Pulling self-avoiding walks from a surface.

Tony Guttmann

ARC Centre of Excellence for Mathematics and Statistics of Complex Systems
Department of Mathematics and Statistics
The University of Melbourne, Australia

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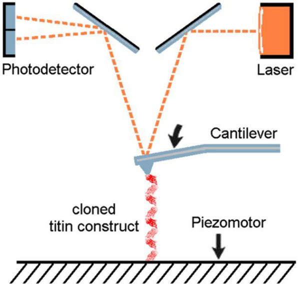
Joint work with Iwan Jensen (Melbourne)
and Stu Whittington (Toronto)

INTRODUCTION

- Techniques such as AFM allow adsorbed polymer molecules to be pulled off a surface. Need theories of adsorbed polymers subject to a force.



PREVIOUS WORK

- Earlier work focussed on random, directed and partially directed walk models. We consider the more realistic SAW model.
- Recently, vR & W established the existence of a phase boundary between an adsorbed phase and a ballistic phase when the force is applied normal to the surface.
- We give the first proof that this phase transition is first-order.

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OUTLINE OF THIS WORK

- We use exact enumeration and series analysis techniques to identify this phase boundary for SAWs on the square lattice.
- We give precise estimates of various critical points.
- And various critical exponents.
- A combination of three ingredients
- Ne rigorous results.
- Faster algorithms giving extended series data
- New numerical techniques.

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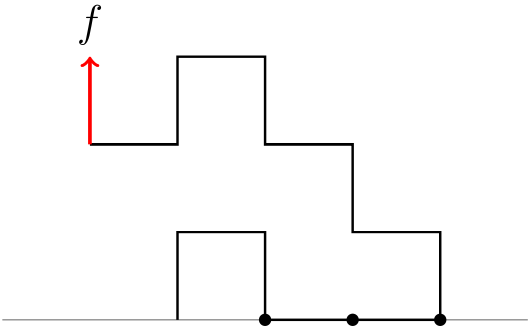

Notation and definitions

- Square lattice: vertex coordinates (x_i, y_i), $i = 0, 1, 2, \ldots n$.
- c_n is the number of n-step SAWs.
- $$\lim_{n\to\infty} n^{-1} \log c_n = \log \mu$$
  exists (HM54), where μ is the *growth constant* of SAWs.
- A *positive walk* is a SAW that starts at the origin and has $y_i \geq 0$ for all $0 \leq i \leq n$. Cardinality c_n^+.
- $$\lim_{n\to\infty} n^{-1} \log c_n^+ = \log \mu. \quad \text{(W75)}$$
- Vertices of a positive walk with $y_i = 0$ are *visits* to the surface, (by convention we exclude the vertex at the origin).

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PARTITION FUNCTION AND VARIABLES a AND y

- The walk has *height* h if $y_n = h$.
- $c_n^+(v, h)$ is card. of positive walks of n steps, v visits, height h.
- The partition function is

$$C_n(a, y) = \sum_{v,h} c_n^+(v, h) a^v y^h. \tag{1}$$

- ϵ is the energy associated with a visit and f is the force applied normally at the last vertex,

$$a = \exp[-\epsilon/k_B T] \quad \text{and} \quad y = \exp[f/k_B T] \tag{2}$$

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- So $\kappa(a)$ is non-analytic at $a = a_c^o$.
- For $a < a_c^o$, $\langle v \rangle = o(n)$. For $a > a_c^o$, (the adsorbed phase,)

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MORE GENERAL MODEL

- For the two variable model, vRW2013 proved the existence of the free energy

$$\psi(a, y) = \lim_{n \to \infty} n^{-1} \log C_n(a, y).$$

- Further, $\psi(a, y)$ is a convex function of $\log a$ and $\log y$ and

$$\psi(a, y) = \max[\kappa(a), \lambda(y)].$$

- This implies that there is a *free phase* when $a < a_c^o$ and $y < y_c^o$ where $\langle v \rangle = o(n)$ and $\langle h \rangle = o(n)$, and a strictly monotone curve $y = y_c(a)$ through the point (a_c^o, y_c^o) separating two phases:
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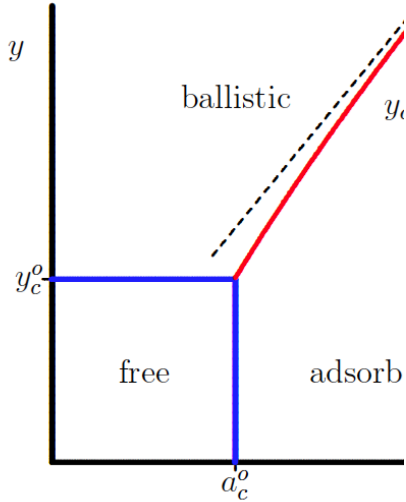
SCHEMATIC PHASE DIAGRAM. (VAN RENSBURG & WHITTINGTON)



IMPROVED ALGORITHM

- The algorithm is based on the CEG (1993) SAW algorithm.
- The TM algorithm keeps track of the way partially constructed SAWs are connected to the left of a cut-line.
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Geometry of rectangle

- We count the number of walks in rectangles $W \times L$ unit cells.
- A spanning walk has length at least $W + L$ steps.
- We add contributions from all rectangles of width $W \leq W_{\max}$, and length $W \leq L \leq 2W_{\max} - W + 1$
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EXAMPLE OF A SAW IN A RECTANGLE

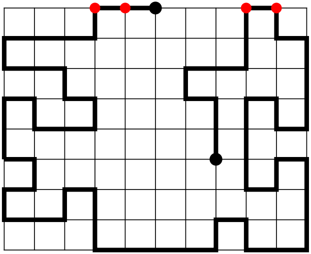

Figure: An example of a self-avoiding walk on a 10×8 rectangle. The walk is tethered to the surface, has the end-point at $h = 5$ and four vertices (other than the start-point) in the surface.

Basic idea: Any SAW has exactly two end-points.

OUTLINE OF THE ALGORITHM

Cutting the SAW by a vertical line (dashed), the SAW is broken into pieces to the left and right of the cut-line. On *either* side of the line are a set of arcs connecting two edges on the cut-line and at most two line pieces connected to the end-points of the SAW.

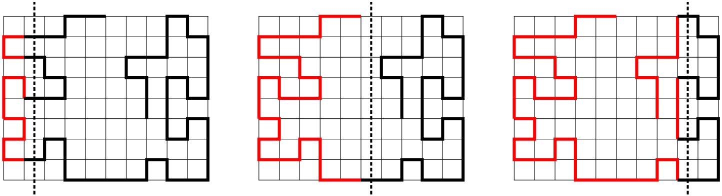

Figure: Examples of cut-lines through the SAW such that the signature of the incomplete section to the right of the cut-line (black lines) contains, respectively, two, one and no free edges.

MOVING THROUGH THE RECTANGLE–BUILDING THE TM

- At every stage a configuration of occupied edges along the cut-line can be described in two ways.
- The edges are connected forming either arcs or line pieces to the left or right of the cut-line.
- Moving the cut-line from left to right we can keep track of how the pieces are connected to the left (the past). This is the traditional TM.
- Tracking how edges can be connected to the right of the cut-line so as to form a valid SAW (the future), is the basis of the new algorithm.
- Looking at a given SAW and cut-line, the partial SAW to the right of this line consists of a number of arcs connecting two edges and at most two *free* edges which are not connected to any occupied edge on the current cut-line.

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LABELING RULES

- Any configuration along the cut-line can thus be represented by a set of edge states $\{\sigma_i\}$, where

$$\sigma_i = \begin{cases} 0 & \text{empty edge,} \\ 1 & \text{lower edge,} \\ 2 & \text{upper edge.} \\ 3 & \text{free edge.} \end{cases}$$

  Reading from bottom to top, the signature S along the cut-lines of the SAW above are, respectively, $S = \{030010230\}$, $S = \{300000000\}$, and $S = \{102001002\}$.

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Updating after a boundary move

- The most efficient implementation of the algorithm involves moving the cut-line so as to build up the lattice vertex by vertex.
- The sum over all contributing graphs is calculated as the cut-line is moved through the lattice.
- For each configuration of edges we keep a generating function G_S for partial walks with signature S.
- Clearly, G_S is a polynomial $G_S(x,a)$ where x, a is conjugate to the number of steps/surface vertices.
- Update: Each source signature S (before the boundary move) generates a few new target signatures S' as $k = 0, 1$ or 2 new edges are inserted with $m = 0$ or 1 surface visits.
- This leads to the update $G_{S'}(x,a) = G_{S'}(x,a) + x^k a^m G_S(x,a)$.
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Modifications for this problem

- We force the SAW to have a free end at the top of the rectangle.
- We must consider all rectangles with $W \leq n + 1$.
- The number of signatures grows exponentially with W. Hence we must minimize the length of the cut-line for optimality.
- The rectangles are broken into two sub-sets, $L \geq W$ and $L < W$.
- For $L < W$ rectangles have start-point on the left-most border.
- To keep track of the height h, the end-point must be in a row h units from the surface, Then repeat for all h.
- We calculated the number of SAW up to length $n = 59$.
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Analysis. No surface interaction, $a = 1$

- We have anaysed the series using differential approximants when $a = 1$, corresponding to no surface interaction.
- For $\log y < 0$, $\lambda(y) = \log \mu$ while for $\log y > 0$, $\max[\log \mu, \log y] \leq \lambda(y) \leq \log \mu + \log y$.

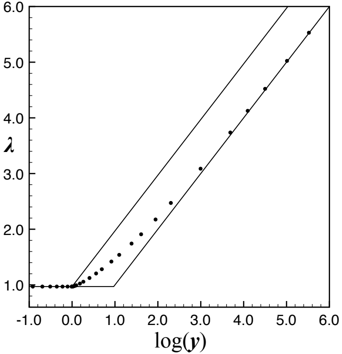

Figure: The free energy $\lambda(y)$, with bounds

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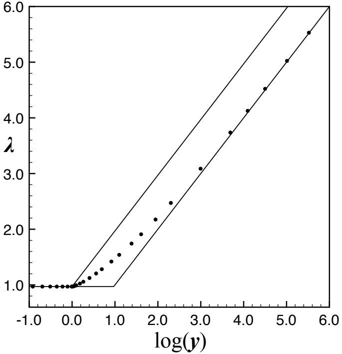

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NO SURFACE INTERACTION, $a = 1$ – MORE DETAILS

$$H(x,y) = \sum_n C_n(1,y)x^n = \sum_n e^{\lambda(y)n+o(n)}x^n$$

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NO SURFACE INTERACTION, $a = 1$ – STILL MORE

- At $y = 1$ the series is well behaved. The critical point $= 1/\mu$, the exponent is $\gamma_1 = 61/64$ (TASAW), as one expects.
- For $y < 1$, $x_c(y)$ remains unchanged at $1/\mu$, but the exponent estimates decrease rapidly with y, settling at at $\gamma_{1,1} = -3/16 = -0.1875$.
- For $y > 1$, $x_c(y)$ mon. dec. as y inc. The sing. is a simple pole.
- The analysis is exquisitely sensitive to the value of y near $y = 1$. This gives us a method for confirming that $y_c = 1$.
- $1/\mu = 0.379052277751$, with uncertainty in the last digit. We vary our estimate of y_c until we get agreement with $1/\mu$.
- This turns out to be at $y_c = 0.9999995 \pm 0.0000005$.
- Now $y_c \geq 1$, plus the numerical result, suggests $y_c = 1$.
- In summary: For $y > y_c$, the exponent is 1. For $y = y_c$ it is $\gamma_1 = 61/64$, and is $\gamma_{1,1} = -3/16$ for $y < y_c$.

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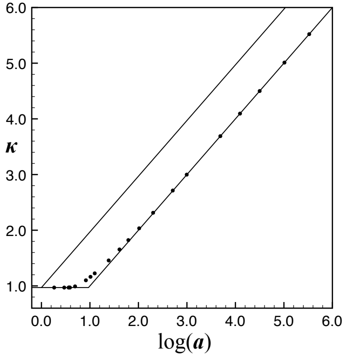

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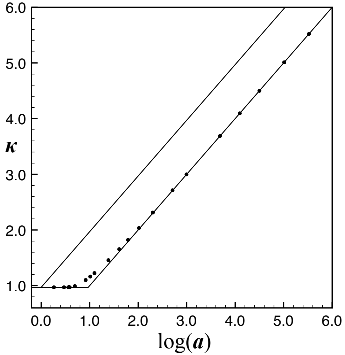

Figure: The free energy $\kappa(a)$, with bounds.

NO APPLIED FORCE, $y = 1$ – FIND a_c.

- The best exisiting estimate of a_c is $a_c = 1.77564$ (BGJ12).
- The series analysis is exquisitely sensitive to the value of a near a_c. This gives us a method for estimating a_c.
- $1/\mu = 0.379052277751$, with uncertainty in the last digit. We vary our estimate of a_c until we get agreement with $1/\mu$.
- This turns out to be at $a_c = 1.775615 \pm 0.000005$.
- At a_c the exponent is 1.4539.
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- For $a > a_c$, $x_c(a)$ is monotonically decreasing as a increases. The singularity is a simple pole.
- For $a < a_c$, $x_c(a)$ remains unchanged at $1/\mu$, but the exponent estimates decrease rapidly with a, settling at at $\gamma_1 = 61/64$.
- Finally, with $y = 0$ and $a = a_c$ we expect loops at the special transition, with exponent $\gamma_{11}^{sp} = 13/16 = 0.8125$. Our estimate is 0.816 ± 0.006.
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PHASE DIAGRAM CALCULATION

- Recall that $\psi(a, y) = \kappa(a)$ throughout the adsorbed phase and $\psi(a, y) = \lambda(y)$ throughout the ballistic phase.
- The phase boundary is the locus of points where

$$\kappa(a) = \lambda(y)$$

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- For a given a we calculated $\kappa(a)$ as above, then found the value of y s.t. $\lambda(y) = \kappa(a)$ by interpolation.
- More precisely, we calculated $y = f_1(x_c)$ by using the program Eureqa on our (y, x_c) data, and $a = f_2(x_c)$ from our (a, x_c) data.
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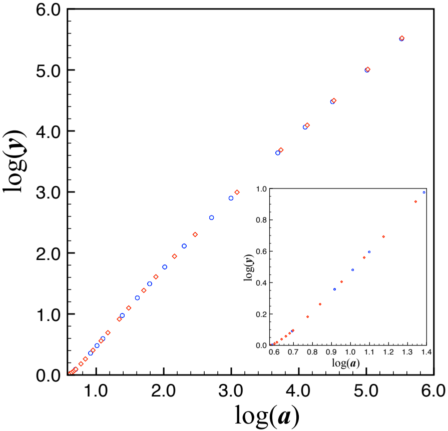
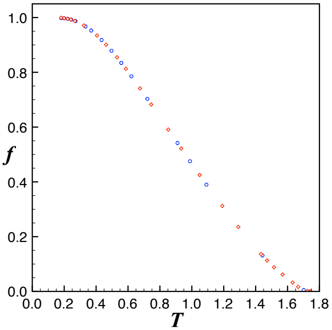


Figure: The phase boundary between the adsorbed and ballistic phases in the $(\log a, \log y)$-plane.

Physical variables

- We can switch to physical variables (force and temperature) using $a = \exp[-\epsilon/k_B T]$ and $y = \exp[f/k_B T]$.
- W.l.o.g we set $\epsilon = -1$ and $k_B = 1$.



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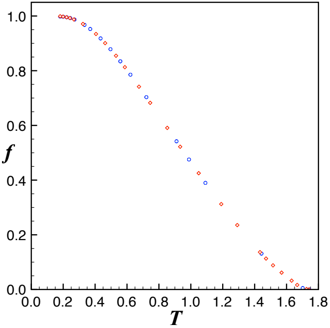

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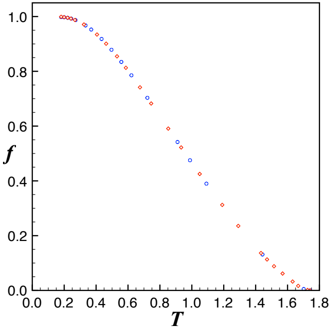

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THE NATURE OF THE PHASE TRANSITION ON THE PHASE BOUNDARY.

- The phase transition from ballistic to adsorbed is first-order.
  Theorem The free energy $\psi(a, y)$ is not differentiable at the phase boundary between the ballistic and adsorbed phases, except perhaps at the triple point (a_c^o, y_c^o).
- At the phase boundary we find a double pole.
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CONCLUSION

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