Random walks

Phys 750 Lecture 17

Random walks

- Deterministic system: given initial conditions, the future is completely determined
- Stochastic system: random transitions between states or random movements along the degrees of freedom
- Stochastic picture is appropriate if we cannot track the individual motion of all particles: e.g., a complicated system interacting with a thermal reservoir

Random walks

- One of the simplest examples is the random walk
- Imagine a particle taking N uncorrelated and randomly determined steps $s_i = \pm 1$
- The total displacement is $x_N = \sum_{i=1}^{N} s_i$
- The total square distance is

$$x_N^2 = \sum_{i=1}^{N} \sum_{j=1}^{N} s_i s_j = N + \sum_{i \neq j} s_i s_j$$

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vanishes on average

$$\langle x_N^2 \rangle = \sum_{i=1}^{N} \sum_{j=1}^{N} \langle s_i s_j \rangle = N + \sum_{i \neq j} \langle s_i s_j \rangle$$

mean over many walks

Random walks

- Root mean square behaviour characteristic of diffusion:

$$\langle x^2 \rangle = 2Dt, \quad \sqrt{\langle x^2 \rangle} \sim \sqrt{t}$$

- Robust with respect to
  - spatial dimension, details of the lattice/continuum
  - most step modifications: e.g., variable step size $x \to x + \xi$ with $\xi \in [-1, 1]$; or with ξ drawn from a nonuniform distribution

Random walks

- Fourth moment of the standard random walk:

$$x_N^4 = \sum_{i=1}^{N} s_i^4 + 3\sum_{i=1}^{N}\left[s_i^2 \sum_{j\neq i} s_j^2\right]$$

- Average over many walks gives

$$\langle x_N^4 \rangle = N + 3N(N-1) = 3N^2 - 2N$$

- Variance of the variance grows linearly with walk length

$$\sqrt{\langle x_N^4 \rangle - \langle x_N^2 \rangle^2} \sim \sqrt{2}N$$

Random walks

- Separation of two typical walkers grows with N
- No single walk behaves like the average walk
- Central limit theorem:
  - a large number of independent random variables with finite mean and variance will be normally distributed

$$x_N^{(1)} = s_1^{(1)} + s_2^{(1)} + \cdots + s_N^{(1)}$$

$$\vdots$$

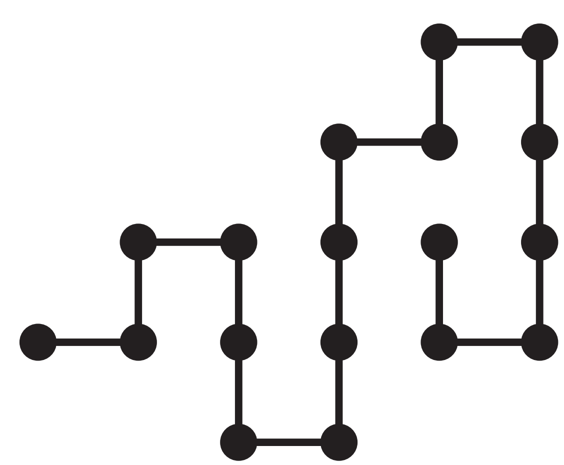
$$x_N^{(k)} = s_1^{(k)} + s_2^{(k)} + \cdots + s_N^{(k)}$$

$$(x_N^{(1)}, x_N^{(2)}, \ldots x_N^{(k)}) \leftarrow e^{-x^2/2\sigma^2}$$

$$\sigma^2 \sim N$$

Self-avoiding walks

- In the conventional random walk, each step is statistically independent
- But interactions and other physical constraints may require models that depend on the path history
- E.g., a polymer is a large molecule of chained structural units (monomers); monomers cannot occupy the same region of space



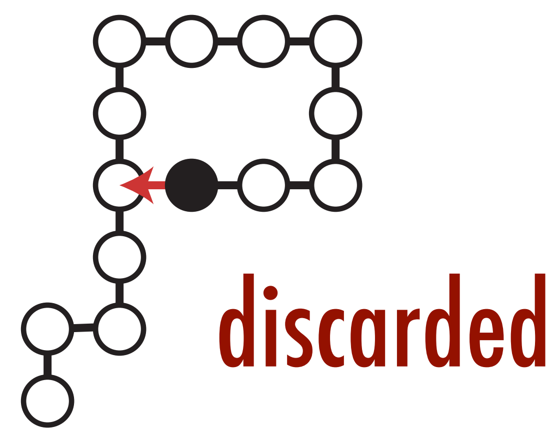
Self-avoiding walks

- Self-avoidance (the "excluded volume constraint") is equivalent to an infinitely strong short-ranged repulsion
- Hence SAWs travel farther afield than convention walks
- Modified power law: $\sqrt{r^2} \sim At^\nu$ with $\nu > 1/2$
  - $\nu = 3/4$ in 2D
  - $\nu \doteq 0.59$ in 3D

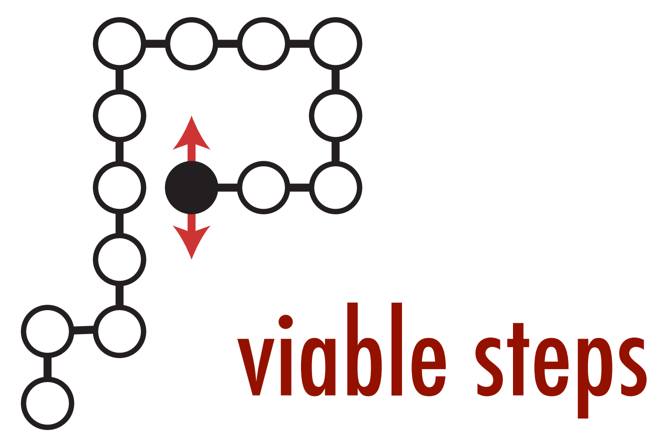
dimensional dependence is a new feature

Self-avoiding walks

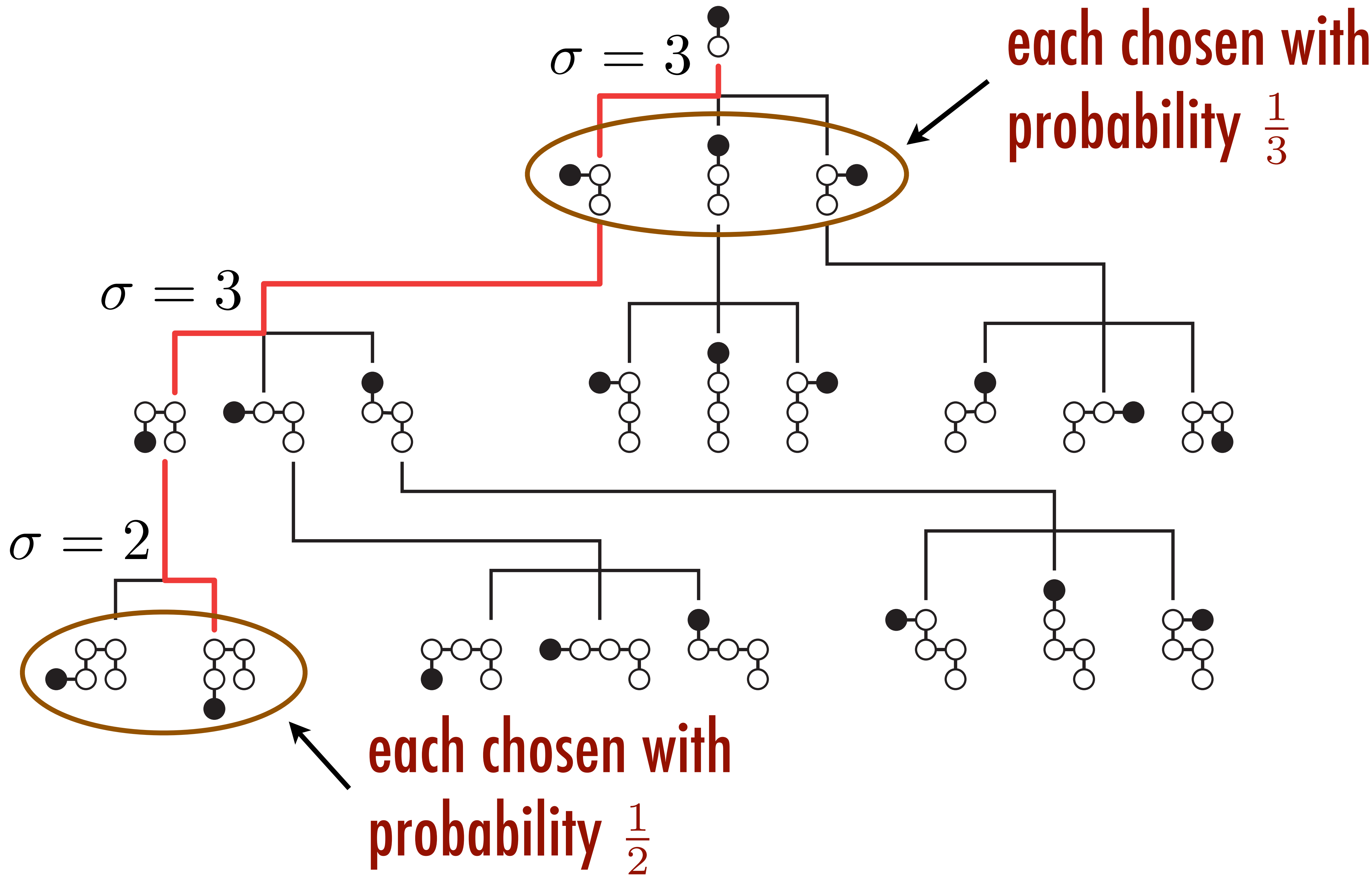
- Self-avoiding walks are difficult to generate: algorithms that grow walks randomly, step by step ($x_N \to x_{N+1}$) suffer from either high attrition or bias
- If we choose from all of the $\sigma = 3$ non-backtracking steps, there is a good chance of self-intersection



- If we choose from only the $\sigma \leq 3$ viable steps, then the walk is giving preference to some configurations



Self-avoiding walks



Self-avoiding walks

- Bias can be eliminated by re-weighting each walk according to

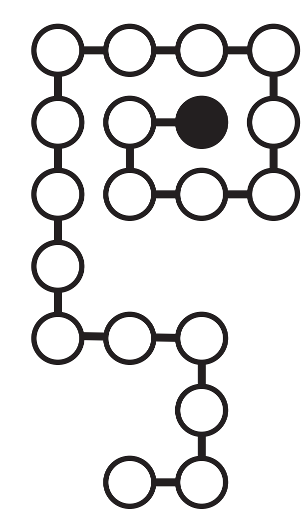
$$w_N = \prod_{i=1}^{N} \frac{1}{\sigma_i}$$

large fluctuations in magnitude (fp issue)

- Measurement of the properties of the N–step walk then corresponds to the weighted average

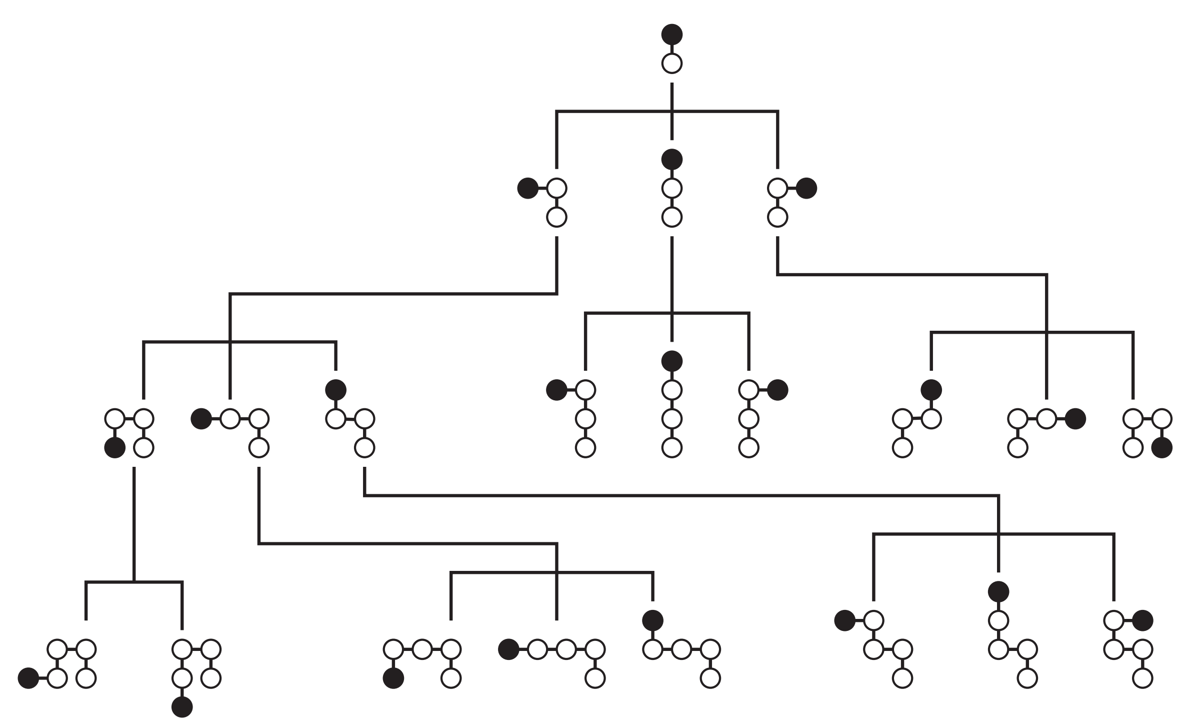
$$\langle O_N \rangle = \frac{\sum_k O_N^{(k)} w_N^{(k)}}{\sum_k w_N^{(k)}}$$

- The problem of attrition through self-trapping remains



Enumeration of SAWs

- An alternative is to exhaustively catalogue all possible configurations
- Systematic construction of the SAW tree using depth-first or breadth-first search algorithms



Enumeration of SAWs

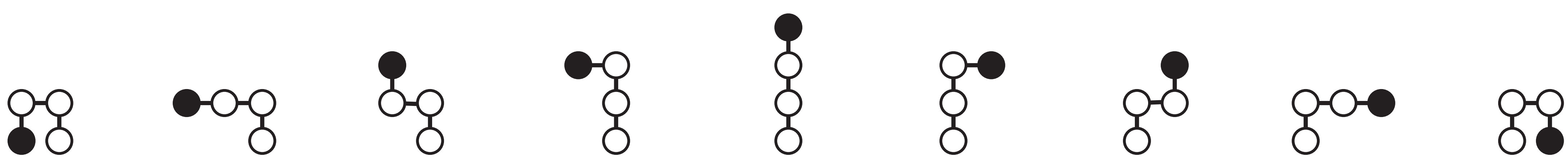
- When all configurations are known, the weights are trivial and measurements correspond to simple averages:

$$\langle O_N \rangle = \frac{\sum_k O_N^{(k)} w_N^{(k)}}{\sum_k w_N^{(k)}} \xrightarrow{w=1} \frac{1}{K_N} \sum_{k=1}^{K_N} O_N^{(k)}$$

- The denominator reverts to K_N, the number of possible walks at level N

Enumeration of SAWs

- Example: measuring $O = r^2$ for the 3-step walk



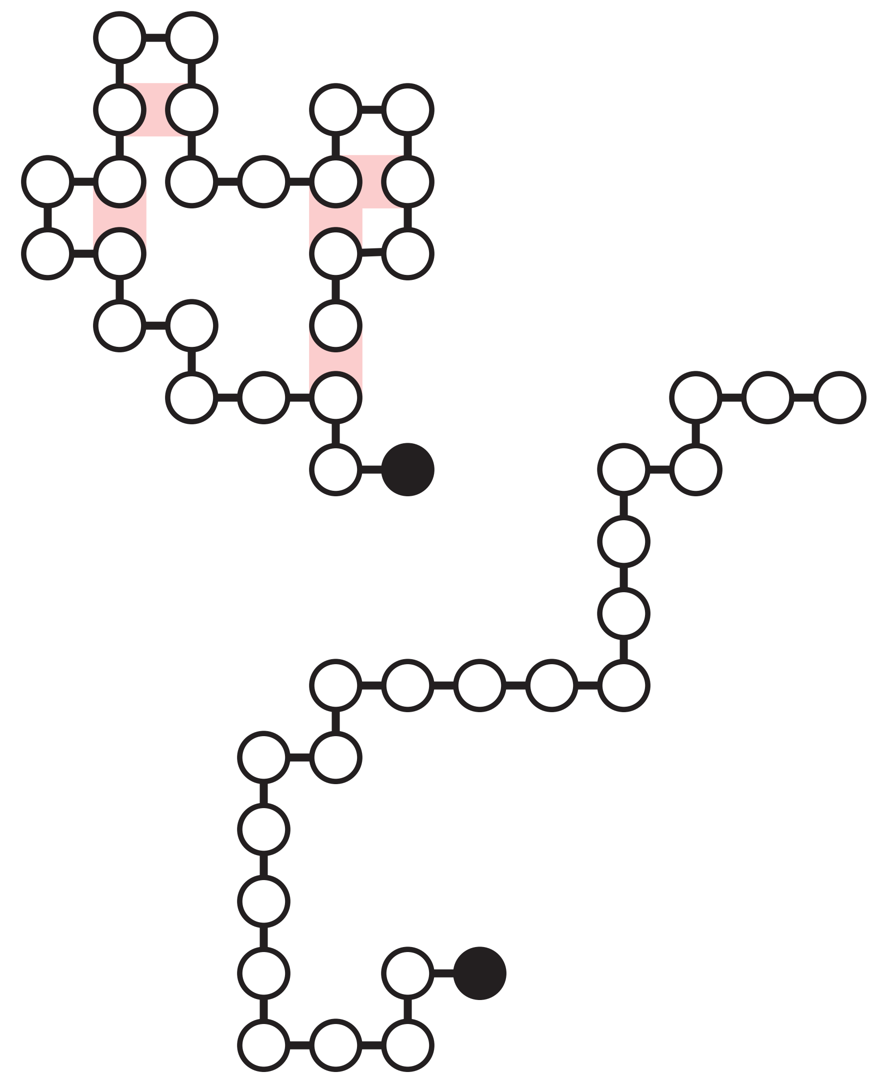
$$\frac{1w+5w+5w+5w+9w+5w+5w+5w+1w}{w+w+w+w+w+w+w+w+w}$$

- Equal weights ($w = 1$) lead to an average

$$\langle r^2_{N=3} \rangle = \frac{9+5\times 6+2\times 1}{9} = \frac{41}{9} \doteq 4.56$$

Interacting SAWs

- How do we handle interactions?
- What if the walks aren't purely random, but instead are influenced by nearest neighbour forces (e.g., van der Waals between monomers)?
- Easiest to treat this in the canonical ensemble (assuming a heat bath fixed at temperature T)



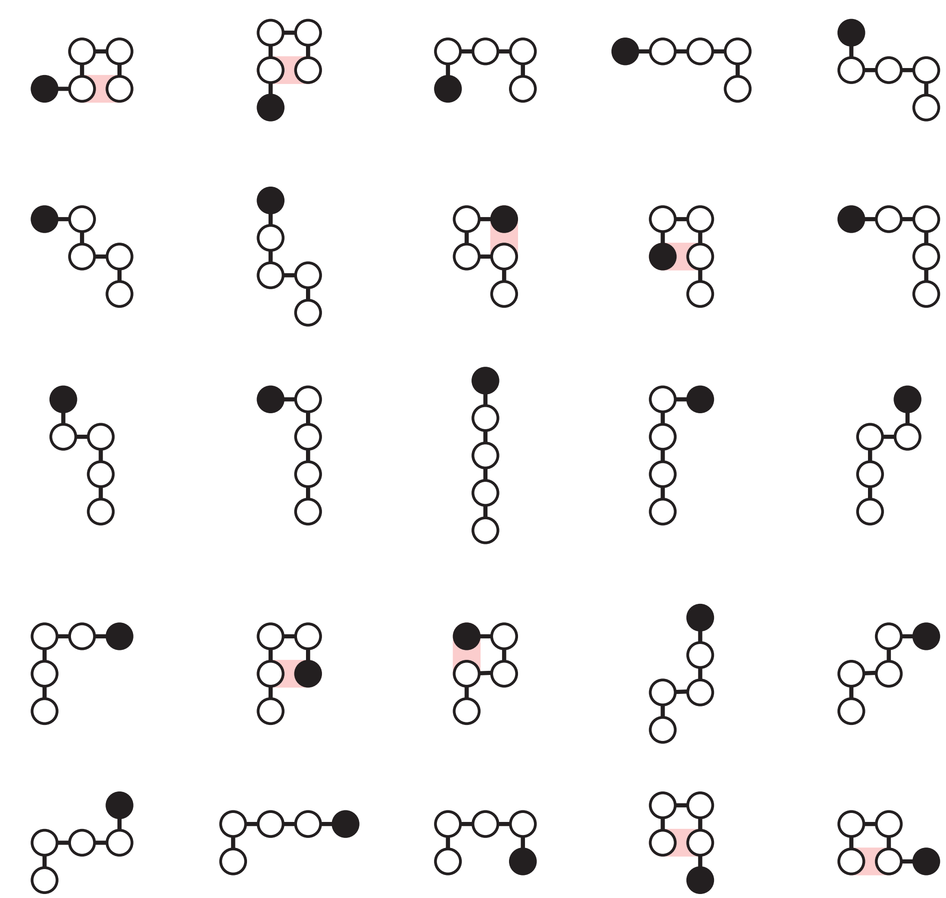
Interacting SAWs

- Introduce Boltzmann weights:

$$\langle O \rangle = \frac{\sum_k O_k w_k}{\sum_k w_k} \xrightarrow{w_k = e^{-\beta E_k}} \frac{1}{Z} \sum_k O_k e^{-\beta E_k}$$

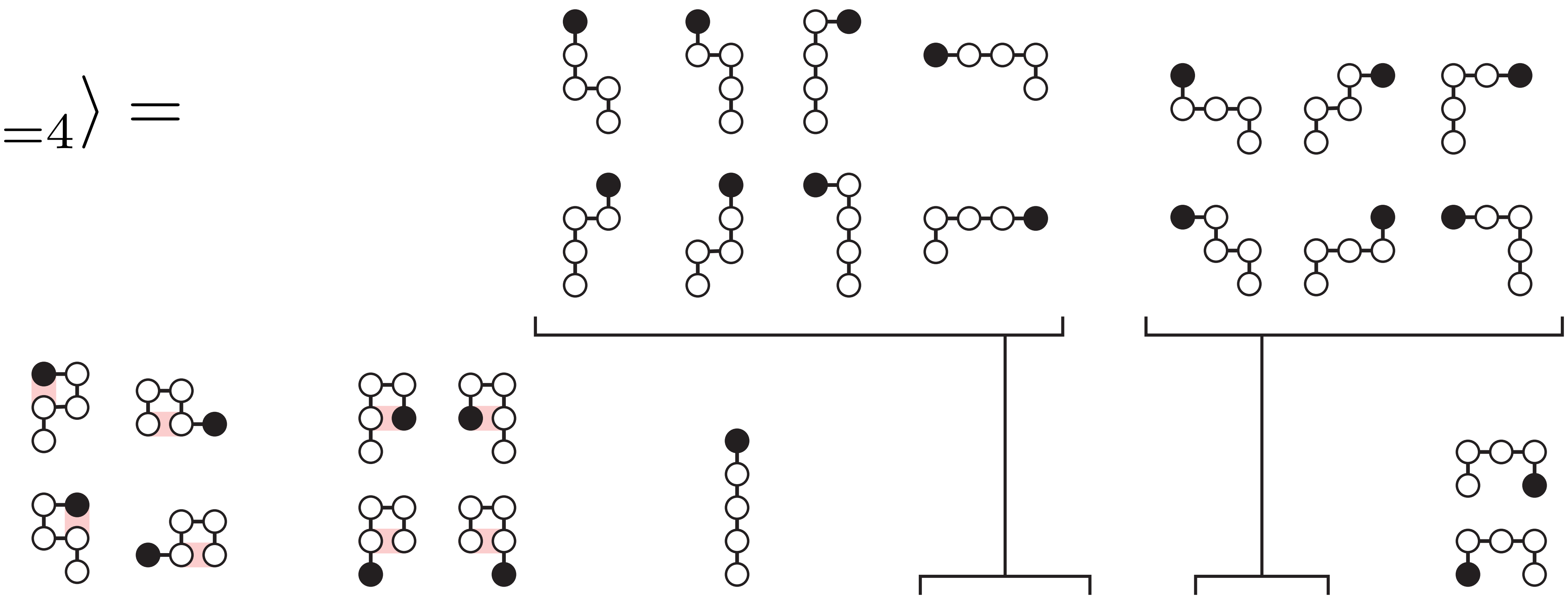
- Example: 4-step walk with configurational energy given by the number of monomers that are neighbours without being adjacent in the chain

$$E_k = -n_k V$$



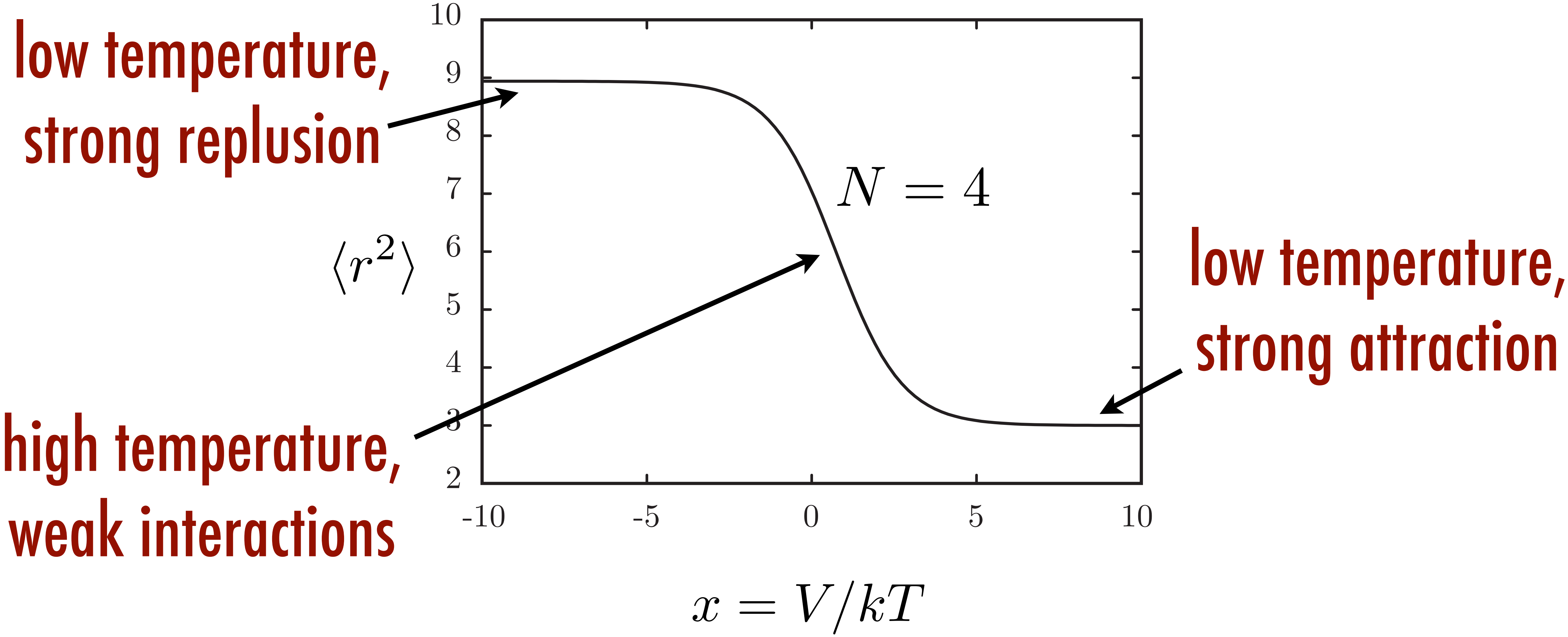
Interacting SAWs

- Group by contribution in $x = \beta V$



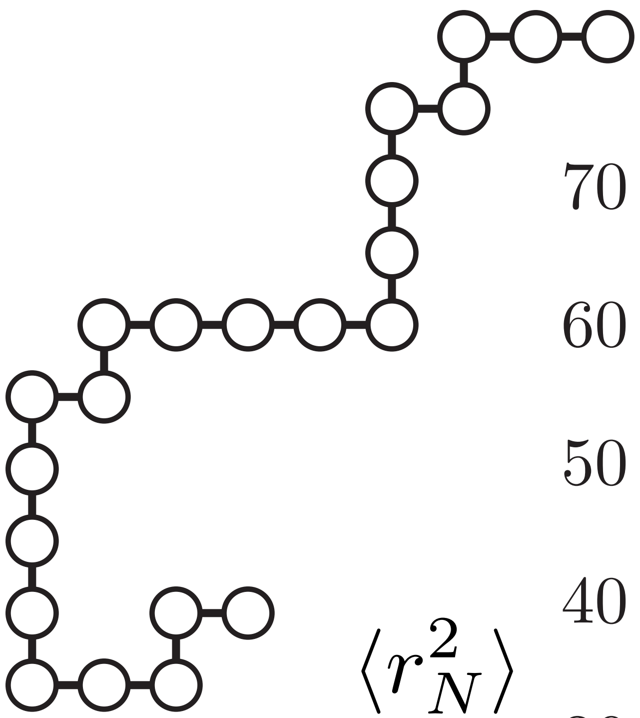
$$\langle r^2_{N=4} \rangle = \frac{4\times 4e^x + 2\times 4e^x + 16\times 1 + 10\times 8 + 8\times 6 + 4\times 2}{3e^x + 5e^x + 1 + 8 + 6 + 2}$$

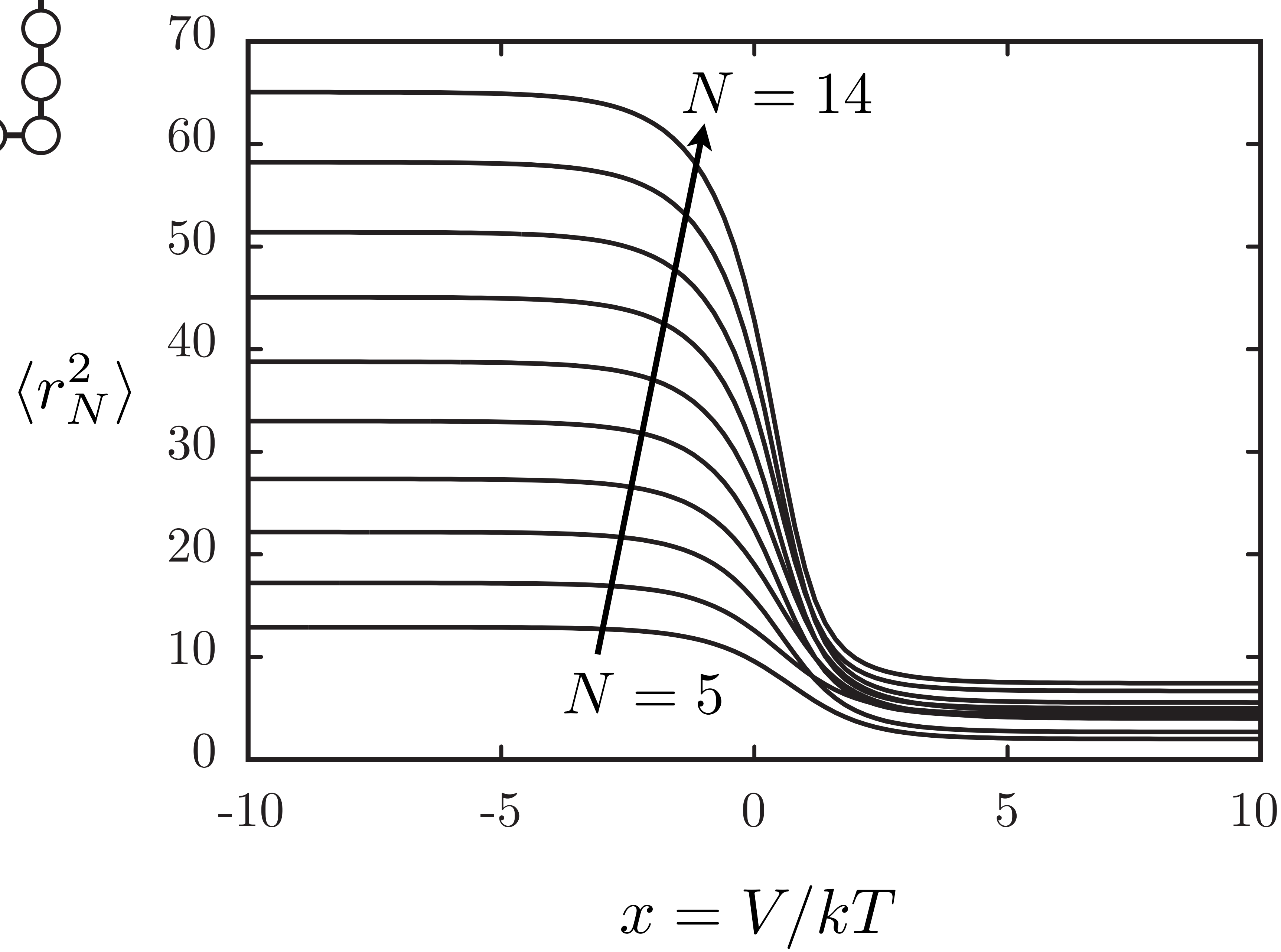
Interacting SAWs

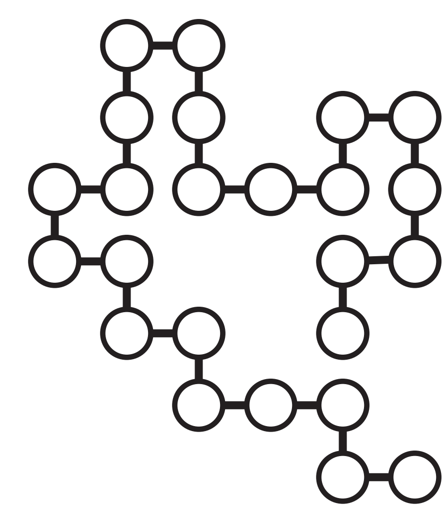


$$\langle r^2_{N=4} \rangle = \frac{24e^x + 152}{8e^x + 17} \to \begin{cases} \frac{24}{8} = 3 & \text{if } x \to \infty \\ \frac{176}{25} \doteq 7.04 & \text{if } x \to 0 \\ \frac{152}{17} \doteq 8.94 & \text{if } x \to -\infty \end{cases}$$

Interacting SAWs







Interacting SAWs