SAW in a box

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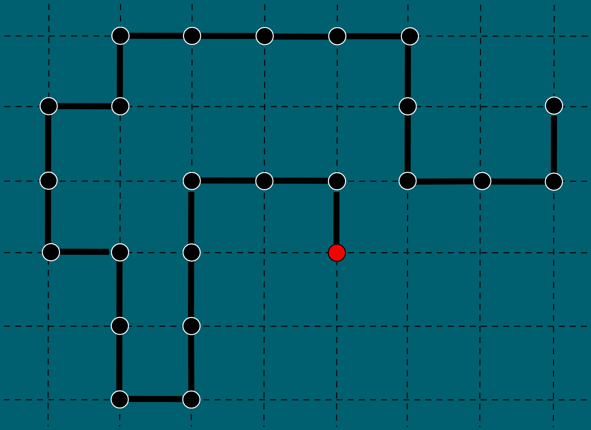
Square lattice Self-avoiding walks (SAW)

A square lattice SAW



A SERIES OF SAW PROBLEMS

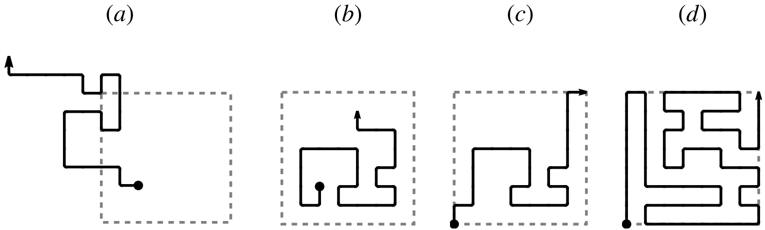


Figure: Example SAWs with increasing degree of confinement to a box of side length $L = 8$. (a) Unconfined, (b) confined to the box (our model), (c) crossing a square and (d) a Hamiltonian path crossing a square.

SAW without any restriction

- Let the number of them be denoted $w(n)$
- It is known that the growth constant exists (Hammersley 1957)

$$\mu = \lim_{n\to\infty} w(n)^{1/n}$$

- with a best estimate of μ most recently $\mu = 2.63815853032790(3)$ (Jacobsen, Scullard and Guttmann, 2016)
- It is expected that

$$w(n) \sim A\mu^n n^{\gamma-1}$$

where $\gamma = 43/32$.

Size of a SAW

The "size" of the SAW scales as

$$\langle R^2(n)\rangle \sim An^{2\nu}$$

In two-dimensions ν is known exactly to be $3/4$ for non-dense polymers and this has been confirmed numerically to high precision (Clisby 2010).
All measures of size should behave similarly: end-to-end distance, radius of gyration and maximum span $L(n)$, so

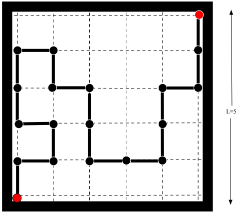
$$L(n) \sim Cn^{\nu}$$

SAW crossing a Square I

- Now consider SAWs with end points fixed at two opposing vertices of a square of side L bonds and all sites of the walk lie within or on the boundary of the square where

$$2L \leq n \leq L^2 + 2L$$

- This problem has a long history too: Whittington and Guttmann 1990, Madras 1995 and Bousquet-Mélou, Guttmann and Jensen 2005 and Knuth 1976 introduced a similar problem



SAW crossing a Square III

Let the number of such SAW be s_L . It has been proven (Abbott and Hanson 1978 and Whittington and Guttmann 1990) that the limit

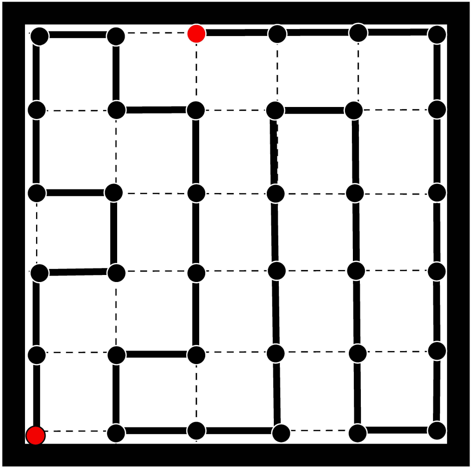
$$\lambda_S = \lim_{L\to\infty} s_L^{1/L^2}$$

exists so that $s_L = \lambda_S^{L^2+o(L^2)}$
The best estimate of this growth constant (Bousquet-Mélou, Guttmann and Jensen 2005) $\lambda_S = 1.744550(5)$
The average number of steps $N(L)$ is expected to scale as

$$N(L) \sim CL^{1/\nu}$$

with $\nu = 3/4$

HAMILTONIAN WALKS I



HAMILTONIAN WALKS II

Walks that visit every vertex of a finite patch of lattice are known as Hamiltonian
Let the number of such walks be h_L and the limit

$$\mu_H = \lim_{L\to\infty} h_L^{1/L^2}$$

exists and has been estimated as $\mu_H = 1.472801(1)$ (Bousquet-Mélou, Guttmann and Jensen 2005)
Note: Whether the walks start and finish at opposite corners is not relevant.

SAW WITH LENGTH FUGACITY

Length fugacity

Consider weighting the length by a fugacity e^{β} with $-\infty < \beta < \infty$.

For SAW in the bulk consider the grand partition function

$$G_w(\beta) = \sum_{n=0}^{\infty} w(n) e^{\beta n},$$

which converges for $\beta < -\log \mu$.
Note that

$$\langle n \rangle = \frac{\partial \log G_w(\beta)}{\partial \beta}$$

is finite when G_w is finite and diverges as a simple pole.

SAW crossing a square with length fugacity

For walks that cross a square define the partition function

$$Z^{(S)}(\beta)_L = \sum_n s_L(n) e^{\beta n}$$

and we can define the free energy as the limit

$$f^{(S)}(\beta) = \lim_{L\to\infty} \frac{1}{L^2} \log Z^{(S)}(\beta)_L$$

Note

$$f^{(S)}(0) = \log \lambda_S$$

PREVIOUS RIGOROUS BOUNDS

Previous rigorous results and bounds on the free energies are summarized as

$$f^{(S)}(\beta) = 0, \quad \text{for } \beta < -\log \mu$$

$$\log \mu_H + \beta \leq f^{(S)}(\beta) \leq \log \mu + \beta, \quad \text{for } \beta \geq -\log \mu$$

Self-avoiding walks in a box I

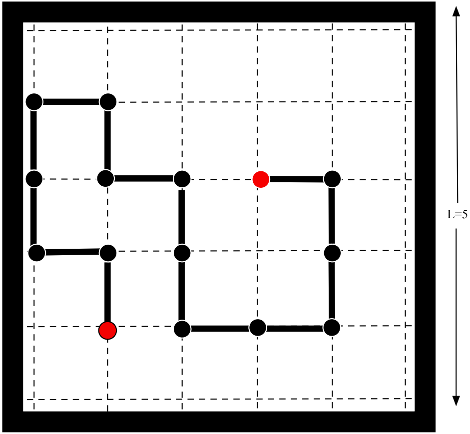
Our problem:

SAW in a box of side length L without restriction of their endpoints

$$Z_L^{(B)}(\beta) = \sum_n c_L(n) e^{\beta n},$$

where $c_L(n)$ is the number of walks of length n that fit in the box and e^β is the fugacity of each step.
It is useful to also consider the number of walks $\hat{c}_L(n)$ that are unique up to translation with the corresponding partition function $\hat{Z}_L^{(B)}(\beta)$

Self-avoiding walks in a box II



Self-avoiding walks in a box III

We define the free energy in a similar way to walks that cross a square as

$$f^{(B)}(\beta) = \lim_{L\to\infty} \frac{1}{L^2} \log Z_L^{(B)}(\beta)$$

and similarly for $\hat{f}^{(B)}(\beta)$
It can be easily seen that if the limit $\hat{f}^{(B)}(\beta)$ exists so does $f^{(B)}(\beta)$.

RIGOROUS RESULTS

It can be proved using standard arguments that

$$f^{(B)}(\beta) = \hat{f}^{(B)}(\beta) = 0 \quad \text{for } \beta < -\log\mu$$

and

$$\log\mu + \beta \geq f^{(B)}(\beta) = \hat{f}^{(B)}(\beta) \geq f^{(S)}(\beta) \geq \log\mu_H + \beta \quad \text{for } \beta \geq -\log\mu.$$

FREE ENERGY BOUNDS

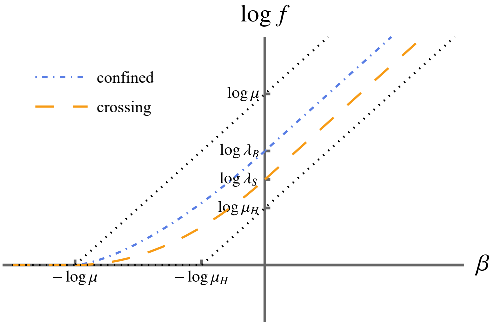


Figure: The free energies of confined SAW models. We do not know that the free energy for our model of confined SAW is strictly greater than that of SAW that cross a square. The top and bottom dotted lines mark bounds derived from unconstrained SAWs and Hamiltonian paths, respectively.

Scaling quantities

We define the average density via a derivatve

$$\rho(\beta) = \frac{\partial f^{(B)}(\beta)}{\partial \beta}.$$

Standard critical scaling implies the existence of an exponent α

$$f^{(B)}(\beta) \sim |\beta - \beta_{\mathrm{c}}|^{2-\alpha}, \quad \beta \to \beta_{\mathrm{c}}^{+},$$

and that

$$\rho(\beta) \sim |\beta - \beta_{\mathrm{c}}|^{1-\alpha}, \quad \beta \to \beta_{\mathrm{c}}^{+}.$$

FINITE SIZE SCALING: DENSITY

For finite L

$$\rho_L = \frac{\partial f_L}{\partial \beta} = \frac{\langle n \rangle}{L^2}$$

and finite size scaling suggests that

$$\rho_L(\beta) \sim L^q \psi \left((\beta - \beta_c) L^{1/\nu} \right)$$

Scaling arguments imply

$$q = -(1 - \alpha)/\nu$$

and that $\alpha = 1/2$

FINITE SIZE SCALING: DENSITY

Density Scaling Ansatz

$$\rho_L(\beta) \sim L^{-2/3}\psi\left(\left(\beta - \beta_c\right) L^{4/3}\right).$$

For fixed values of β we have

$$\langle n\rangle(\beta) \sim \begin{cases} A & \text{for } \beta < \beta_c \ , \\ B\,L^{4/3} & \text{for } \beta = \beta_c \ , \\ C\,L^2 & \text{for } \beta > \beta_c \end{cases}$$

with

$$A \sim (\beta_c - \beta)^{-1} \text{ as } \beta \to \beta_c^- \text{ and } C \sim (\beta_c - \beta)^{\frac{1}{2}} \text{ as } \beta \to \beta_c^+$$

The scaling ansatz for the partition function can be written as

$$Z_L^{(B)}(\beta) \sim L^p \phi\left((\beta - \beta_c)\, L^{1/\nu}\right),$$

with scaling argument implying that

$$p = 2 - \eta = \gamma/\nu$$

so that

$$Z_L^{(B)}(\beta_c) \sim BL^{2-\eta}$$

η is predicted to have exact value 5/24 in two dimensions (Nienhuis1982).

Partition Function Scaling Ansatz

$$Z_L^{(B)}(\beta) \sim L^{43/24}\phi\left((\beta - \beta_c)\, L^{4/3}\right),$$

The fixed β scenario is

$$Z_L^{(B)}(\beta) \sim \begin{cases} D(\beta) & \text{for } \beta < \beta_c \ , \\ E\, L^{43/24} & \text{for } \beta = \beta_c \ , \\ \exp\left(f^{(B)}(\beta)\left[L^2 + o\left(L^2\right)\right]\right) & \text{for } \beta > \beta_c \ . \end{cases}$$

with

$$D \sim (\beta_c - \beta)^{-43/32} \text{ as } \beta \to \beta_c^-$$

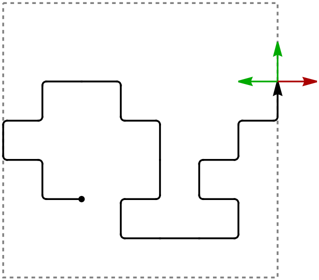


Figure: A sample SAW of length $n = 24$, considered to be confined in a bounding box of side length $L = 7$. The possible next steps are shown with arrows; the only restriction is that the step to the right is forbidden if the limit for the simulation was chosen to be $L_{\max} = 7$.

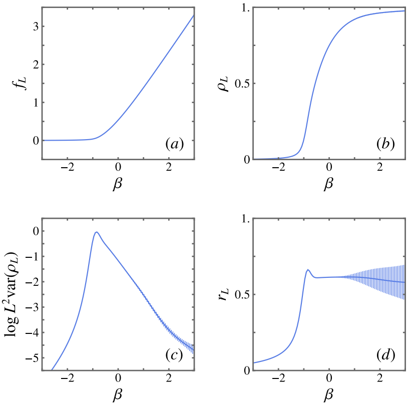


Figure: Thermodynamic quantities for SAWs confined to a box of size $L = 9$. Plots show (a) the free energy f_L, (b) the density ρ_L, (c) the logarithm of the variance $L^2 \mathrm{var}(\rho_L)$, and (d) the average size r.

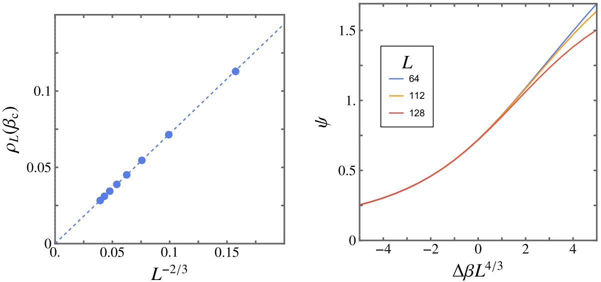


Figure: (a) The critical density $\rho_L(\beta_c)$ plotted against the expected scaling $L^{-2/3}$ and (b) the scaling function $\psi(x)$ for confined SAWs.

OUR EXPONENT ESTIMATES: ν AND α

We fitted the data to our scaling form at $\beta = \beta_c$ assuming $\nu = 3/4$ yielding the critical exponent

$$\alpha = 0.4996(8)$$

Then we considered the crossover exponent in the scaling variable so obtain the estimate

$$\nu = 0.756(4)$$

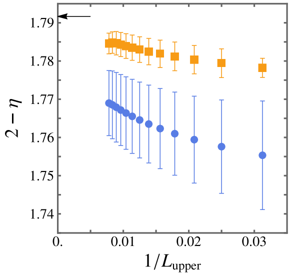


Figure: The critical exponent of the confined SAW partition function $Z_L(\beta_c)$ versus the upper bound of the range of L values used to fit the data, with (top) and without (bottom) a correction-to-scaling term.

OUR EXPONENT ESTIMATES: η

We fitted the data to our scaling form at $\beta = \beta_c$ yielding the critical exponent

$$2 - \eta = 1.785(3)$$

to be compared to the conjectured value of $43/24 = 1.791\dot{6}$

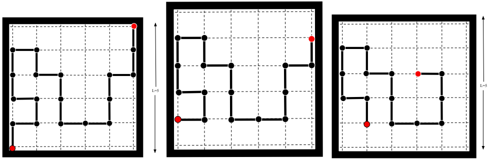
SIMULATING HAMILTONIAN WALKS

Monte Carlo Backbite Algorithm (clisby.net)

- Moves go back to ”Monte Carlo studies of polymer chain dimensions in the melt” by Marc L. Mansfield, J. Chem. Phys. 77, 1554 (1982)
- “Secondary structures in long compact polymers” by Richard Oberdorf, Allison Ferguson, Jesper L. Jacobsen and Jané Kondev, Phys. Rev. E 74, 051801 (2006)
- An aside: no proof of ergodicity
- Let’s use the moves for a different purpose ...

SAW in a Box with Three Endpoint Conditions

1. walks whose endpoints lie at opposing corners of the square counted as s_L;
2. walks whose endpoints lie on opposing sides of the square counted as d_L;
3. walks whose endpoints lie anywhere inside the square (or on the boundary) counted as a_L.



THE LIMIT OF INTEREST

We are interested in the existence of the limit

$$\lambda_A = \lim_{L\to\infty} a_L^{1/L^2} \ .$$

and comparing its value to the previously considered

$$\lambda_S = \lim_{L\to\infty} s_L^{1/L^2} = 1.744550(5) \ .$$

One can in fact prove that

$$\lambda_A = \lambda_S$$

Start of the proof

Let us further define the number of walks whose endpoints lie anywhere inside a square of side ℓ that span the square in at least one direction: in this way they are walks whose minimal bounding box is of side ℓ and these have cardinality m_ℓ with the convention $m_0 = 1$. Denote by $\widehat{m}_L$ the union of the sets counted by m_ℓ for $0 \leq \ell \leq L$. Hence

$$\widehat{m}_L = \sum_{\ell=0}^{L} m_\ell$$

and

$$s_L \leq d_L \leq m_L \leq \widehat{m}_L \leq a_L \ .$$

Importantly can also argue that

$$a_L \leq (L+1)^2 \widehat{m}_L \leq (L+1)^3 m_L \ .$$

Our comparisons

So

$$m_L \leq a_L \leq (L+1)^3 m_L \ .$$

Hence, if we can show that

$$\lambda_M = \lim_{L\to\infty} m_L^{1/L^2}$$

exists then λ_A exists and $\lambda_A = \lambda_M$
Moreover if we can also prove

$$\lambda_M = \lambda_S$$

we will have our result

$$\lambda_A = \lambda_S$$

So need to compare

walks with end points anywhere to those at opposite corners where the bounding box is a square of side L

STRATEGY

- Start with walks whose end points are anywhere inside the box
- Move the endpoints to the sides of the box
- bound the number of configurations that lead to a unique configuation with endpoints on the sides of the box

Backbite moves

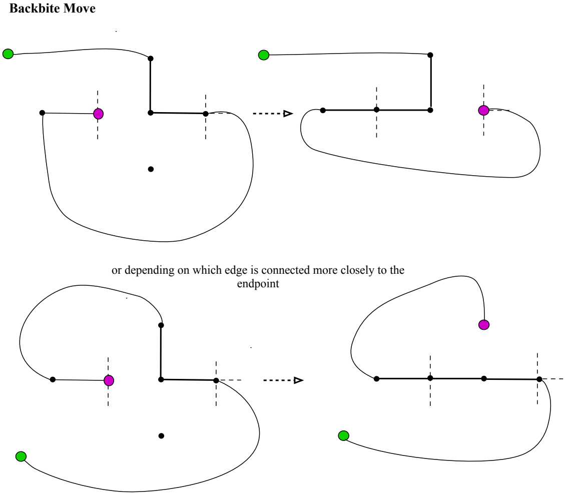


Figure: The backbite move from the Hamiltonian walk algorithm

End attack moves

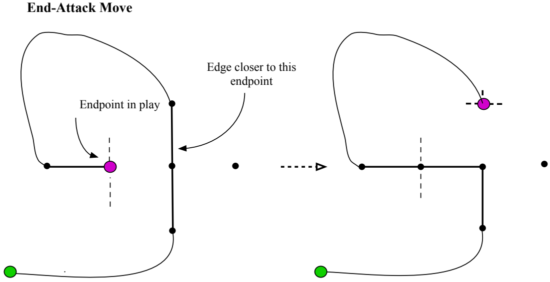


Figure: The end-attack move

Changing the length moves

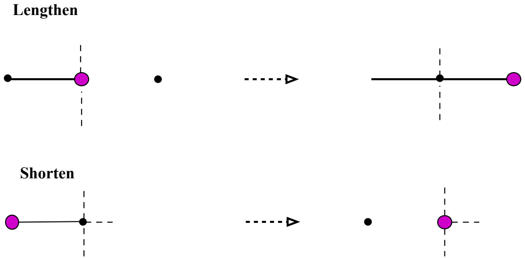


Figure: The lengthening and shortening moves.

ANTECEDENTS

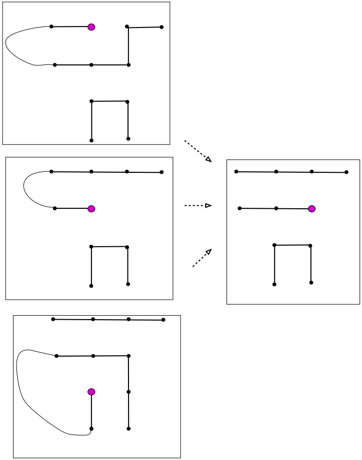


Figure: On the left are the three possible antecedents of the configuration on the right when moving the endpoint to the right

Final bounds

Consider the antecedents whose left endpoint reach the boundary after b moves, then the total is a sum over values of $b \leq L$. Hence the total number of antecedents is bounded for $L \geq 2$ by

$$\sum_{b=0}^{L} 3^b \sum_{r=0}^{L-b} 3^r = \frac{1}{2} \sum_{b=0}^{L} 3^b (3^{L-b+1} - 1) < \frac{1}{2}(L+1)3^{L+1} \, .$$

Hence we have

$$s_L \leq m_L \leq \frac{1}{2}(L+1)3^{L+1} s_L$$

and the results (λ_M exists and $\lambda_M = \lambda_S$) follow by raising each to the power $1/L^2$ and taking the limit $L \to \infty$. Hence

$$\lambda_A = \lambda_S$$

FULL ASYMPTOTICS

From series analysis we conjecture that the number of such walks A_L, for both problems, behaves as

$$A_L \sim \lambda_A^{L^2+bL+c} \cdot L^g,$$

where $\lambda_A = 1.7445498 \pm 0.0000012$, $b = -0.04354 \pm 0.0005$, $c = -1.35 \pm 0.45$, and $g = 3.9 \pm 0.1$.