Exact solution of some new planar polygon models.
Plus aspects of a ”new” SAW model.

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An absolutely classical problem in enumerative combinatorics and in statistical mechanics, and *inter alia* in theoretical chemistry is the enumeration of self-avoiding walks and polygons on a two- or three-dimensional lattice.

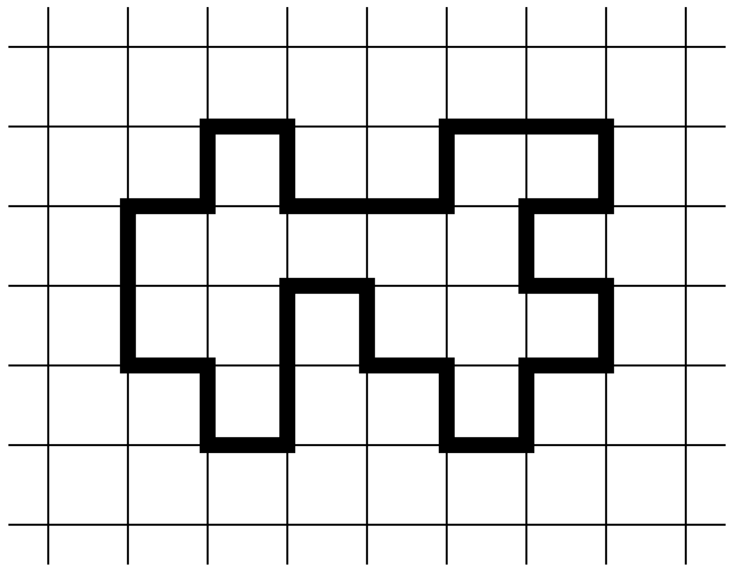


Figure 1: A typical SAP on $\mathbb{Z}^2$

- The key question asked is, quite simply, how many SAW or SAP are there of length n-steps, equivalent up to a translation?
- In the absence of a closed form solution, much effort has been devoted to finding the answer to the above question for simpler models.
- All of the solved, simpler models have a differentiably finite generating function (otherwise called holonomic).
- Such functions satisfy a linear ODE with polynomial coefficients.
- SAP do not (Rechnitzer), and nor do SAW (not proved, but true).
- This distinction applies to a much broader class of problems than just SAW and SAP.

- For example, the Ising model. Specific heat and magnetisation are known (and are D-finite), while the susceptibility is not known (and is not D-finite).
- Here we consider two previously unsolved problems, that of three-choice polygons and staircase polygons with staircase holes, and one new (and still unsolved problem), prudent SAW and SAP.

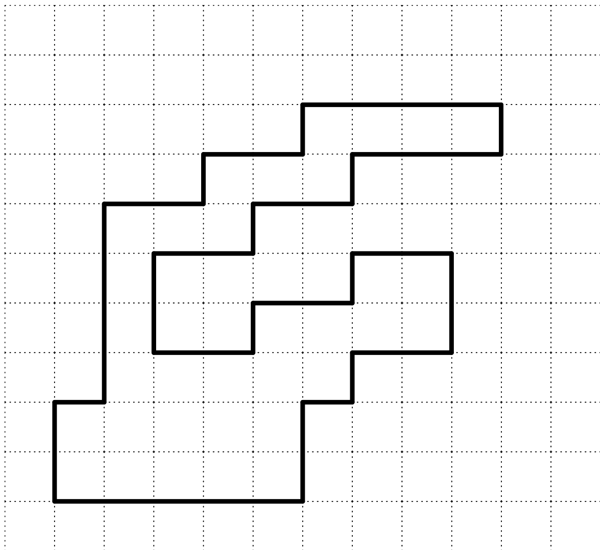


Figure 2: A 3-choice polygon

- We obtain the perimeter generating function of three-choice polygons and staircase polygons with staircase holes.
- We comment on the area generating function, and two-variable (area-perimeter) generating functions.
- Prudent SAW were introduced by Turban and Debierre in physics and by Pascal Préa in the mathematics literature. More recently it has been carefully studied by Enrica Duchi. They are conjectured to be non-D-finite, but may be solvable.
- At the very least, we already have a polynomial time algorithm for their series expansion.

- Three-choice SAW were introduced by Manna in 1984.
- They were defined to be SAW on the square ($\mathbb{Z}^2$) lattice, such that after an E step, the next step could only be N or E, while after a W step, the next step could only be S or W.
- This constraint is in addition to the SAW constraint.
- It is easy to prove that the number of such n-step SAW equivalent up to a translation, grows as $t_n = \mu^{n+o(n)}$.
- Whittington showed that μ, the growth constant, is exactly 2.

- Thus the number of n-step 3-choice SAW t_n grows as $t_n = 2^{(n+o(n))}$ where we don't have a clear idea of the sub-dominant behaviour, unlike normal SAW on the same lattice.
- The polygon version of this problem was first considered by Conway, Delest and Guttmann in 1997.
- They gave a polynomial time algorithm for generating such polygons, and demonstrated this by generating polygons with perimeter up to 506 steps (250 coefficients).
- The 3-choice rule generates staircase polygons with multiplicity $2n$, and *imperfect* staircase polygons with multiplicity 2 as they can be rotated through 180 deg .

- Let $T(x,y) = \sum_{m\geq 0, n\geq 0} t_{m,n} x^n y^m$ be the o.g.f. of 3-choice polygons by semi-perimeter.
- Then $T(x,y) = \sum_{n\geq 0} x^n T_n(y)$ where the generating function for 3-choice polygons with $2n$ vertical bonds, $T_n = \frac{P_n(y)}{Q_n(y)}$ is rational.
- Then we observed, and later M. Bousquet-Mélou proved, that

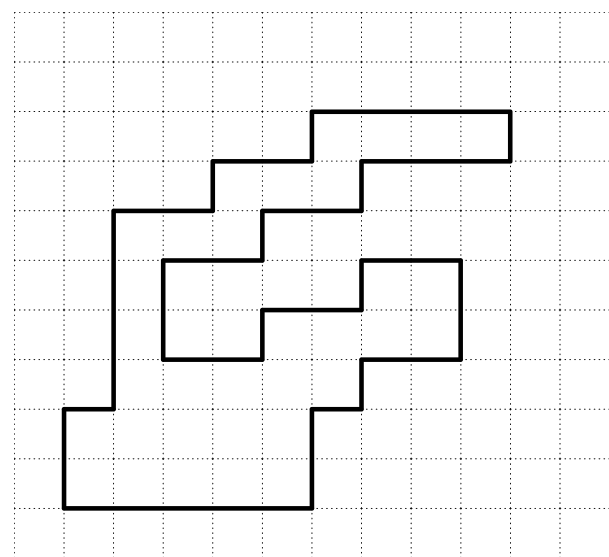
$$Q_n(y) = (1-y)^{2n-1}(1+y)^{(2n-7)_+} \qquad n \quad \text{even}$$

$$Q_n(y) = (1-y)^{2n-1}(1+y)^{(2n-8)_+} \qquad n \quad \text{odd}$$

.

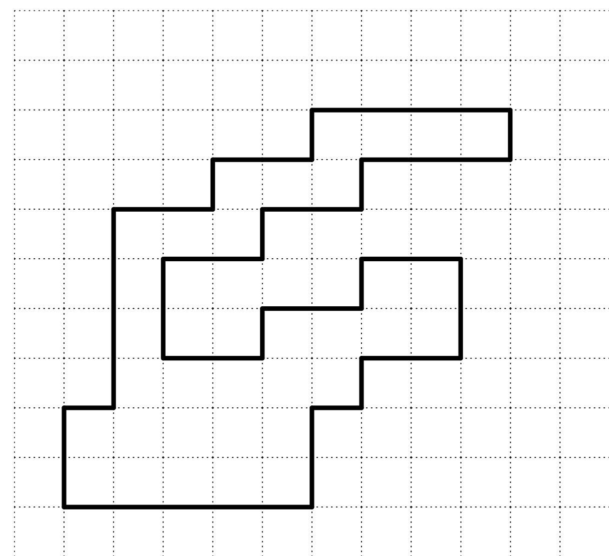
- Unfortunately, we don't know the numerators, apart from their value at 0 and -1 (MBM).

- The enumeration of imperfect staircase polygons can be set up as a sum over determinants, using the Gessel-Viennot idea, but it is a five-fold sum, with constraints over three additional indices, and so is entirely unmanageable.



- However, the fact that it is a finite determinant (4 by 4) means that the generating function corresponding to each determinant in the sum is D-finite, and by the closure properties of D-finite functions under addition, so is the solution.
- But a search for the generating o.d.e. based on 250 terms was not successful.
- One of the problems was the lack of adequate software to search for huge, large order, o.d.e's.
- Solved by a MMA routine written by Jean-Marie Maillard and colleagues, and some inspired guesswork.

3-choice polygons may be staircase polygons (occurring with multiplicity $2n$) or *imperfect* staircase polygons, occurring with multiplicity 2, illustrated below:



The generating function satisfies an 8th order homogeneous, linear o.d.e., which is Fuchsian,

$$\sum_{i=0}^{8} P_i(x) f^{(i)}(x) = 0,$$

where

$$P_8(x) = 32x^8(1+x)(4+x^2)(16+4x+7x^2)(x-1)^8 Q^{(8)}_{[25]}(x)$$

$$P_7(x) = 16x^7(x-1)^7 Q^{(7)}_{[31]}(x)$$

$$P_6(x) = 16x^6(x-1)^6 Q^{(6)}_{[32]}(x)$$

$$P_5(x) = 24x^5(x-1)^5 Q^{(5)}_{[33]}(x)$$

$$P_4(x) = 30x^4(x-1)^4 Q^{(4)}_{[34]}(x)$$

$$P_3(x) = 15x^3(x-1)^4 Q^{(3)}_{[34]}(x)$$

$$P_2(x) = 90x^2(x-1)^4 Q^{(2)}_{[34]}(x)$$

$$P_1(x) = 180x(x-1)^4 Q^{(1)}_{[34]}(x)$$

$$P_0(x) = 180x(x-1)^4 Q^{(0)}_{[33]}(x)$$

and $Q_{[n]}$ denotes a polynomial of degree n and we've normalized the growth constant to 1.

- The 25 zeros of $Q^{(8)}_{[25]}(x)$ are apparent singularities.
- The indicial equation at $x = 1$ gives exponents
  -1/2, -1/2, 0, 1/2, 1, 3/2, 2, 3
  and at $x = -1$
  0, 1, 2, 3, 4, 5, 6, 13/2.
- Analysis of such high order ODEs, given indicial equations with repeated roots, with roots separated by integers, and with integer values, is enormously cumbersome.
- Even after the correct singularity structure is identified, to determine the amplitude of the singularity is a very complex task.

- We can simplify the 8th order differential operator.
- We first found three solutions of the ODE, each corresponding to an order one differential operator.
- We denote these $L_i^{(1)}$, with $i = 1..3$.
- We found that our 8th order differential operator can be decomposed as $L^{(8)} = L^{(5)} L_1^{(1)} L_2^{(1)} L_3^{(1)}$.
- Calculating the Wronskian of $L^{(5)}$ shows that it is further decomposable, and we find $L^{(5)} = L^{(3)} L^{(2)}$.
- This then allows us to write down the form, in an appropriate global basis of solutions, of the 8×8 matrix representing the differential Galois group of $L^{(8)}$.
- To determine the asymptotics one would need to calculate non-local connection matrices between solutions at different points. This is a huge task for such a large differential operator.

- Instead, we have developed a numerical technique that avoids all these difficulties.
- We assume the most general form allowable by the indicial equation, with all possible powers of logarithms.
- Then we generate a large number of coefficients (100,000 to start with).
- Then we fit successive $k-$tuples of coefficients to the k unknowns in the general fit, and observe the convergence.
- Then we discard the absent terms and repeat the process, giving better convergence for the remainder.

Analysis of the indicial equation, coupled with the numerical technique described, enabled us to give the asymptotic form of the coefficients

$$t_n = \frac{1}{\sqrt{n}} \sum_{i \geq 0} \left(\frac{a_i \log n + b_i}{n^i} + (-1)^n \left(\frac{c_i}{n^{7+i}} \right) \right).$$

The first two amplitudes a_i and b_i correspond to the "physical" singularity, the third, c_i corresponds to a non-physical singularity, analogous to the anti-ferromagnetic singularity seen in combinatorial magnetic models (e.g. the Ising model, or SAW) on loose-packed lattices.

We have obtained the amplitudes a_i, b_i and c_i for $i \leq 16$ with a precision of at least 60 digits, based on a careful analysis of the first 100,000 terms of the generating function. These can be generated by Mathematica in less than 10 minutes.

In CDG the authors gave a combinatorial argument that suggested that the dominant term is $\mathrm{O}(\log n/\sqrt{n})$ and further that $a_0 = const./\pi^{3/2}$. A numerical study, based on 250 terms, led to the conjecture that the constant was $12\sqrt{3}$. The numerical study above confirms all these conclusions with a precision of 100 decimal digits.

- Is it a proof? No.
- But since we've proved the solution is D-finite, if we could bound the degree of the ODE from the determinantel formulation, we would have a proof.
- Is it correct? Indubitably. We have 200 independent confirmations.

- We have also looked at the area generating function. For staircase polygons the area generating function is given by

$$A(q) = \sum_{n \geq 1} a_n q^n = \frac{J_1(1,1,q)}{J_0(1,1,q)},$$

where $J_i = \sum_{n \geq 0} \frac{(-1)^n q^{(n+i)(n+i+1)/2}}{(q)_n^2 (1-q^{n+1})^i}, \qquad i = 0, 1.$

- Based on a 500 term series, our analysis suggests that the solution is of the form $\frac{F(q)+G(q)/\sqrt{1-q\eta}}{[J_0(1,1,q)]^2}$. That is to say, the leading singularity occurs at $q = 1/\eta$, where η is the first zero of $J_0(1,1,q)$, and F and G are regular in the neighbourhood of $q = 1/\eta$.
- The solution is not, however, of the simple product form as found for staircase polygons.
- We can see this by constructing Padé approximants of steadily increasing order, which don't stabilise.

Prudent SAW.

A (regular) SAW never revisits a previously visited lattice site. To reduce the danger of this potentially calamitous event prudent SAW never try to even walk towards a previously visited site. That is to say, if the extension of a proposed step would intersect a previously visited site, the step is forbidden. This ensures that such a walk is self-avoiding.

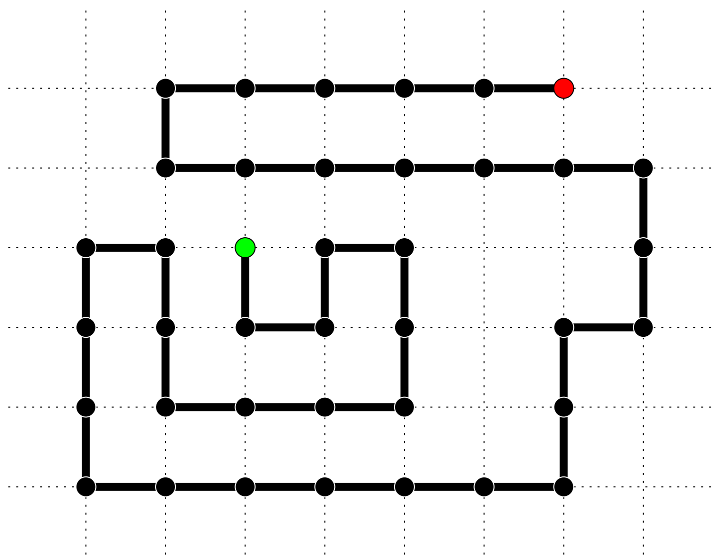


Figure 3: A prudent SAW

We can also define a polygon version of prudent SAW by defining a prudent SAP to be a prudent SAW whose end-point is adjacent to its starting point.

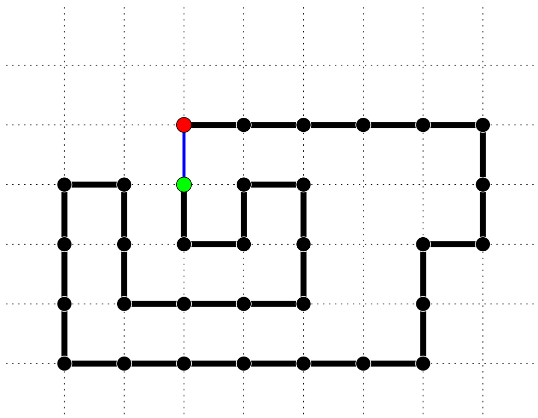


Figure 4: A prudent SAP

The key aspect of this definition is that the end point of the walk is always on the perimeter of the minimal bounding rectangle.

- The model was introduced in the physics literature by Loïc Turban and Jean-Marc Debierre in 1987.
- They called it a self-directed walk.
- Their Monte Carlo studies convincingly showed that $\nu = 1/2$, where ν is the exponent defining the mean-square end-to-end distance, through $\langle R^2 \rangle_n \sim const.n^{2\nu}$.
- They also gave an argument that the exponent $\gamma = 1$, where γ is the exponent governing the sub-dominant growth of the number of such walks, $c_n \sim const.\mu^n n^{\gamma-1}$. This implies a simple pole for the dominant singularity of the generating function.

- The model was introduced independently in the mathematics "literature", in an unpublished manuscript by Pascal Préa, in the '90s.
- It was recently (FPSAC2005) taken up by Enrica Duchi (Université Paris 7).
- She considered two simplifications.
- In the first, the subsequence of steps WS and SW is forbidden. Such walks always end on the north or east edge of the bounding rectangle.
- Duchi obtained the generating function, which is rational.

- The number of such SAW are found to grow as $\mu^n n^g$ with $\mu = 2.48119...$ (the root of $1 - 2t - 2t^2 + 2t^3$) and $g = 0$ (equivalently, $\gamma = 1$ as argued for the unsimplified model by Turban and Debierre), so the generating function has a simple pole.

- A less restrictive simplification, in which a WS sequence is forbidden if the walk visits the top of its bounding box, or a WN sequence if the walk visits the bottom of its bounding box, is also solved by Duchi.
- A much uglier algebraic generating function (of degree 4) is obtained, but it still has a simple pole, with $\mu = 2.498785..$

- The unrestricted problem has not been solved, though Duchi obtained a pair of functional equations which can be iterated to produce the series coefficients in polynomial time.

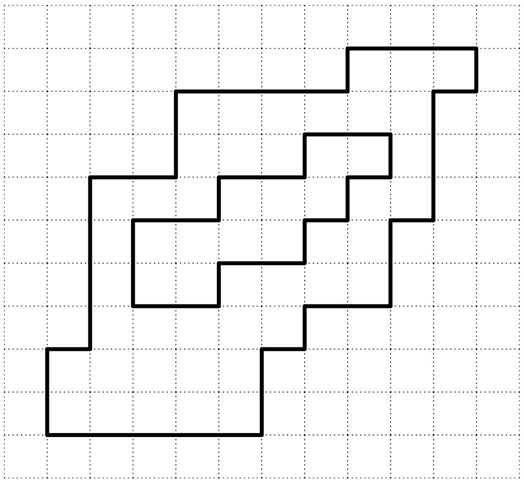
- A very preliminary series analysis suggests that the number of such walks behaves as $\mu^n n^g$ with $\mu = 2.5...$ and $g \geq 0$. It should be possible to significantly improve these estimates!

- No series for prudent SAP has yet been generated, though this is under development.

- We have also calculated the anisotropic generating function Let $P(x,y) = \sum_{m\ge 0, n\ge 0} t_{m,n} x^n y^m$ be the o.g.f. of prudent SAW by perimeter.
- Then $P(x,y) = \sum_{n\ge 0} x^n R_n(y)$ where the generating function for prudent SAW with n vertical bonds, $R_n = \frac{P_n(y)}{Q_n(y)}$ is rational.

- We find that $Q_n(y)$ is given by a product of cyclotomic polynomials.
- As n increases, so does the degree of the largest occurring cyclotomic polynomial.
- If this behaviour persists, the generating function P cannot be D-finite.
- We believe that this is the case.

- Turning now to staircase polygons with an arbitrary staircase hole, these are staircase polygons which contain a (fully enclosed) staircase polygon.



- It is clear that these can be viewed as two 3-choice polygons with common bonds deleted. Thus it is not surprising that their generating o.d.e. is similar in size and structure, and even analytic properties.
- The generating function was also found to satisfy an 8th order homogeneous, linear o.d.e.

$$\sum_{i=0}^{8} P_i(x) f^{(i)}(x) = 0,$$

where

$$P_8(x) = 32x^8(1+x)(4+x^2)(16+4x+7x^2)(x-1)^8 Q^{(8)}_{[22]}(x)$$

$$P_7(x) = 16x^7(x-1)^7 Q^{(7)}_{[28]}(x)$$

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$$P_5(x) = 24x^5(x-1)^5 Q^{(5)}_{[30]}(x)$$

$$P_4(x) = 30x^4(x-1)^4 Q^{(4)}_{[31]}(x)$$

$$P_3(x) = 15x^3(x-1)^3 Q^{(3)}_{[32]}(x)$$

$$P_2(x) = 45x^2(x-1)^2 Q^{(2)}_{[33]}(x)$$

$$P_1(x) = 90x(x-1) Q^{(1)}_{[34]}(x)$$

$$P_0(x) = 90x Q^{(0)}_{[34]}(x)$$

and $Q_{[n]}$ denotes a polynomial of degree n.

A similar factorization of the 8th order differential operator into a third order, a second order and three first order differential operator as was obtained for three-choice polygons has been found for this problem too.

A similar analysis of the indicial equation enabled us to give the asymptotic form of the coefficients

$$s_n = 1024 + \frac{1}{\sqrt{n}} \sum_{i \geq 0} \left(\frac{a_i \log n + b_i}{n^i} + (-1)^n \left(\frac{c_i}{n^{7+i}} \right) \right).$$

The singularity structure is similar to that of 3-choice polygons, apart from the leading constant, corresponding to a dominant simple pole singularity. The next term has amplitude $a_0 = -6144\sqrt{3}/\pi^{3/2}$.

In this case too we have estimated the amplitudes a_i, b_i and c_i for $i \leq 16$ with a precision of at least 60 digits, based on a similar analysis of the first 100,000 terms of the generating function.

- We have also performed a similar analysis of the area generating function.
- Based on a 500 term series, our analysis suggests that the solution is of the form $\frac{F(q)+G(q)\sqrt{1-q\eta}}{[J_0(1,1,q)]^2}$.
- That is to say, the leading singularity occurs at $q = 1/\eta$, where η is the first zero of $J_0(1,1,q)$, and F and G are regular in the neighbourhood of $q = 1/\eta$.

The motivation for studying punctured staircase polygons is to proceed iteratively toward the scaling function of polyominoes. They have a perimeter ogf with zero radius of convergence.

- We review the situation for staircase polygons with holes (Guttmann, Jensen, Wong, Enting 2000) and the two-variable area-perimeter generating function and scaling function for staircase polygons and SAP (Richard, Guttmann and Jensen 2004).

- van Rensburg and Whittington studied the area generating function of SAP in $\mathbb{Z}^2$ with k punctures. Writing the area generating function

$$A^{(k)}(q) = \sum_{n>0} a_n^{(k)} q^n \sim D^{(k)}(q) + E^{(k)}(q)(1 - \kappa^{(k)} q)^{-\beta_k},$$

for a k-punctured SAP, they proved that $\kappa^{(k)} = \kappa^{(0)} = \kappa$, and that if the exponent exists, $\beta_k = \beta_0 + k$.

- In GJWE, the perimeter o.g.f. was considered,

$$P^{(k)}(x) = \sum_{n>0} p_{2n}^{(k)} x^n \sim B^{(k)}(x) + C^{(k)}(x)(1 - (\mu^{(k)})^2 x)^{2-\alpha_k}.$$

- They proved that $\mu^{(k)} = \mu^{(0)} = \mu$, and that if the exponent exists, $\alpha_k = \alpha_0 + 1.5k$, though this was not proved, just conjectured on the basis of an heuristic argument.

- For polyominoes, if one classifies them by the number of punctures, it can be proved that the growth constant is $\kappa \approx 3.97087 < \tau \approx 4.06259$, where κ is the growth constant for SAP enumerated by area, and τ is the growth constant for polyominoes, enumerated, of course by number of cells (i.e. area).

- For k-punctured polyominoes we find

$$a_n^{(k)} = [q^n]A^{(k)}(q) = \kappa^n n^{k-1} \sum_{i \geq 0} a_i^{(k)}/n^i.$$

- We also proved that, if the exponent exists, it increases by 1 per puncture.

- Notice too that the correction terms go down by a whole power, unlike the situation for punctured polygons.

- For regular polyominoes, we proved in GJO that the perimeter generating function has zero radius of convergence.
- The perimeter is defined to be the perimeter of the boundary plus the perimeter of any holes.
- If p_{2n} denotes the number of polyominoes, d.u.t.a.t, with perimeter $2n$, we proved that $p_{2n} = (2n)^{n/2+o(n)}$.
- In fact we prove

$$\lim_{n\to\infty} \frac{\log p_{2n}}{2n\log 2n} = \frac{1}{4}.$$

- An attempt to study the quasi-exponential generating function with coefficients $r_n = p_n/(n/4)!$ was equivocal.
- For that reason, studying punctured staircase polygons was considered a controlled route to determine the two-variable, area-perimeter generating function of polyominoes.

We briefly review the properties of the two-variable area-perimeter generating function for both staircase polygons and SAP.

- Let $p_m(n)$ be the number of staircase polygons or *rooted* SAP per site on an infinite lattice, with perimeter m enclosing area n. In 1991 Fisher, Guttmann and Whittington proved that the free energy

$$\lim_{m \to \infty} \frac{1}{m} \log \sum_n p_{m,n} q^n := \kappa(q)$$

  exists and is finite for all values of $q \leq 1$.

- Further, $\kappa(q)$ is log-convex and continuous for these values of q and is infinite for $q > 1$.

- The two-variable generating function is

$$P(x,q) = \sum_{x,q} p_{m,n} x^m q^n,$$

- It was proved that for $q < 1$, $P(x,q)$ converges for $x < \mathrm{e}^{-\kappa(q)}$.
- For $q > 1$, $P(x,q)$ converges only for $x = 0$. The expected phase diagram is shown below:

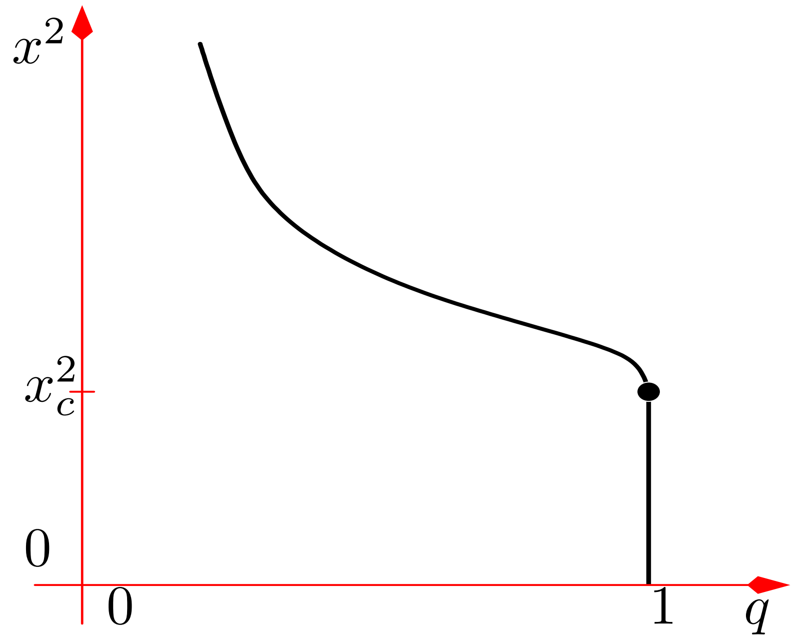

Figure 5: The phase diagram showing the phase boundary $x_c(q)$.

- Below the phase boundary, the polygons are ramified objects, closely resembling branched polymers.
- As q approaches unity, they fill out more, and become less string-like. At $q = 1$ one has pure SAP.

- For $q > 1$ the polygons become “fat”, indeed they become convex polygons (OP) ’99, with their average area scaling as the square of their perimeter.
- Fisher et al. obtained rigorous upper and lower bounds on the shape of the phase boundary, and the locus of the actual phase boundary was estimated numerically from extrapolation of SAP enumerations by area and perimeter.
- The corresponding phase diagram for staircase polygons can be determined exactly, and is qualitatively similar.
- In the extended phase $q = 1$, the mean area of polygons $\langle a \rangle_m$ of perimeter m grows asymptotically like $m^{3/2}$, whereas it grows like m in the deflated phase $q < 1$.
- In the limit $q \to 0$ the generating function is dominated by polygons of minimal area.

- Since for SAPs these polygons may be viewed as branched polymers, the phase $q < 1$ is also referred to as the *branched polymer phase*.
- This change of asymptotic behaviour is reflected in the singular behaviour of the perimeter and area generating function.
- Typically, the line $q = 1$ is a line of finite essential singularities for $x < x_c$.
- The line $x_c(q)$, where $P(x, q)$ is singular for $q < 1$, is typically a line of logarithmic singularities.
- For branched polymers in the continuum limit, the logarithmic singularity has been recently proved by Bridges and Imrie.

- Of special interest is the point $(x_c, 1)$ where these two lines of singularities meet. The behaviour of the singular part of the perimeter and area generating function about $(x_c, 1)$ is expected to take the special form

$$P(x,q) \sim P^{(reg)}(x,q) + (1-q)^{\theta} F((x_c - x)(1-q)^{-\phi}), \qquad (x,q) \nearrow, \tag{1}$$

  where $F(s)$ is a *scaling function* of combined argument $s = (x_c - x)(1-q)^{-\phi}$, commonly assumed to be regular at the origin, and $\theta = 1/3$ and $\phi = 2/3$ are *critical exponents*.

- The scaling function and exponents are provably correct for staircase polygons and universally accepted for *rooted* SAP.

- For unrooted SAP $\theta = 1$, and we must add a q dependent constant of integration, $C(q) = \frac{1}{6\sigma\pi}(1-q)\log(1-q)$, recently discovered by Richard et al.

- For staircase polygons, we have

$$F(s) = \frac{1}{8}\frac{d}{ds}\log \mathrm{Ai}\left((4\sqrt{2})^{\frac{2}{3}} s\right) \tag{2}$$

- Working with *rooted* SAP, the conjectured form of the scaling function is

$$F^{(r)}(s) = \frac{x_c}{\pi\sigma}\frac{d}{ds}\log \mathrm{Ai}\left(\frac{\pi}{x_c}(2E_0)^{\frac{2}{3}} s\right) \tag{3}$$

- The conjectured form of the scaling function is then obtained by integration and is

$$F(s) = \frac{1}{\pi\sigma}\log \mathrm{Ai}\left(\frac{\pi}{x_c}(2E_0)^{\frac{2}{3}} s\right) \tag{4}$$

with exponents $\theta = 1$ and $\phi = 2/3$.

- The parameters for the square lattice are $\sigma = 2$ and $x_c = 0.379052277757(5)$. The parameters for the hexagonal lattice are $\sigma = 2$ and $x_c = 1/\sqrt{(2+\sqrt{2})}$ (known exactly from the work of Nienhuis) and for the triangular lattice $\sigma = 1$ and $x_c = 0.2409175745(3)$.

- We still have some way to go to understand the polyomino phase diagram, but feel this is the correct route.
- In conclusion, we have obtained the o.d.e. for the generating function, by perimeter, of 3-choice and 1-punctured staircase polygons.
- We have obtained some numerical estimates of the critical properties of prudent polygons, and indicated that the generating function is not D-finite.
- It still remains to obtain results for the area generating function, and to unravel the phase diagram of polyominoes.