Efficient implementation of connectivity changing moves for dense polymers

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- Monte Carlo algorithms may allow for dramatically better sampling rates for equilibrium systems.

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- Will now give an example: the pivot algorithm for self-avoiding walks.

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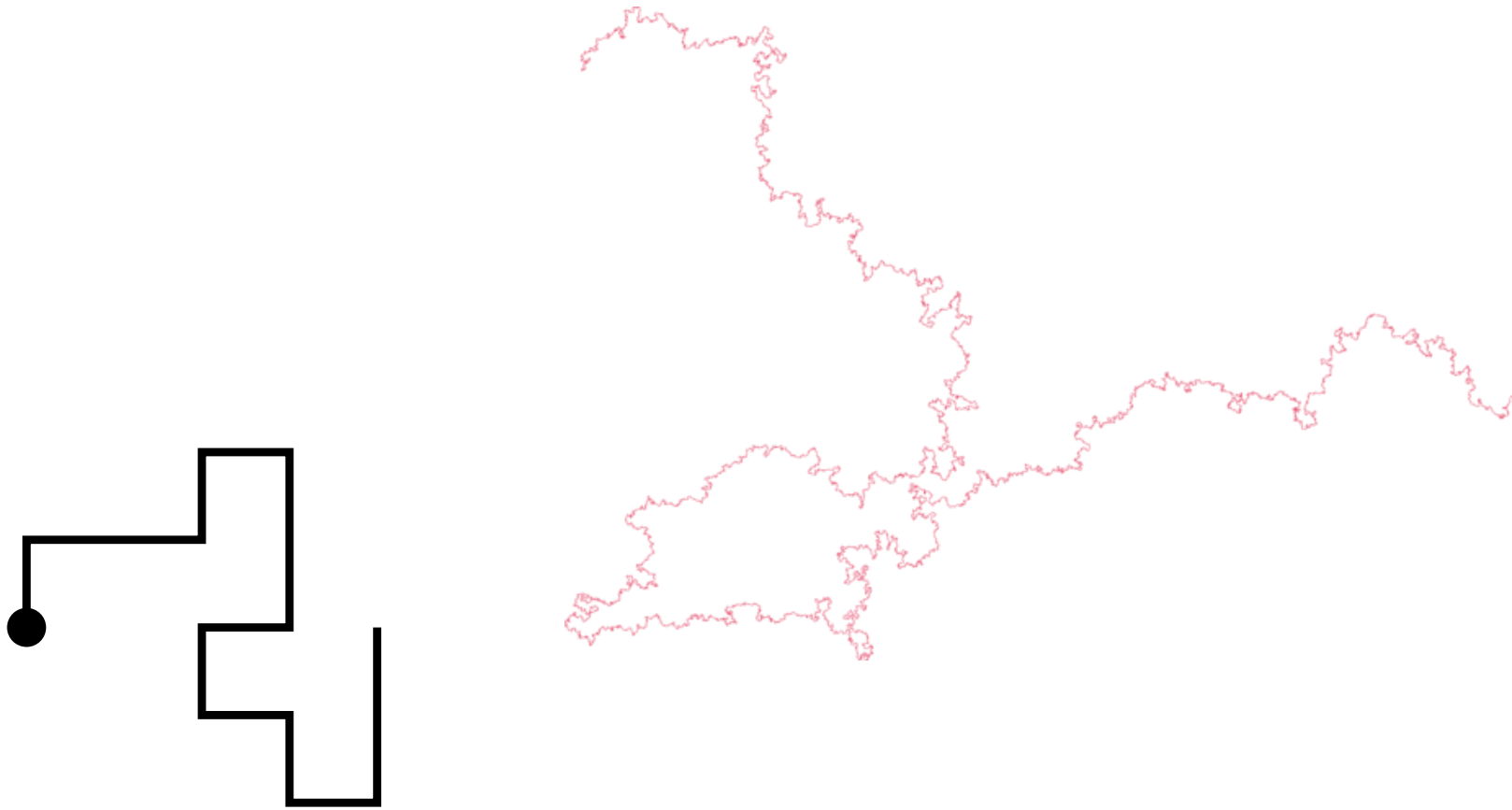
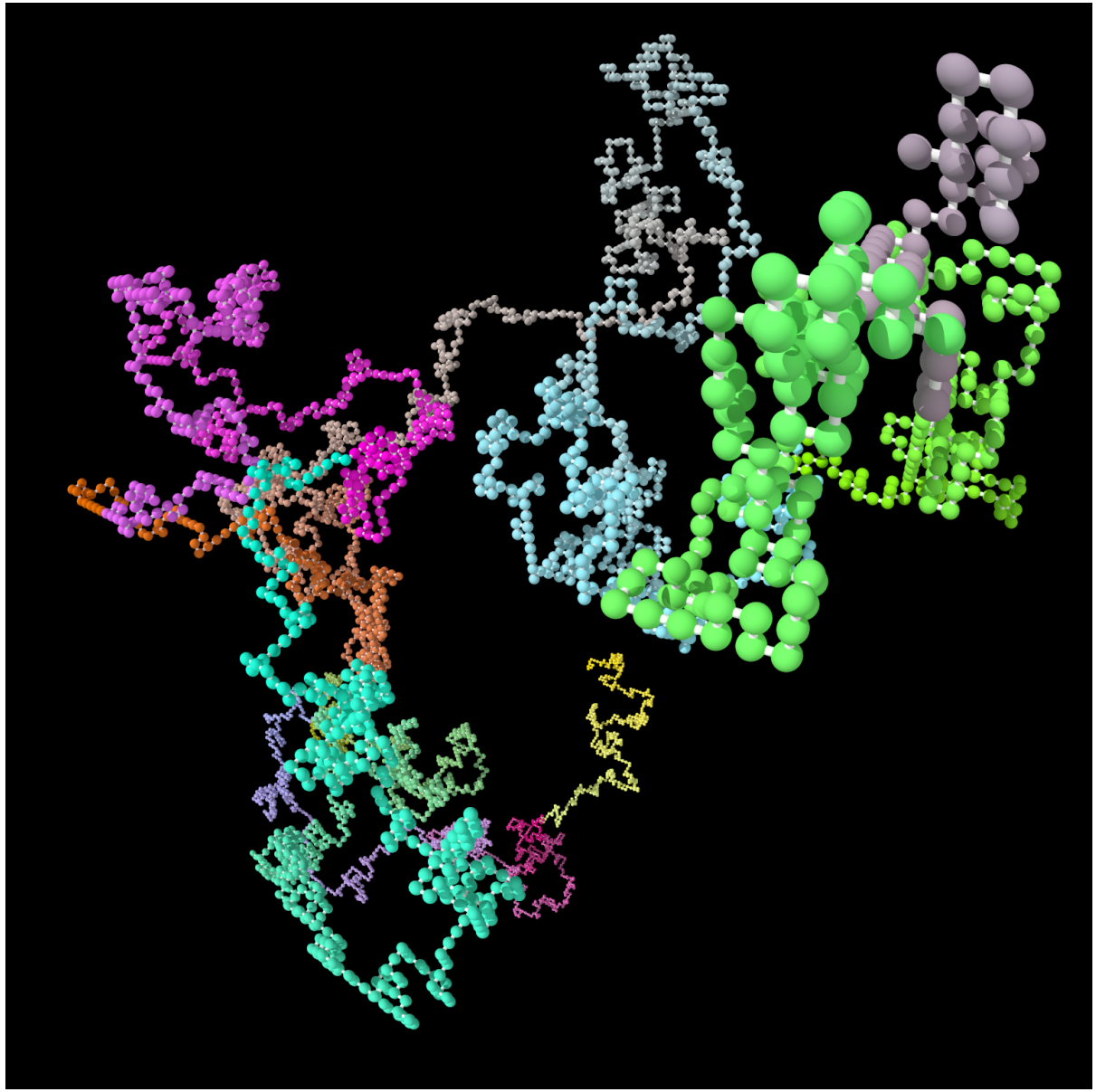
- Graph: typically $\mathbb{Z}^d$, but sometimes random networks, percolation clusters.
- Models dilute solution of polymers in a good solvent.



Self-avoiding walks of 15 and 2^{25} steps.



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- Mean-squared end-to-end distance for SAWs of length N:

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- Flory exponent ν is universal; same for SAWs and real world polymers.

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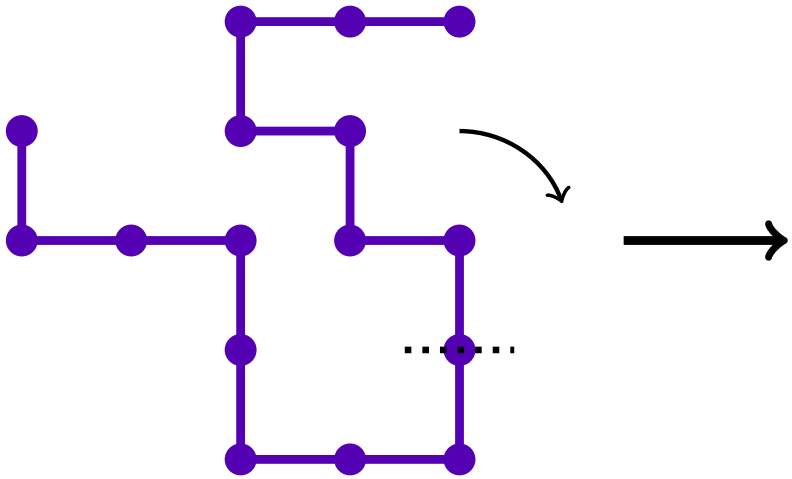
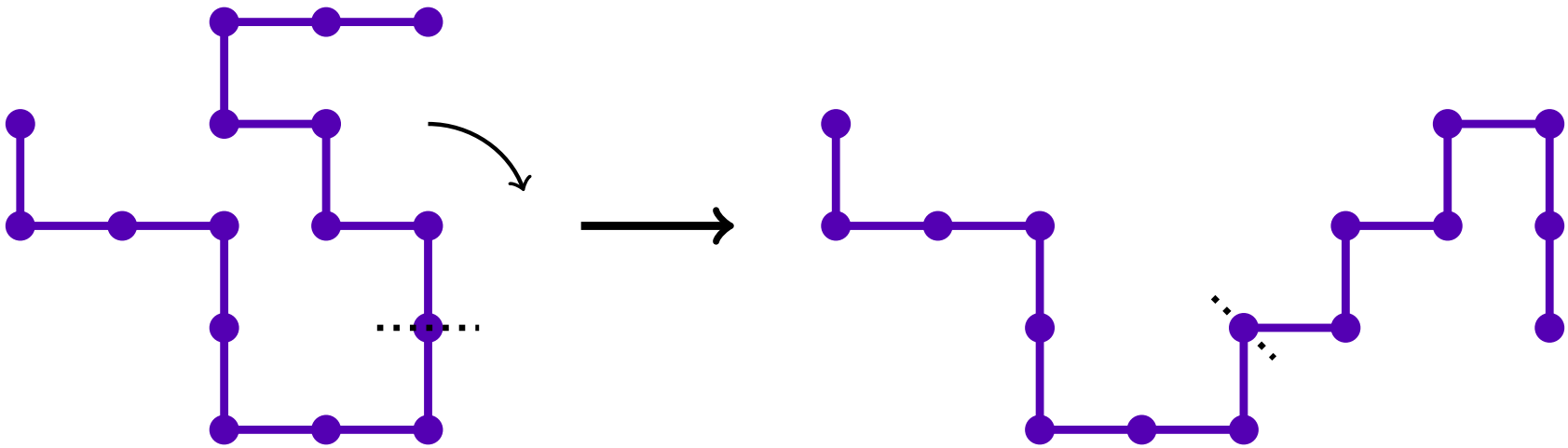


Example pivot move



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- In fact, don't need to write down! CPU time $O(N^{0.74})$[4].
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- Bookkeeping can be handled efficiently in binary tree structure $O(\log N)$[5].

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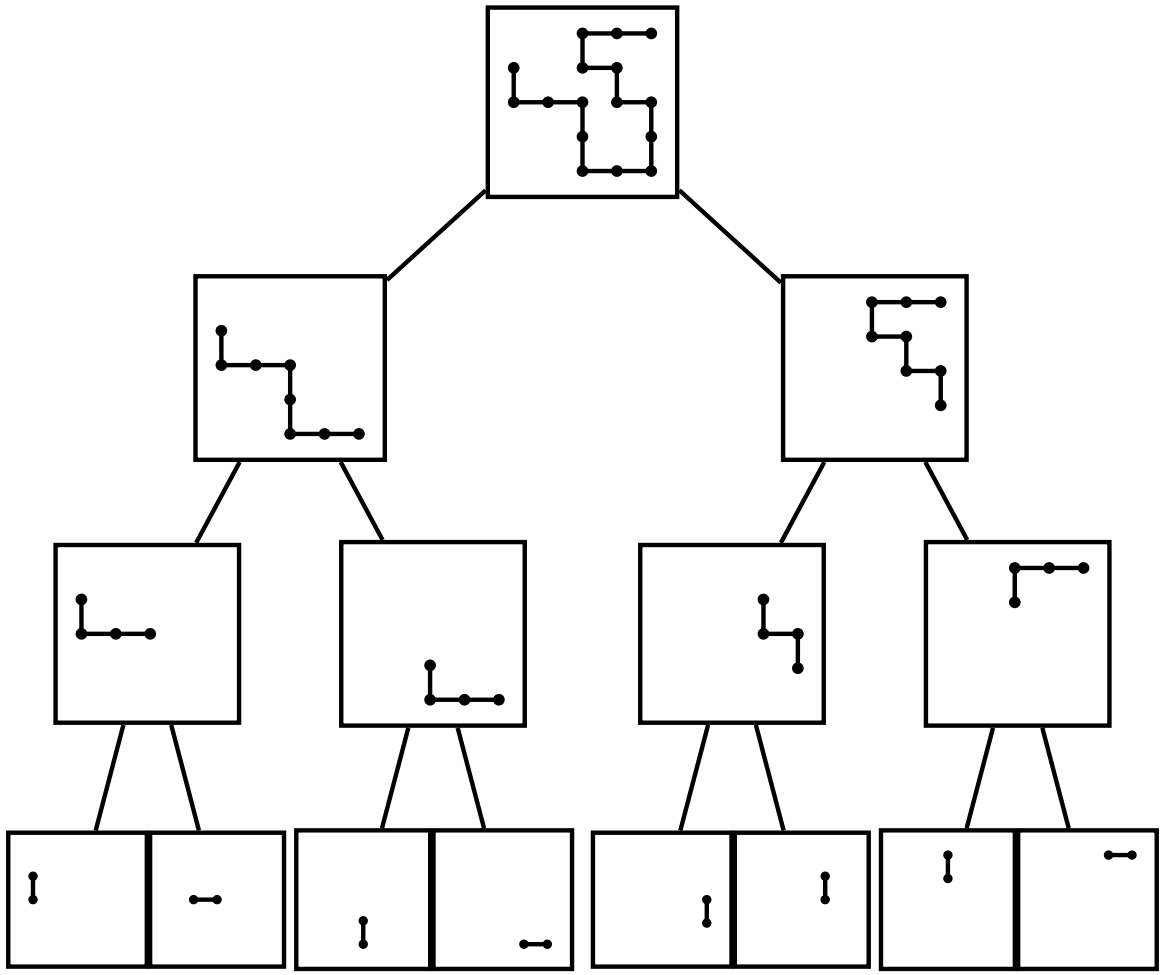

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- *Global effect* for *local cost*.

Results

- Simulations of SAWs with up to 1 billion monomers.

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- Can we find a fast global move for dense polymers?

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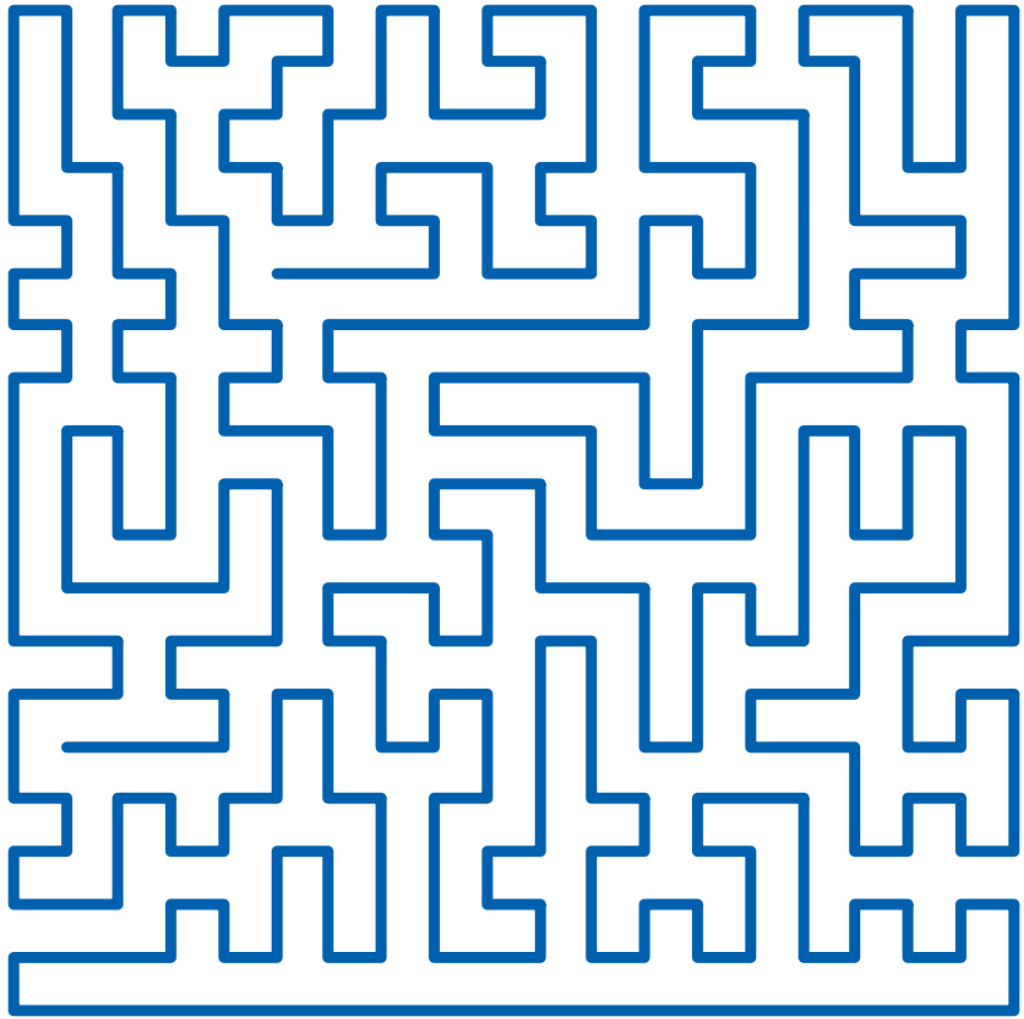

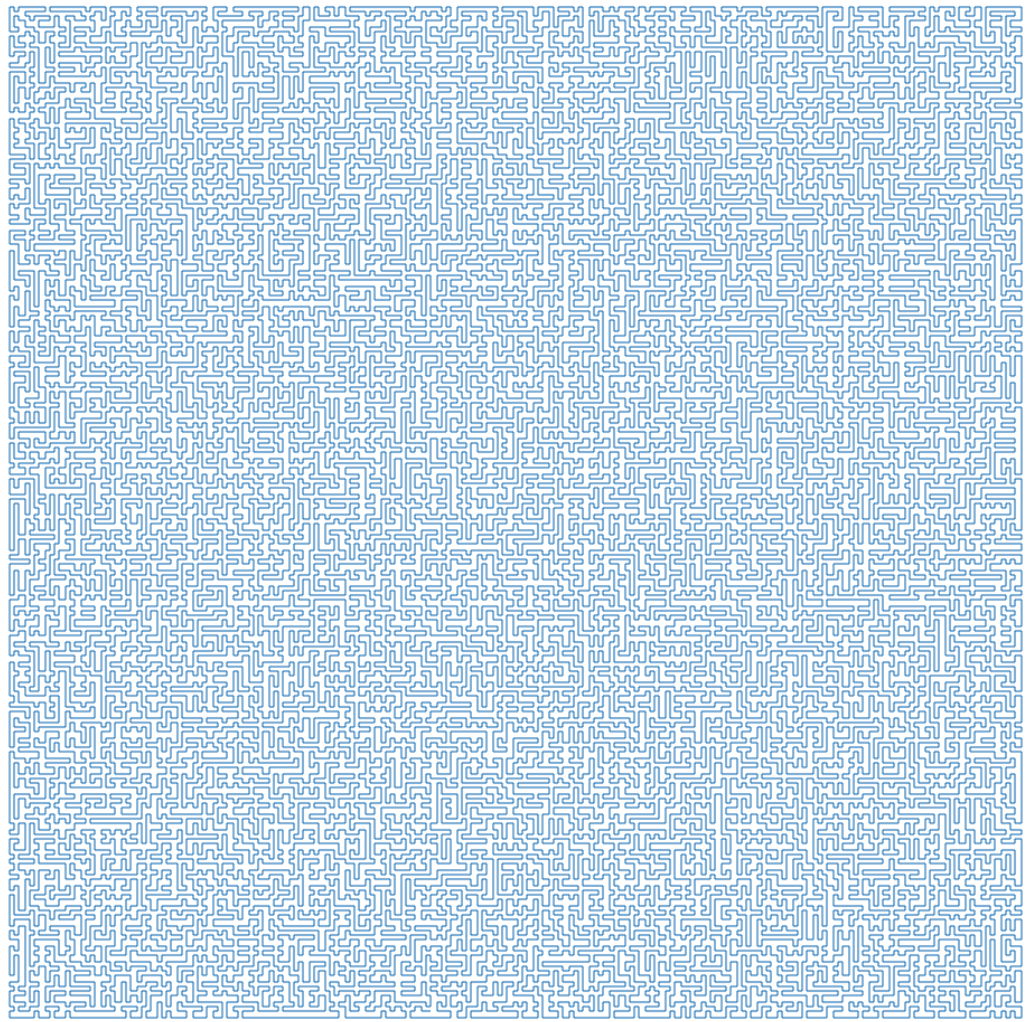

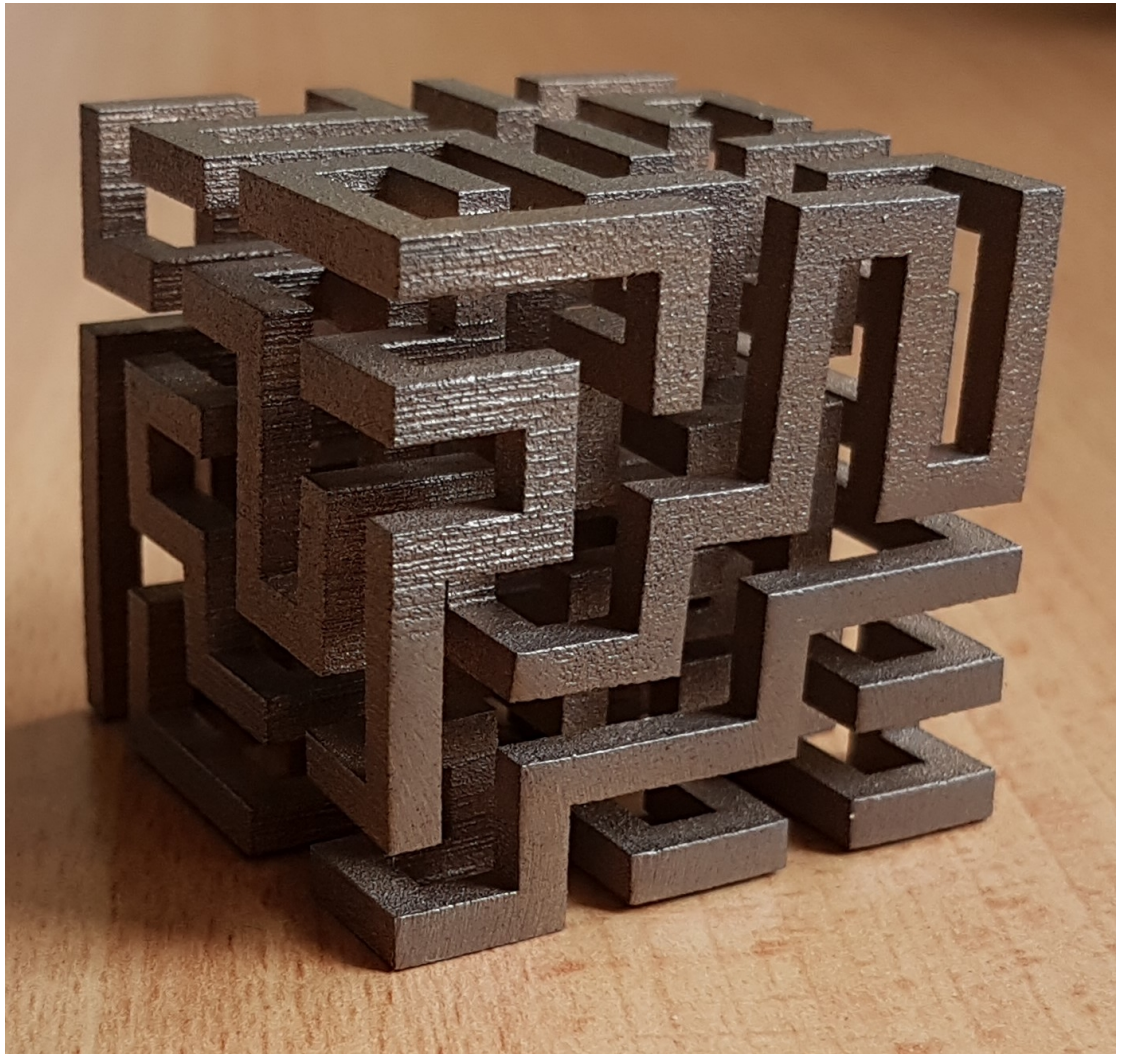

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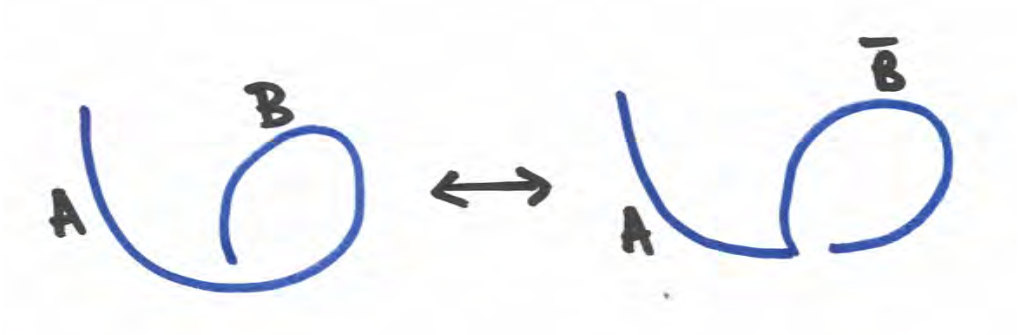
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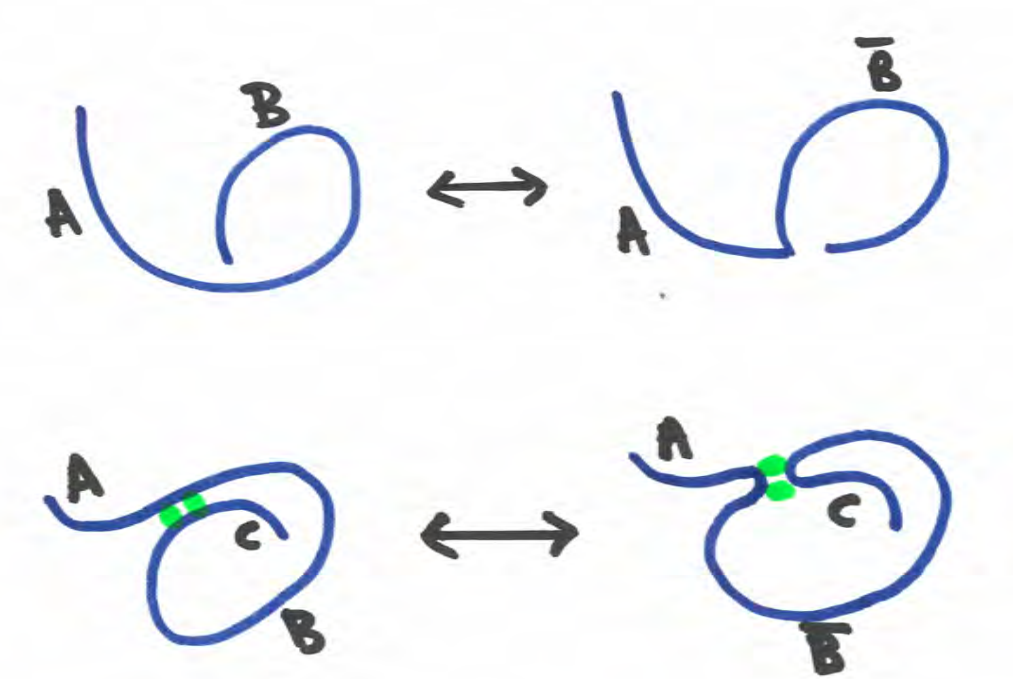
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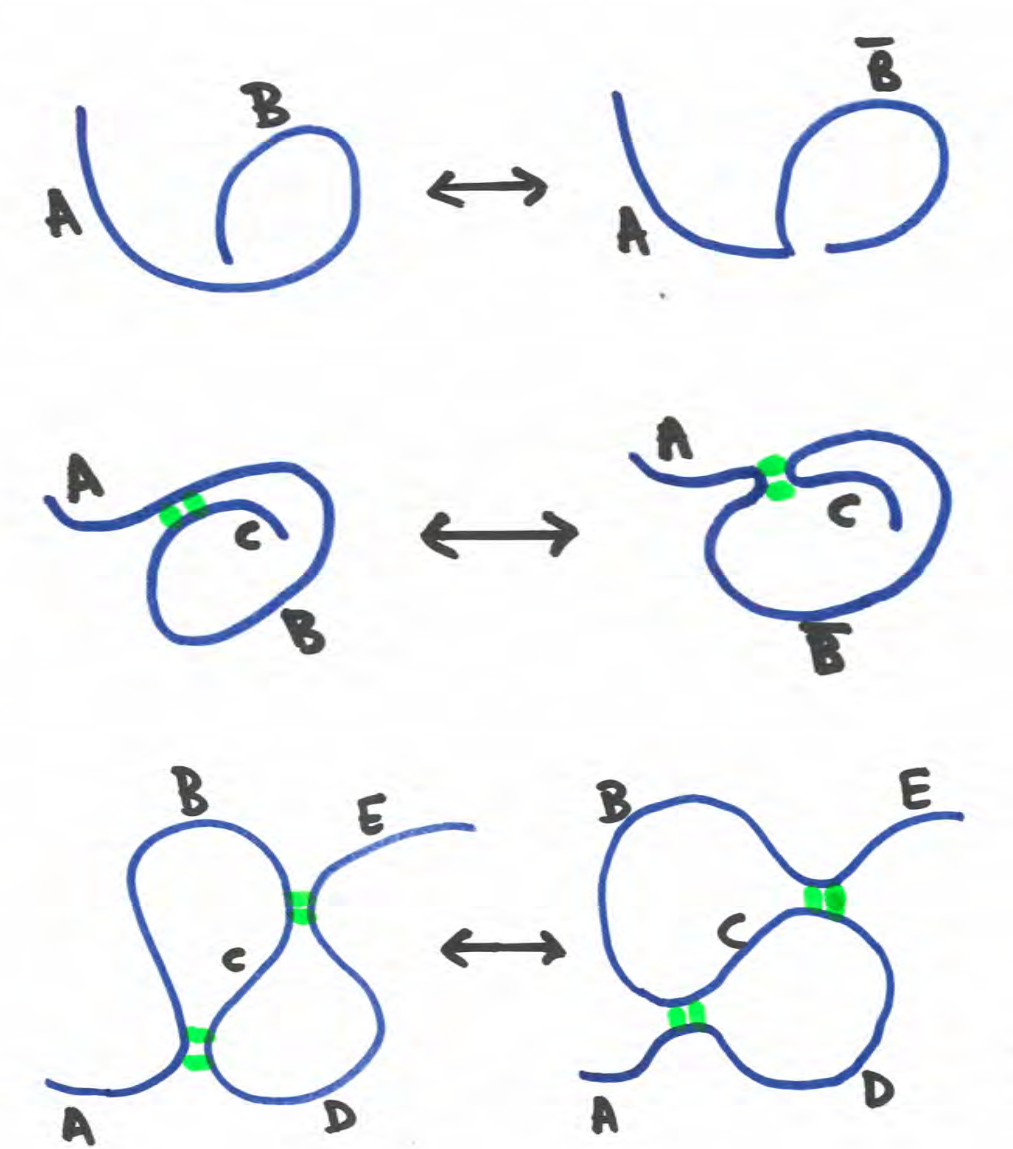
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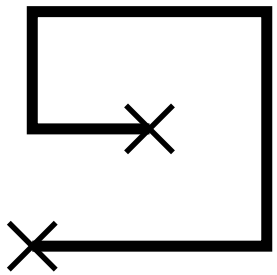
Backbite moves for sampling Hamiltonian paths.



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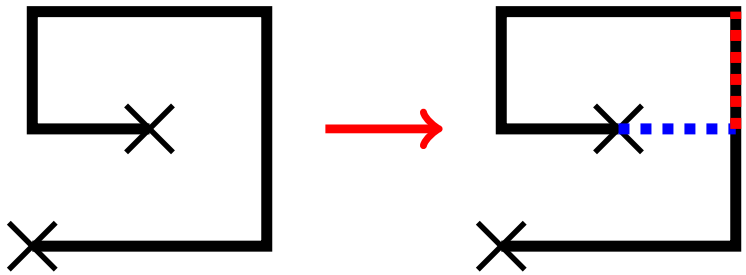

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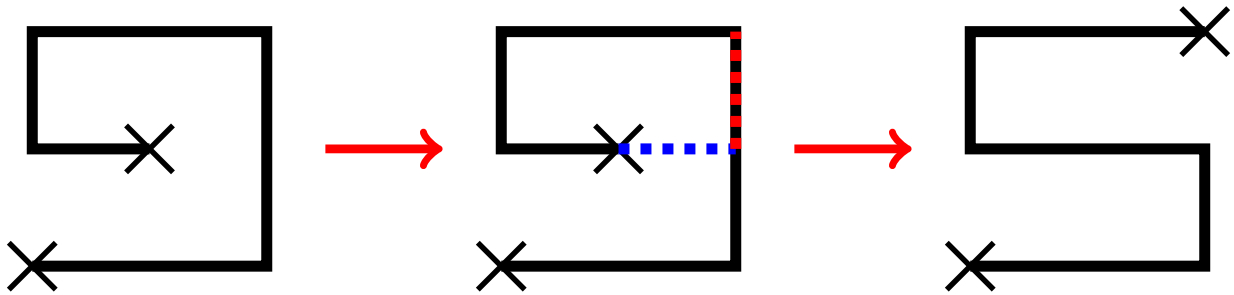

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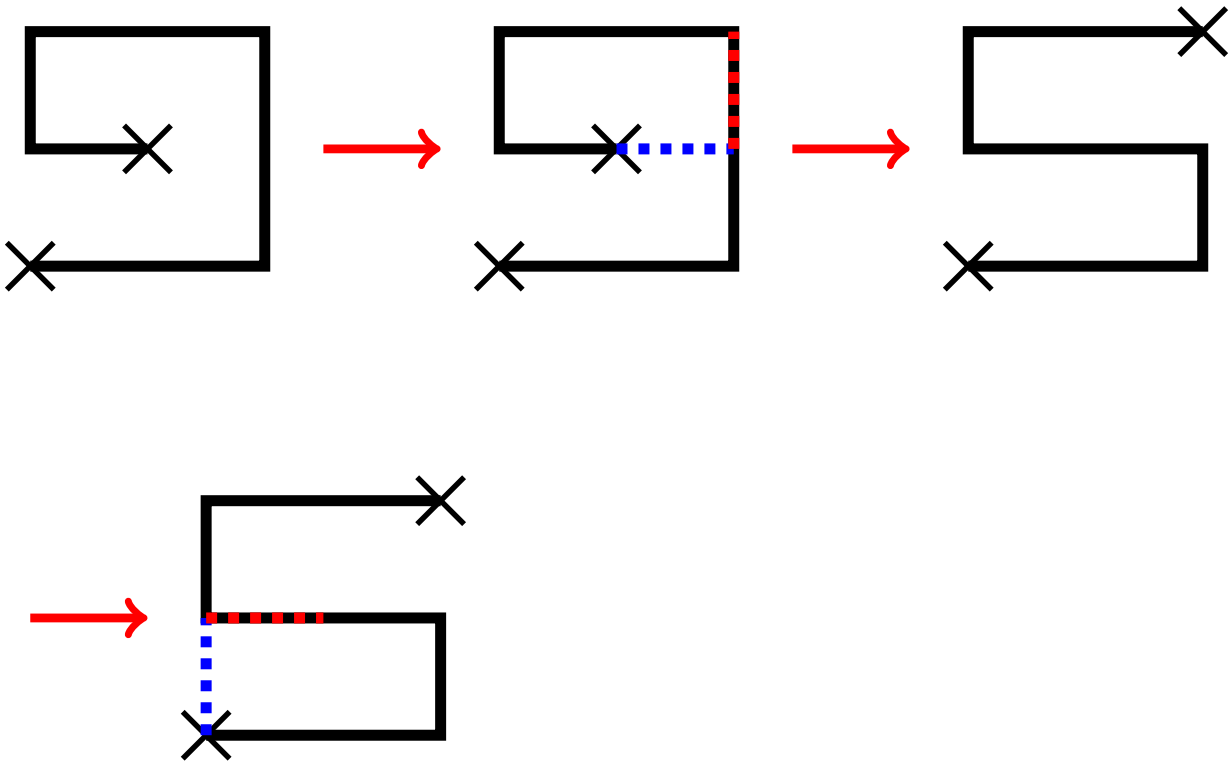

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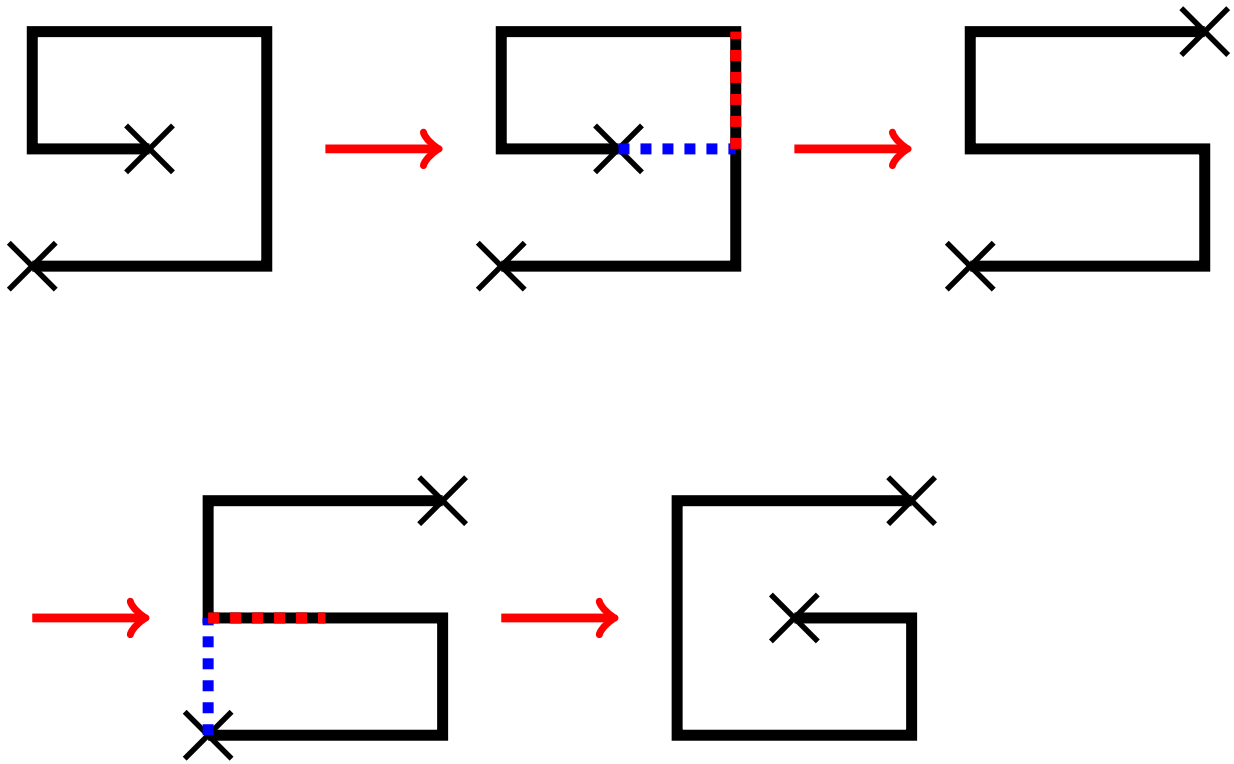

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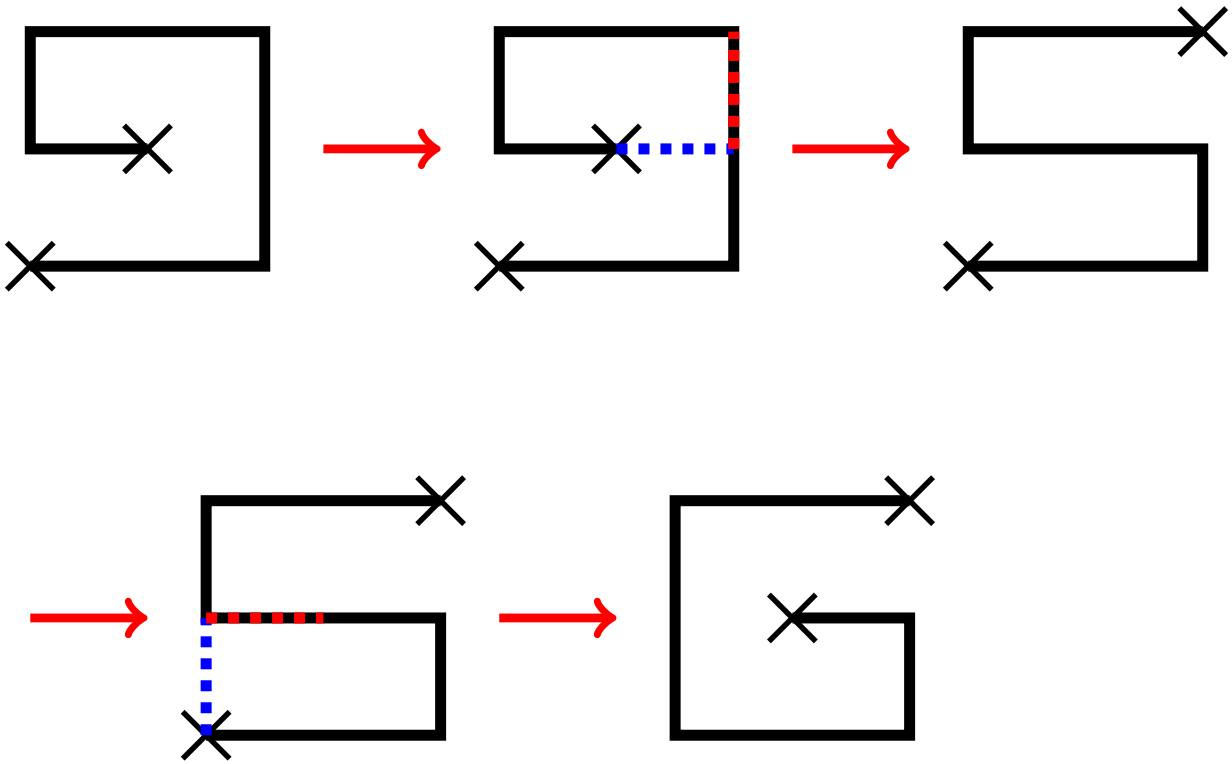

Each time we make a backbite move we create a loop, delete the edge which completes the loop, and *reverse* the orientation of the remaining edges of the loop.

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- Are the moves fast?
  - For a loop of length N, naive implementation of backbite move takes CPU time $O(N)$ as it requires reversal of N steps.

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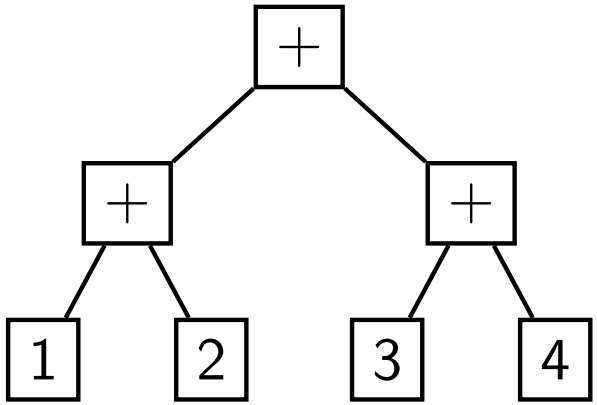
- Use binary tree data structure with *time reversal* as our symmetry operation, with bookkeeping for determining neighbours.

Backbite move

- For the simple cubic lattice, loops are of mean size $O(N)$.
- $\Rightarrow$ mean CPU time per backbite move $O(N)$.
- But, like with SAW, we don't need to explicitly "write down" each step of the walk, just need to be able to store information about structure, and find neighbours of walk ends.
- Use binary tree data structure with *time reversal* as our symmetry operation, with bookkeeping for determining neighbours.
- Can generalise to other moves for dense polymers, e.g. bond rebridging.

Time reversal symmetry elements in the binary tree nodes.



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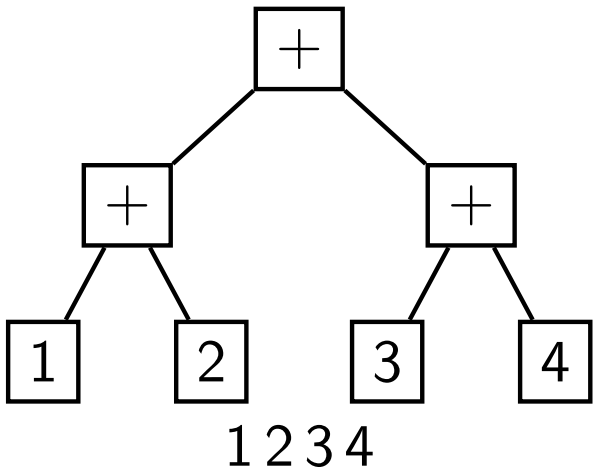

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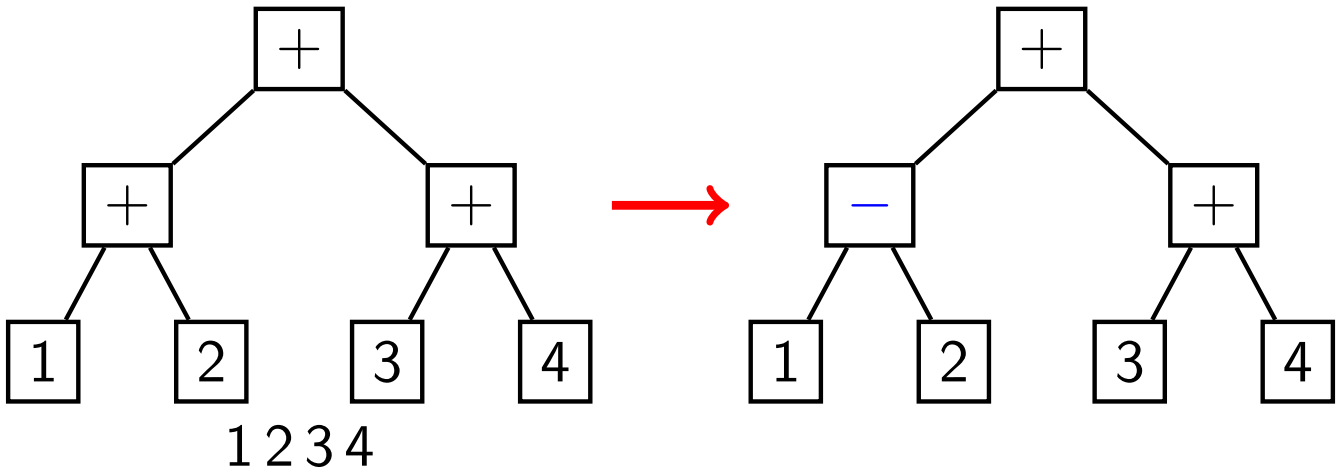

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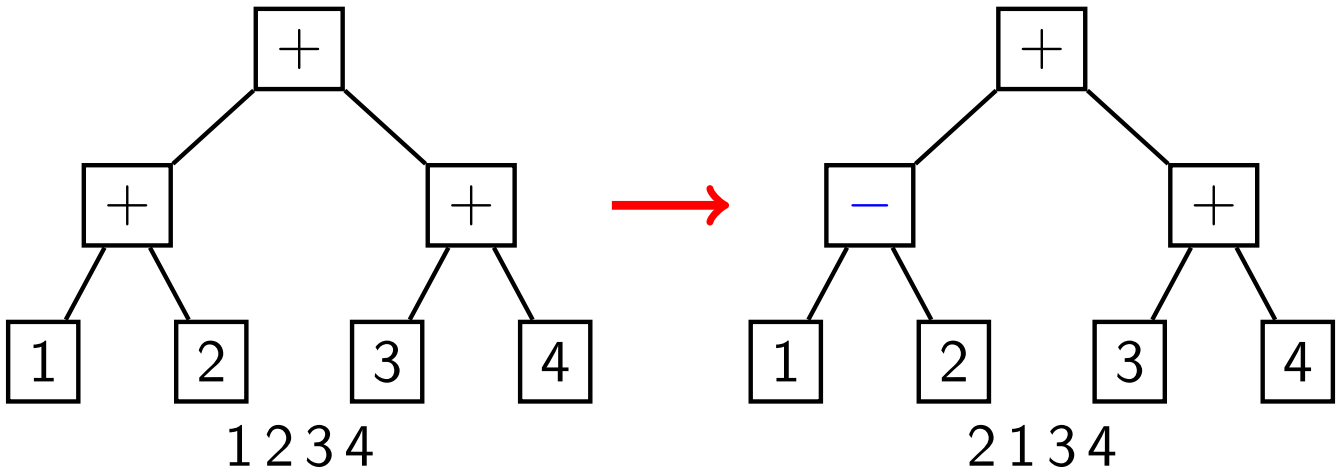

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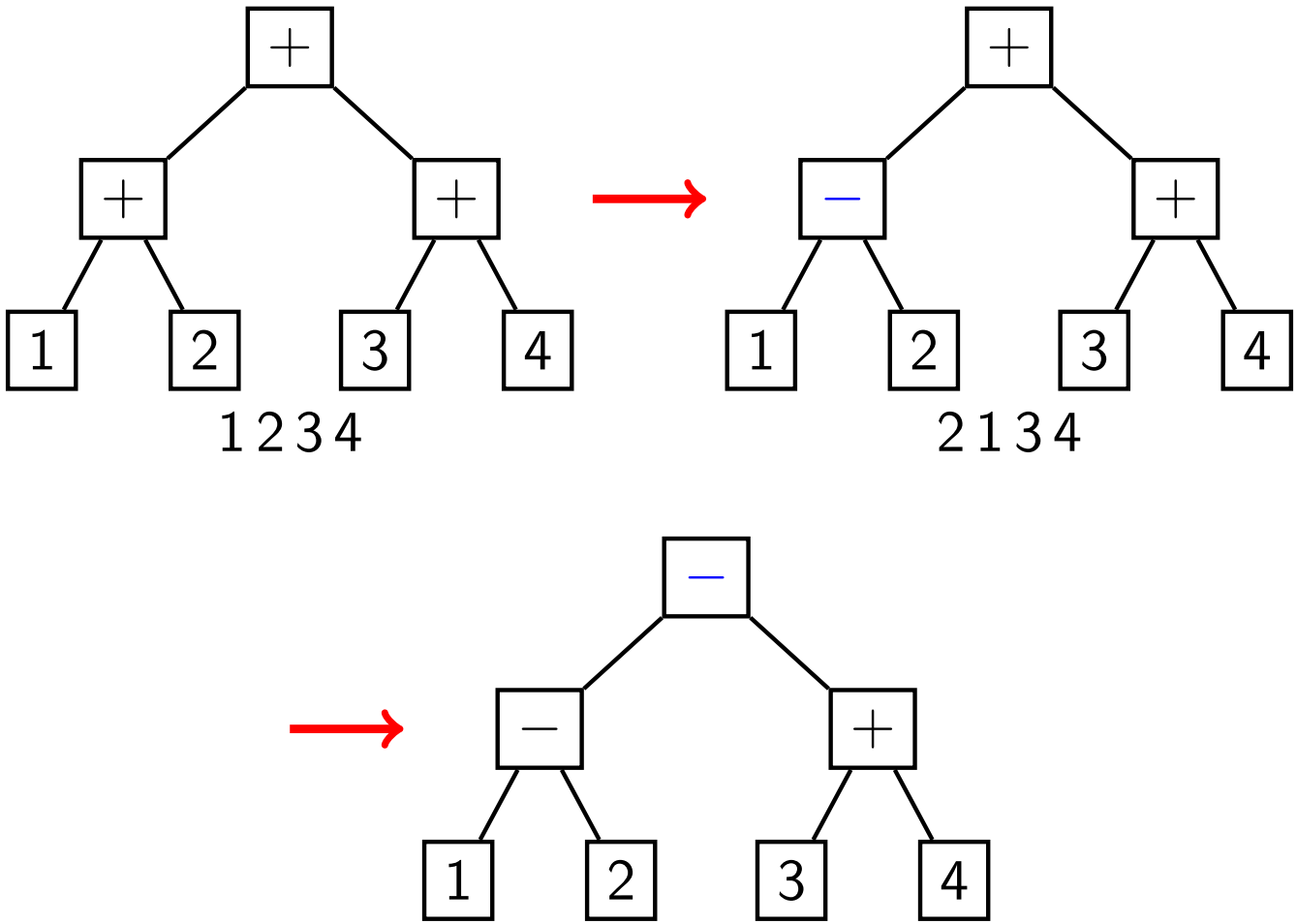

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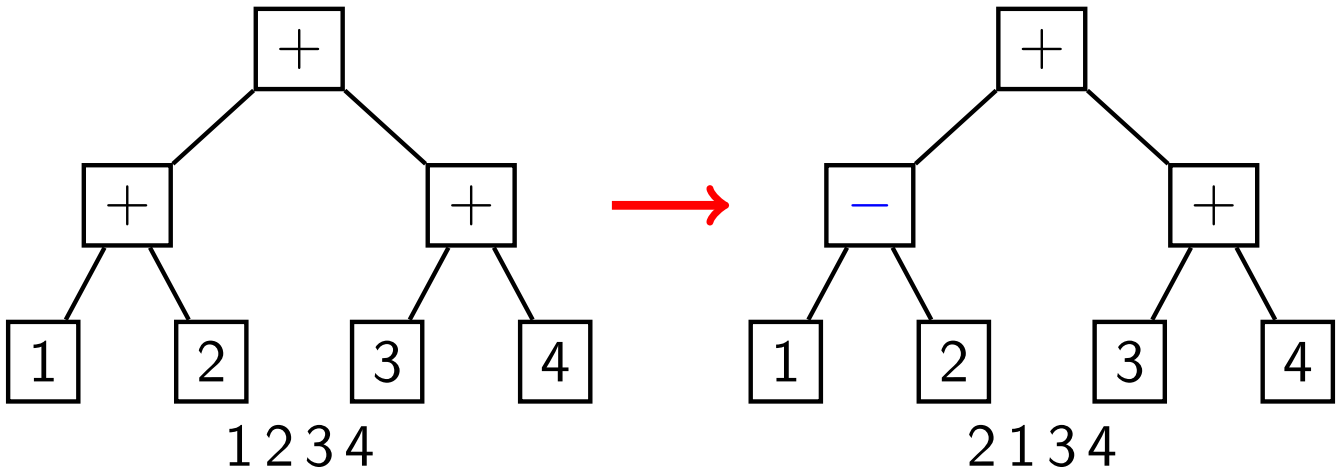

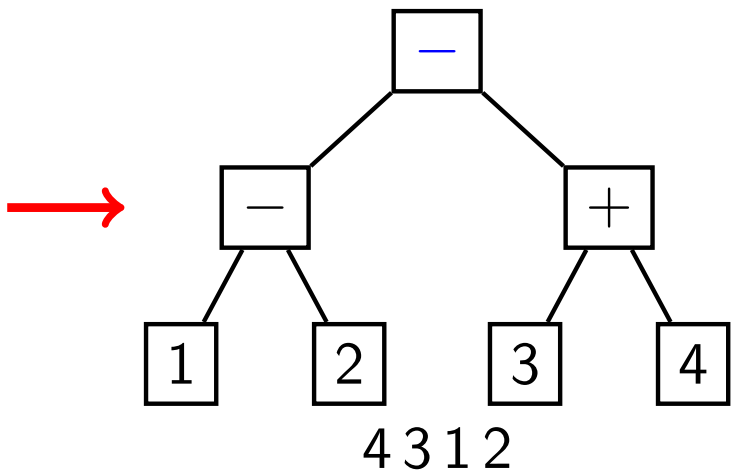

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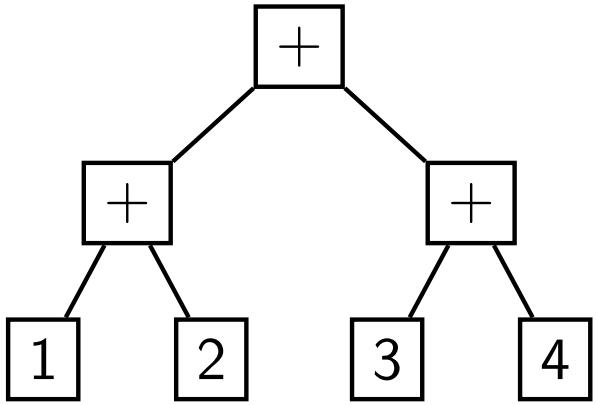

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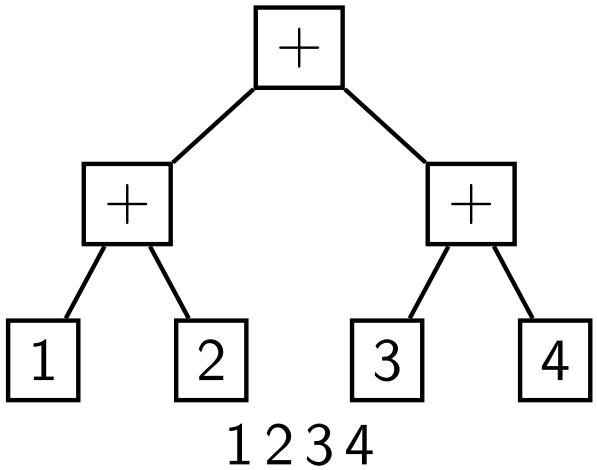

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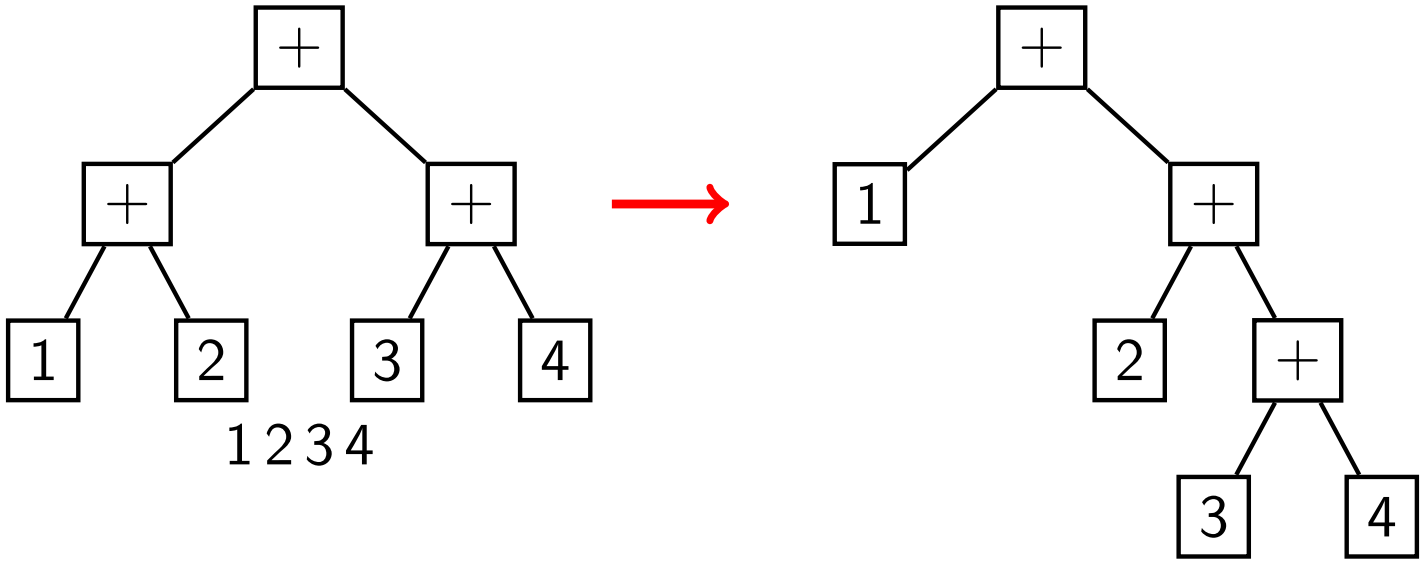

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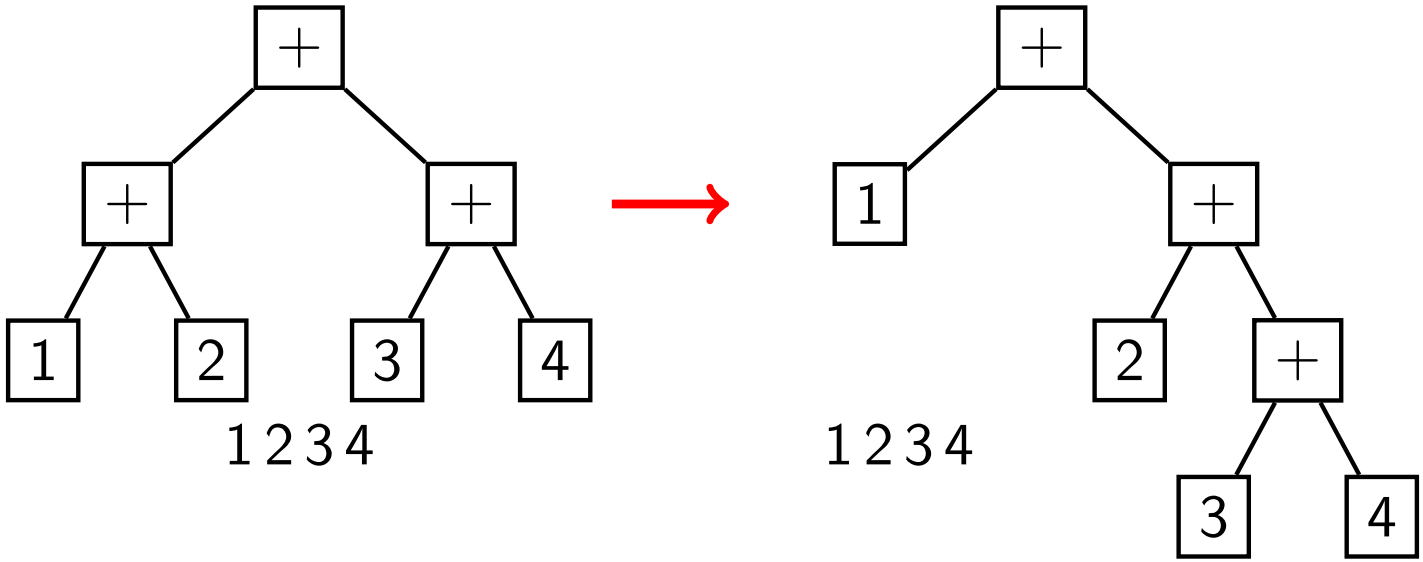

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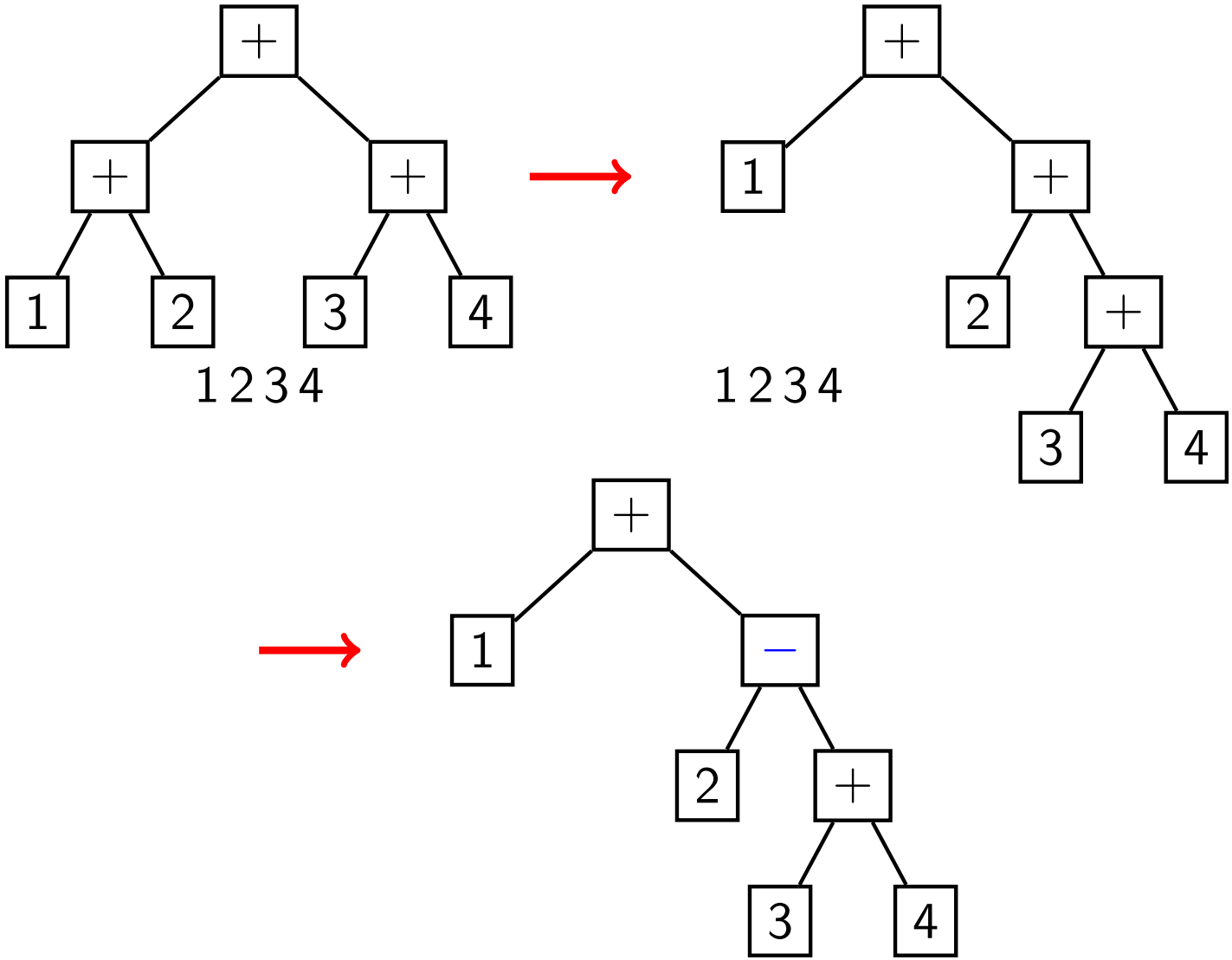

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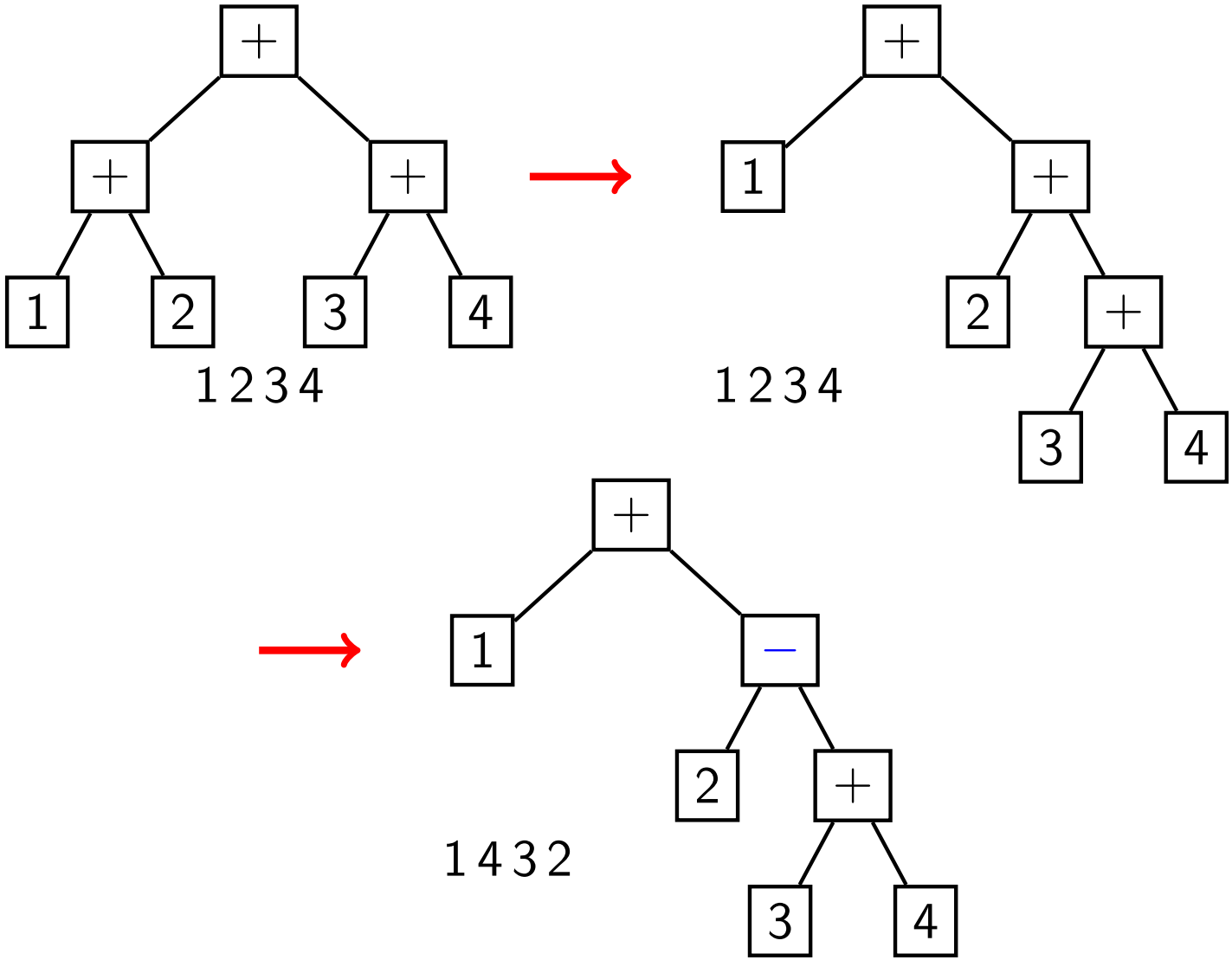

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- What if we use periodic boundary conditions? (PBC)

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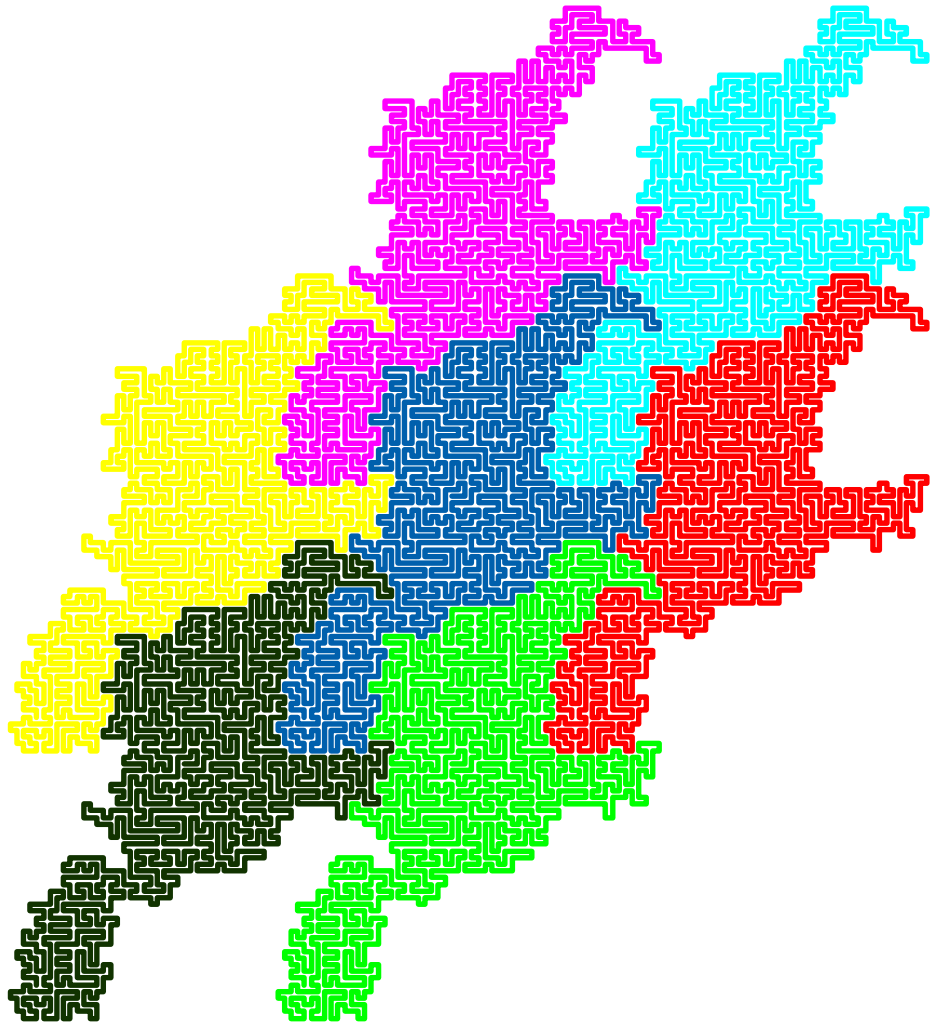
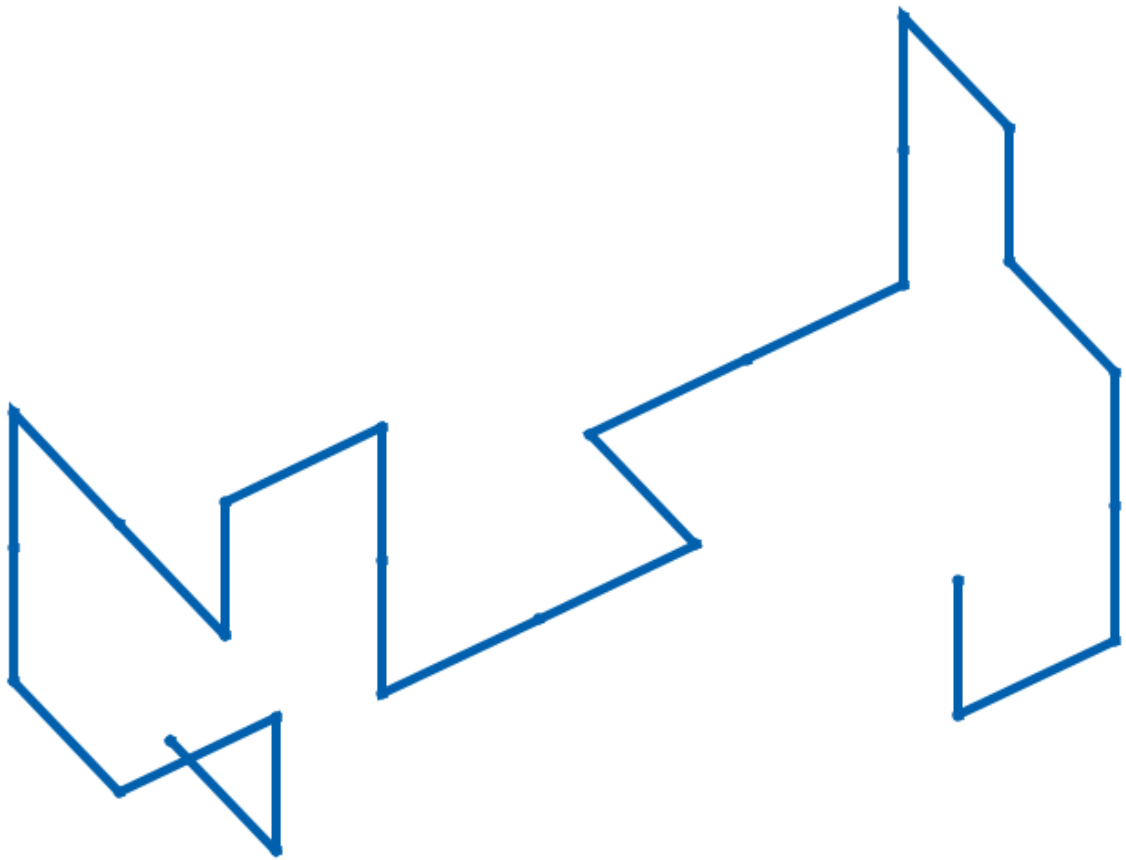
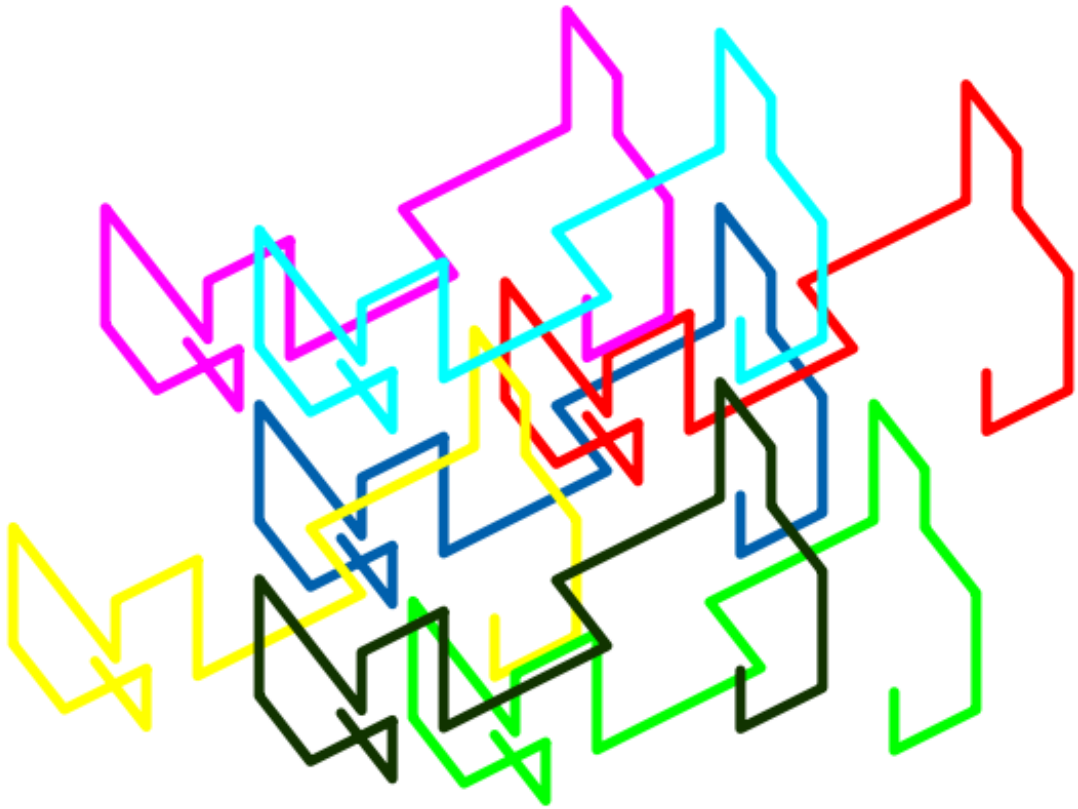
- In 2d, $k = O(N)$ and walks wind around $O(1)$ times. In 3d, $k = O(N^{2/3})$ and walks wind around $O(N^{1/3})$ times.



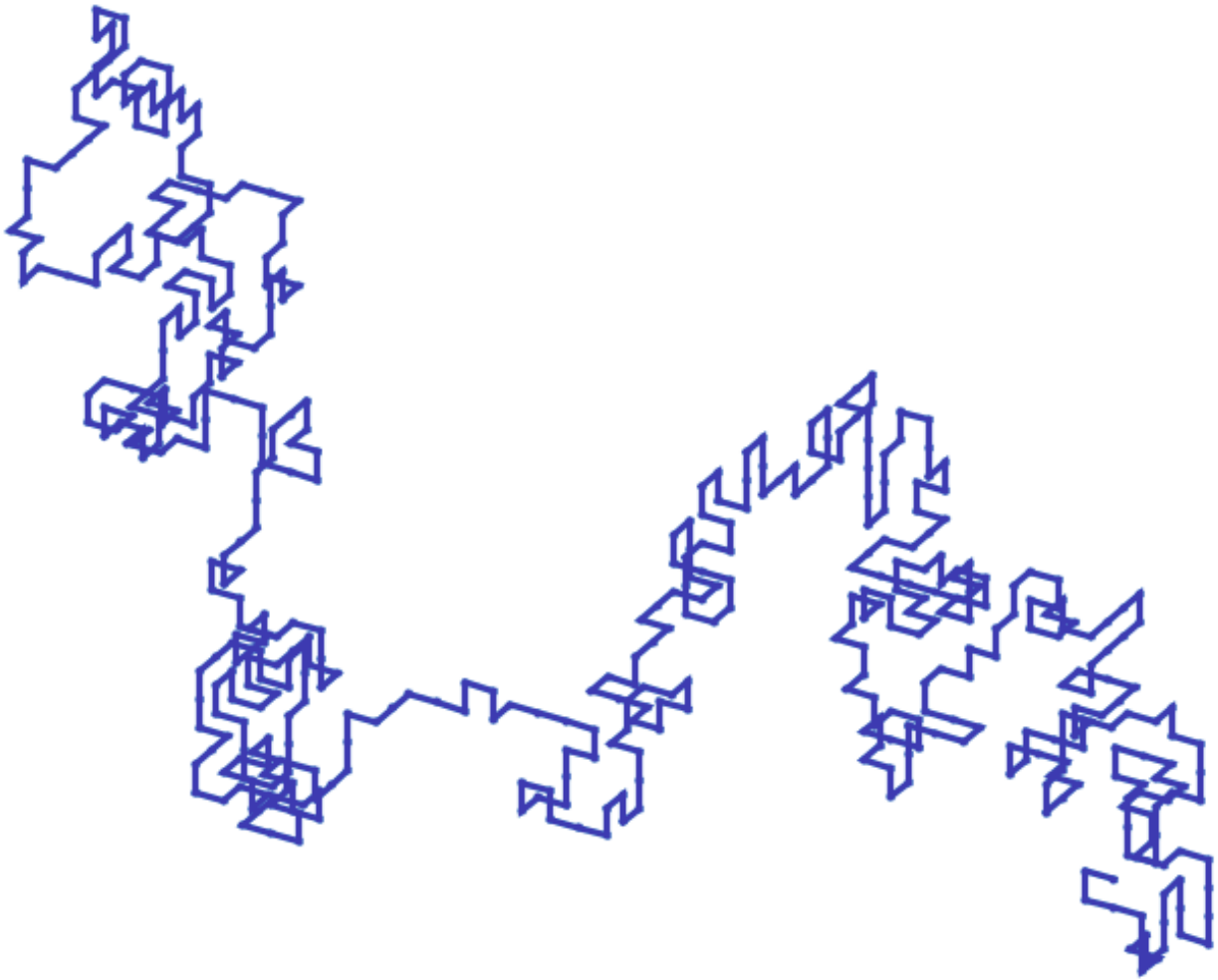
40×40 grid, with copies from winding. Random walk behaviour competing with space-filling nature (remains disc like).



$3 \times 3 \times 3$ grid.

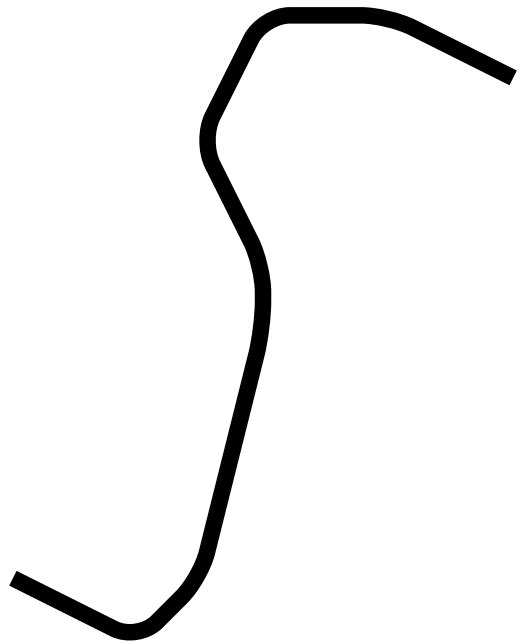


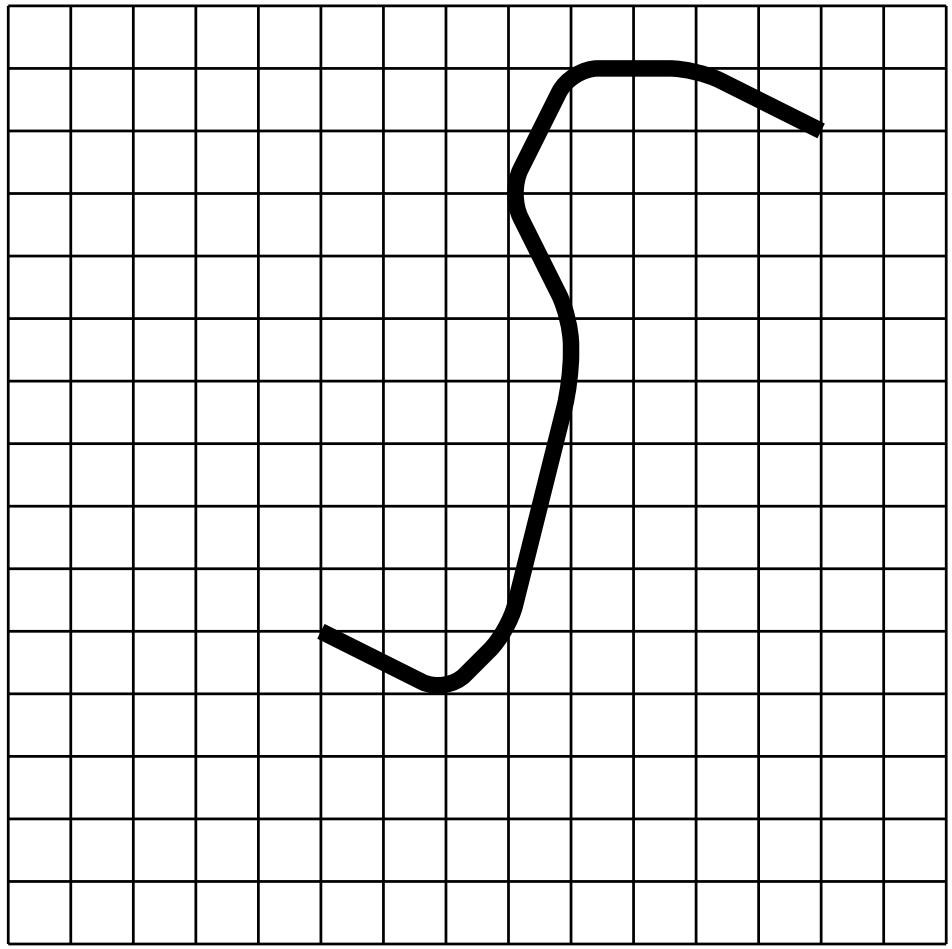
$3 \times 3 \times 3$ grid, with copies from winding around.



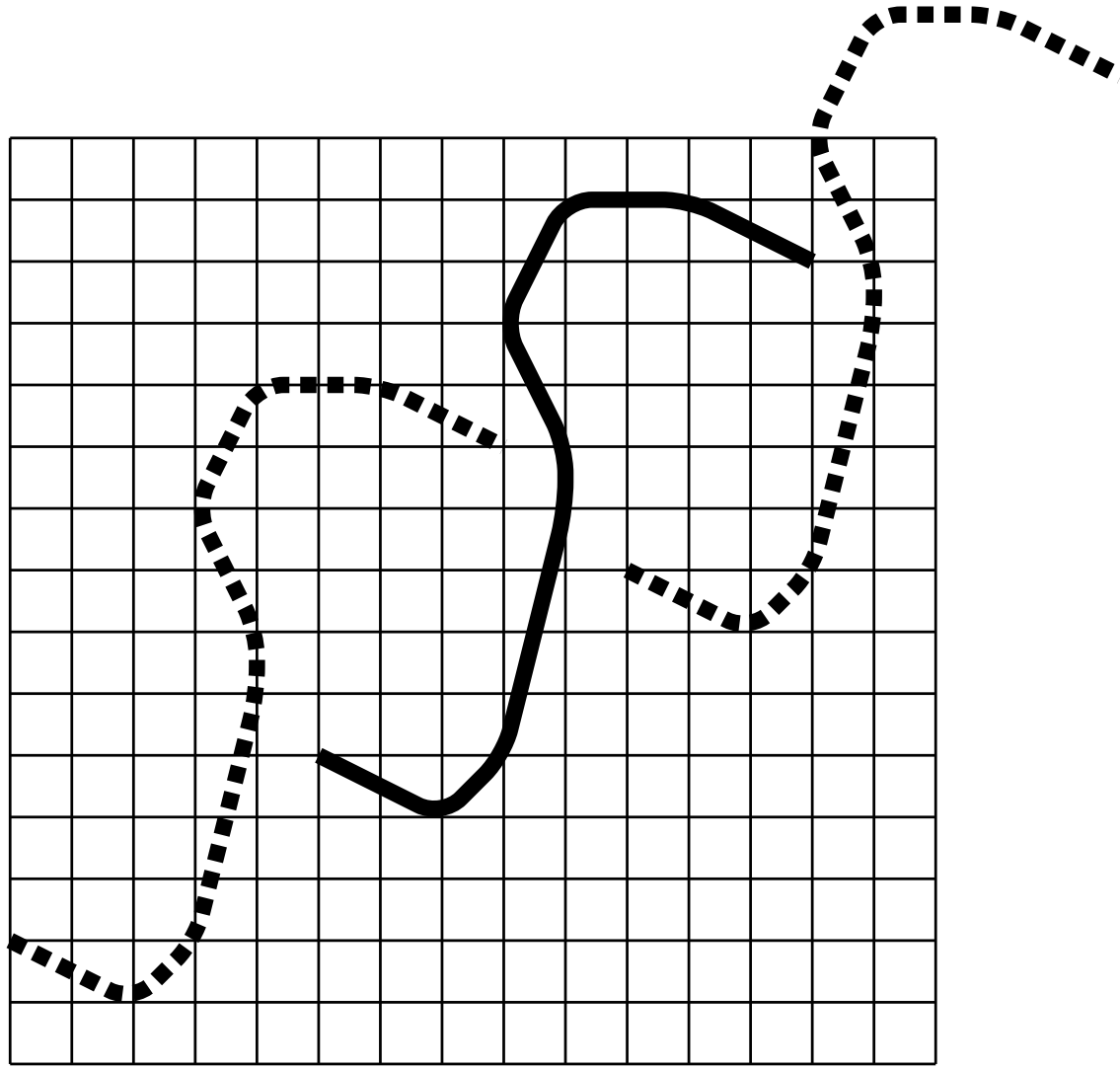
$8 \times 8 \times 8$ grid; random walk behaviour clearly observable.

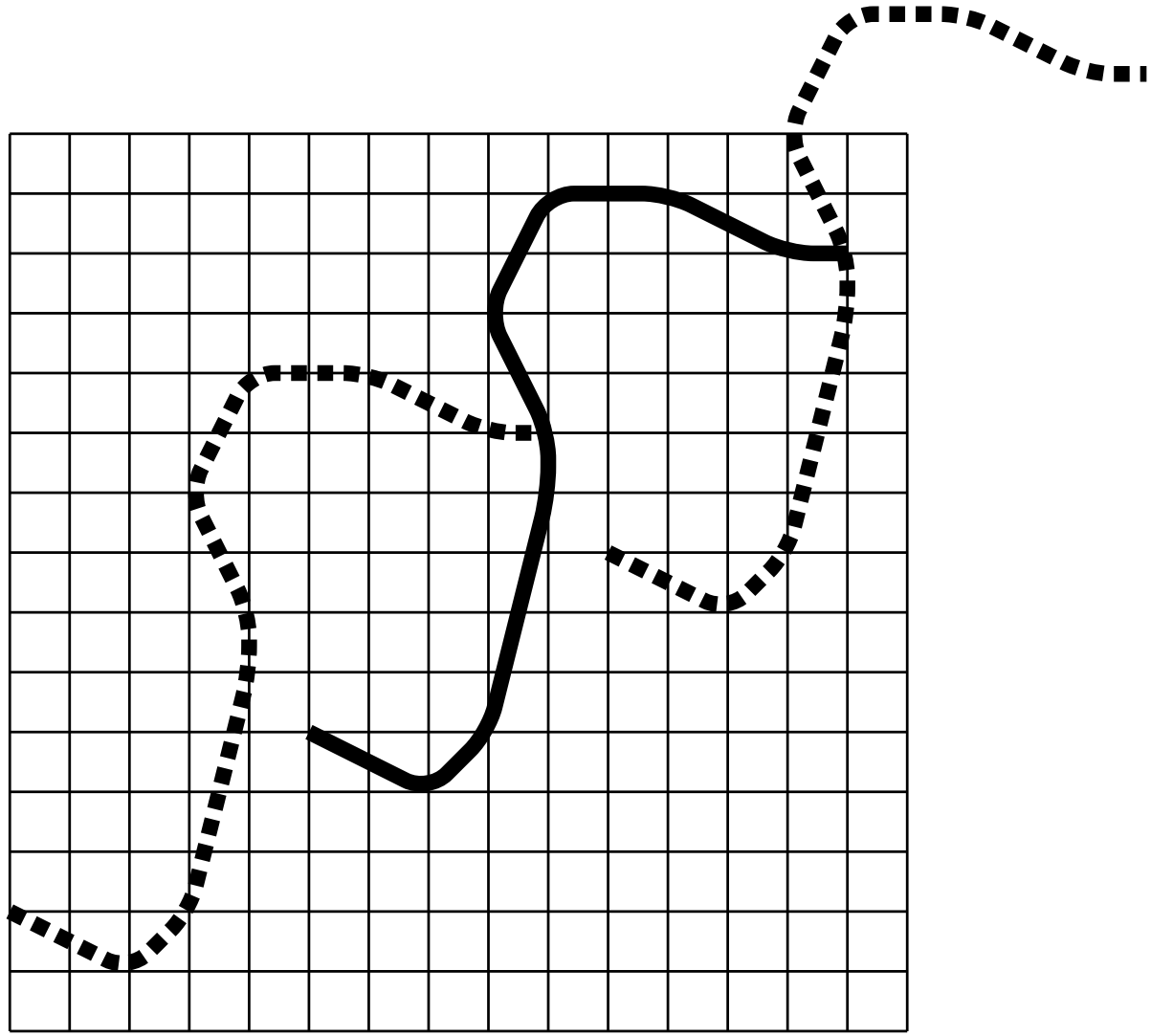
What are backbite moves like when we use PBC?

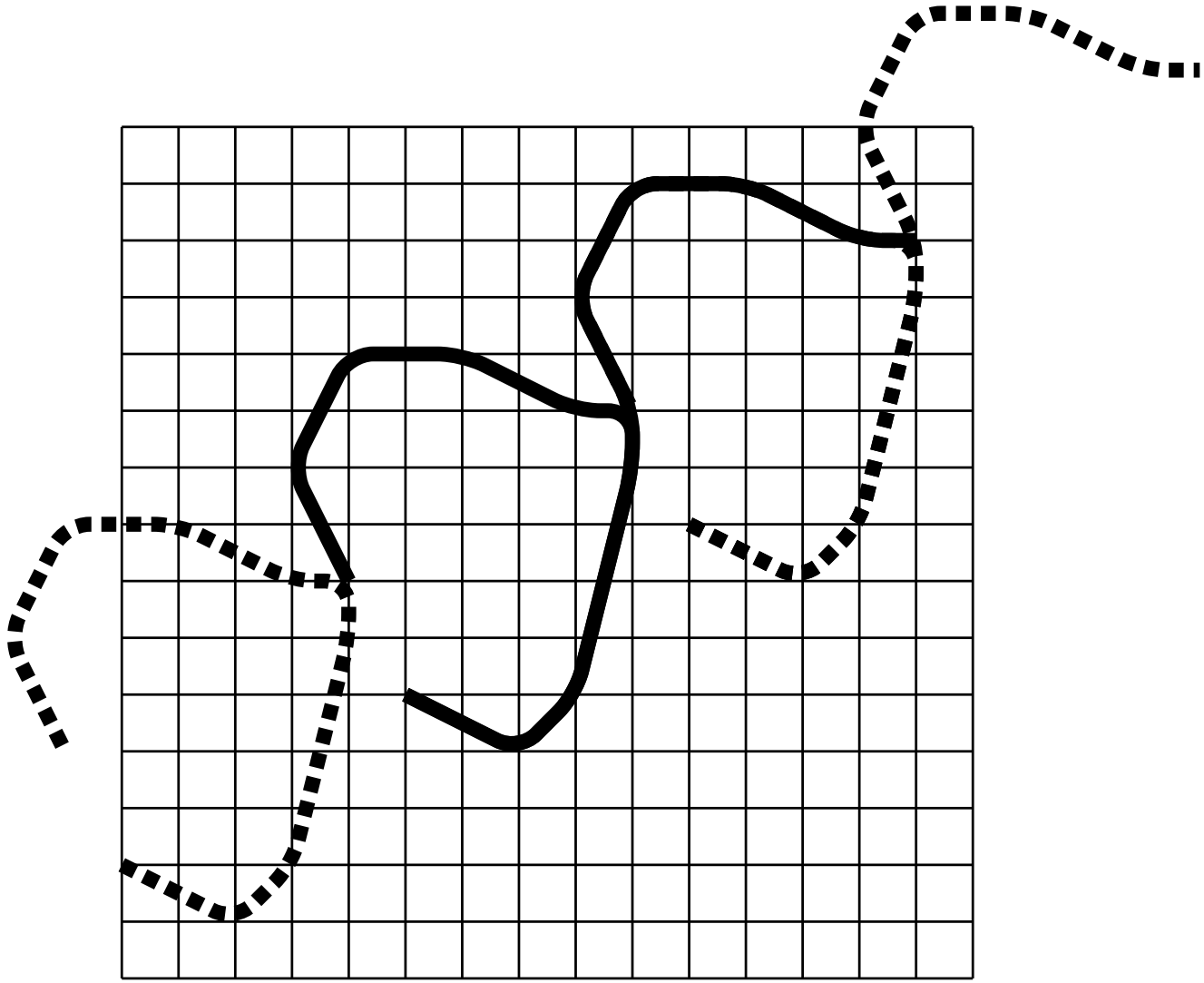


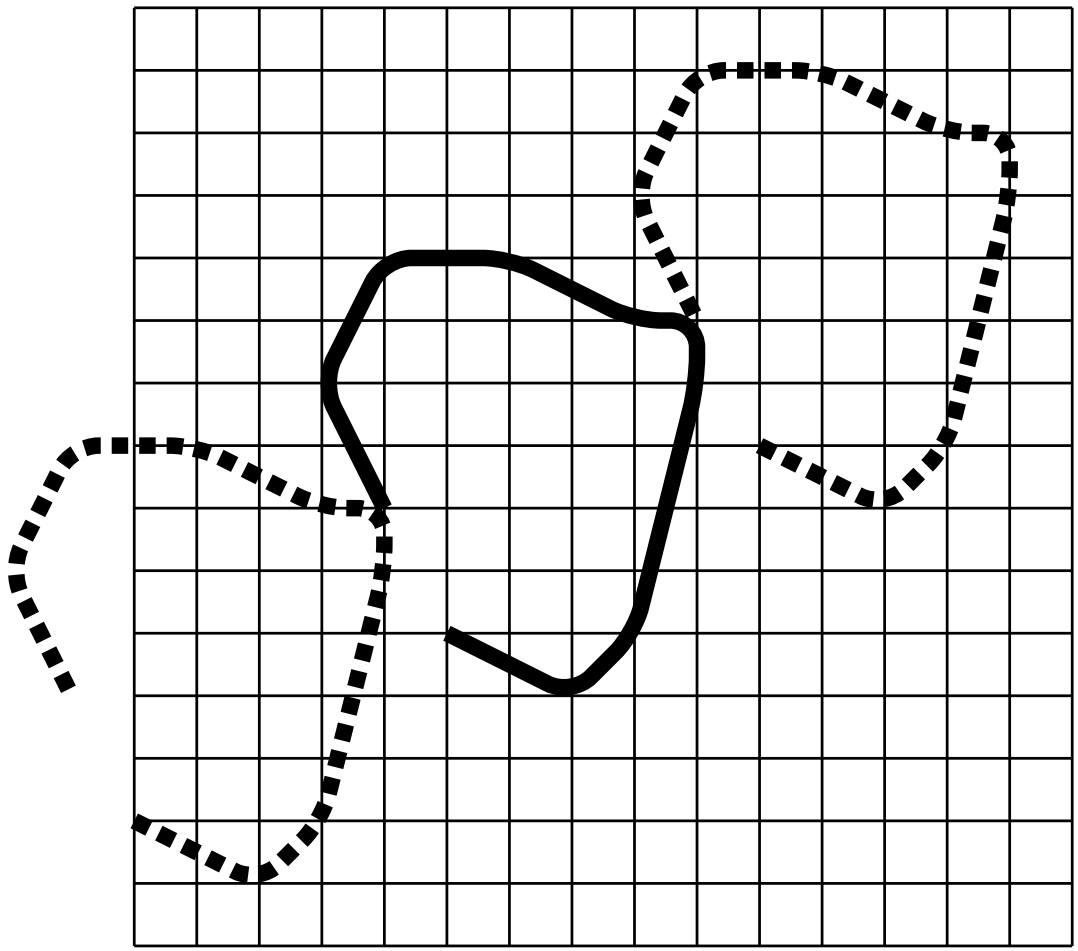


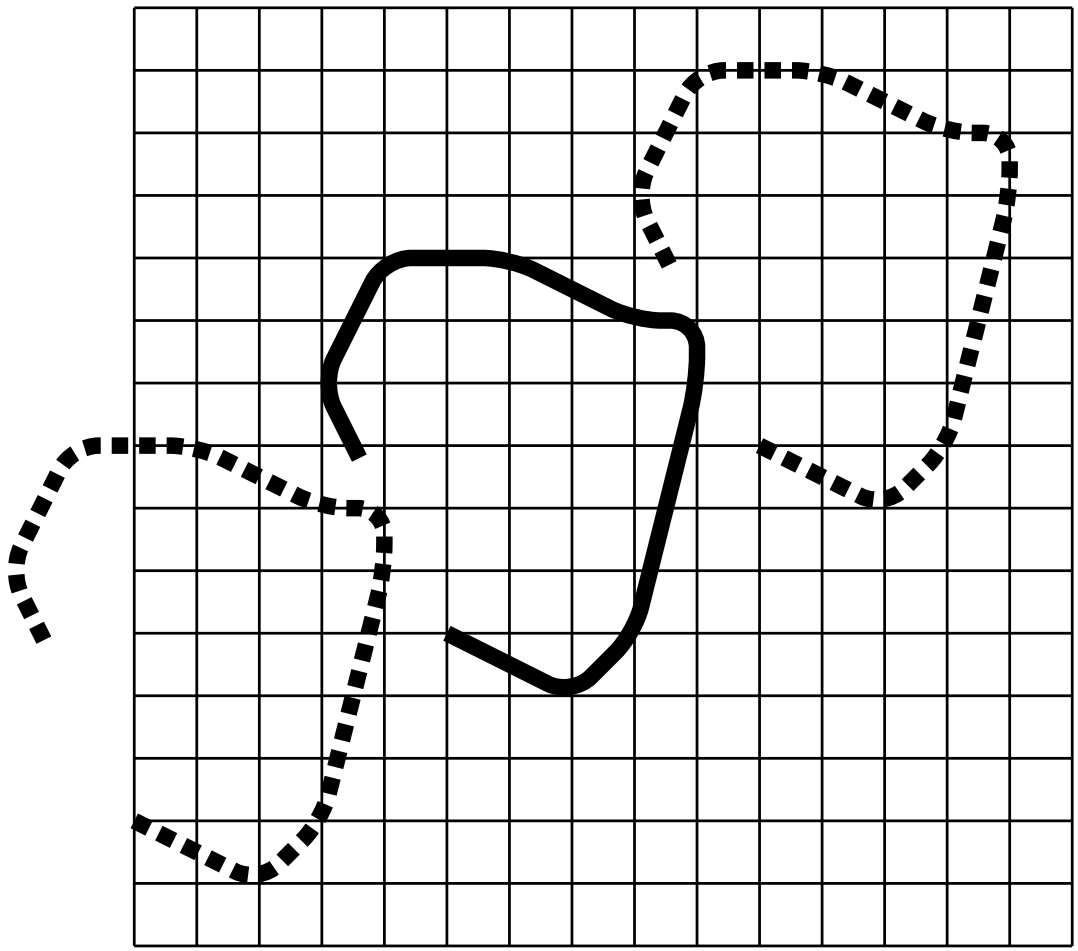
N.B.: 2d representation is a bit misleading, because phenomenon of random walk diffusion winding around multiple times occurs for $d > 2$.

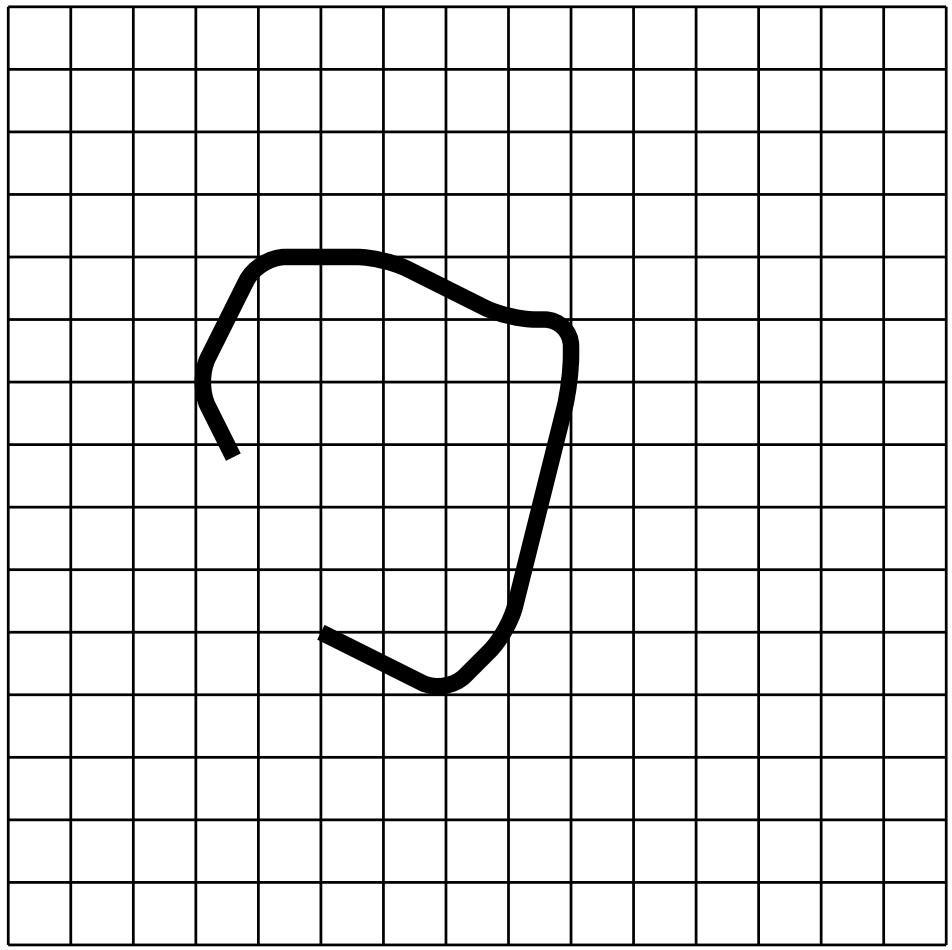


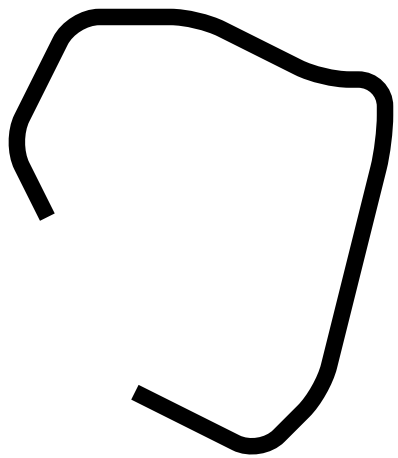


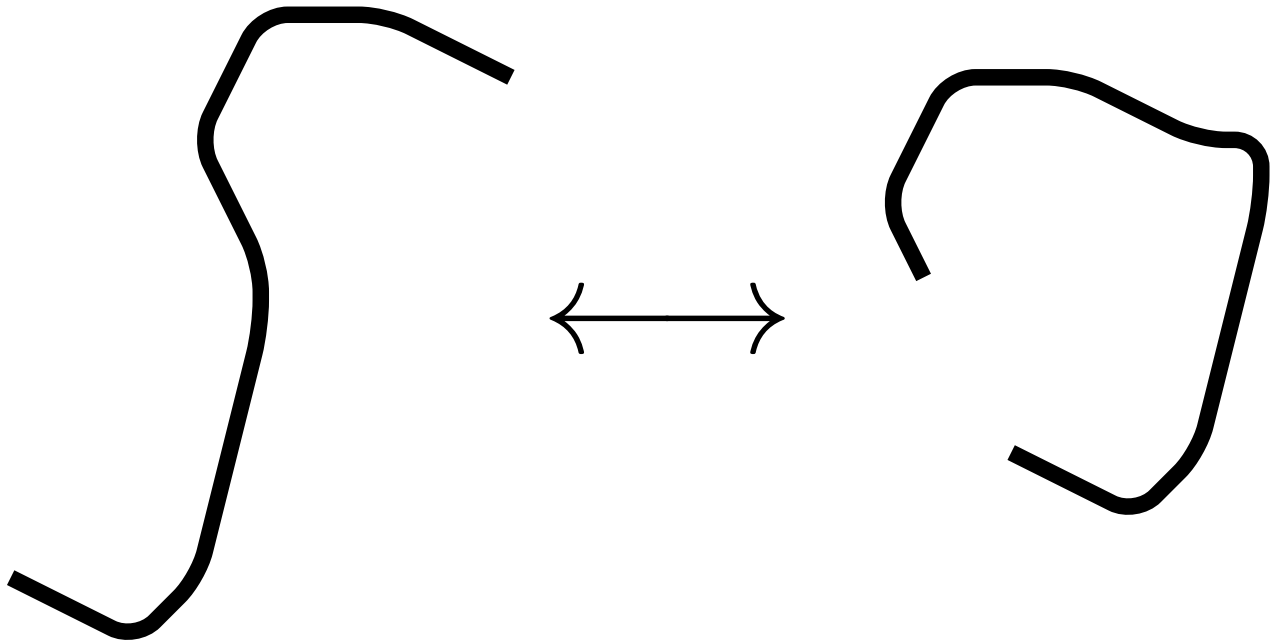












With PBC, endpoints can shift by even multiples of the boundary length with each backbite move.

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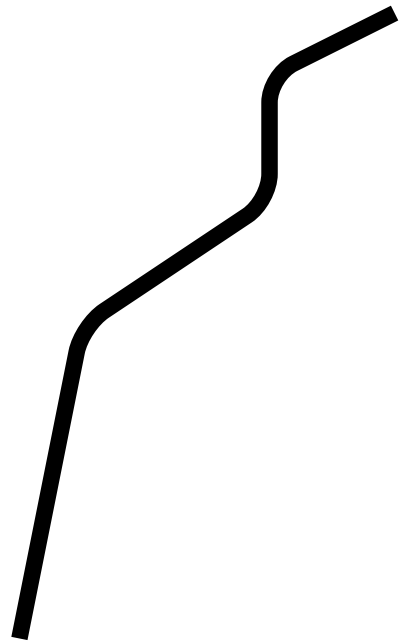

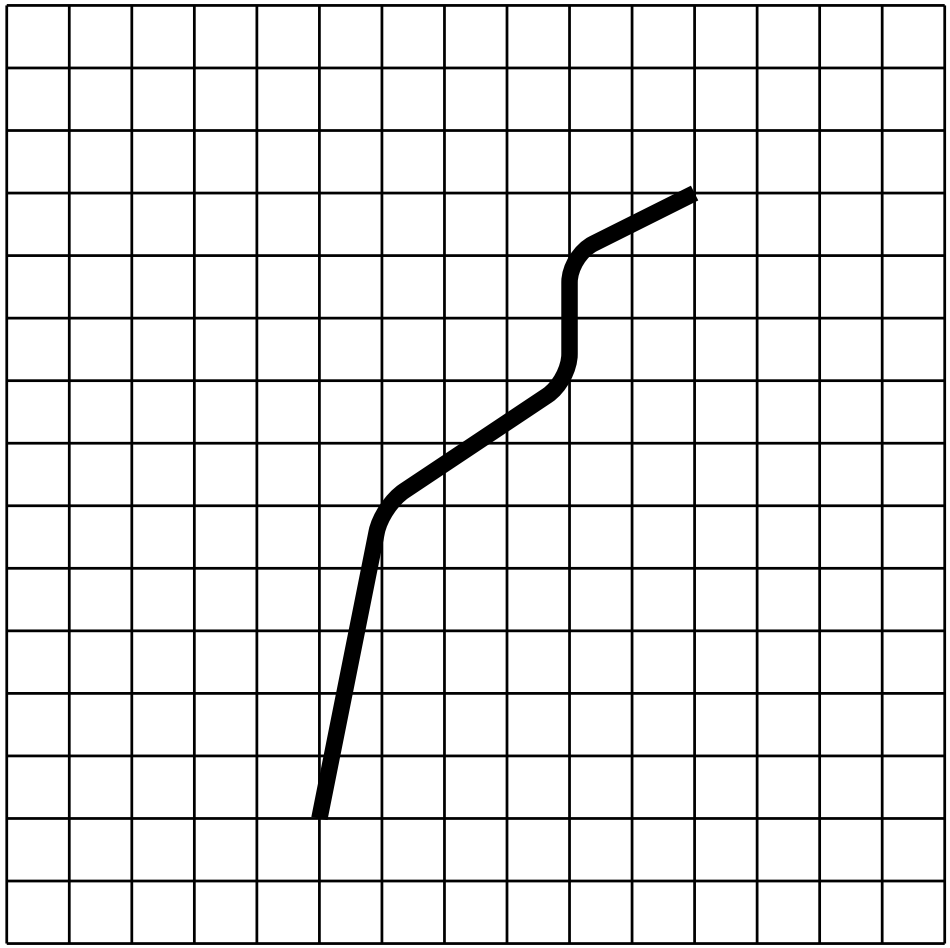

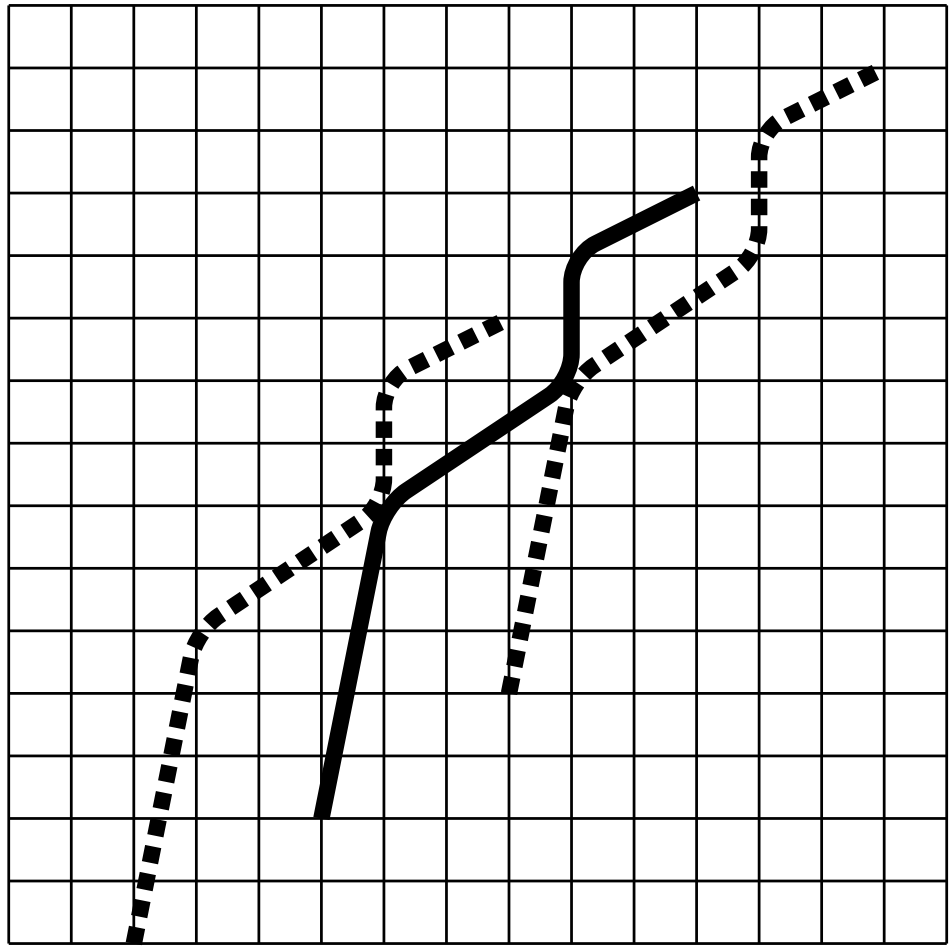

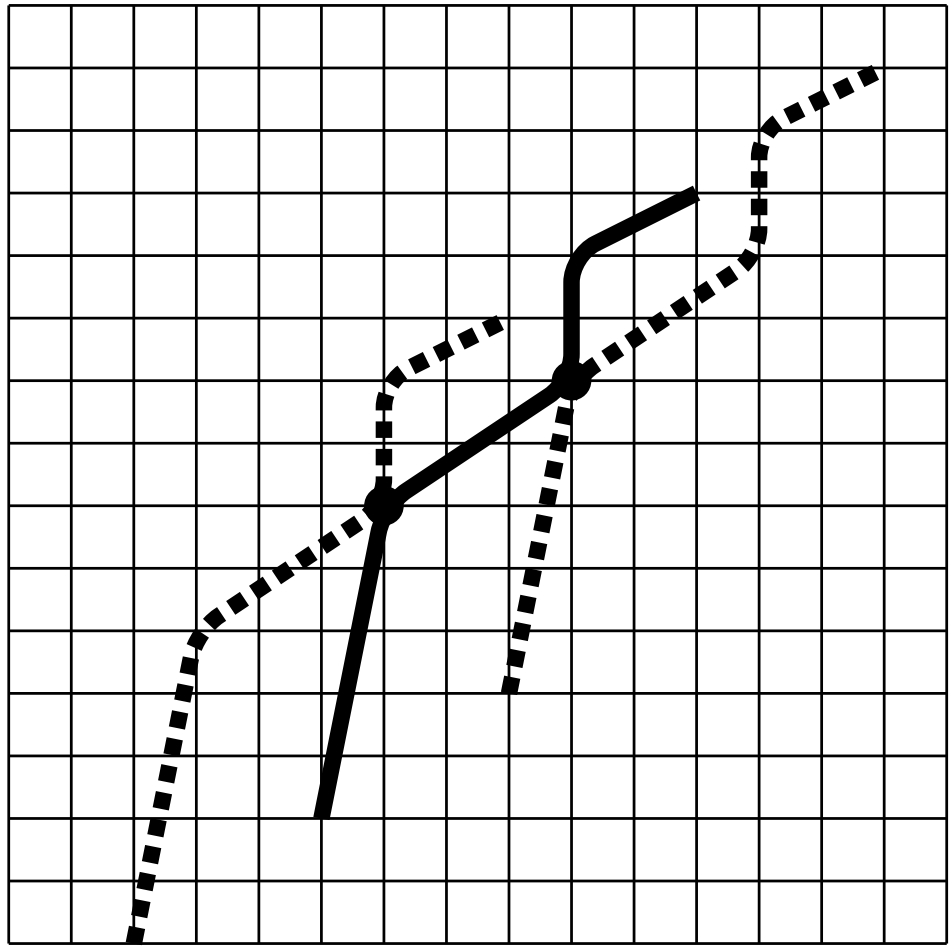

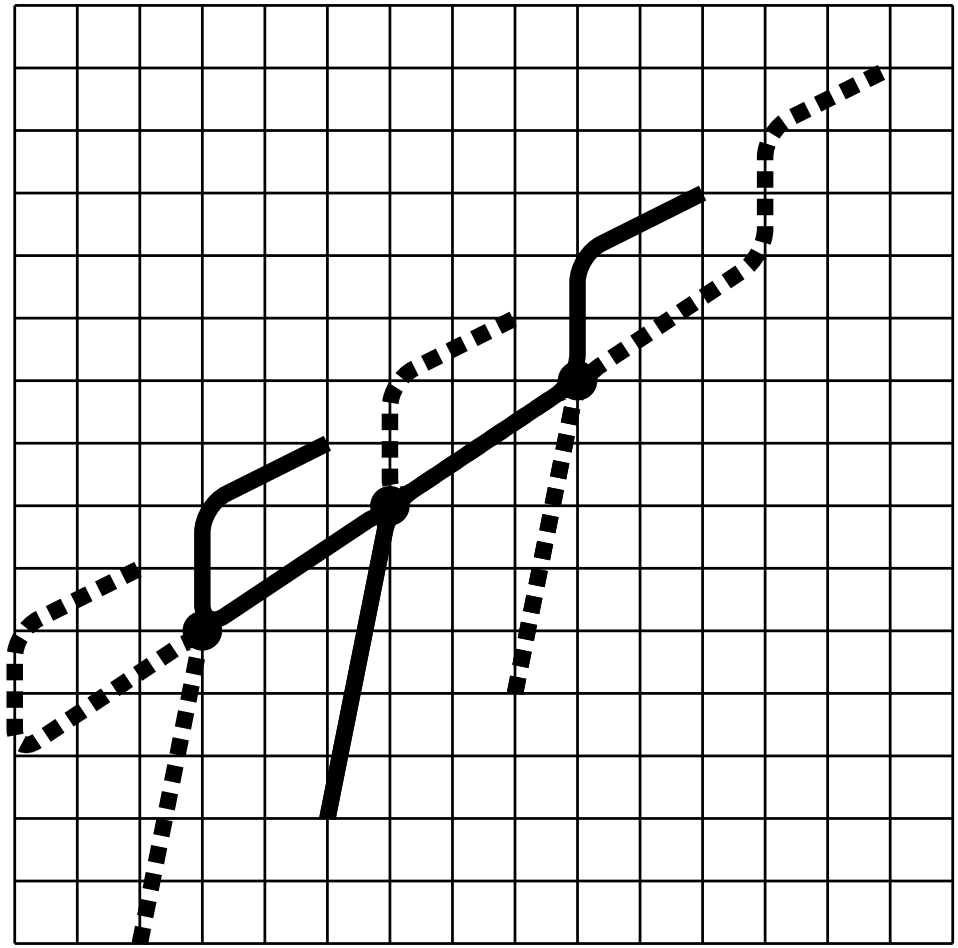

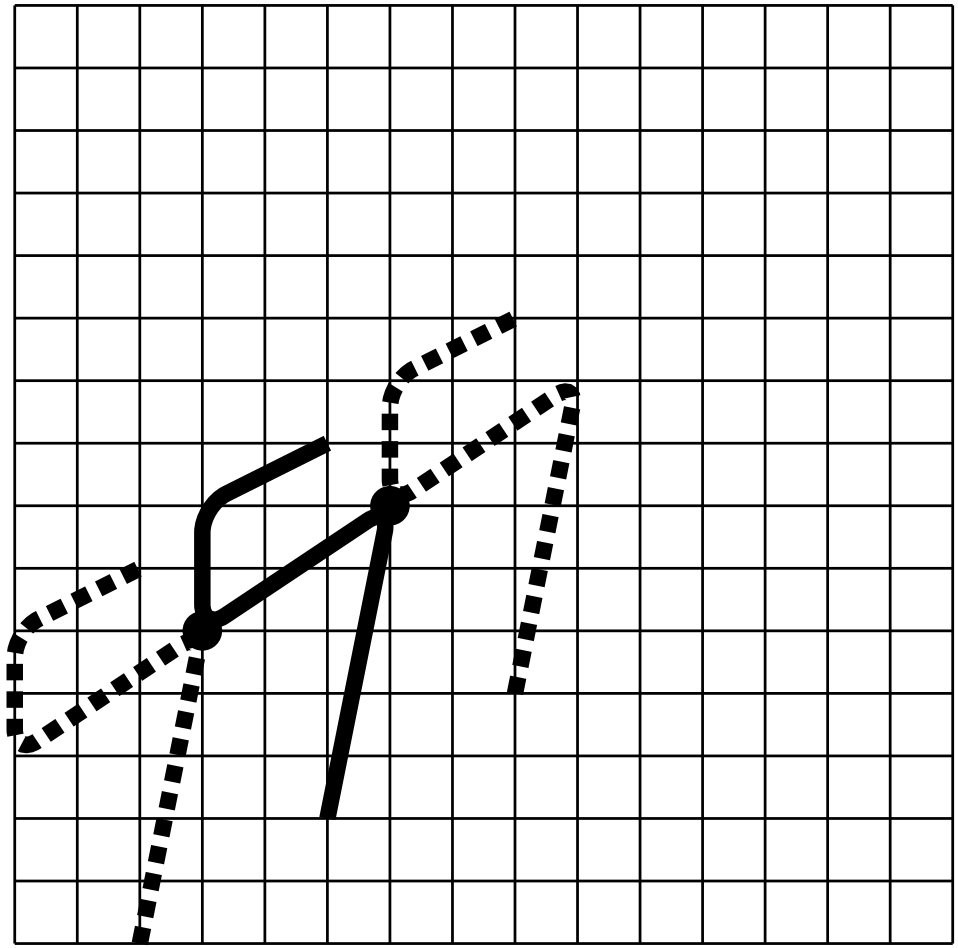

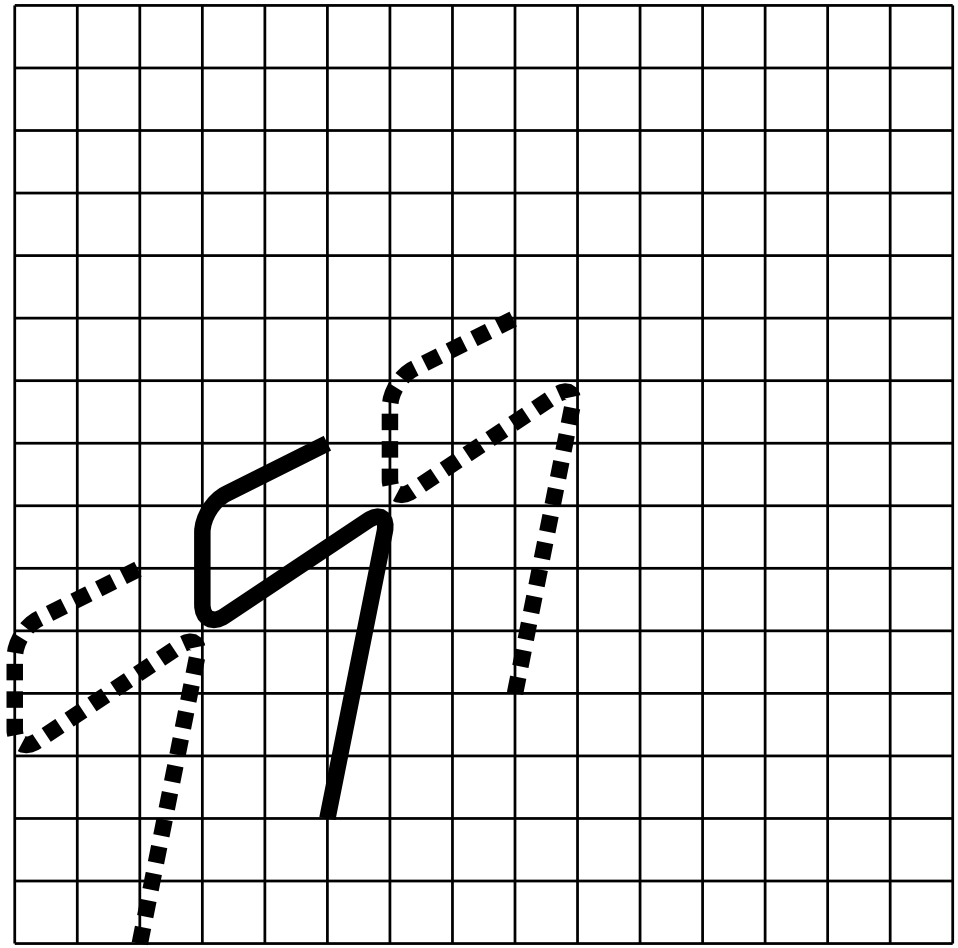

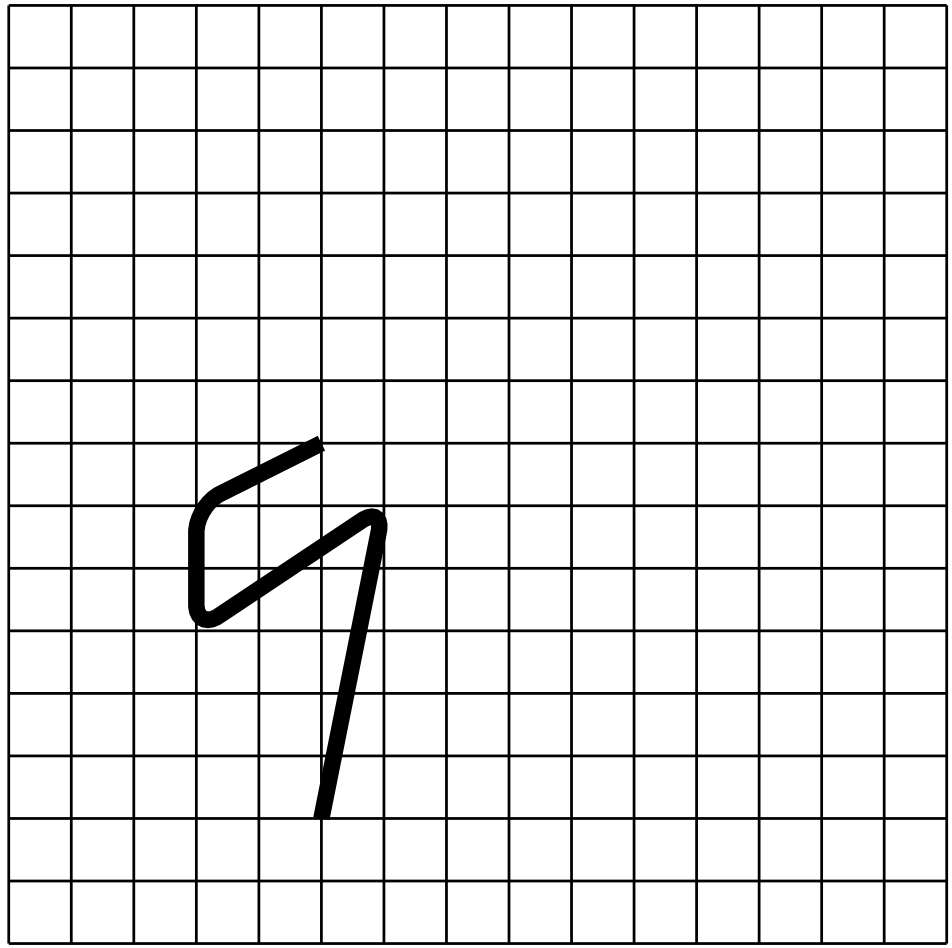

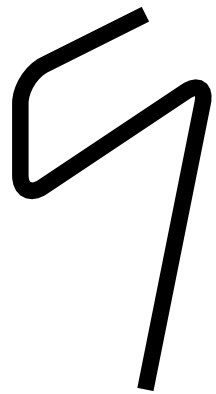

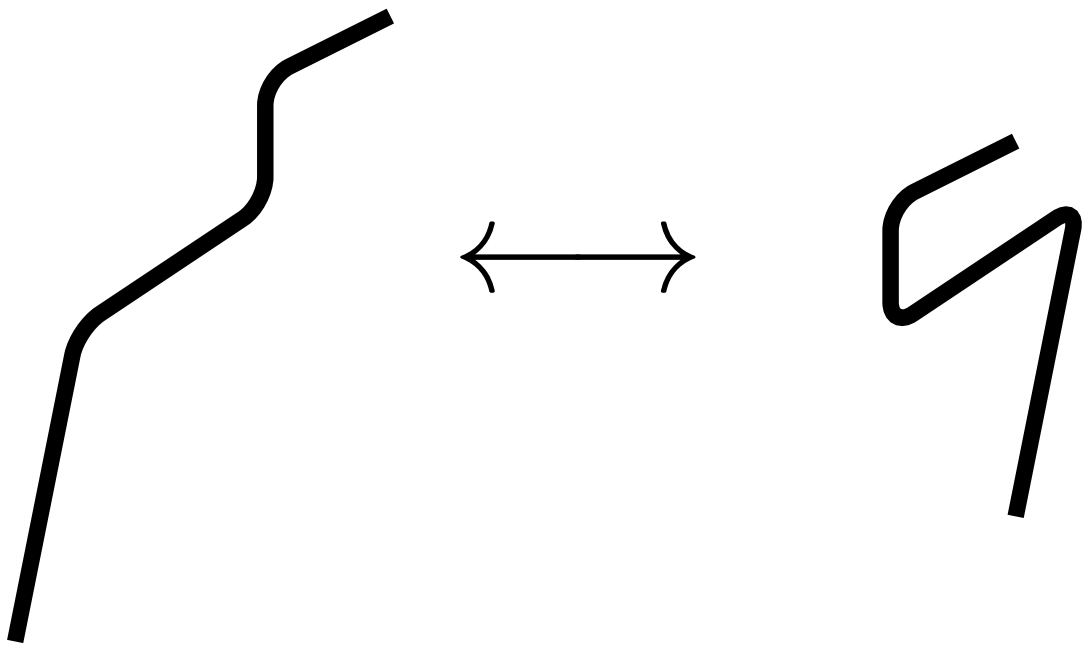

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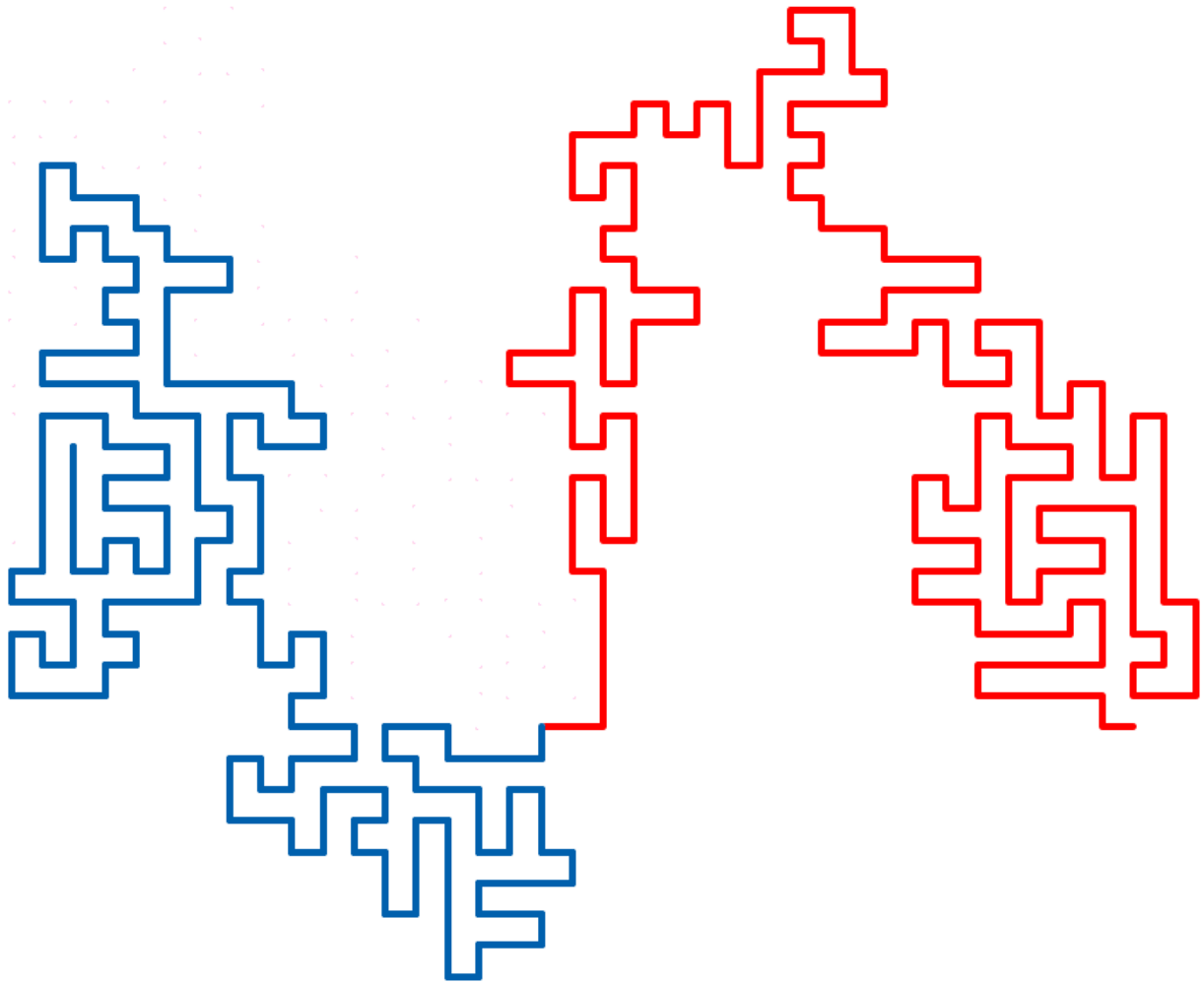

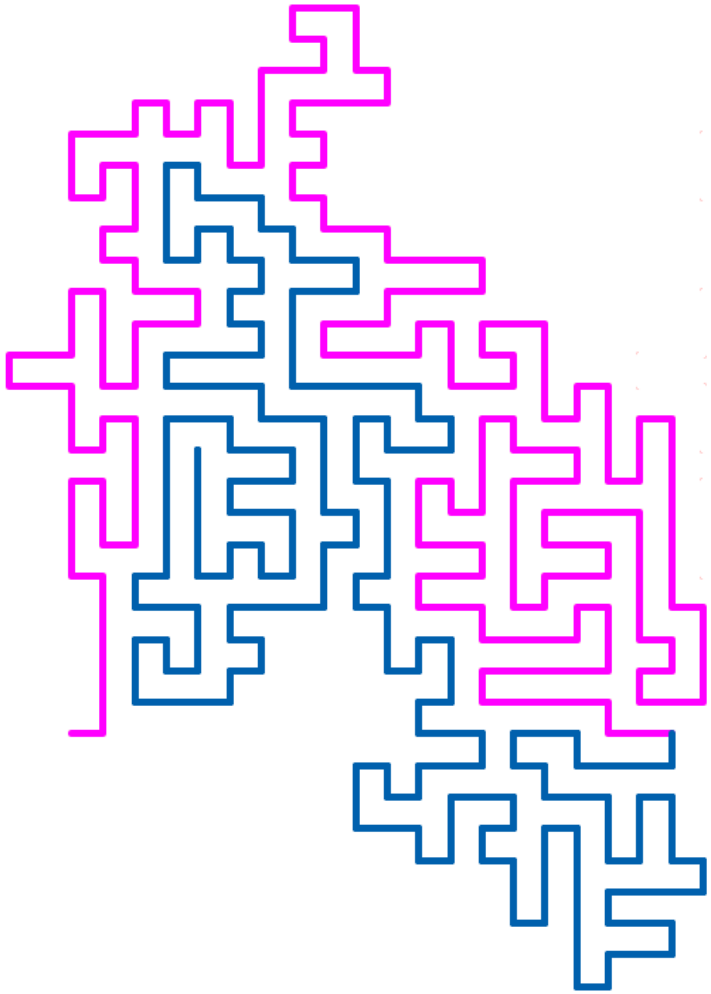

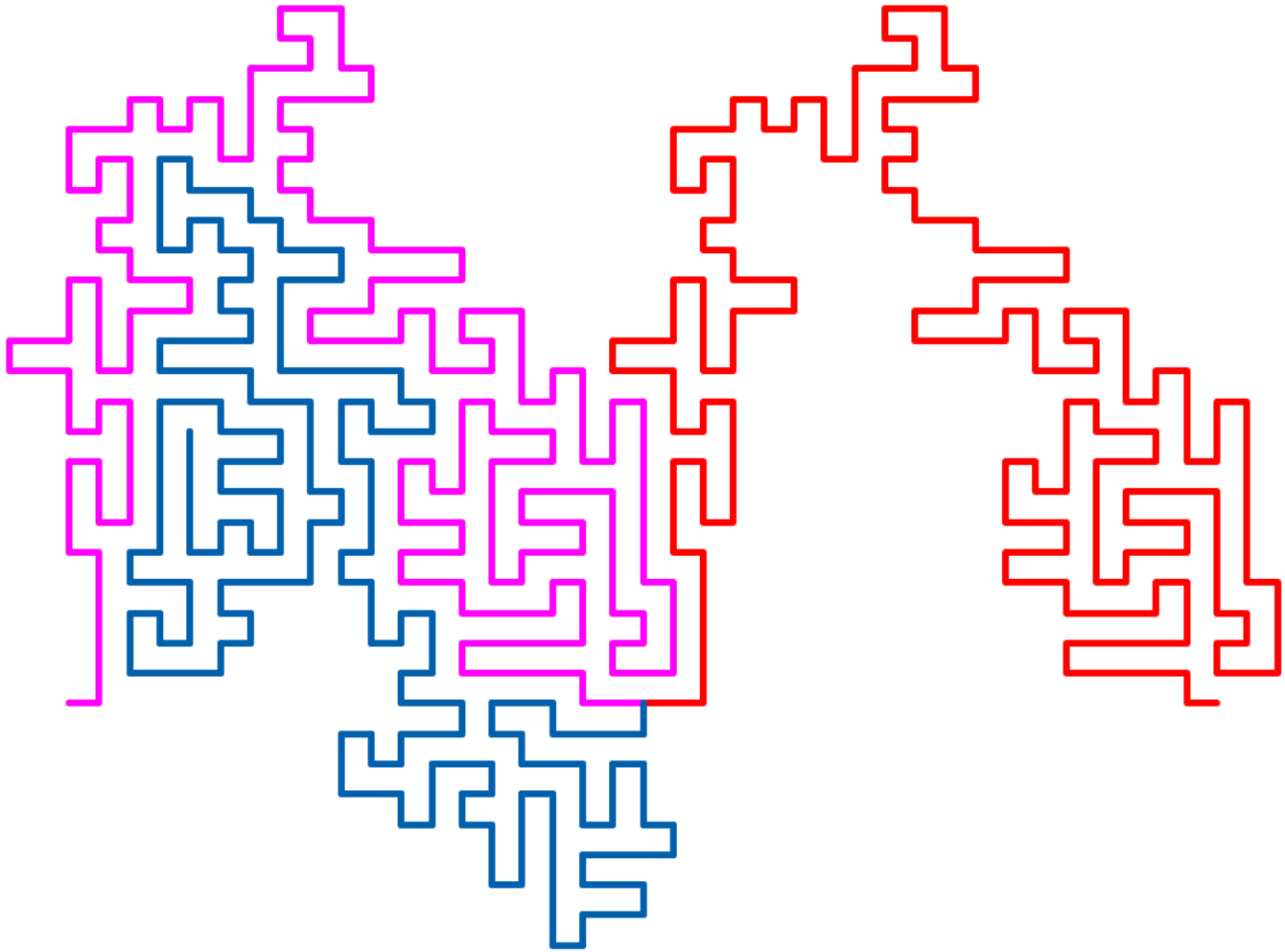

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- Key question: what is $\tau_{\mathrm{int}}(R_{\mathrm{E}}^2)$?
- In large N limit, do periodic boundary conditions for a single polymer correspond to a single polymer in the midst of a melt?

Future work

- Study bond correlations within chain. (Use periodic boundary conditions?)
- Combine Monte Carlo with molecular dynamics to study dynamics. E.g., melts of rings are quite poorly understood, and their dynamics are even slower than for linear polymers as reptation is not possible.
- Develop efficient algorithms for other cases, e.g. θ-transition? Semi-dilute regime? Explicit solvent?
- Continuum models.
- Copolymers, star polymers, and many more applications.

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- Can we find additional useful moves?

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- Hamiltonian path search problem for a graph is a special case of the traveling salesman problem.[10]

[9] S. Lin/B. W. Kernighan: An Effective Heuristic Algorithm for the Traveling-Salesman Problem, in: Oper. Res. 21 (1973), pp. 498–516.

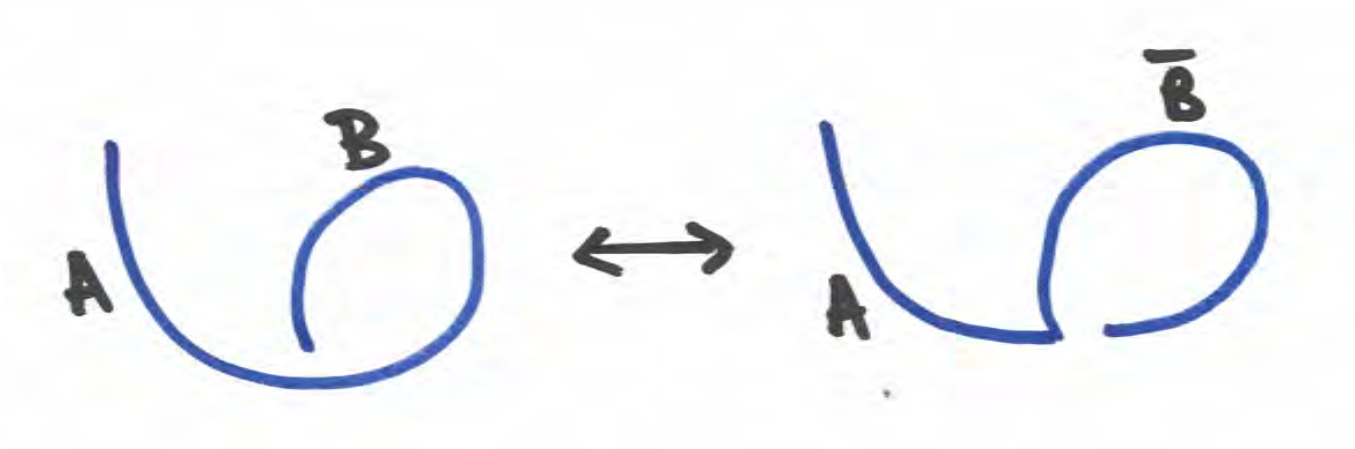
[10] Pouya Baniasadi et al.: Deterministic Snakes and Ladders Heuristic for the Hamiltonian cycle problem, in: Mathematical Programming Computation 6 (2014), pp. 55–75.

Alternate representation of connectivity changing moves

- Can we find additional useful moves?
- Long history of algorithms to find optimal paths for the traveling salesman problem.
- Lin-Kernighan heuristic[9] involves 2-opt and 3-opt connectivity changing moves. No lattice, so these moves are represented differently.
- Hamiltonian path search problem for a graph is a special case of the traveling salesman problem.[10]
- Any further insight if we abstract away the underlying lattice?

[9] S. Lin/B. W. Kernighan: An Effective Heuristic Algorithm for the Traveling-Salesman Problem, in: Oper. Res. 21 (1973), pp. 498–516.

[10] Pouya Baniasadi et al.: Deterministic Snakes and Ladders Heuristic for the Hamiltonian cycle problem, in: Mathematical Programming Computation 6 (2014), pp. 55–75.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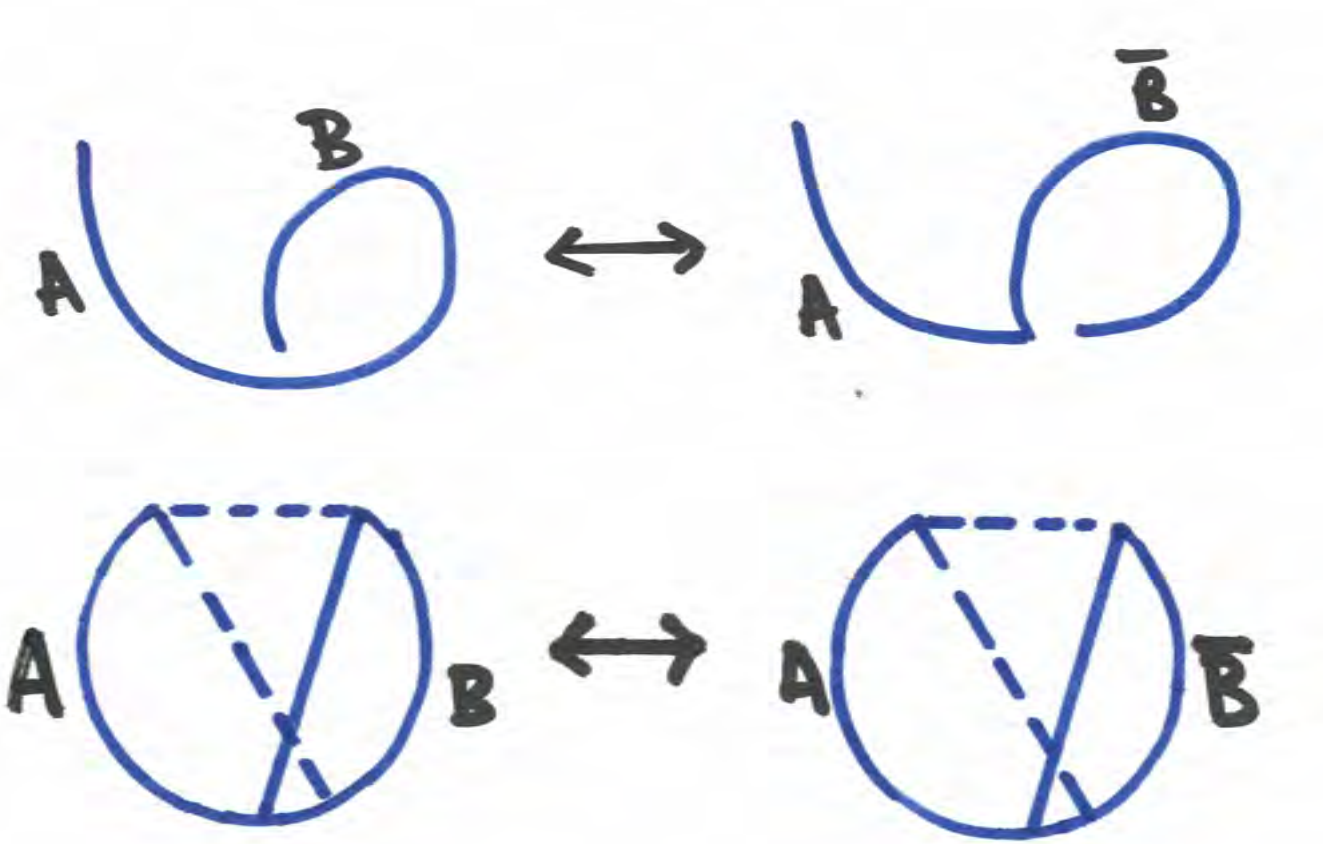
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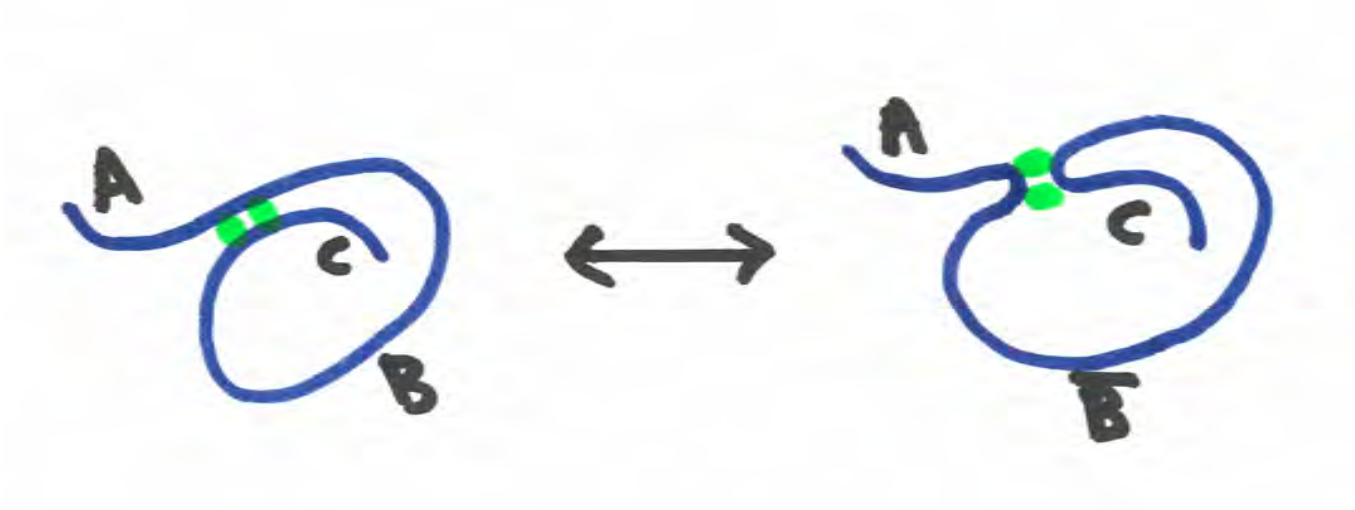
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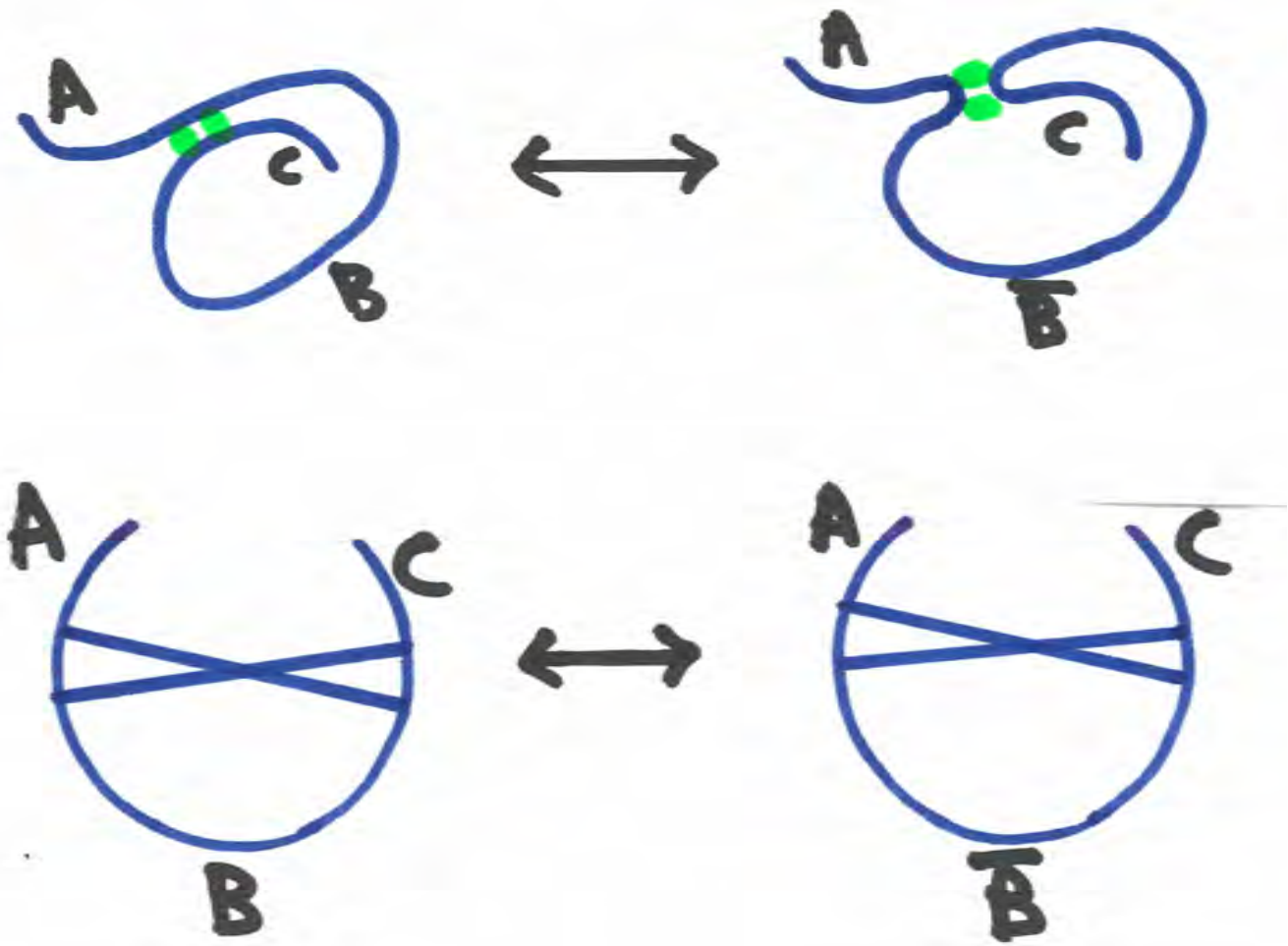
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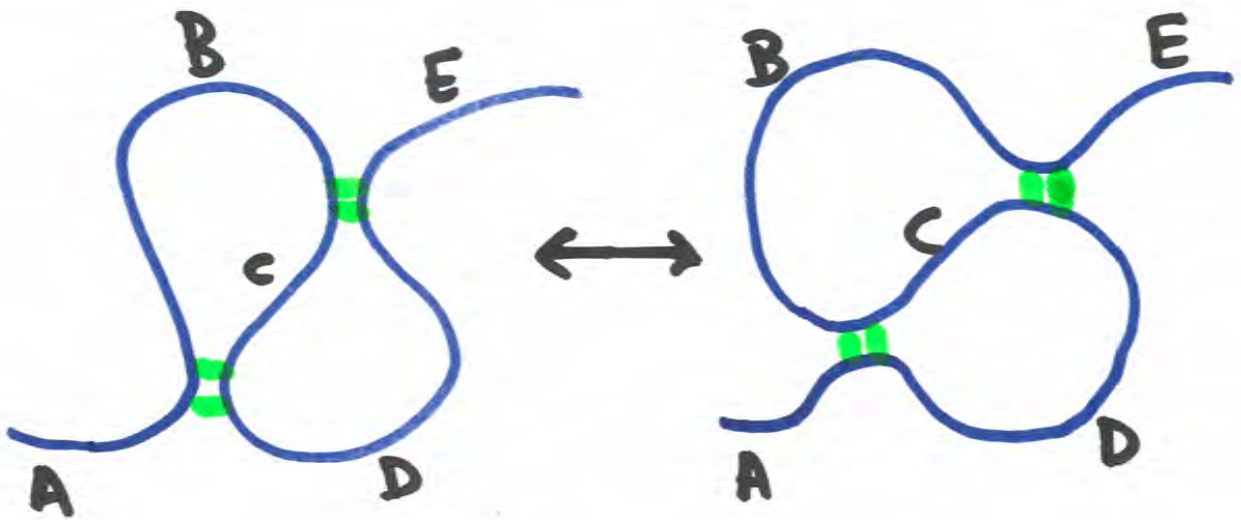
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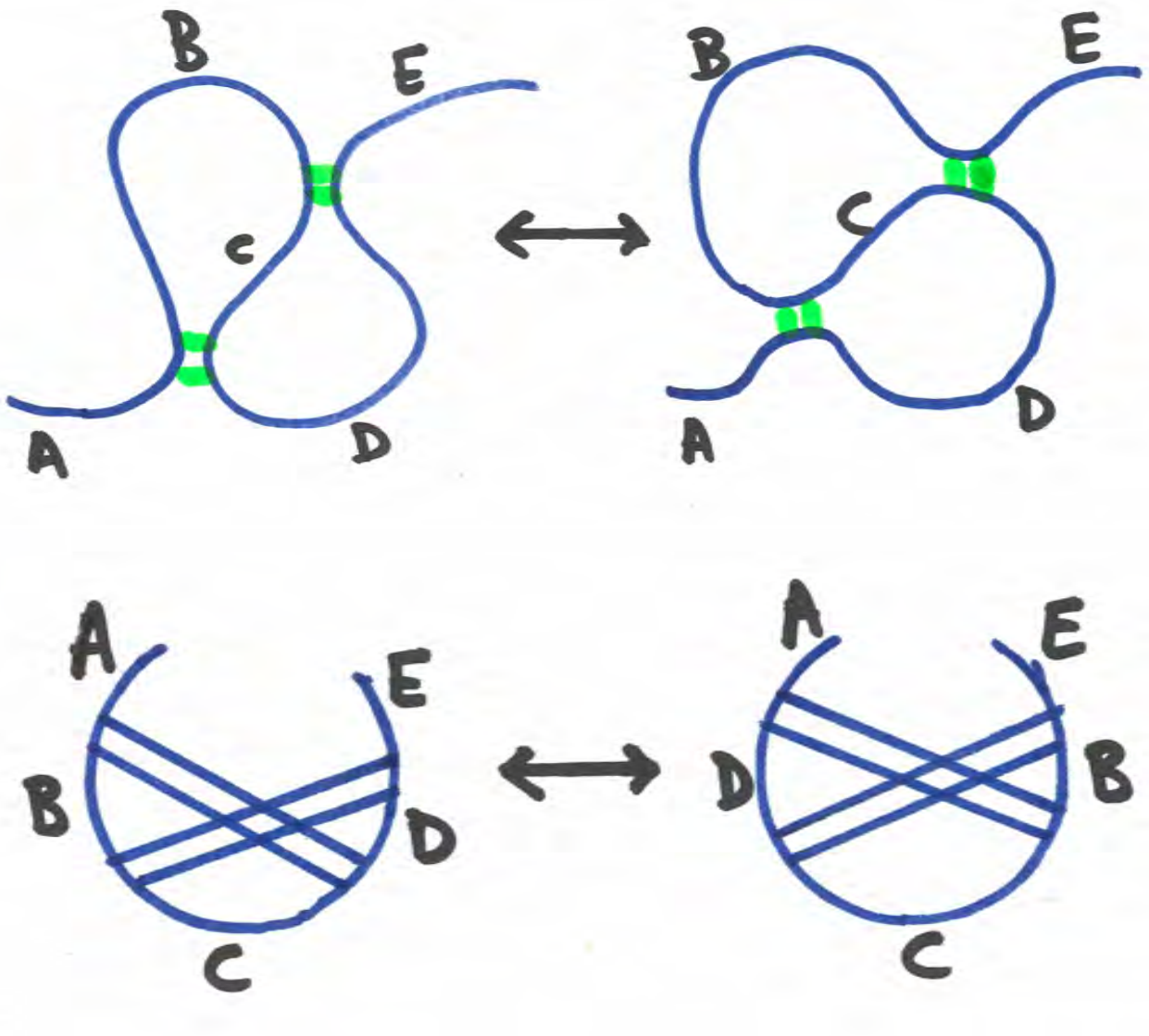
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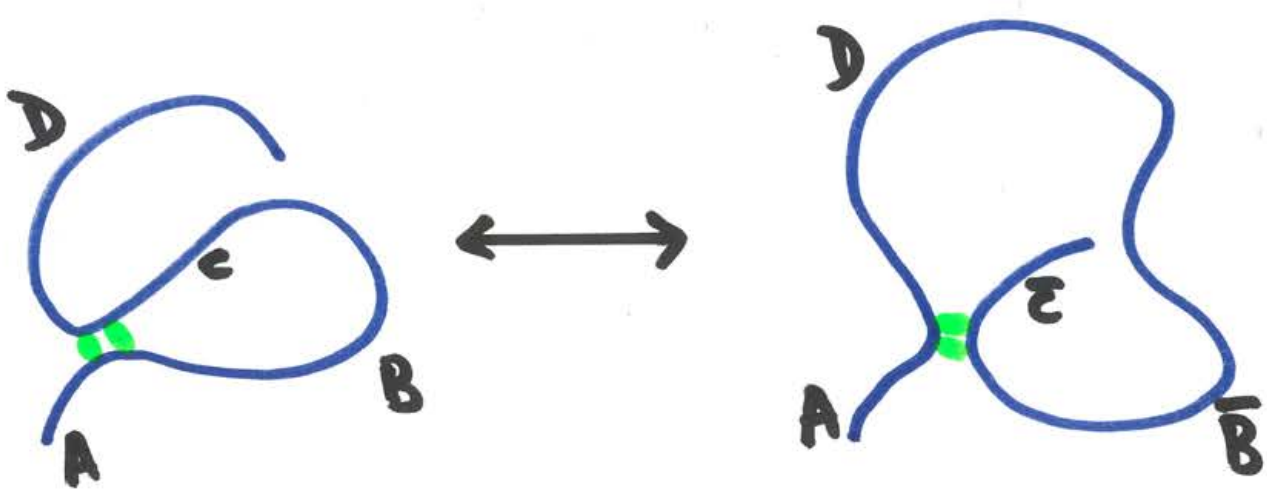
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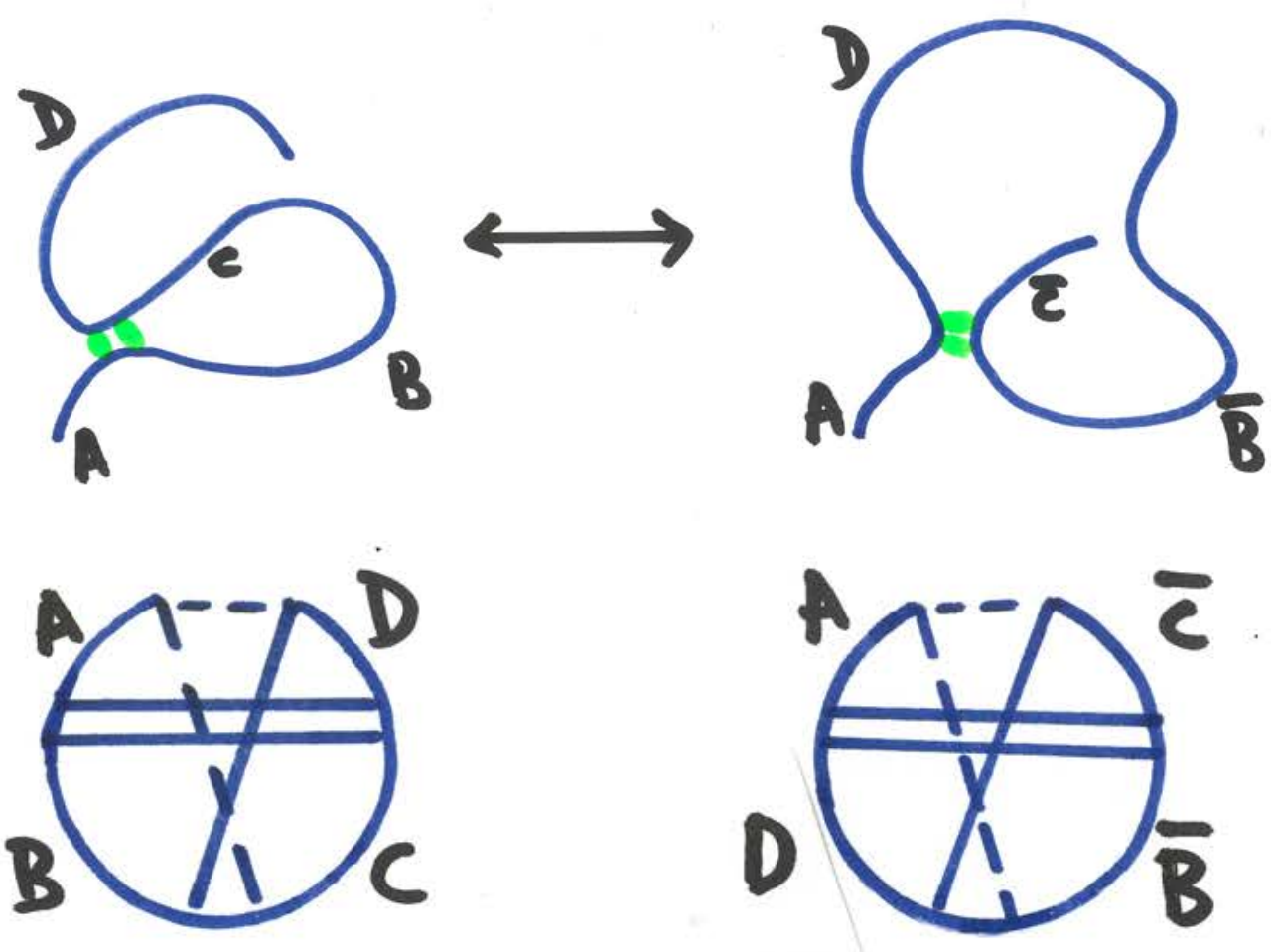
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Alternate representation of connectivity-changing moves

- Abstracts away the lattice. Instead, think about transformations, and then determine which lattices are commensurate with those moves.

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- One insight from this point of view so far: combination of backbite and rebridging may allow preferential sampling of moves close to the end. (Desirable for efficiency in 2d.)

Alternate representation of connectivity-changing moves

- Abstracts away the lattice. Instead, think about transformations, and then determine which lattices are commensurate with those moves.
- One insight from this point of view so far: combination of backbite and rebridging may allow preferential sampling of moves close to the end. (Desirable for efficiency in 2d.)
- Also, makes it easier to understand effect of moves, and how to implement them, as tree representation encodes linear information.

Computational efficiency

$d = 2$, $N = 10^9$

- Pr(success) $= 0.0189$
- 4-5 microseconds per pivot attempt
- 250 microseconds per pivot success

$d = 3$, $N = 10^9$

- Pr(success) $= 0.098$
- 9 microseconds per pivot attempt
- 90 microseconds per pivot success

$d = 4$, $N = 10^9$

- Pr(success) $= 0.50$
- 30 microseconds per pivot attempt
- 60 microseconds per pivot success