SAW in a box

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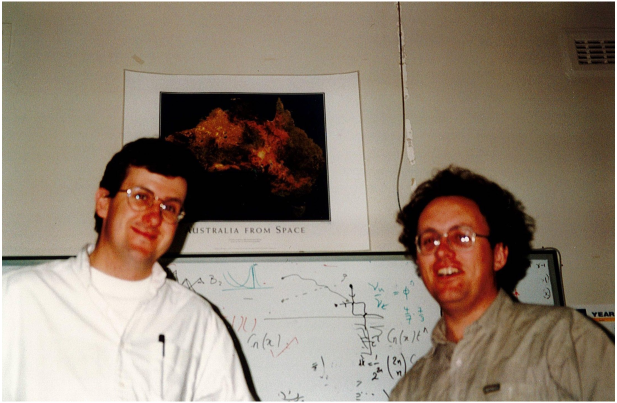
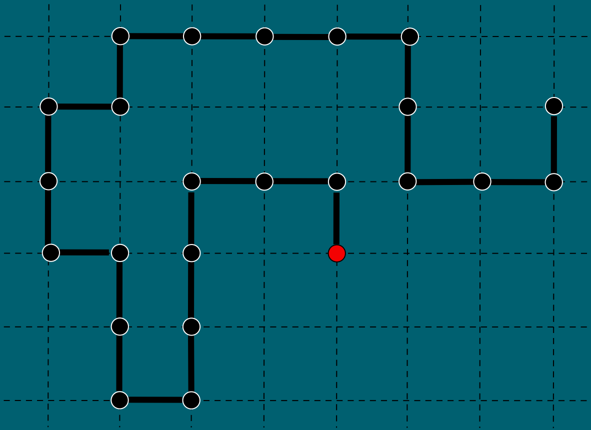

USTRALIA FROM SPACE

MOTIVATIONS

- rigour/simulation/scaling
- scaling arguments
- asymptotic matching: crossover scaling form is consistent with fixed parameter scaling
- polymers in mesoscopic pores

Square lattice Self-avoiding walks (SAW)

A square lattice SAW



A series of SAW problems

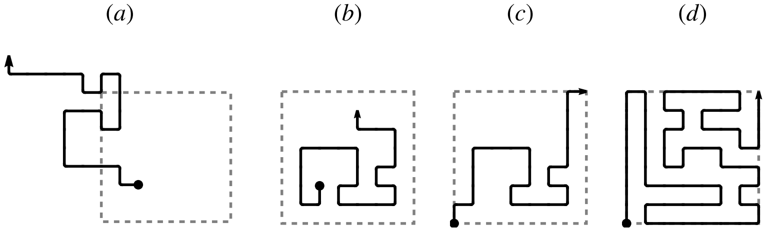


Figure: Example SAWs with increasing degree of confinement to a box of side length $L = 8$. (a) Unconfined, (b) confined to the box (our model), (c) crossing a square and (d) a Hamiltonian path crossing a square.

SAW without any restriction

- The problem we all know: Self-avoiding walks on the square lattice of length n without further 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

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

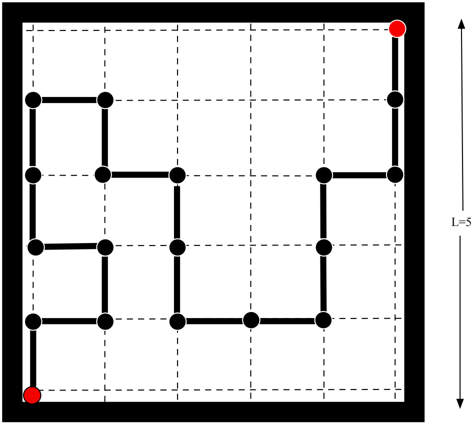
In two-dimensions ν is known exactly to be $3/4$ for non-dense polymers and this has been confirmed numerically to high precision (Clisby 2010).
All measures of size should behave similarly: end-to-end distance, radius of gyration and maximum span $L(n)$, so

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

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
- $$2L \leq n \leq L^2 + 2L$$
- 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
- Recent extensions to links by Janse van Rensburg and Orlandini 2021

SAW crossing a Square lattice II



SAW crossing a Square III

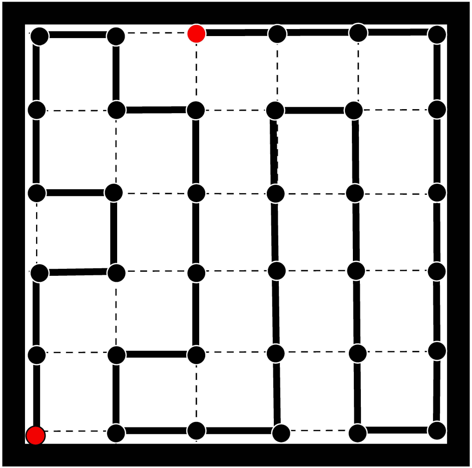
Let the number of such SAW be s_L . It has been proven (Abbott and Hanson 1978 and Whittington and Guttmann 1990) that the limit

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

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

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

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

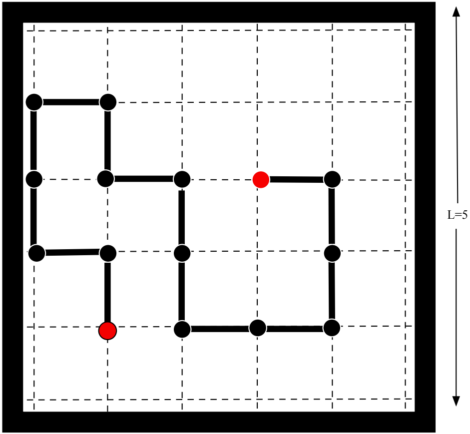
Our problem:

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

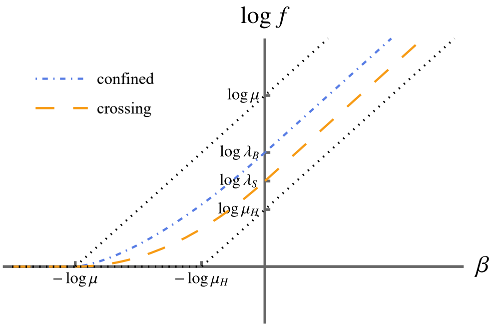


Figure: The free energies of confined SAW models. We do not know that the free energy for our model of confined SAW is strictly greater than that of SAW that cross a square. The top and bottom dotted lines mark bounds derived from unconstrained SAWs and Hamiltonian paths, respectively.

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

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

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

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

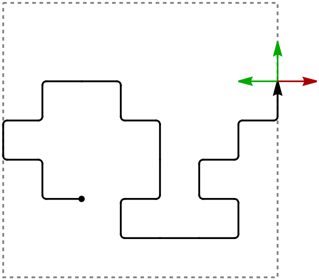


Figure: A sample SAW of length $n = 24$, considered to be confined in a bounding box of side length $L = 7$. The possible next steps are shown with arrows; the only restriction is that the step to the right is forbidden if the limit for the simulation was chosen to be $L_{\text{max}} = 7$.

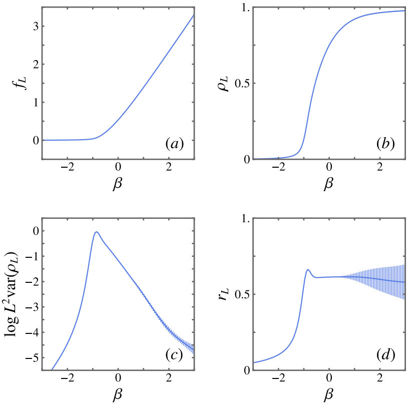


Figure: Thermodynamic quantities for SAWs confined to a box of size $L = 9$. Plots show (a) the free energy f_L, (b) the density ρ_L, (c) the logarithm of the variance $L^2\mathrm{var}(\rho_L)$, and (d) the average size r.

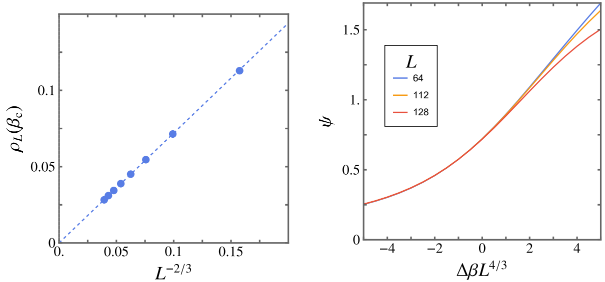


Figure: (a) The critical density $\rho_L(\beta_c)$ plotted against the expected scaling $L^{-2/3}$ and (b) the scaling function $\psi(x)$ for confined SAWs.

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

$$\nu = 0.756(4)$$

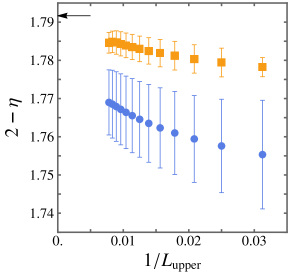


Figure: The critical exponent of the confined SAW partition function $Z_L(\beta_c)$ versus the upper bound of the range of L values used to fit the data, with (top) and without (bottom) a correction-to-scaling term.

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 $43/24 = 1.791\dot{6}$

- Introduce a model of polymers in mesoscopic pores
- In context of unrestricted SAW and SAW crossing a square
- Some rigorous bounds
- Scaling theory
- Monte Carlo confirmation
- What is the value of λ_B? Is it the same as λ_S?
- Are the free energies for walks in a box and crossing a square the same?