Random and self-avoiding walks

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- What do we know about them?

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- In *Nature*, on 27 July 1905 Karl Pearson asked *A man starts from a point O and walks l yards in a straight line; he then turns through any angle whatever and walks another l yards in a second straight line. He repeats this proces n times. I require the probability that after n of these stretches he is at a distance between r and $r + \delta r$ from his starting point.*

What are random walks?

- The question was answered the following week by Lord Rayleigh, who pointed out the connection between this problem and an earlier paper of his (Rayleigh) published in 1880 concerned with sound vibrations. Rayleigh pointed out that, for large values of n, the answer is given by

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- You'll recognise this as having the shape of a normal distribution, centred at the origin.

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- In *Nature*, on 10 August 1905 Karl Pearson wrote, in relation to Rayleigh's letter and reference to his earlier work: *I ought to have known it, but my reading of late years has drifted into other channels, and one does not expect to find the first stage of a biometric problem provided in a memoir on sound.* He went on to comment on the solution:

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- *The lesson of Lord Rayleigh's solution is that in open country the most probable place of finding a drunken man who is at all capable of keeping on his feet is somewhere near his starting point.*

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- Then he solved the more difficult case when $n/2$ steps are in the x direction, and $n/2$ steps are in the y direction.
- Finally, he removes this restriction and produces the required result.

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- In the 1980s this problem was revived as a model for the travelling of micro-organisms possessing flagella.

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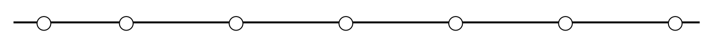

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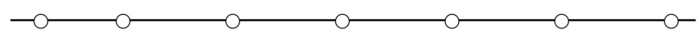

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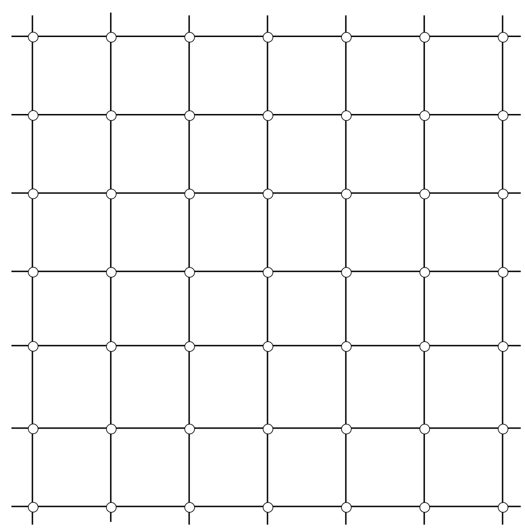

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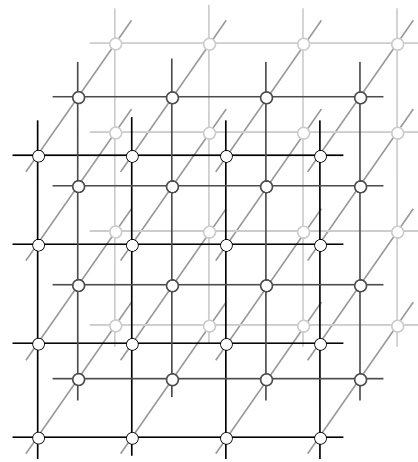

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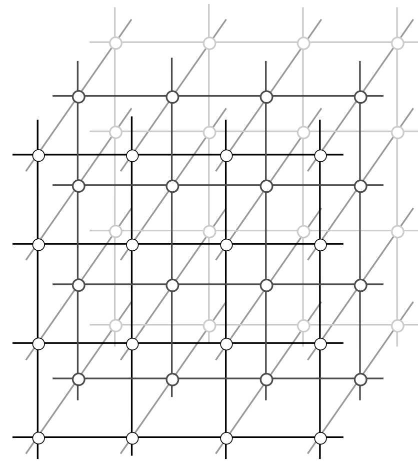

- On a (2d) square grid, the walker moves N, S, E or W with probability 1/4, and in general, on a d-dimensional lattice, the walker moves in one of the $2d$ possible directions with equal probability $1/2d$. Hence the number of possible n step random walks is $c_n = (2d)^n$.

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- Surprisingly—or at least, non-obviously–the answer is yes for $d = 1$ and $d = 2$, but no for $d \geq 3$.

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- Then the next step is either back to the origin (with probability $1/2$), or to “2”, also with probability $1/2$.
- In the latter case, the walker must return to “1” before he/she can return to “0”. The walker, upon returning to “1”, can then go to “0” or move off to the right again.

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- It follows that

$$R = \frac{1}{2} + \frac{1}{4}R + \frac{1}{8}R^2 + \cdots + \frac{R^2}{2^{m+1}} + \cdots .$$

Proof for $d = 1$ continued.

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- This is just a geometric series, summing which gives $2R = \frac{1}{1-R/2}$. Cross-multiplying gives $2R(1 - R/2) = 1$ or $R^2 - 2R + 1 = (R-1)^2 = 0$.

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- Thus the walker will return absolutely certainly to the origin.
- In three dimensions the probability of return is given by a very difficult integral. It evaluates to 0.340537...

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- This took 37 years to get into “simple” closed form:

$$m_3 = \frac{\sqrt{6}}{32\pi^3}\Gamma(\frac{1}{24})\Gamma(\frac{3}{24})\Gamma(\frac{5}{24})\Gamma(\frac{7}{24}) = 1.5163860591\cdots$$

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- There is a close connection between random walks and Brownian motion.
- Note that walks have no *history*. The next step depends only on the walker’s current position. Such a process is called a *Markov process*.

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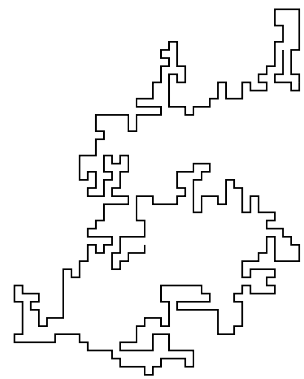

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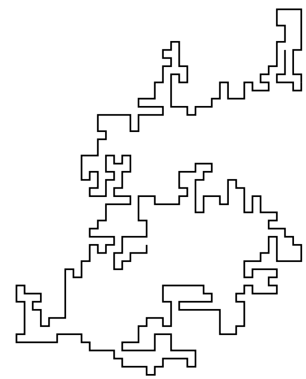

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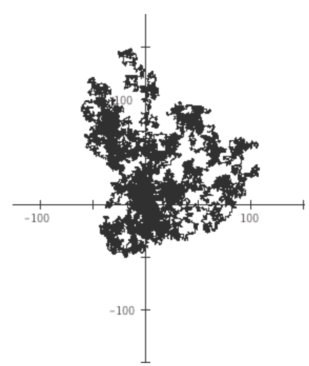

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- The questions we want to answer include the following: How many n-step SAW are there? How big are they?
- The difficulty relates to the fact that we have (for $d > 1$) lost the Markovian property.

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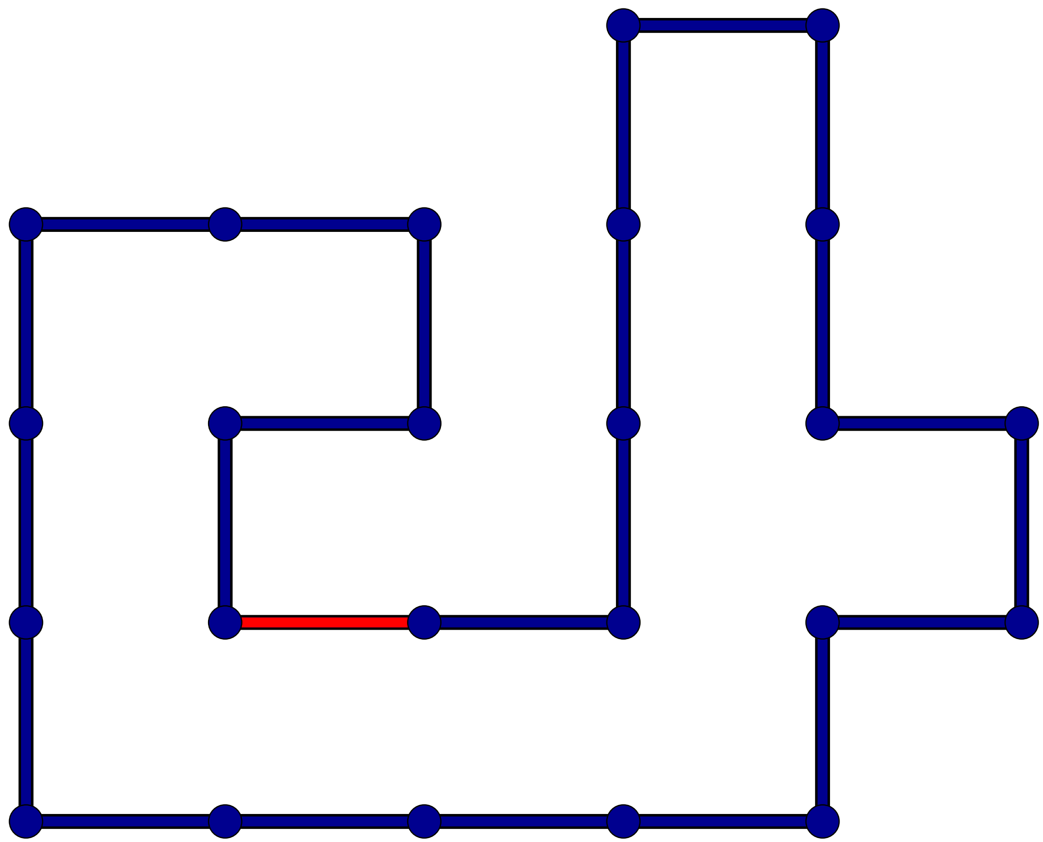

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- Examples range from paint to polyethylene.

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- Those made of identical units are called *homopolymers,*
- Those made of more than one unit are called *heteropolymers* or *copolymers*.
- Chemists are traditionally interested in local properties, notably the specific chemical properties, while physicists are interested in the global properties, and mathematicians are interested in exact solutions, or proving properties that the solution must satisfy, even if we can't find it.

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- The idealisation as random or more usually *self-avoiding* walks on a lattice has become ubiquitous.
- The self-avoiding property reflects the fact that two monomers cannot occupy the same point in space.
- The measure of a polymer is given by properties such as the number of monomers (its length), or the average distance from one end to the other.

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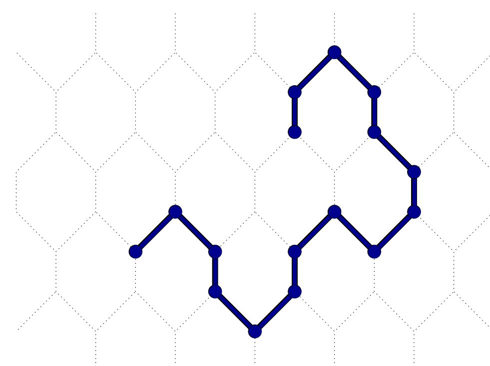

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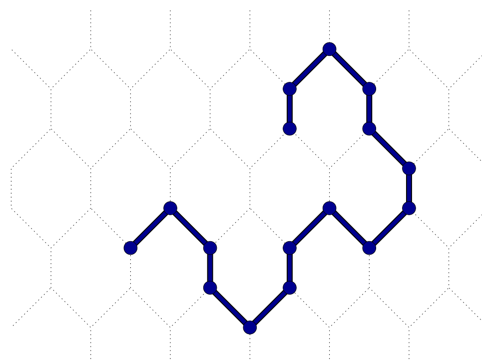

- Unfortunately it is trivial in one dimension, and unsolved in higher dimensions.

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- On the square grid, clearly $c_1 = 4$, $c_2 = 12$ and $c_3 = 36$.

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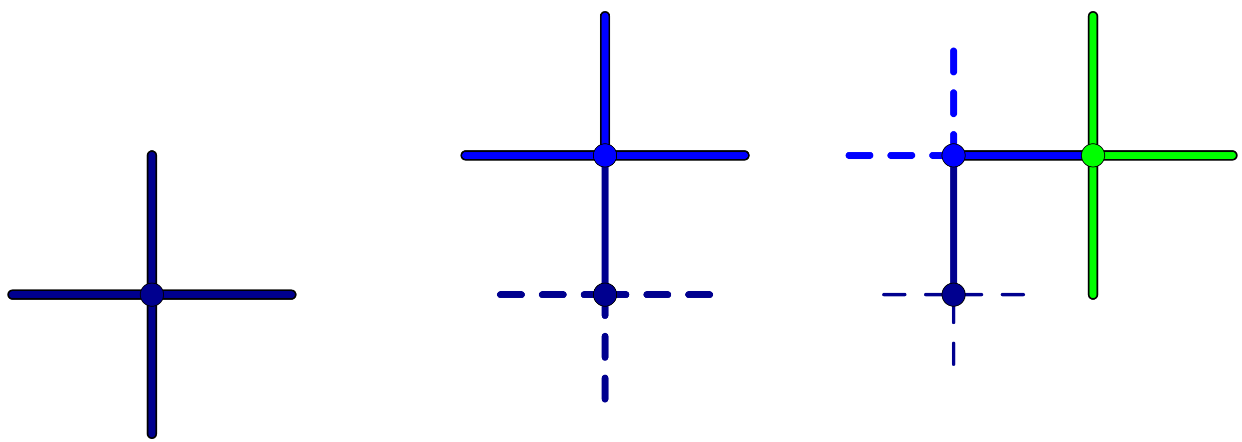

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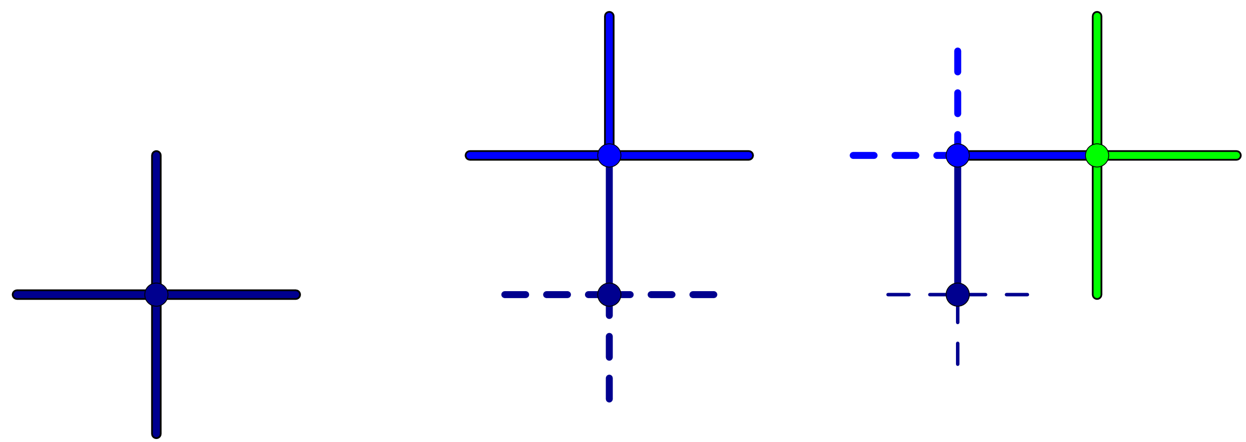

- $c_4 = 100$ rather than 108 as SAW constraint first enters.

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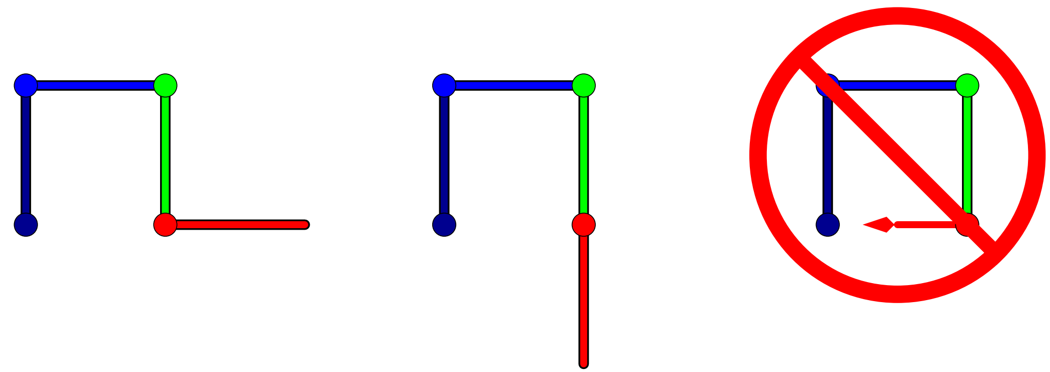

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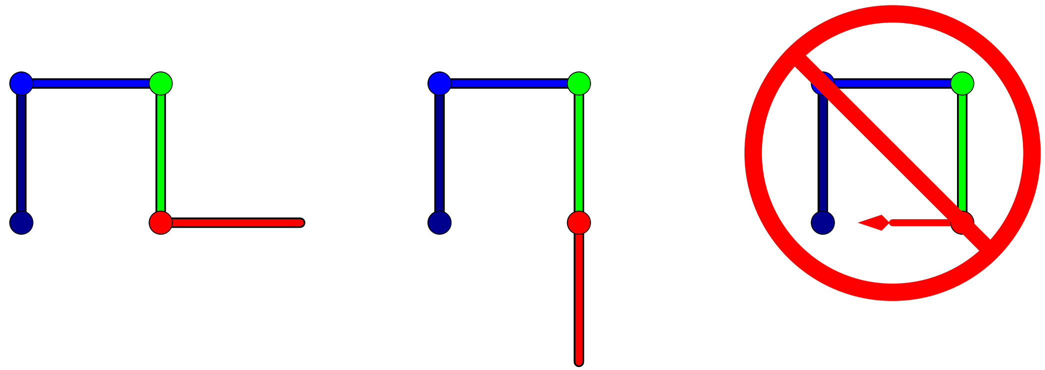

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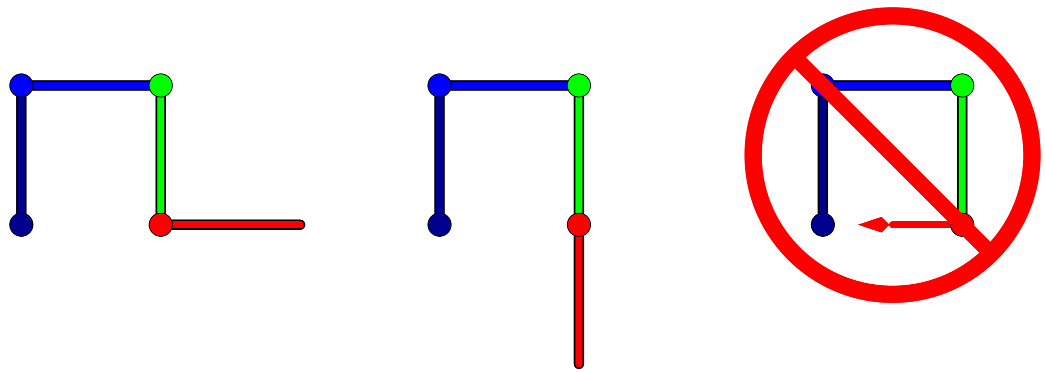

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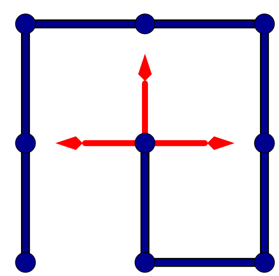

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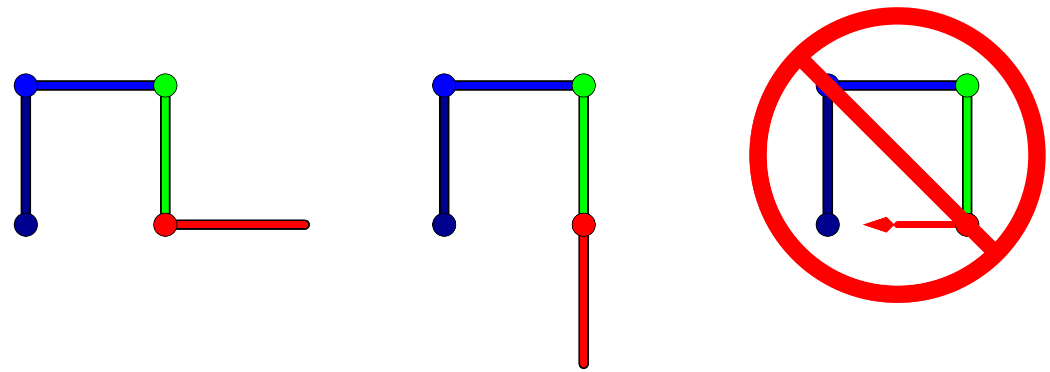

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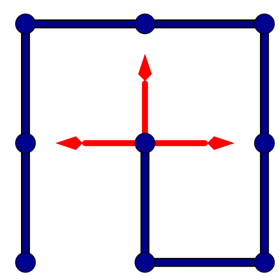

- On the square lattice, the mean number of steps of a self-trapping walk is about 71.

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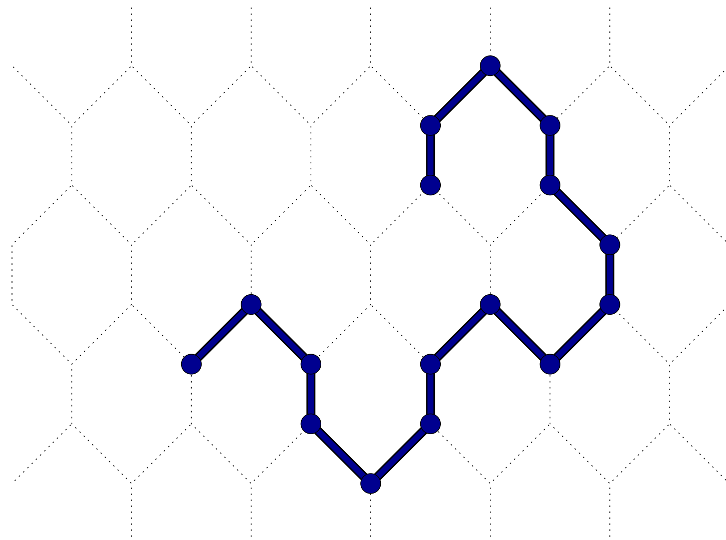
- Recall, on a square grid, for random walks, $c_n = 4^n$. Hence $\mu_{random} = 4$.
- If we forbid immediate reversals, $c_n = 4 \times 3^{n-1}$, so $\mu_{no-reversal} = 3$ in that case.

Values of μ

An argument due to Nienhuis ('82) yields
$\mu_h = \sqrt{2+\sqrt{2}} \approx 1.8477..$ for SAWs on the hexagonal lattice.
(Here, $\mu_{rand.} = 3$, and $\mu_{no-rev.} = 2$.)



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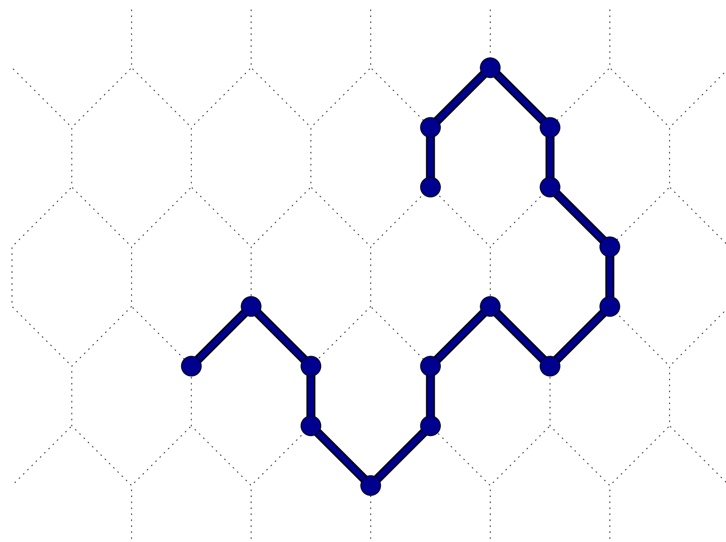

Status: Universally believed, but not proved.

Properties relating to *number* and *size*

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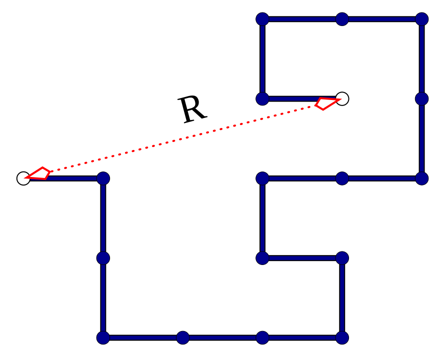

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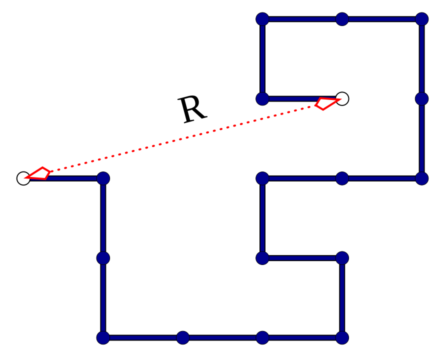

- This measures the *size* of a SAW. Like γ, ν is also lattice independent.

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- This is intuitively reasonable. The SAW constraint causes the walk to “spread out.”

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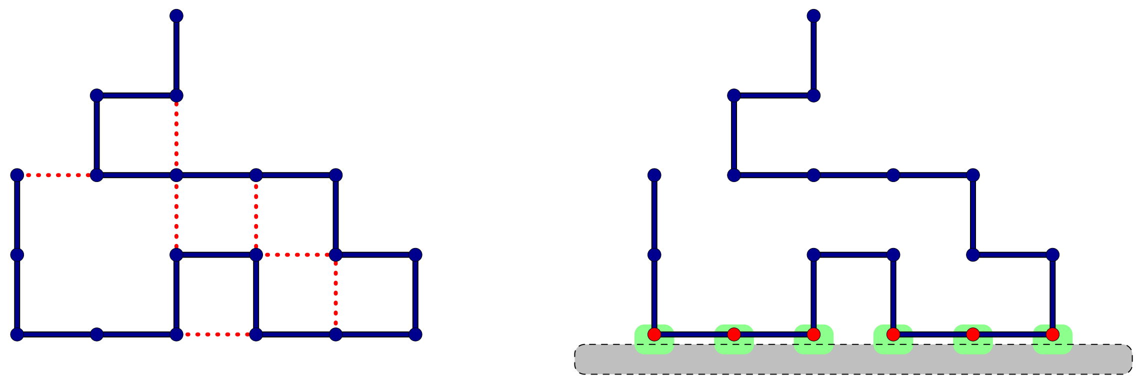

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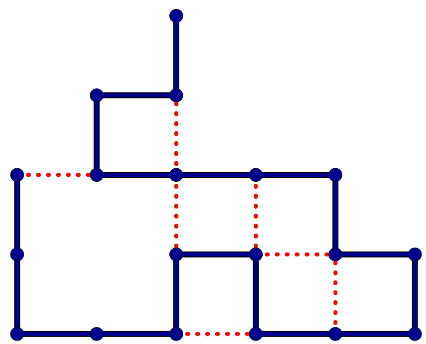

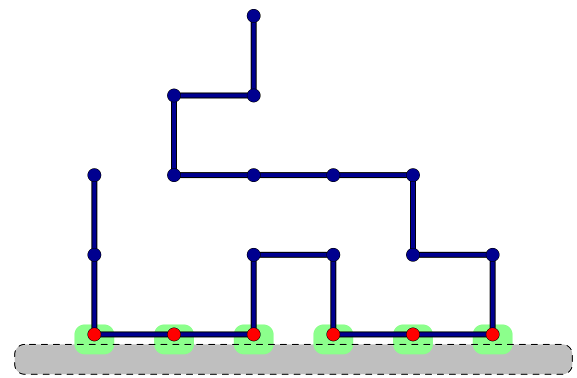

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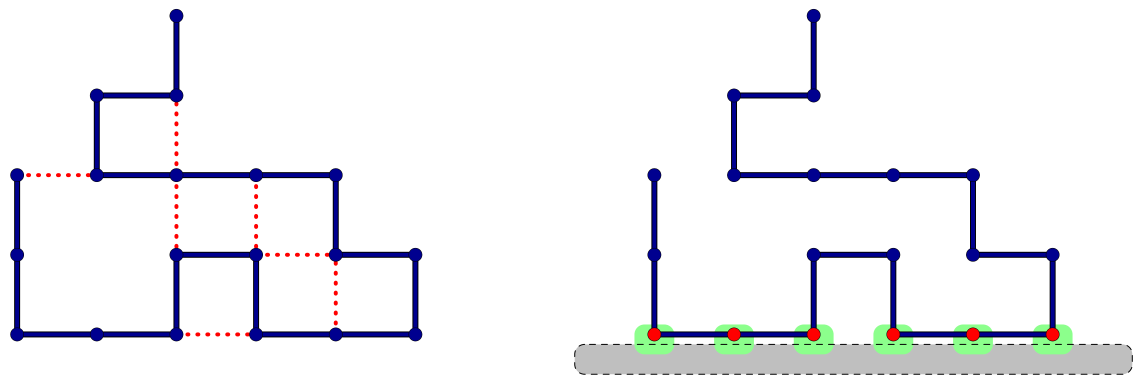

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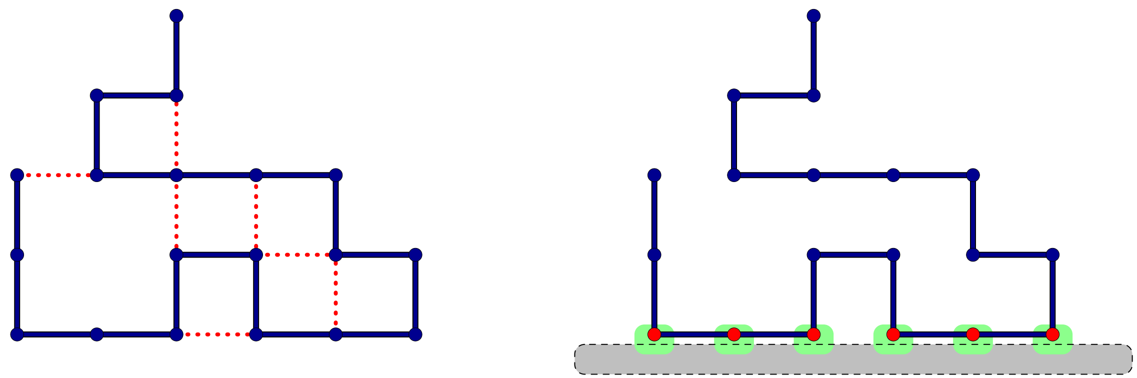

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- We usually ask how the size varies with these interactions.

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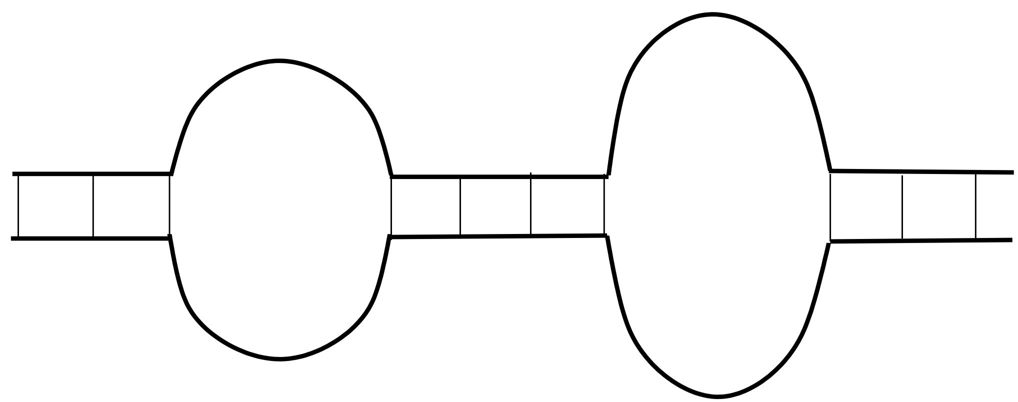

Figure 3: Schematic representation of denatured chain structure

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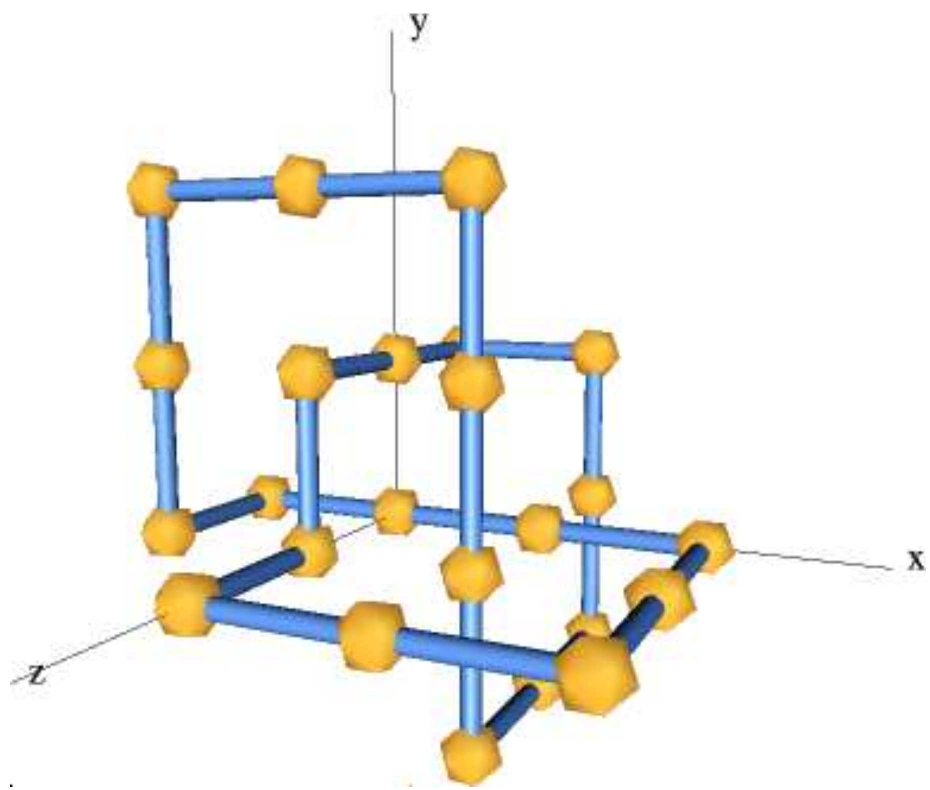
- Because they enclose an area or volume, we can study pressure induced phenomena, which occur in biological molecules.
- The fact that we are dealing with loops means the concept of *knottedness* can be studied. The theory of knots in polymers is an important and active subject in its own right.

Knots

There is a lot of literature devoted to *knotted walks* and *polygons.* These model knots in polymers, and in particular DNA. Here is a *trefoil* in three-dimensional space.



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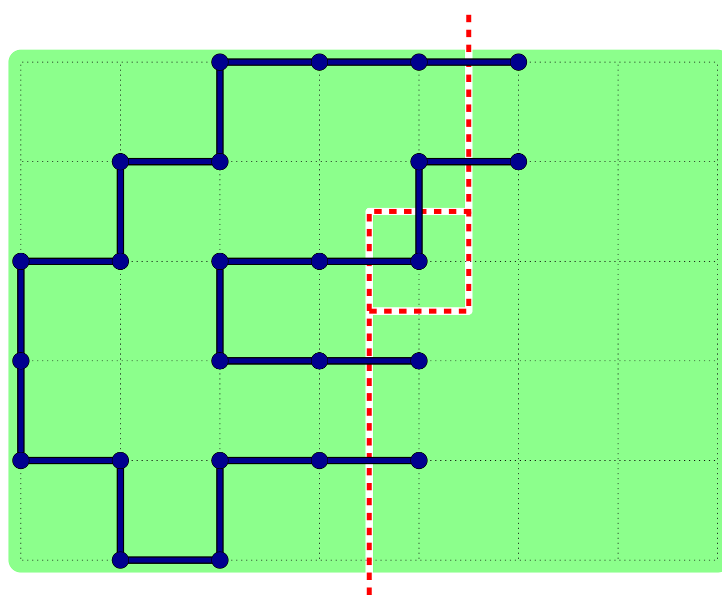

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- The FLM plus TM is the best way to enumerate lattice objects in two dimensions. Works in higher dimension, but implementation is difficult

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The End/Fin

Thank you for your attention.