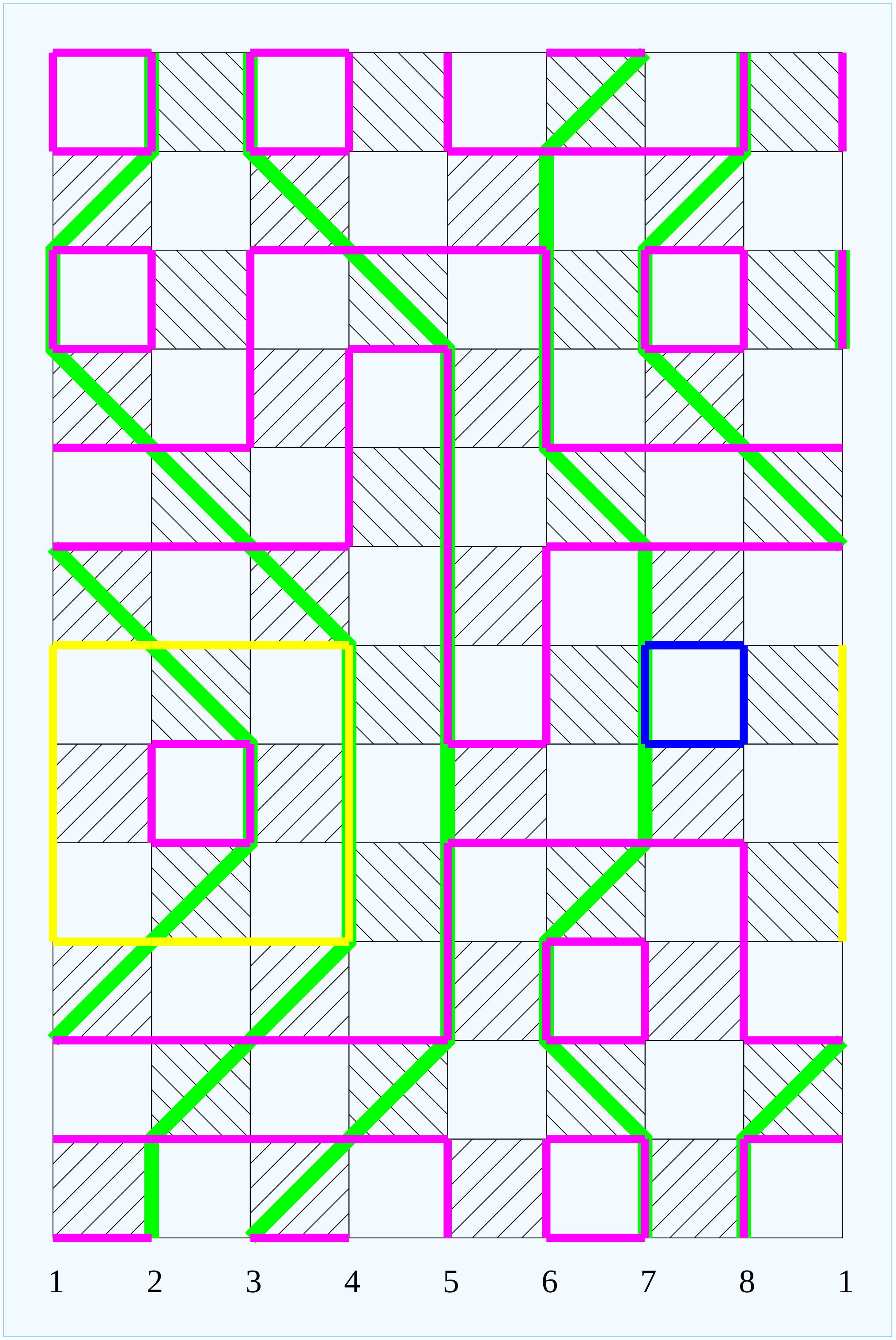

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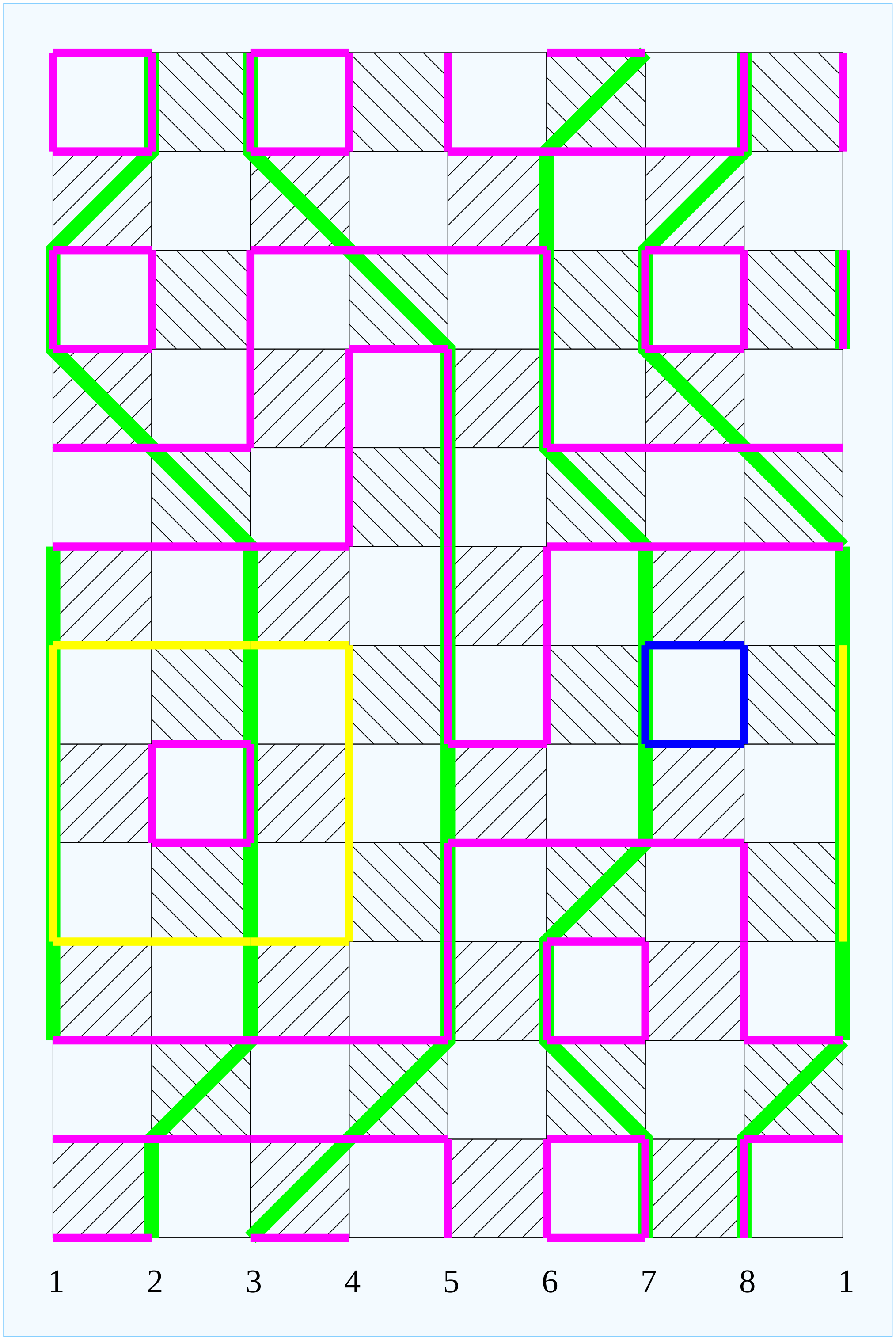

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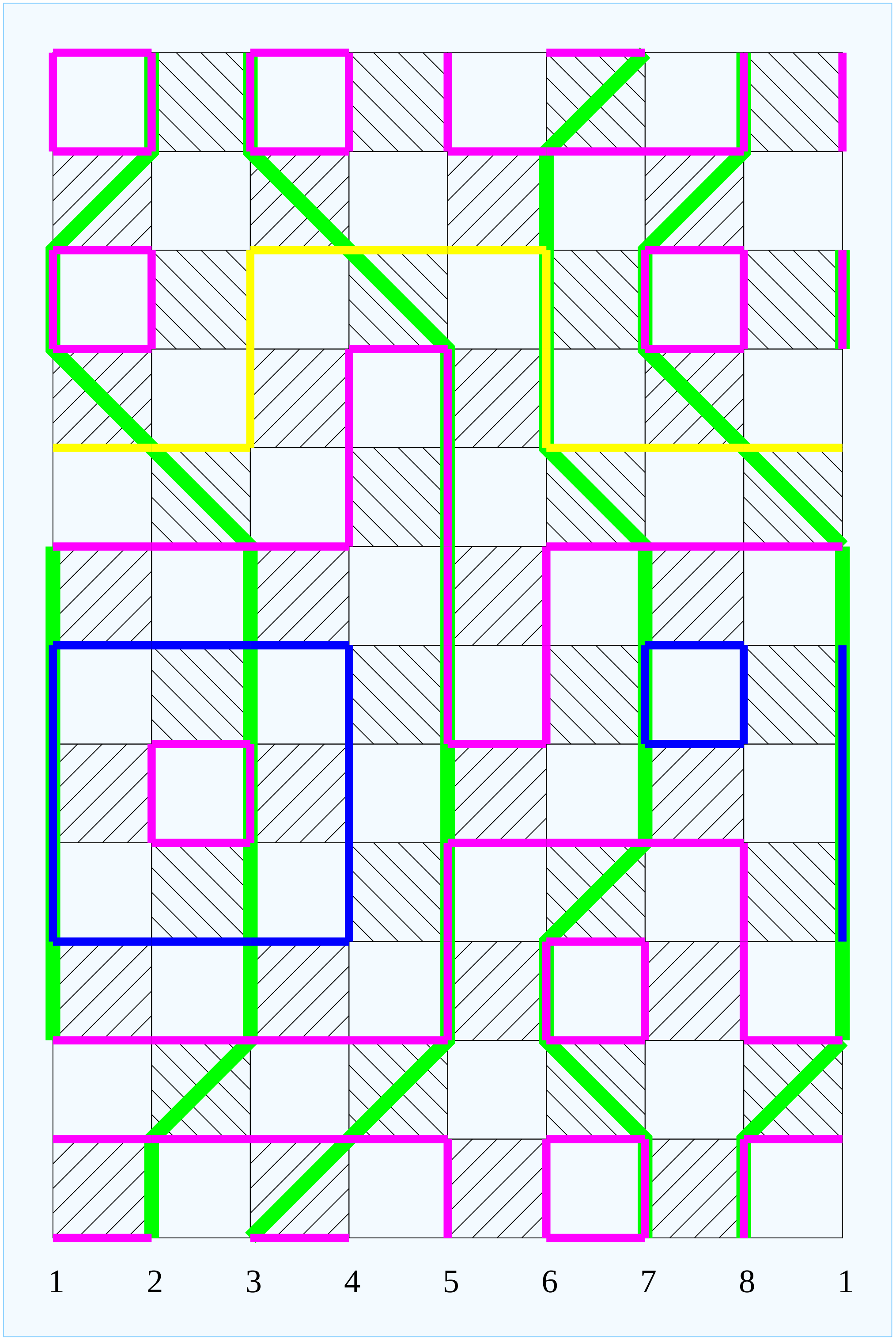

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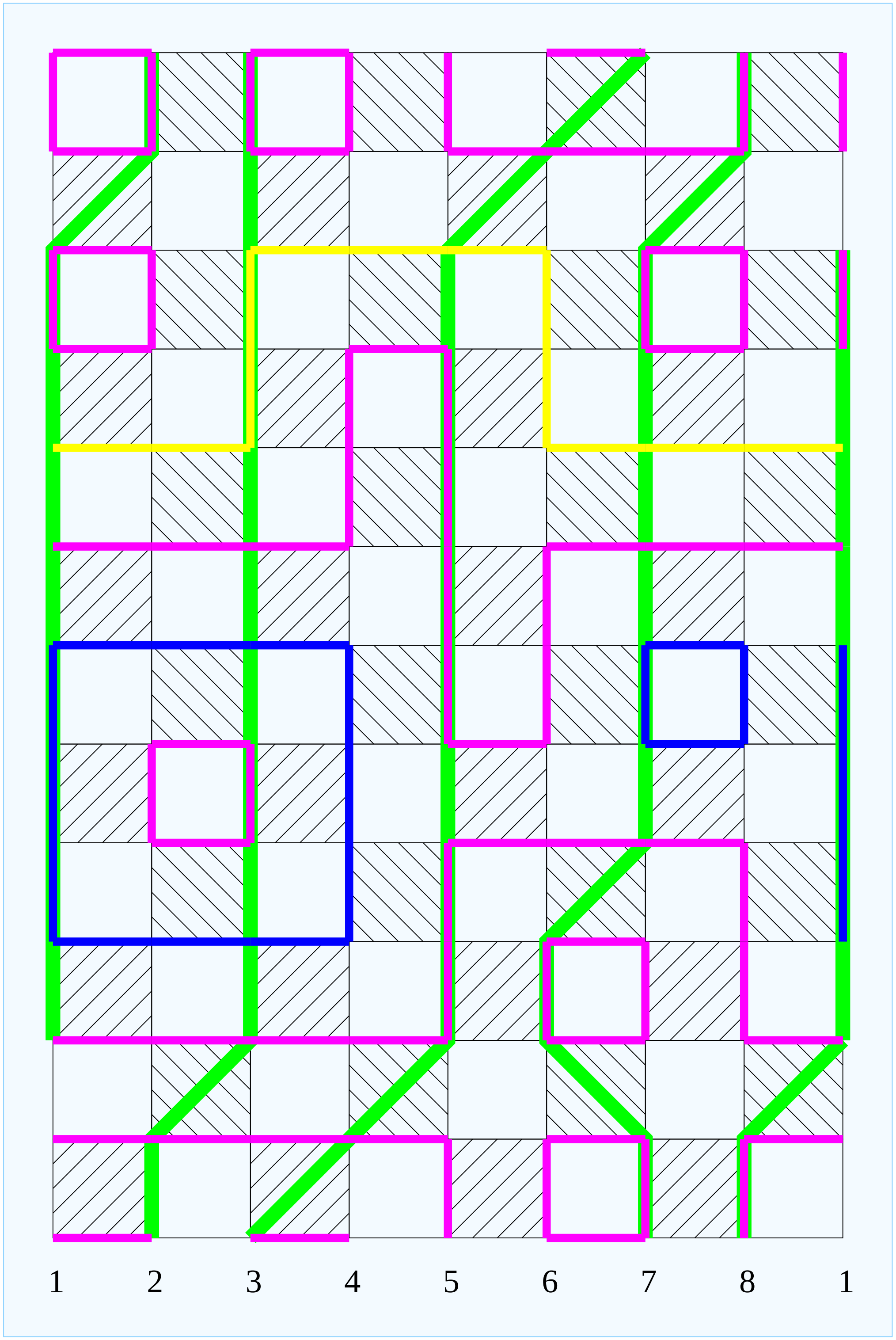

All S_T^z states accessible

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

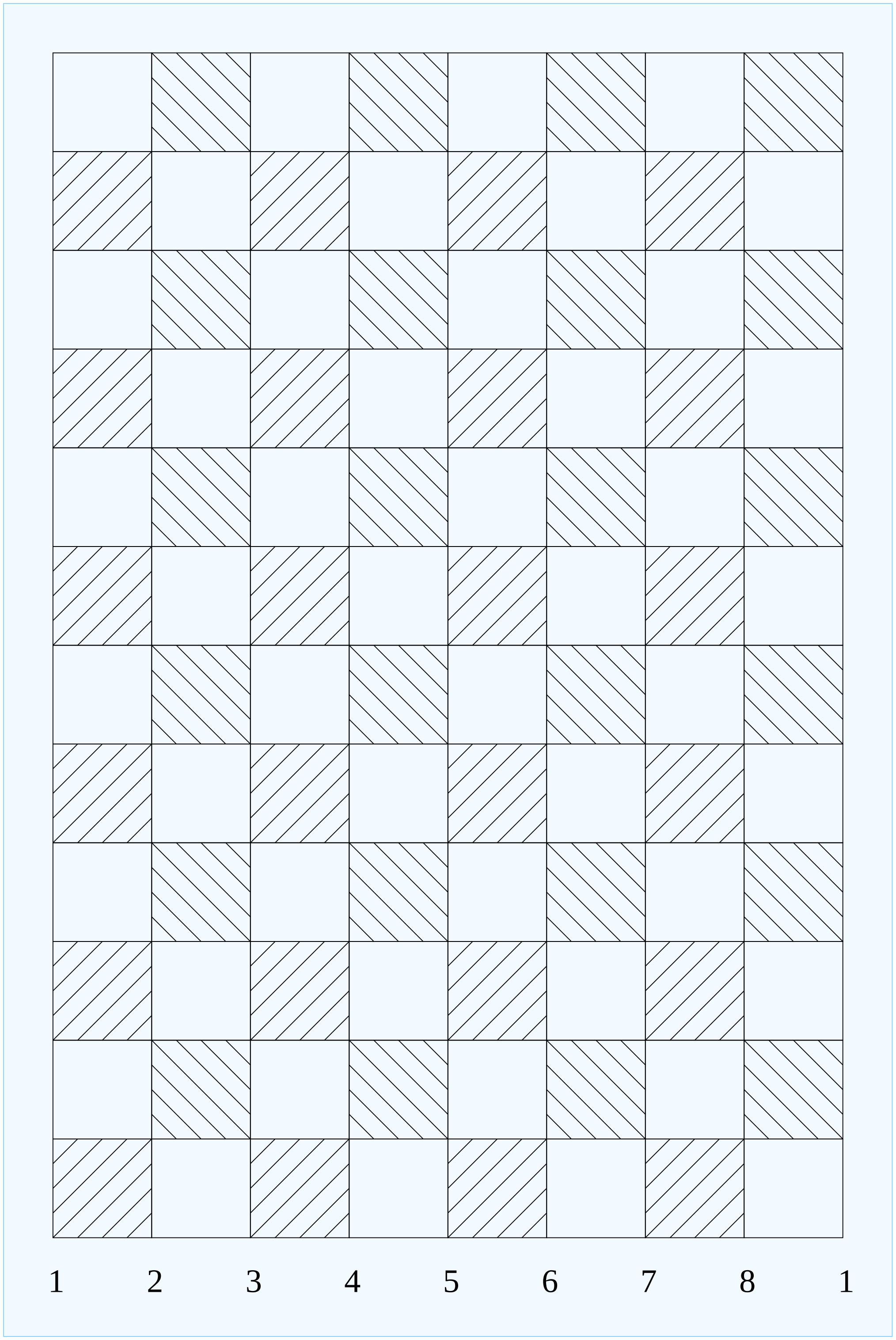
All S^z_T states accessible

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

Loops

Active loops

World lines



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Active loops

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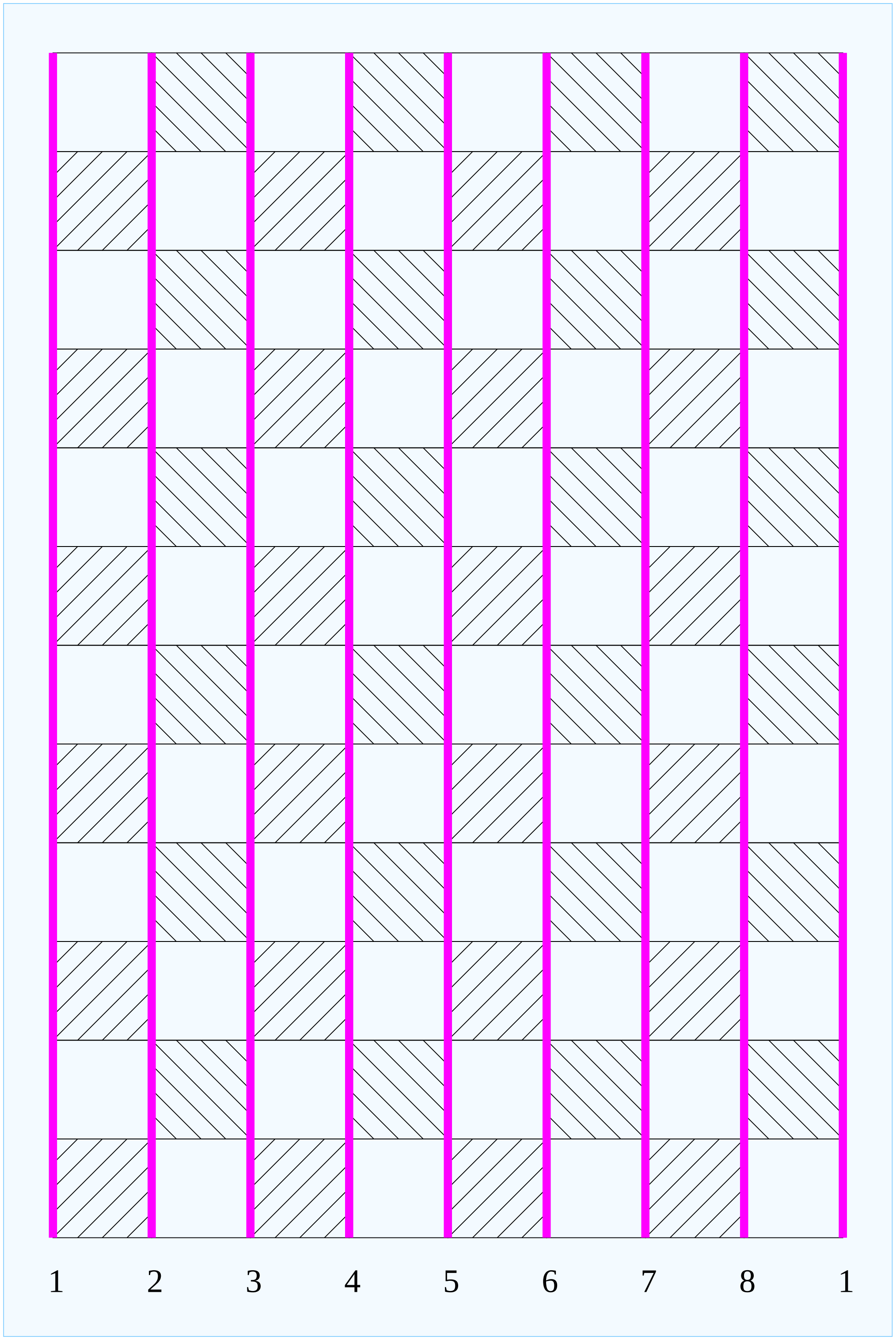

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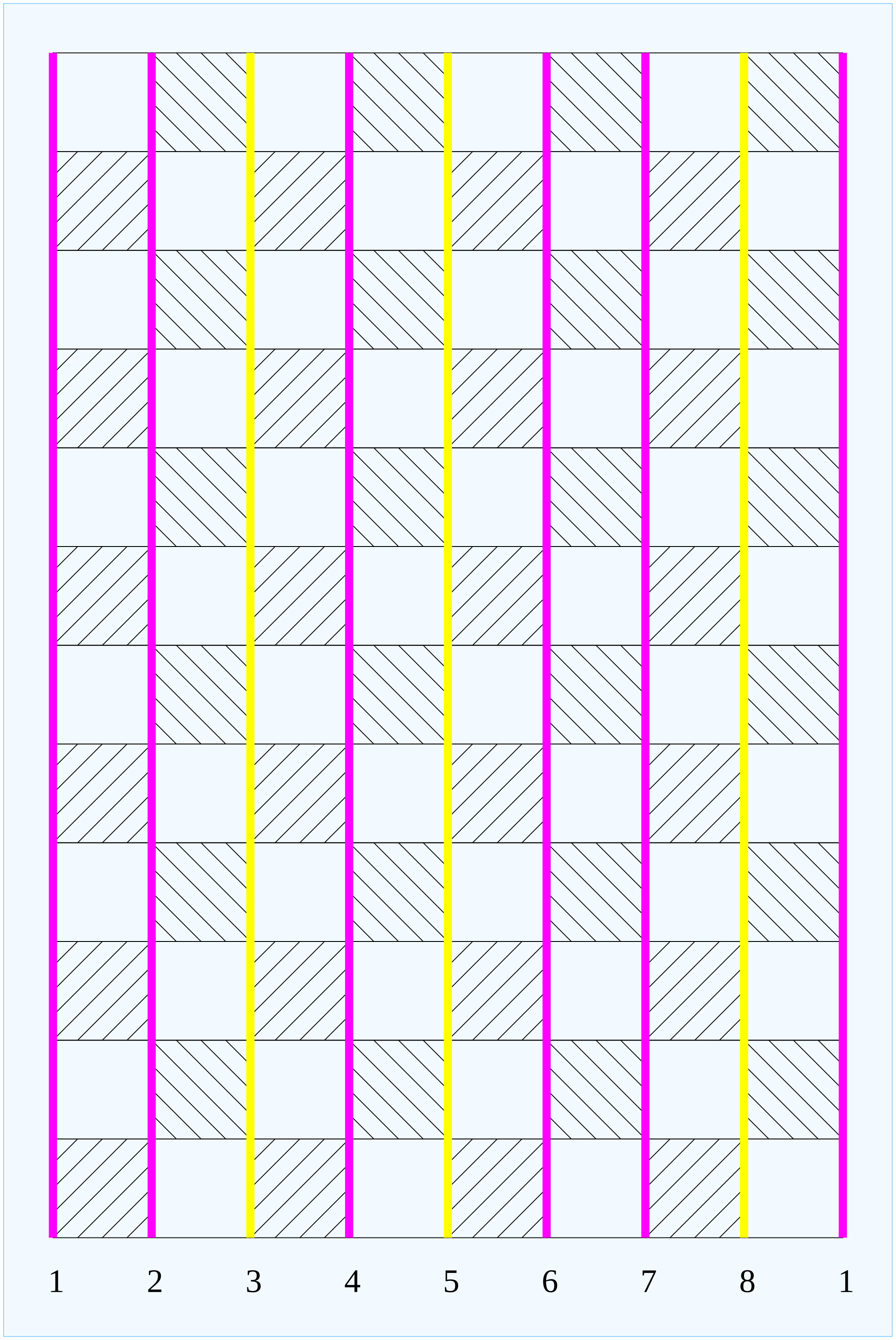

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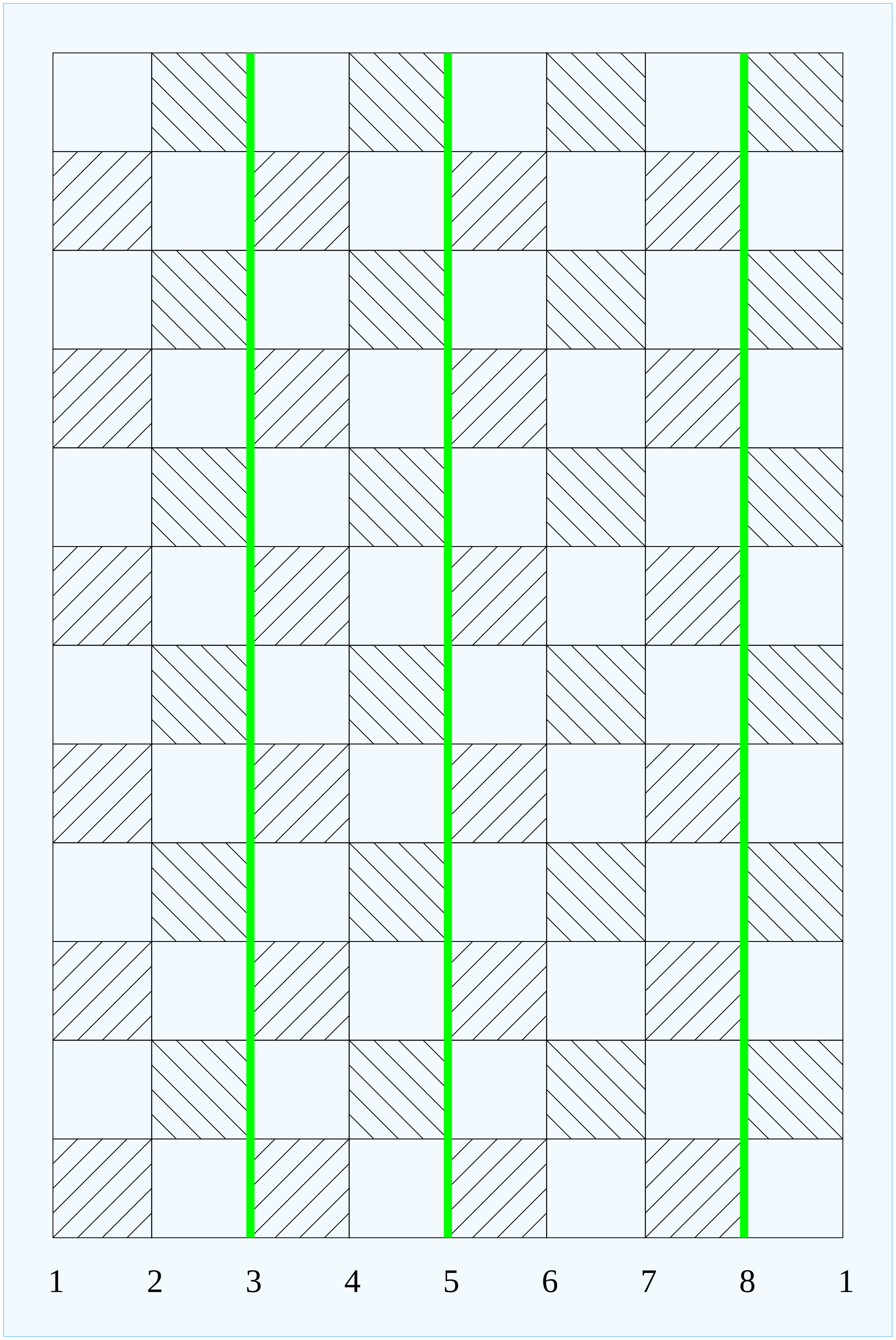
Active loops

World lines



Change of winding numbers are possible

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World lines

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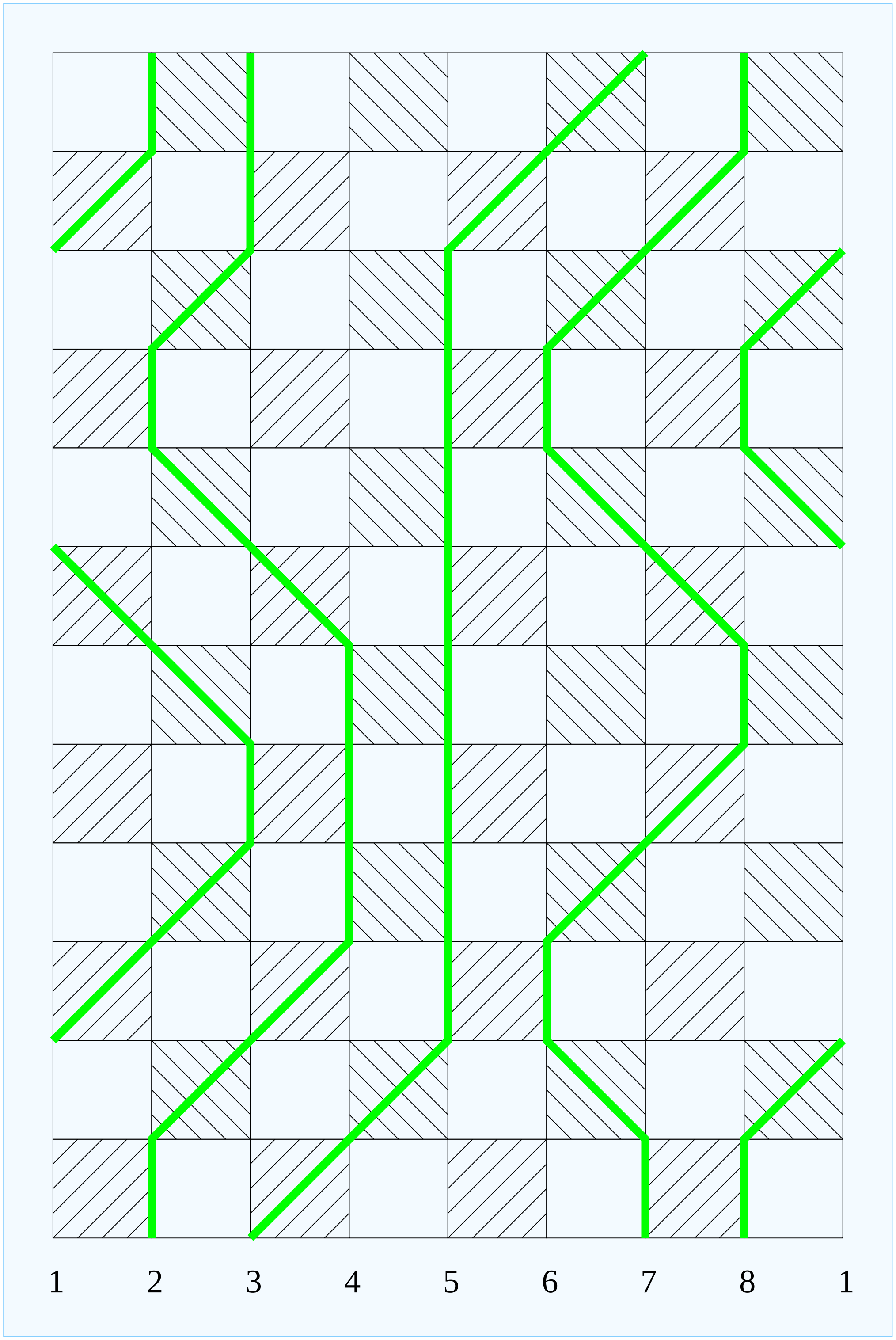
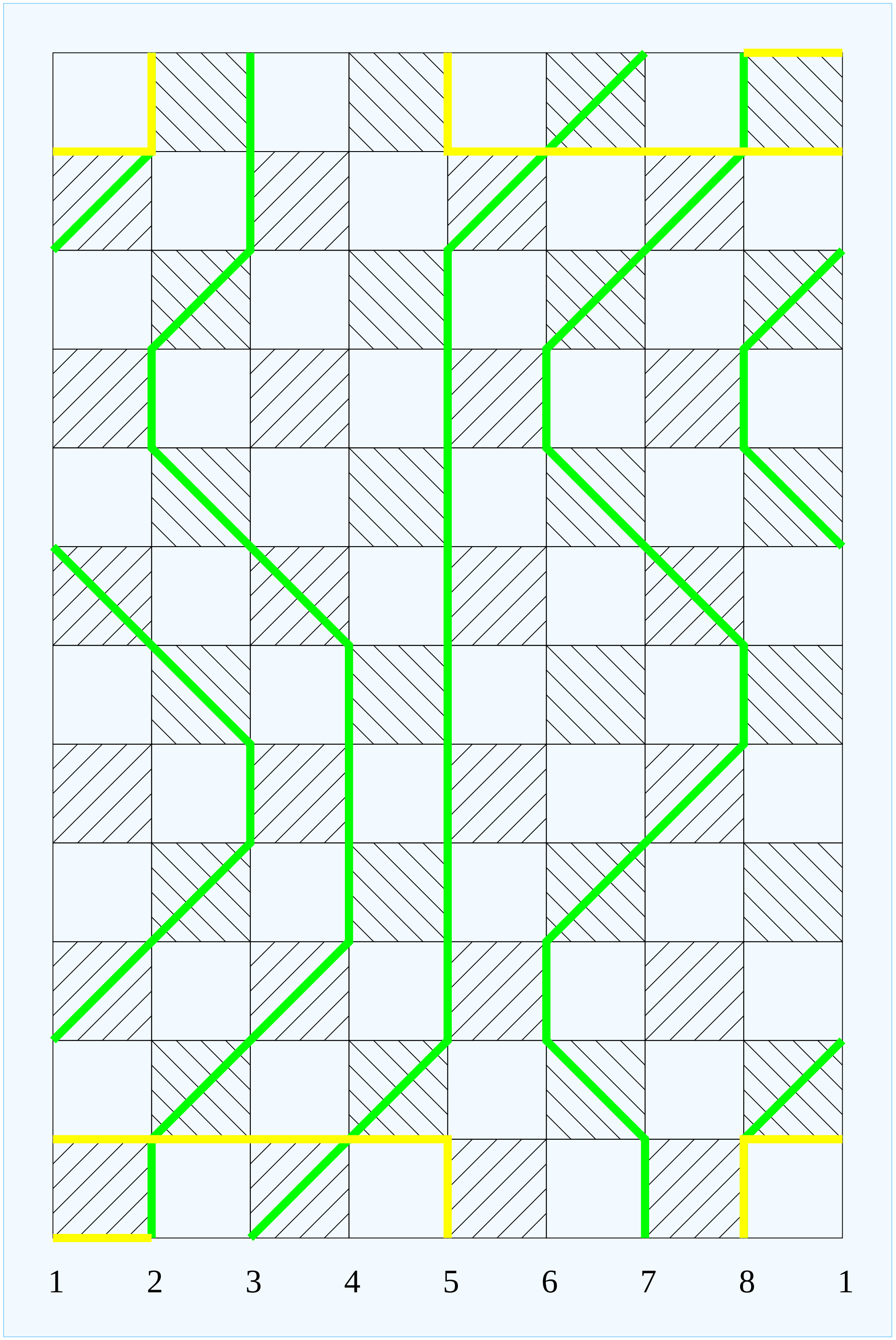


Change of winding numbers are possible

↪ Simulations are ergodic

World lines

Active loops

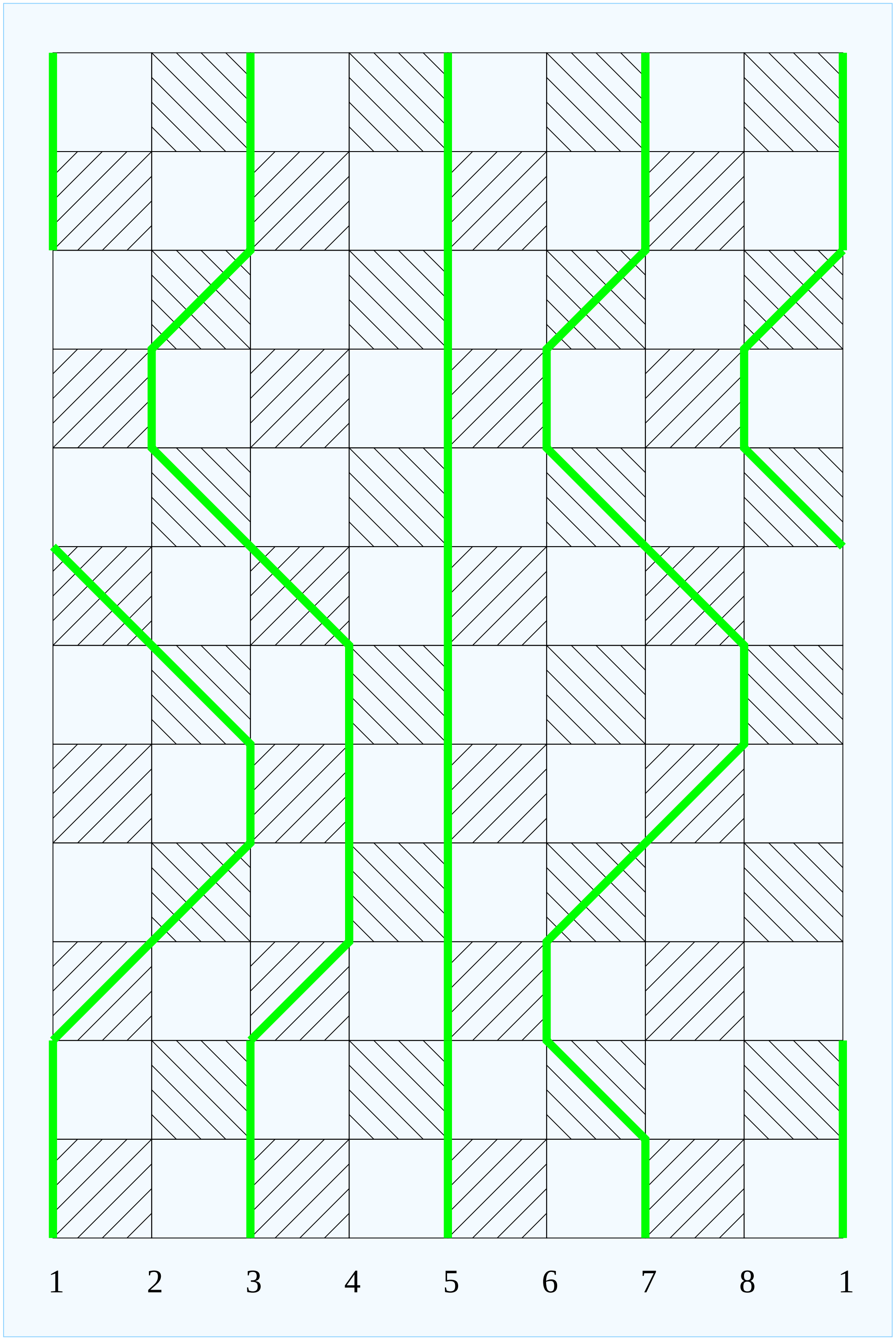


Change of winding numbers are possible

↪ Simulations are ergodic

World lines

Active loops



Change of winding numbers are possible

↪ **Simulations are ergodic**

World lines ▬

Active loops ▬

Short autocorrelation times.