PARTIALLY CONVEX LATTICE VESICLES: METHODS AND RECENT RESULTS

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ABSTRACT

We review the methods and results achieved recently for some lattice models of vesicles in two dimensions, which are defined by the restriction of partial convexity. These models provide an alternate testing ground for the scaling and universality hypotheses to the more intricate Ising model. The scaling functions can be calculated, in addition to the exponents, and we conclude that all the most complex models fall into one universality class. We also present, as a pedagogical example of the methods, the scaling behaviour of a model not previously studied in this fashion.

Interest in two dimensional lattice models of closed fluctuating membranes (or vesicles) has come from at least two primary sources: the first physical and the second combinatorial. One was stimulated by the work of Leibler, Singh and Fisher[1] which, from a physical perspective, investigated, amongst other things, the critical phenomena (scaling behaviour) associated with such a model[2]. The geometric model underlying this study was that of self-avoiding polygons, where the scaling of quantities in perimeter and area was sought. (There are other properties, excluded in this review, such as rigidity, that affect the behaviour of model vesicles.)

One method of attack on self-avoiding walk problems in general has been to simplify the model so as to give a system that is mathematically tractable. It is this approach, and the outcomes, that are the subjects of this review. In particular, we are focussed upon self-avoiding polygon models that have been restricted by imposing some degree of convexity.

As is usual in science this group of models has also been investigated for a completely unrelated reason: they represent geometrically many formal languages of computer science[3] and are basic objects of study in combinatorics[4]. Of course, the motivations stem from a different view of the problem but nonetheless similar functions are sought. The enumeration of the number of such objects of given area and perimeter is the goal here and the associated asymptotics are not considered. However, the search for the most compact solution of the associated generating functions has provided important impetus for new methods of solution.

Further interest in these models comes from an association with low temperature approximations to correlations in the Ising model[5,6] and, from one member of the group, in relation to wetting transitions[7,8].

The models considered are classes of (partially) convex polygons on the square lattice. We call a polygon partially convex if any line of a given orientation intersects the polygon at most twice. By choosing the orientation to be vertical we define the class of column-convex polygons, and we call a polygon convex if it is column- and row-convex.[a] Equivalently, a polygon is convex if it has the same perimeter as its bounding rectangle.

Clearly, the largest class of partially convex polygons is given by column-convex polygons, and all partially convex polygons can be seen as "directed", a property that will be essential for their theoretical analysis. In order to put further restrictions onto the partially convex polygons, we first use this "directedness" to decompose any such polygon into an upper and a lower walk. These walks are partially directed, and restricting the allowed upper and lower walks defines new subclasses. We shall in particular be interested in the cases in which the upper and lower walks are restricted to be either

(i) horizontal walks (only steps to the right),
(ii) fully directed walks (being either, only steps to the right and up (NE) or alternately, only steps to the right and down (SE)), or
(iii) partially directed self-avoiding walks (no steps to the left).

These walks already generate various classes of polygons. Naturally, one can define numerous other directed walks, for instance by allowing only one vertical step at a time, leading to commonly called *restricted* models, or by using alternating partially directed walks, where subsequent vertical segments of steps have to point in the opposite direction.

We now list a few examples of the classes of polygons we can generate, see figure 1. For example, joining two horizontal walks with two vertical lines leads to rectangles, joining a horizontal walk with a fully directed walk leads to Ferrer diagrams, and joining a NE-fully directed walk with a SE-fully directed walk gives stack polygons. More complex classes of polygons are

[a]The notion of partial convexity is a bit unusual, as diagonal convexity is an even stronger restriction leading to the class of staircase polygons (a proper subclass of "convex" polygons) and the only truly convex polygons are rectangles.

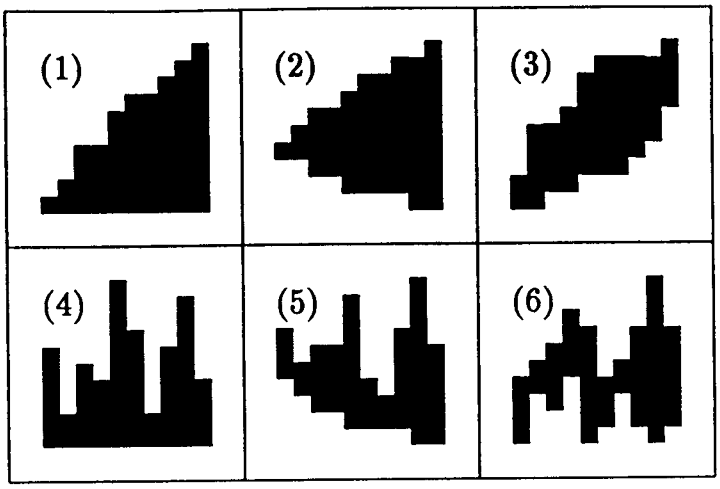

Fig. 1. Typical configurations for a selection of partially convex vesicle models. (1) Ferrer diagrams, (2) stack polygons, (3) staircase polygons, (4) bar-graph polygons, (5) directed column-convex polygons, (6) column-convex polygons.

(a) staircase polygons (skew-Ferrer diagrams), (ii) with (ii)
(b) bar-graph polygons, (i) with (iii)
(c) directed column-convex polygons, (ii) with (iii)
(d) column-convex polygons, (iii) with (iii)

All the polygons in this list are in the same universality class. The simpler models of Ferrer diagrams, stack polygons and, even simpler, rectangles, lie in other universality classes.

For each of these models, we define the generating function as follows. Let $c_m^{n_x,n_y}$ be the number of polygonswith $2n_x$ horizontal steps and $2n_y$ vertical steps which enclose an area of size m. (Clearly the numbers of horizontal and vertical steps are even.) We then define the polygon generating function $G(x,y,q)$ to be

$$G(x,y,q) = \sum c_m^{n_x,n_y} x^{n_x} y^{n_y} q^m \, . \tag{1}$$

In the case of staircase polygons, for example, one can now write the generating function as a sum over the height of each column r_i and the allowed overlap s_i between the columns,

$$\begin{aligned} G(x,y,q) &= \sum_{n=1}^{\infty} x^n \sum_{r_1=1}^{\infty} (yq)^{r_1} \sum_{s_1=1}^{r_1} y^{-s_1} \sum_{r_2=s_1}^{\infty} (yq)^{r_2} \\ &\quad \cdots \sum_{s_{n-1}=1}^{r_{n-2}} y^{-s_{n-1}} \sum_{r_n=s_{n-1}}^{\infty} (yq)^{r_n} \end{aligned} \tag{2}$$

By introducing a variable vertical lattice spacing a and formally taking the limit $a \to 0$ one can define a semi-continuous version of each of these models, where the length of the vertical steps is allowed to assume positive real values. For example, the generating function G_{cont} for the semi-continuous version of the staircase polygons can be written as

$$G_{cont}(x,y,q) = \sum_{n=1}^{\infty} x^n \int_0^{\infty} dr_1 \, (yq)^{r_1} \int_0^{r_1} ds_1 \, y^{-s_1} \int_{s_1}^{\infty} dr_2 \, (yq)^{r_2} \dots \int_0^{r_{n-2}} ds_{n-1} \, y^{-s_{n-1}} \int_{s_{n-1}}^{\infty} dr_n \, (yq)^{r_n} \quad (3)$$

Formally, we have

$$G_{cont}(x,y,q) = \lim_{a\to 0} \frac{1}{a} G(a^2 x, y^a, q^a) \quad (4)$$

It is the singularity structure of these generating functions that shall interest us. We will now briefly sketch its general form for this class of models (for details see Brak *et al*[9]). For simplicity, consider the generating function

$$G(x,q) = G(x,x,q) = \sum_{m,n} c_m^n x^n q^m \quad (5)$$

where c_m^n is the number of polygons with perimeter $2n$ and area m. We further write

$$A_m(x) = \sum_n c_m^n x^n \qquad \text{and} \qquad P_n(q) = \sum_m c_m^n q^m \quad (6)$$

so that $A_m(y)$ and $P_n(q)$ are the generating functions for polygons with fixed area and perimeter respectively.

Let us consider q as a parameter and x the variable. Then G is a power series in x with coefficients $P_n(q)$ and its radius of convergence, $x_c(q)$, is given by

$$x_c(q) = \lim_{n\to\infty} P_n(q)^{-\frac{1}{n}}. \quad (7)$$

The existence of this limit can be shown using sub-multiplicative inequalities[10,11]. A plot of the radius of convergence $x_c(q)$ as a function of q is of the generic form shown in figure 2.

Alternatively one can fix x and consider G as a function of q with radius of convergence $q_c(x)$. For polygon models, the generating function is singular along the line $q = 1$ between $x = 0$ and some point $x_t = x_c(1)$. The point (q_t, x_t) is an example of a "tricritical" point[9], at least mathematically, where $q_t = q_c(x_t)$. For polygon models $q_t = 1$.

The generating function $G(x, 1)$ only generates the polygons by perimeter. For all the above models it is an algebraic function and hence has a branch point with exponent γ_u at x_t, that is

$$G(x,1) \sim A\,(x_t - x)^{-\gamma_u} \qquad \text{as} \qquad x \to x_t^- \, . \quad (8)$$

For $x = x_t$, the generating function has a branch point-like singularity in q at q_t, but with a different exponent, γ_t where γ_t is defined through

$$G(x_t,q) \sim B(1-q)^{-\gamma_t} \qquad \text{as} \qquad q \to q_t^- \, . \quad (9)$$

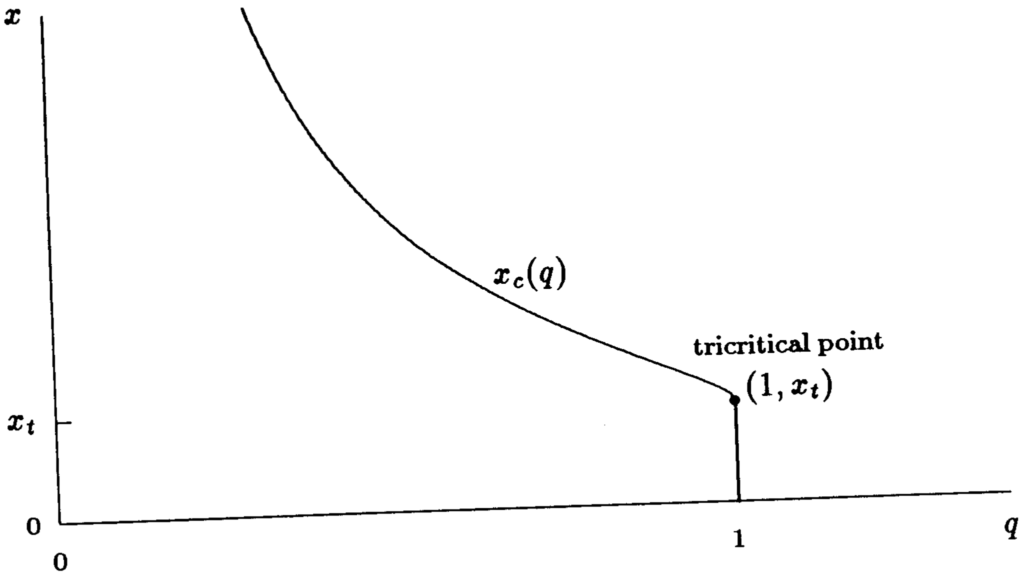

Fig. 2. The schematic form of the radius of convergence of the area-perimeter generating function for vesicle models.

These two different asymptotic behaviours can be combined into a scaling function f, where

$$G(x,q) \sim (1-q)^{-\gamma_t} f\left(\{1-q\}^{-\phi}\{x_t - x\}\right) \tag{10}$$

with

$$f(z) \sim \begin{cases} z^{-\gamma_u} & \text{if } z \to \infty \\ 1 & \text{if } z \to 0. \end{cases} \tag{11}$$

where ϕ is called the tricritical crossover exponent and $\gamma_u = \gamma_t/\phi$.

One further behaviour of G begs attention: the shape of the $x_c(q)$ curve in the neighbourhood of the tricritical point. For $x_c(q) < x_t$ it is just a straight line, however for $x_c(q) > x_t$ it is expected that

$$x_c(q) - x_t \sim (q_t - q)^{1/\psi} \qquad \text{as} \qquad q \to q_t^- \tag{12}$$

with a shape exponent ψ which is related to the crossover exponent ϕ via $\psi = 1/\phi$. Moreover, identification of ψ with the singularity $2-\alpha$ in the free energy $(-\lim_{n\to\infty} \frac{1}{n} \log P_n(q))$, where α is the specific heat exponent, leads to the tricritical scaling relation linking this exponent to the crossover exponent via[9]

$$2 - \alpha = \frac{1}{\phi}\,. \tag{13}$$

In what follows, we will describe the various methods used to enumerate the number of configurations of these polygon models by deriving expressions for their generating functions.

Temperley[12] introduced a recurrence relation method to find the generating function of these polygon models which has been successfully utilised in recent years[13,14,11]. Zwanzig and Lauritsen investigated an interacting walk model of alternating vertical segments in discrete and continuous forms with transfer matrix and integral equation methods. The semi-continuous systems for walks[15] and vesicles[16] have been now successfully tackled with an extension of Temperley's method to semicontinuous systems. Given that it is now recognised that all these methods are similar we shall only describe the method for the discrete model explicitly.

Essentially, the configurations are partitioned into configurations with fixed height to their left. Then, one can easily derive an infinite recurrence relation by constructing configurations G_r of height r by concatenating a column of height r in all possible ways to configurations of heights r'. In the case of staircase polygons, where we denote G_r by S_r, we get

$$S_r(x,y,q) = xq^r \left(y^r + \sum_{s=1}^{r} y^{r-s} \sum_{r'=s}^{\infty} S_{r'}(x,y,q) \right) \tag{14}$$

By expanding in x it is possible to view this equation as a transfer matrix equation, so one could now proceed by studying its spectrum. However, it turns out that one can in fact solve for the generating functions S_r explicitly, by using an Ansatz which leads to q-series. In the semi-continuous case this equation is an integral equation. The type of Ansatz necessary is more easily seen when one transforms this equation into a difference equation,

$$S_{r+2} - q(1+y)S_{r+1} + q^2 y S_r = -xq^{r+2} S_{r+1} \,. \tag{15}$$

Either equation can be solved using a generalisation (needed since these equations do not have constant coefficients) of an exponential Ansatz (μ^r):

$$S_r = \mu^r \sum_{m=0}^{\infty} c_m(q) q^{mr} \tag{16}$$

Summing $S = \sum_r S_r$ leads after some transformations to the solution

$$S(x,y,q) = y\left(\frac{J(qx,y,q)}{J(x,y,q)} - 1\right) \qquad \text{with} \qquad J(x,y,q) = \sum_{n=0}^{\infty} \frac{(-qx)^n q^{\binom{n}{2}}}{(q,qy;q)_n} \,, \tag{17}$$

where we have used the q-product notation

$$(x_1, x_2, \ldots, x_k; q)_n = \prod_{m=0}^{n-1} (1 - x_1 q^m)(1 - x_2 q^m) \ldots (1 - x_k q^m) \,. \tag{18}$$

The difference equation becomes a differential equation in the semi-continuous analogue. This differential equation is none other than Bessel's and the function $J(x,y,q)$ is a q-generalisation of a Bessel function. This calculation generalises for the other models, although it gets more and more cumbersome, leading to a full-page formula in the case of column-convex polygons[16].

However, if one considers the generating function

$$G(\lambda) = G(\lambda; x, y, q) = \sum_{r=1}^{\infty} G_r(x, y, q)\lambda^r \tag{19}$$

one can write down functional equations instead of recurrence relations and it turns out that this is a unifying way of solving all these models[17]. The functional equations are all linear and of the general form

$$G(\lambda) = x\left\{a(\lambda) + b(\lambda)G(1) + c(\lambda)G(\lambda q) + d(\lambda)\frac{\partial G}{\partial \lambda}(1)\right\} \tag{20}$$

for which the general solution can be given explicitly. In the case of column-convex polygons, the most compact solution so far reads[17]

$$G(x, y, q) = y\frac{(1-y)H(x, y, q)}{1 + K(x, y, q) + yH(x, y, q)}, \tag{21}$$

with

$$H(x, y, q) = \frac{xq}{(1-y)(1-yq)} + \sum_{n\geq 2} \frac{(-1)^{n+1}x^n(1-y)^{2n-4}q^{\binom{n+1}{2}}(y^2q)_{2n-2}}{(q)_{n-1}(yq)_{n-2}(yq)_{n-1}^2(yq)_n(y^2q)_{n-1}}, \tag{22}$$

and

$$K(x, y, q) = \sum_{n\geq 1} \frac{(-1)^n x^n(1-y)^{2n-3}q^{\binom{n+1}{2}}(y^2q)_{2n-1}}{(q)_n(yq)_{n-1}^3(yq)_n(y^2q)_{n-1}}. \tag{23}$$

Clearly this solves the combinatorial problem of giving a closed form solution of the generating function (and thus a polynomial time algorithm to compute the coefficients). However, it is almost unfeasible to extract from these q-series the singular behaviour of the generating functions. One could think of working directly with the functional equations, but they become singular at $\lambda = 1$ and $q = 1$. On the other hand, it is known that at $q = 1$ the generating functions are algebraic. It turns out that there is an alternate approach of deriving functional equations which leads to non-linear equations[18].

The technique for deriving the functional equations is to use a geometrical partition of the set of all polygons into disjoint subsets. These subsets are chosen such that they enable one to give construction rules that can be transformed into equations for the corresponding generating functions. A related method for the derivation of functional equations based on the theory of algebraic languages has been developed[19,20,21].

These equations can then in principle be used to solve for the generating function. As we shall see, one can also extract information about the singularity structure of the generating function directly from the functional equations. As they are well behaved near $q = 1$ one can employ a singular perturbation expansion.

The partition is constructed as follows: one set of the partition will be a set P_1 of "inflated" polygons, i.e. polygons which are generated from the set P of all polygons by increasing the height of each column by one (replacement of x by qx) and thereby increasing the number of vertical perimeter bonds by 2 (multiplication by y), leading to the equation

$$P_1(x,y,q) = P(qx,y,q)y\,. \tag{24}$$

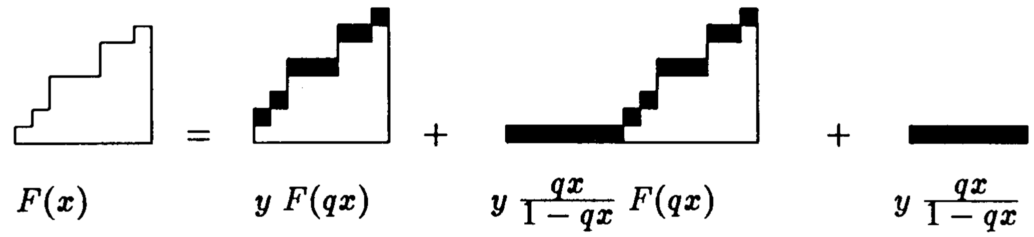

Fig. 3. The diagrammatic form of the functional equation for Ferrer diagrams.

As an example, let us consider Ferrer diagrams. The partition due to the inflation process is represented in figure 3. If we inflate Ferrer diagrams we have to correct by adding a row of height one to the left, leading to the functional equation

$$F(x,y,q) = \frac{y}{1-xq}\left(xq + F(xq,y,q)\right) \tag{25}$$

which for $q = 1$ reduces to

$$F(x,y,1) = \frac{xy}{1-x-y} \tag{26}$$

Now we assume the existence of an asymptotic expansion of P at $q = 1^-$, and we get as the first correction term

$$\frac{\partial F}{\partial q}(x,y,1) = \frac{xy(1-y)(1-x)}{(1-x-y)^3} \tag{27}$$

This is already enough information to give us the critical exponents for this class of polygons. Firstly, we note that at $q = 1$ the generating function diverges with an exponent $\gamma_u = 1$. Secondly, it follows from tricritical scaling that the partial derivative diverges with an exponent $\gamma_u + \Delta$, with a gap exponent $\Delta = 1/\phi$. Therefore we have a complete set of thermodynamic exponents,

$$\gamma_u = 1, \quad \gamma_t = \frac{1}{2}, \quad \phi = \frac{1}{2}, \quad \alpha = 0\,. \tag{28}$$

In order to get the complete scaling behaviour, we can now take the semi-continuous limit as described above, resulting in a differential equation for $f(x) = F_{cont}(x,y,q)$,

$$x\varepsilon f'(x) = (x-\tau)f(x) + x \quad \text{with} \quad \varepsilon = -\log q\,, \quad \tau = -\log y\,, \tag{29}$$

which has as solution

$$f(x) = \exp\left(\frac{x}{\varepsilon} + \frac{\tau}{\varepsilon}\log(\frac{x}{\varepsilon})\right)\ \gamma(\frac{\tau}{\varepsilon}+1, \frac{x}{\varepsilon}) \tag{30}$$

where $\gamma(a,x) = \int_0^x e^{-t}t^{a-1}dt$ is the incomplete Gamma function. From this solution the exponents above can be confirmed. This solution could also be extracted from the Temperley-like method described previously.

Alternatively, one can extract the complete scaling function directly from the differential equation[18], using the method of dominant balance. We first transform the critical point to the origin,

$$-\varepsilon(t+\tau)p'(t) = tp(t) + (t+\tau)p^2(t) \quad \text{where} \quad p(t) = \frac{1}{f(t+\tau)} \tag{31}$$

Substituting $p = \varepsilon^{\theta}\bar{p}$ and $t = \varepsilon^{\phi}\bar{t}$, we now look for the dominating terms in this equation for $\varepsilon \to 0$. This yields $\theta = \phi = \frac{1}{2}$, and we get a differential equation for the asymptotically dominant part as

$$-\tau\bar{p}'(\bar{t}) = \bar{t}\bar{p}(\bar{t}) + \tau\bar{p}^2(\bar{t}). \tag{32}$$

Solving this equation and fixing the arbitrary constant by using asymptotic matching with the solution for $\varepsilon = 0$ results in the scaling solution

$$F(x,y,q) \sim \sqrt{\frac{\pi\tau}{2\varepsilon}}\exp\left(\frac{(\tau-x)^2}{2\varepsilon\tau}\right)\operatorname{erfc}\left(\frac{\tau-x}{\sqrt{2\varepsilon\tau}}\right) \tag{33}$$

Again this result could have been found, via the Temperley-like method, directly from the solution itself with greater effort!

This has been a particularly simple example, with the functional equation being, in fact, still linear. For the more complicated models, however, one gets non-linear equations. The simplest case is for staircase polygons,

$$S(x,y,q) = \{S(qx,y,q) + qx\}\{y + S(x,y,q)\}\ , \tag{34}$$

with the complexity of the equations growing as one proceeds to more complicated models.

The introduction of the non-linearity changes the universality class of the generating function, which leads to another set of exponents and a different scaling function. However, it turns out that a large group of models, containing bar-graph, staircase, directed column-convex, and column convex polygons, are all in the same universality class. These exponents and scaling function are therefore generic for directed models. In particular, we get for the exponents at the tricritical point

$$\gamma_u = -\frac{1}{2}, \quad \gamma_t = -\frac{1}{3}, \quad \phi = \frac{2}{3}, \quad \alpha = \frac{1}{2}\ . \tag{35}$$

For staircase polygons, we found[16] the scaling function is

$$S(x,x,q) \sim a + b\nu^{-1/3}\,\frac{\mathrm{Ai}'(c\nu^{2/3}(1-\sigma))}{\mathrm{Ai}(c\nu^{2/3}(1-\sigma))} \tag{36}$$

where

$$\sigma = \frac{\sqrt{x}}{\log(x^{-1/2})}\ , \nu = \frac{\log(x)}{\log(q)}\ , \tag{37}$$

Ai(x) is the Airy function and the prime denotes differentiation. The value $\sigma = 1$ defines the tricritical point and note that as $q \to 1$ we have $\nu \to \infty$.

The amplitudes of the scaling function for staircase polygons are

$$a = \log(x^{-1/2})\ ,\ b = 2^{1/3}\log(x^{-1/2}) \text{ and } c = 2^{-2/3}(1+\sigma)\ . \tag{38}$$

For column-convex polygons it was found[16] that the identical scaling form holds with

$$a = \frac{2}{17}(5-2\sqrt{2})\log(x^{-1/2}),\ b = \frac{4}{289}(19+6\sqrt{2})\log(x^{-1/2}),\ c = (1+\sigma)/2 \tag{39}$$

with

$$\sigma = \frac{2\sqrt{x}}{\log(x^{-1/2})} \tag{40}$$

and ν unchanged.

In summary, all the models listed in the introduction ((a) to (d)) have this scaling solution around their tricritical-like points. We therefore conclude that they all fall into one universality class. We point out that the solutions of the staircase and column-convex models are in terms of *different* functions while their scaling solutions are essentially the same. All the models can be solved for their generating functions using the Temperley-like method while the scaling solution can be extracted, as described above, from functional/differential equations. (The semi-continuous staircase generating function can be found explicitly in terms of Bessel function which, in turn, can be shown directly to give the scaling solution[16].)

The simpler Ferrer diagram and stack polygon models lie in a different universality class. (The semi-continuous and scaling solutions of the generating function for Ferrer diagrams have not been previously given.) Rectangles and convex polygons lie in further universality classes. (Rectangles have the exponents $\gamma_u = 2$, $\phi = 1/2$ or $\gamma_u = 1$, $\phi = 1$ depending on whether the fugacities are symmetric or asymmetric respectively.)

We have presented a class of models that can be solved completely around a tricritical-like point with non-trivial results. The scaling form, in addition to the exponents, can be extracted. Several interrelated methods of solution have been summarised which include recurrence, differential, and linear and non-linear q-functional equations. These models are then some of the only non-trivial statistical mechanical models that can be solved to give scaling functions as in the Ising model. Also, since several different models can be solved, the universality hypothesis has been tested.

Future work lies in at least two directions. The first is the solution of the end-to-end distance generating functions and related scaling solutions. The second lies in an attempt to see how the models might be altered to change the universality class. We note however that the full self-avoiding polygon vesicle model also has a crossover exponent $\phi = 2/3$. Moreover, rooted self-avoiding polygons[22] have precisely the exponents given in (35). This intriguing observation begs the question: 'Is the scaling function for rooted self-avoiding polygons the same as in the partially convex class?'

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