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Pulled directed lattice paths

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Abstract
The generating functions of models of directed walks pulled by an external force f are determined using the kernel method. These paths are models of linear polymers subject to an external force. The generating function is related to the generating function of ballot paths, and has an unexpected and non-physical singularity for the model of Dyck paths pulled at its central vertex. In each model the force–extension curve is determined exactly, and has a sigmoid shape partially given by $C\tanh(cf)$ if f is the applied force and where c and C are the model-dependent constants. This result is consistent with previous results for models of pulled directed paths, and also with data obtained from the numerical simulation of self-avoiding walk models of linear polymers.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The experimental phenomenon of forced-induced polymer localization and delocalization has seen renewed interest in recent years [16, 17, 25] and this has in turn spawned a renewed activity in the theoretical modelling of polymer adsorption under externally applied forces. For example, numerical studies in [22, 23, 26] examine the behaviour of self-avoiding walk models of polymers pulled by externally applied forces, while directed path and partial directed path models were analysed in [1, 3, 27, 28].

Directed lattice paths have long served as models of polymer entropy [11, 32]. These models are in many cases exactly solvable so that the singular nature of limiting free energies and the structure of phase diagrams can be exactly calculated (see for example [10]). These models have also been used to explore a variety of polymer phenomena; for example directed path models are examined in [6, 14, 19, 20, 29], while Motzkin path models of polymer adsorption and collapse were analysed in [4]. Examples of models of directed vesicles or directed lattice polygons can be found in [5].

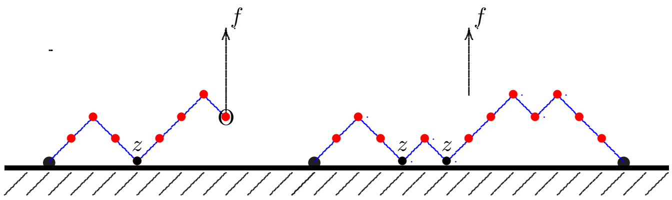

Figure 1. Two models of adsorbing directed paths pulled by an external force. On the left-hand side a path fixed at its first vertex is pulled away from the adsorbing line by an externally applied force at its last vertex. On the right-hand side is a Dyck path with both endpoints fixed being pulled away from the adsorbing line by an externally applied force averaged over the entire path. In both these models the visits of the path are weighted by a parameter z; for large values of z the paths are adsorbed, and for small values of z it is desorbed. These models were considered in [27, 28], where it was shown that there are adsorption–desorption transitions due to the parameter z and a ballistic phase for large (pulling) values of the external force. In [1] the elastic response of these paths was examined by the calculation of force–extension curves. For $z = 1$ the paths are in the desorbed phase, and this is the situation which is considered here.

Directed path models of a polymer pinned at an interface and pulled by optical tweezers (see reference [12]) were examined in [27], and were further generalized in [1] by examining force–extension relations for models of adsorbing Dyck paths and partially directed paths [3]. In particular, the generating functions and force–extension curves were determined for the models in figure 1 in [1, 27].

The models in figure 1 are of directed paths in the positive half-space $Y \geqslant 0$ and adsorbing onto the boundary $Y = 0$ with the interaction parameter z. These are *adsorbing directed paths* [14]: on the left a model of a directed path with first vertex fixed in the horizontal line and with an external force f applied vertically on the last vertex is illustrated. The path has a length n and the number of visits it makes to the horizontal line is v while height of its final vertex is h. The generating function of the model is [27, 28]

$$H(z, f, t) = \sum_{n,v,h} c_n(v, h) t^n z^v \, \mathrm{e}^{hf} = \frac{4t}{(2 - z(z - \sqrt{1-4t^2}))(2t - \mathrm{e}^f(1 - \sqrt{1-4t^2}))}, \qquad (1)$$

where $c_n(v, h)$ is the number of paths of length n, with v visits in the adsorbing line and final vertex at height h. The generating variable t generates edges, z generates visits and the external force f is conjugate to the height h.

The model on the right-hand side in figure 1 is more interesting. The external force f is not applied at a given central vertex in the path, but it is instead averaged over vertices along the entire path. The generating function of such *stitched Dyck Paths* was obtained in [1], and is given by

$$S(z, f, t) = \frac{16t^2}{((2 - z(1 - \sqrt{1-4t^2}))^2(4t^2 - \mathrm{e}^f(1 - \sqrt{1-4t^2})^2)}. \qquad (2)$$

This generating function was obtained by finding a second-order functional recurrence which can be explicitly solved.

If the force in the model on the right in figure 1 is applied at a particular vertex (say at the middle vertex), then it becomes far more difficult to determine the generating function. In this paper, I consider this particular situation for a Dyck path pulled in the middle, as illustrated in figure 2. I shall simplify the model by putting the adsorption parameter $z = 1$. The generating

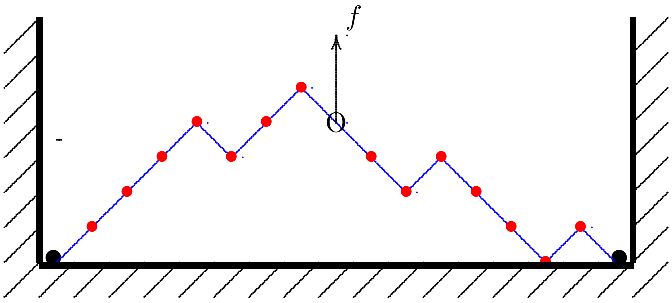

Figure 2. A Dyck path pulled at its central vertex by an external force f. Positive values of f correspond to forces acting vertically up. Negative values of f correspond to forces acting vertically down. For positive values of f, the central vertex is pulled away from the boundary, while it is pushed into the boundary if f is negative.

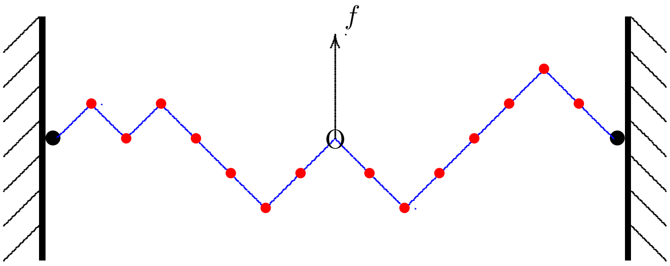

Figure 3. A directed path with fixed endpoints pulled by a force f at its central vertex. Positive values of f correspond to forces acting vertically up. Negative values of f correspond to forces acting vertically down.

function will be determined by a constant term formulation of a more general model, which I shall solve using the obstinate kernel method [2, 13].

A simpler implementation of this approach is demonstrated first on the model of a directed path pulled in the middle, and illustrated in figure 3. In this model both endpoints of the path are fixed in the line $Y = 0$, and the path is pulled by an external force f in the middle. For positive values of f the path is pulled up, and for negative values it is pulled down.

The generating function of the model in figure 3 has an intimate relation with Legendre polynomials, and I show in particular that it is given by

$$g_0(t; f) = \frac{1}{\sqrt{1 - 4t^2 \cosh f + 4t^4 \sinh^2 f}}. \tag{3}$$

An additional result is a proof of the following combinatorial identity:

$$\sum_{n=0}^{\infty} \left[\sum_{j=0}^{n} \binom{n}{j}^2 a^j \right] b^n = \frac{1}{\sqrt{1 - 2b\,(a+1) + b^2\,(a-1)^2}}. \tag{4}$$

The method of proof is via a constant term formulation of the generating function of the paths in figure 3. The selection of the constant term gives the generating function $g_0(t, f)$ as a series over Legendre polynomials from which the identity follows.

The radius of convergence t_c of the generating function $g_0(t, f)$ in the t-plane defines the limiting free energy per edge of the path. This is given by

$$\mathcal{F}_0(f) = \log[2\cosh(f/2)]. \tag{5}$$

The mean extension (or height) of the midpoint of the path per unit length is given by $\langle h\rangle = \frac{d\mathcal{F}_0(f)}{df} = [\tanh(f/2)]/2$. This should be compared with equation (6) in [1] for the force–extension curve of a single path pulled at its end point; inverting that equation for $T = 1$ (below the critical adsorption temperature) gives $\langle h\rangle = (e^{2f} - 1)/(e^{2f} + 1) = \tanh(f)$.

The presence of a hard wall in the model in figure 2 poses significantly more difficult challenges. Let $G(Z; f)$ be the generating function of these paths, with Z conjugate to the visit of the central vertex (where the force is applied) to the hard wall.

If the generating function $G(Z; f)$ is generalized so that $G(1; f)$ is the constant term of the generating function of a more general model of pairs of directed paths, then $G(Z; f)$ can be determined using the obstinate kernel method. This generalized formulation gives a generating function which satisfies an algebraic recurrence, and selection of the constant term gives the following theorem.

Theorem 1. *If α is any root of the quadratic polynomial in a:*

$$a - t^2(a + e^{-f})(a + e^f) = 0, \tag{6}$$

and the function $F_0(y)$ is given by

$$F_0(y) = \frac{e^f y^2}{t^2}\left(\frac{1}{4} - \frac{1}{2\pi}E(4t^2)\right) + t^2(e^f y^2 - 1)\sum_{j=1}^{\infty}\sum_{k=0}^{j-1}\frac{1}{j+1}\binom{2j}{j}\binom{2j+1}{k}(e^f y^2)^{j-k}t^{4j}, \tag{7}$$

where $E(a)$ is a complete elliptic integral of the second kind, then the generating function $G(1; f)$ is formally given by

$$G(1; f) = \frac{F_0(\sqrt{\alpha}) - F_0(\sqrt{1/\alpha})}{e^f t^2(\alpha - 1/\alpha)} \tag{8}$$

for values of t within a circle in the complex t-plane determined by the radius of convergence of $F_0(\sqrt{\alpha})$ and $F_0(\sqrt{1/\alpha})$.

This result should be compared to the generating function of pulled Dyck paths (with $z = 1$) in equation (2), and the roots α in theorem 1 are related to the singularities of the generating function $g_0(t; f)$ in equation (3).

A corollary of the above is the following combinatorial identity involving Catalan numbers: this identity arises when the function $F_0(y)$ is given a complex argument.

Theorem 2. *If C_n is the n-Catalan number, then*

$$\sum_{n=0}^{\infty} C_n^2 a^n = \frac{E(4\sqrt{a})}{\pi a} - \frac{(1-16a)K(4\sqrt{a})}{2\pi a} - \frac{1}{4a},$$

where $K(a)$ and $E(a)$ are complete elliptic integrals of the first and second kind, respectively. In particular, it is the case that $F_0(ie^{-f/2}) = -t^2\sum_{n=0}^{\infty} C_n^2 t^{2n}$.

The limiting free energy per edge in this model can also be determined from the above; it is given by

$$\mathcal{F}(f) = \begin{cases}\log 2, & \text{if } f < 0;\\ \log[2\cosh(f/2)], & \text{if } f \geqslant 0.\end{cases} \tag{9}$$

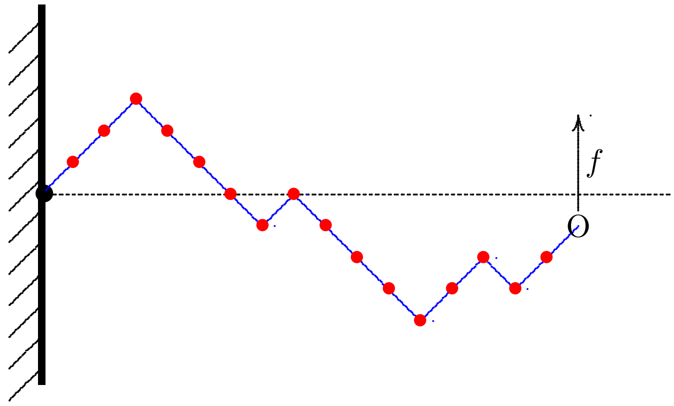

Figure 4. A directed path pulled vertically at its last vertex. The force–extension curve in this model is $\langle h\rangle = \tanh f$, where $\langle h\rangle$ is the average height of the last vertex from the X-axis. The elastic response of this path is given by $R(f) = f/\tanh f$ so that $|R(f)| \geqslant 1$ for all f and $|R(f)| \sim |f|$ asymptotically.

This shows that $\mathcal{F}(f)$ is singular when $f = 0$, separating a phase of paths with positive mean extension per edge for $f > 0$ given by $\langle h\rangle = \frac{d\mathcal{F}(f)}{df} = [\tanh(f/2)]/2$ from a phase with zero mean extension per edge when $f \leqslant 0$. This signals a phase transition at the critical value $f_c = 0$ of the applied force to a ballistic phase for the forces $f > 0$.

Observe that if $T = 1$ in equation (16) in [1], then inverting the equation gives $\langle h\rangle = [\tanh(f/2)]/2$ for $f > 0$. In other words, pulling the path at its middle vertex (as in this paper), or pulling it from an averaged position (as in [1]) gives the same force–extension curves.

The model in figure 2 is related to models of osculating paths and vicious paths [8, 9, 30, 31], and also to models of staircase polygons [5] and random walks in the quarter plane [13]. Our approach will be similar to the method for three osculating walkers in [9].

Both the models in figures 2 and 3 are already solved in the sense that the number of paths, in each case, can be written down using binomial coefficients. For example, the number of paths in the model in figure 2 can be determined from either equation (2.1) in [21], or equation (4.156) in [19]. Directly computing the generating function from these expressions, using computer algebra packages (for example Maple 12 [24]) produces a series over generalized hypergeometric functions about which little is apparently known.

It is remarkable that the expressions for the limiting free energies obtained above are similar to those for the free energy of directed paths with north-east and south-east steps from the origin of the lattice, and pulled in a vertical direction by the last vertex. This model is illustrated in figure 4 and the number of such paths of length n ending at height h above the X-axis is given by the binomial coefficient

$$c_n(h) = \binom{n}{\frac{n+h}{2}}. \tag{10}$$

Observe that there is a parity effect, if n is even, then h must be even, and if n is odd, then h is odd. Thus, the partition function can be found directly:

$$Z_n(f) = \sum_h c_n(h)\, e^{fh} = (e^f + e^{-f})^n. \tag{11}$$

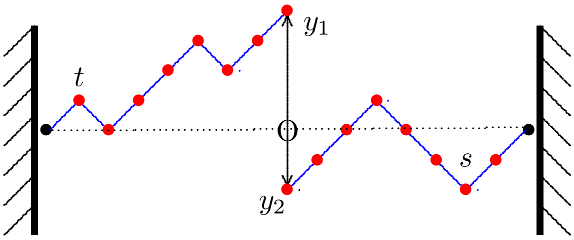

Figure 5. Two directed paths starting in the opposite boundaries and stepping towards the line midway between the boundaries. The paths terminate when they step onto the halfway line between the boundaries. The *heights* of the endpoints of the walks in the halfway line are generated by the variables y_1 and y_2. Paths in the model in figure 3 are generated in this model when the endpoints of the two paths meet on the halfway line—in the generating function this will correspond to the selection of constant term.

The generating function of this model can be explicitly computed to be

$$G(t, f) = \sum_n \sum_h c_n(h)\,\mathrm{e}^{fh} t^n = \frac{1}{1 - 2t\cosh f}, \tag{12}$$

and the result is that the limiting free energy per vertex is given by

$$\mathcal{F}(f) = \log[2\cosh f]. \tag{13}$$

This shows that $\mathcal{F}$ is analytic in f and the force–extension curve of the path is given by $\langle h\rangle = \tanh f$. The elastic response of the path is defined by $R(f) = f/\tanh f$ and note that $R(0) = 1$ and $R(f) \geqslant 1$ for all f and that $|R(f)| \sim |f|$ asymptotically.

I conclude the paper with a few final comments in section 4.

2. A directed path pulled in the middle

In this section, I show how to use a constant term formulation to determine the generating function of the model in figure 3. Note that the pair of paths have a combined even length $2n$ and the number of paths with the middle vertex at height $h = 2j - n$ from the X-axis is given by $c_n(2j - n) = \binom{n}{j}^2$. In other words, this is the number of pairs of directed paths from the origin of length n both ending at height $2j - n$.

I shall now determine the generating function of this model by selecting the constant term of a more general generating function. Consider instead the model in figure 5 of two paths with free endpoints starting in the walls of the slit and stepping towards the middle. North-east and south-east steps in the first path are generated by t and vertical displacement from the horizontal line by y_1.

Similarly, north-west and south-west steps in the second path are generated by s and vertical displacement from the horizontal line is generated by y_2.

The generating function $h(y_1, y_2)$ of the (combined) pairs of paths in figure 5 satisfy the recurrence relation given by

$$h(y_1, y_2) = 1 + (ty_1 + t/y_1)(sy_2 + s/y_2)h(y_1, y_2), \tag{14}$$

so that $h(y_1, y_2)$ is either the set of trivial paths composed of one vertex each, or is a pair of paths obtained by appending a single edge to the paths generated by $h(y_1, y_2)$: the factor $(ty_1 + t/y_1)$ appends a north-east edge (ty_1) or a south-east edge (t/y_1) to the path on the left, while $(sy_2 + s/y_2)$ appends a north-west edge (sy_2) or a south-west edge (s/y_2) to the path on the right.

If $h(y_1, y_2)$ is known, then the generating function of the model in figure 3 can be determined by putting $y_1 = e^{f/2}y$ and $y_2 = e^{f/2}/y$ and then determining the constant term (CT—this is the term independent of y) of $h(e^{f/2}y, e^{f/2}/y)$.

In other words, the generating function of the model in figure 3 is given by

$$g_0(s, t; f) = \mathrm{CT}[h(e^{f/2}y, e^{f/2}/y)], \tag{15}$$

where CT is an operator which selects the terms *independent* of y in $h(e^{f/2}y, e^{f/2}/y)$.

Proceed by solving for h in equation (14). Substituting $y_1 = e^{f/2}y$ and $y_2 = e^{f/2}/y$ then gives the expression

$$h(e^{f/2}y, e^{f/2}/y) = \sum_{n=0}^{\infty}(e^f + y^2 + y^{-2} + e^{-f})^n T^n, \tag{16}$$

where $T = st$.

Factor the coefficient of T^n in the above as follows:

$$(e^f + y^2 + y^{-2} + e^{-f})^n = y^{-2n}(y^2 + \alpha_+)^n(y^2 + \alpha_-)^n, \tag{17}$$

where α_+ and α_- are determined from the roots of the quartic $y^4 + 2y^2(e^f + e^{-f}) + 1$ in y and is given by

$$\alpha_\pm = \tfrac{1}{2}\sqrt{(e^f + e^{-f})^2 - 4} \pm \tfrac{1}{2}(e^f + e^{-f}). \tag{18}$$

Observe that

$$[\alpha_+\alpha_-] = 1, \qquad \text{and} \qquad [\alpha_+/\alpha_-] = e^{-2f}. \tag{19}$$

Expanding the powers in equation (17) and collecting the constant terms shows that

$$\begin{aligned}\mathrm{CT}[(\alpha_+ + y^2 + y^{-2} + \alpha_-)^n] &= \sum_{j=0}^{n}\binom{n}{j}\binom{n}{n-j}\left(\sqrt{\frac{\alpha_+}{\alpha_-}}\right)^{n-2j} \\ &= {}_2F_1\left([-n,-n],[1];\frac{\alpha_-}{\alpha_+}\right)\left(\frac{\alpha_-}{\alpha_+}\right)^n \\ &= \left(\sqrt{\frac{\alpha_+}{\alpha_-}} - \sqrt{\frac{\alpha_-}{\alpha_+}}\right)^n P_n\left(\frac{\alpha_+ + \alpha_-}{\alpha_+ - \alpha_-}\right),\end{aligned} \tag{20}$$

where $P_n(x)$ is the nth degree Legendre polynomial (see for example 8.916(5) in [15]).

Multiplying by $T^n = s^n t^n$ and summing over n gives the complete generating function. Put $s = t$ in the expression for $g_0(s, t; f)$ to see that

$$\begin{aligned}g_0(t; f) \equiv g_0(t, t; f) &= \sum_{n=0}^{\infty}\left[\sum_{j=0}^{n}\binom{n}{j}^2 e^{(2j-n)f}\right]t^{2n} \\ &= \sum_{n=0}^{\infty}\sinh^n(-f)\, P_n(\coth(-f))\, (2t^2)^n \\ &= \frac{1}{\sqrt{1 - 4t^2\cosh(-f) + 4t^4\sinh^2(-f)}};\end{aligned} \tag{21}$$

see for example 8.921 in [15] for the generating function of Legendre polynomials. This in particular proves equation (4).

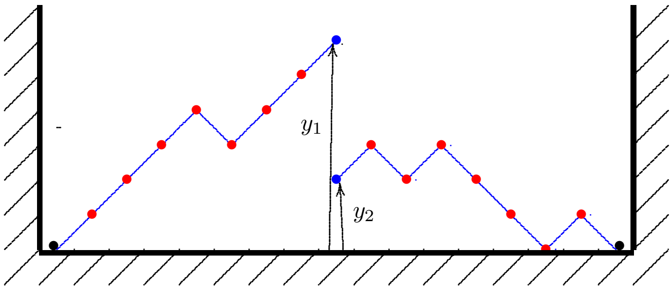

Figure 6. Two directed paths in the half-space $Y \geqslant 0$ starting in the opposite boundaries and stepping towards the line halfway between the vertical boundaries. The paths terminate when they meet the halfway line between the boundaries. The *heights* of the endpoints of the paths in the halfway line are generated by variables y_1 and y_2. The generating function of this model is $g(Z; y_1, y_2)$, where Z generates paths with both endpoints at height zero and in the horizontal hard wall. Paths in the model in figure 2 are counted in this model when the endpoints of the two paths meet on the halfway line—in the generating function this will correspond to the selection of a constant term.

Determining the radius of convergence of $g_0(t; f)$ shows that

$$t_c^2 = \min\left\{\frac{1}{2}\left(\frac{1}{2(\cosh(f) \pm 1)}\right)\right\}, \tag{22}$$

where the minimum is taken over the sign. This finally gives the limiting free energy per edge of the model:

$$\mathcal{F}_0(f) = -\log t_c = \log\sqrt{2\,(1+\cosh(f))} = \log\left[2\cosh(f/2)\right]. \tag{23}$$

The force–extension relation for this model is obtained by taking the first derivative to f, and is given by $\langle h\rangle = [\tanh(f/2)]/2$. This completes the proofs of the claims made in equation (4) and in the introduction.

3. Dyck paths pulled in the middle

Next consider a model of Dyck Paths pulled in the middle. The approach followed here will be similar to that of the previous section. The model is illustrated in figure 2, and as above the path is cut into two independent paths of equal length (see figure 6) in its middle vertex.

In particular, I determine the generating function $g(Z; y_1, y_2)$ of the model in figure 6, where Z is a generating variable conjugate to pairs of paths with both endpoints in the boundary or hard wall. The generating function $G(Z; f)$ of the model in figure 2 can then be determined from the constant term (the term independent of y) in $g(Z; \mathrm{e}^{f/2}y, \mathrm{e}^{f/2}/y)$, following the outline of the method in the previous section.

Our basic approach is to write down a functional recurrence for the model, and then to solve it using the kernel method [7, 8], and in particular the incarnation of this method as the *obstinate kernel method* (see for example [13]).

A functional recurrence for the generating function $g(Z; y_1, y_2)$ of the model in figure 6 is obtained by examining the number of ways each path can be extended by adding edges. A factor of Z will be used to generate the special visit when both the free endpoints of the walks are in the hard wall at $Y = 0$.

Define $\overline{y}_j = 1/y_j$ for $j = 1$ or $j = 2$. Then ty_1 is a north-east edge and $t\overline{y}_1$ is a south-east step in the path on the left in figure 6, while sy_2 is a north-west edge and $s\overline{y}_2$ is a south-west step in the path on the right in figure 6.

The functional recurrence for $g(Z; y_1, y_2)$ is obtained by appending one edge to each of the two paths in figure 6. This gives the recurrence stated below, where I have included comments to justify each set of terms. The letter 'U' represents a 'north-east' or 'north-west' (up)-step, and 'D' represents a 'south-east' or 'south-west' (down)-step in each case. In addition, h_1 is the height of the endpoint of the path on the left and h_2 is the height of the endpoint of the path on the right. The explanatory comments are in square brackets after each term.

$$
\begin{aligned}
g(Z; y_1, y_2) = Z \quad & \text{[The trivial pair]} \\
& + g(Z; y_1, y_2)(tsy_1y_2) \quad \text{[UU for both paths]} \\
& + \Bigg(g(Z; y_1, y_2) - g(Z, 0, y_2) - g(Z; y_1, 0) + g(Z; 0, 0) \\
& - y_1 \left[\frac{\partial g(Z; y_1, y_2)}{\partial y_1} \right]_{y_1=0} - y_2 \left[\frac{\partial g(Z; y_1, y_2)}{\partial y_2} \right]_{y_2=0} \\
& + y_1y_2 \left[\frac{\partial^2 g(Z; y_1, y_2)}{\partial y_1 y_2} \right]_{\substack{y_1=0\\y_2=0}} \Bigg) (ts\overline{y}_1\overline{y}_2 + tsy_1\overline{y}_2 + ts\overline{y}_1y_2) \\
& \text{[DD,UD,DU, for } h_1 > 1 \text{ and } h_2 > 1] \\
& + y_1y_2 \left[\frac{\partial^2 g(Z; y_1, y_2)}{\partial y_1 y_2} \right]_{\substack{y_1=0\\y_2=0}} (Zts\overline{y}_1\overline{y}_2 + tsy_1\overline{y}_2 + ts\overline{y}_1y_2) \\
& \text{[DD,UD,DU, for } h_1 = 1 \text{ and } h_2 = 1] \\
& + \left(y_1 \left[\frac{\partial g(Z; y_1, y_2)}{\partial y_1} \right]_{y_1=0} - y_1y_2 \left[\frac{\partial^2 g(Z; y_1, y_2)}{\partial y_1 y_2} \right]_{\substack{y_1=0\\y_2=0}} \right) \\
& (ts\overline{y}_1\overline{y}_2 + ts\overline{y}_1y_2 + tsy_1\overline{y}_2) \quad \text{[DD,UD,DU, for } h_1 = 1 \text{ and } h_2 > 1] \\
& + \left(y_2 \left[\frac{\partial g(Z; y_1, y_2)}{\partial y_2} \right]_{y_2=0} - y_1y_2 \left[\frac{\partial^2 g(Z; y_1, y_2)}{\partial y_1 y_2} \right]_{\substack{y_1=0\\y_2=0}} \right) \\
& (ts\overline{y}_1\overline{y}_2 + ts\overline{y}_1y_2 + tsy_1\overline{y}_2) \quad \text{[DD,UD,DU, for } h_1 > 1 \text{ and } h_2 = 1] \\
& + (g(Z; y_1, 0) - g(Z; 0, 0))(ts\overline{y}_1y_2) \quad \text{[DU, for } h_1 > 0 \text{ and } h_2 = 0] \\
& + (g(Z; 0, y_2) - g(Z; 0, 0))(tsy_1\overline{y}_2) \quad \text{[UD, for } h_1 = 0 \text{ and } h_2 > 0].
\end{aligned}
$$

Multiplying this by y_1y_2 and collecting terms give the simplified functional recurrence

$$
\begin{aligned}
\left(y_1y_2 - T\left(1+y_1^2\right)\left(1+y_2^2\right)\right) g(Z; y_1, y_2) &= y_1y_2Z + T\left(1 - y_1^2y_2^2\right) g(Z; 0, 0) \\
& - T\left(1+y_1^2\right) g(Z; y_1, 0) - T\left(1+y_2^2\right) g(Z; 0, y_2) \\
& + Ty_1y_2(Z-1) \left[\frac{\partial^2}{\partial y_1\, \partial y_2} g(Z; y_1, y_2) \right] \Bigg|_{\substack{y_1=0\\y_2=0}} + Ty_1^2y_2^2 g(1; 0, 0)
\end{aligned} \tag{24}
$$

for the generating function. Proceed by substituting $Z = 1$ to get a recurrence for $g(y_1, y_2) \equiv g(1; y_1, y_2)$. Simplifying the resulting expression gives

$$
\begin{aligned}
\left(y_1y_2 - T\left(1+y_1^2\right)\left(1+y_2^2\right)\right) g(y_1, y_2) &= y_1y_2 + Tg(0, 0) \\
& - T\left(1+y_1^2\right) g(y_1, 0) - T\left(1+y_2^2\right) g(0, y_2).
\end{aligned} \tag{25}
$$

The *kernel* in equation (25) is

$$K(y_1, y_2) = y_1 y_2 - T\left(1 + y_1^2\right)\left(1 + y_2^2\right), \tag{26}$$

and observe that it is also the kernel of recurrence equation (14) of the model in section 2. Equation (24) cannot be directly solved; for example, substituting $y_1 = 0$ gives a tautology for $g(0, y_2)$. However, note that if (Y_1, Y_2) is a pair such that $K(Y_1, Y_2) = 0$ in equation (25), then expressions involving $g(Y_1, 0)$, $g(0, Y_2)$ and $g(0, 0)$ can be obtained. Thus, proceed by first examining the kernel $K(y_1, y_2)$ before solving for $g(y_1, y_2)$.

3.1. The kernel

Solving for $g(y_1, y_2)$ in equation (25) by the kernel method proceeds by relating y_2 and y_1 such that $K(y_1, y_2) = 0$. This 'killing of the kernel' gives relations involving $g(y_1, 0)$, $g(0, y_2)$ and $g(0, 0)$ from which a solution may be extracted.

Solving for $y_2 = Y_\pm(y_1)$ in $K(y_1, y_2) = 0$ in equation (26) gives pairs $(y_1, Y_\pm(y_1))$ such that $K(y_1, Y_\pm(y_1)) = 0$. The roots are

$$Y_\pm(X) = \frac{X \pm \sqrt{X^2 - 4T^2(1 + X^2)^2}}{2T(1 + X^2)}. \tag{27}$$

Substitution of pairs $(y_1, y_2) = (X, Y_+(X))$ or $(y_1, y_2) = (X, Y_-(X))$ kills the kernel $K(y_1, y_2)$ in equation (25). However, these substitutions alone are not enough to determine $g(y_1, y_2)$, and other pairs (X, Y) which kill the kernel must be generated.

Examination of the roots $Y_\pm(X)$ shows that $Y_+(X)$ is a Laurent series in T, and substitution of a pair $(X, Y_+(X))$ do not give a well-defined power series solution for the generating function. The root $Y_-(X)$ is a formal power series in T, given by the Dyck Path generating function

$$Y_-(X) = \sum_{j=0}^{\infty} \frac{1}{j+1} \binom{2j}{j} (X + 1/X)^{2j+1}\, T^{2j+1}, \tag{28}$$

and pairs $(X, Y_-(X))$ can be substituted to obtain a functional equation relating $g(y_1, 0)$, $g(0, y_2)$ and $g(0, 0)$. The root $Y_-(X)$ is the 'physical root', which gives a legitimate power series counting a certain class of objects.

Direct calculations show that for non-negative values of $X \leqslant 1$,

$$\begin{aligned} &Y_- \cdot Y_+ = 1, && Y_- + Y_+ = [X/(T(1 + X^2))], \\ &(Y_- \circ Y_-)(X) = X, && (Y_- \circ Y_+)(X) = X, \\ &(Y_+ \circ Y_-)(X) = 1/X, && (Y_+ \circ Y_+)(X) = 1/X, \\ &Y_-(X) = Y_-(1/X), && Y_+(X) = Y_+(1/X). \end{aligned} \tag{29}$$

In particular, if one defines the involutions $(X, Y) \to (1/X, Y)$ and $(X, Y) \to (X, 1/Y)$ in view of the above, then direct calculation shows that $K(X, Y) = K(1/X, Y) = K(X, 1/Y) = 0$.

Define $Y_2(y) \equiv Y_-(y)$ to be the physical root. Then $(X, Y) = (y, Y_2(y))$ kills the kernel, and the above shows that other possible kernel killing pairs related to $Y_2(y)$ are $(1/y, Y_2(y))$, $(y, 1/Y_2(y))$ and $(1/y, 1/Y_2(y))$. Since $1/Y_2(y) = Y_+(y)$ is a Laurent series in T, the only appropriate choice amongst these is the pair $(1/y, Y_2(y))$.

These choices give the two kernel killing pairs $(y, Y_2(y))$ and $(1/y, Y_2(y))$. Substitution of these gives the two equations:

$$\begin{aligned} 0 &= yY_2(y) + Tg(0, 0) - T(1 + y^2)g(y, 0) - T(1 + [Y_2(y)]^2)g(0, Y_2(y)), \\ 0 &= (1/y)Y_2(y) + Tg(0, 0) - T(1 + 1/y^2)g(1/y, 0) - T(1 + [Y_2(1/y)]^2)g(0, Y_2(1/y)). \end{aligned} \tag{30}$$

Subtraction of these equations shows that

$$T(1+y^2)g(y,0) - T(1+1/y^2)g(1/y,0) = (y-1/y)Y_2(y). \tag{31}$$

This functional equation must be solved for $g(y,0)$ subject to the requirement that $g(y,0)$ is a formal power series in y. Define $H(y) = T(1+y^2)g(y,0)$; then $H(y)$ is a formal power series in y and satisfies the functional equation

$$H(y) - H(1/y) = (y-1/y)Y_2(y), \tag{32}$$

which is solved in the appendix (see equation (A.1)). The solution is however not unique, but $H(y)$ is a power series in y^2, and if its constant term (independent of y) is stripped away, then a solution is

$$H(y) = \frac{y^2}{T}\left(\frac{1}{4} - \frac{1}{2\pi}E(4T)\right) + T(y^2-1)\sum_{j=1}^{\infty}\sum_{k=0}^{j-1}\frac{1}{j+1}\binom{2j}{j}\binom{2j+1}{k}y^{2j-2k}T^{2j}, \tag{33}$$

where $E(z)$ is a complete elliptic integral of the second kind.[1] Thus, up to an unknown function of T (and independent of y), $T(1+y^2)g(y,0)$ is given by the above, and it remains to extract $g(y,0)$ from this result.

3.2. *Determining* $g(y,0)$

Determining $g(y,0)$ from the result in equation (33) proceeds as follows. Observe that $g(y,0) = g(0,0) + y^2$ (times a function of y), so that one may assume that

$$g(y,0) = g(0,0) + y^2 g_1(y) \tag{34}$$

for some function $g_1(y)$. This assumption implies that $g(1/y,0) = g(0,0) + y^{-2}g_1(1/y)$, and since $H(y) = T(1+y^2)g(y,0) + f(T)$ for some unknown function $f(T)$ independent of y, it follows that

$$H(y) - H(1/y) = T(y^2 - 1/y^2)g(0,0) + (Ty^2)(1+y^2)g_1(y) - (T/y^2)(1+1/y^2)g_1(1/y). \tag{35}$$

The positive power series in y of this is given by equation (33) and is also given by

$$\begin{aligned} H(y) &= (Ty^2)g(0,0) + (Ty^2)(1+y^2)g_1(y) \\ &= (Ty^2)g(0,0) + T(1+y^2)(g(y,0) - g(0,0)) \\ &= T(1+y^2)g(y,0) - Tg(0,0). \end{aligned} \tag{36}$$

In particular, in view of equation (33) this implies that

$$g_1(y) = \frac{H(y) - Ty^2 g(0,0)}{Ty^2(1+y^2)} \tag{37}$$

and the objective is to compute $g(0,0) + y^2 g_1(y) = g(y,0)$ given by

$$g(y,0) = \frac{g(0,0)}{1+y^2} + \frac{H(y)}{T(1+y^2)}, \tag{38}$$

where $H(y)$ is explicitly given by $H(y)$ in equation (33).

[1] The complete elliptic integral of the first and second kinds are respectively defined by

$$K(z) = \int_0^1 \left[\frac{1}{\sqrt{1-z^2t^2}\sqrt{1-t^2}}\right]dt; \qquad E(z) = \int_0^1 \left[\frac{\sqrt{1-z^2t^2}}{\sqrt{1-t^2}}\right]dt.$$

The radius of convergence of both $E(z)$ and $K(z)$ is $|z| = 1$.

3.3. Determining $g(Z; y_1, y_2)$

The solution for $g(y, 0)$ gives a solution for the full generating function $g(1; y_1, y_2) \equiv g(y_1, y_2)$. By equation (25) it follows that

$$g(y_1, y_2) = \frac{y_1 y_2 + T g(0,0) - T\left(1+y_1^2\right) g(y_1, 0) - T\left(1+y_2^2\right) g(0, y_2)}{y_1 y_2 - T\left(1+y_1^2\right)\left(1+y_2^2\right)}, \quad (39)$$

and observe that $g(y, 0) = g(0, y)$ by reflection symmetry of the model. Then substituting $g(y, 0)$ into this from equation (38) shows that

$$g(y_1, y_2) = \frac{y_1 y_2 - T(g(0,0) + H(y_1) + H(y_2))}{y_1 y_2 - T\left(1+y_1^2\right)\left(1+y_2^2\right)}. \quad (40)$$

Since $g(Z; y_1, y_2) = (Z-1) g(0,0) + g(1; y_1, y_2)$, it follows that

$$g(Z; y_1, y_2) = (Z-1) g(0,0) + \frac{y_1 y_2 - T(g(0,0) + H(y_1) + H(y_2))}{y_1 y_2 - T\left(1+y_1^2\right)\left(1+y_2^2\right)}. \quad (41)$$

This gives a solution for $g(Z; y_1, y_2)$ subject to the determination of $g(0, 0)$. Examination of the above indicate that $g(0, 0) \equiv g(1; 0, 0)$ is the term independent of (y_1, y_2) on the right-hand side of equation (40).

3.4. Extracting the constant term

Extracting the constant term in expressions such as equation (40) is necessary to determine the full generating function. In general, I will be concerned with $y_1 = \mathrm{e}^{f/2} y$ and $y_2 = \mathrm{e}^{f/2}/y$, and then I shall extract the constant term (that term independent of y) in the generating function $g(\mathrm{e}^{f/2} y, \mathrm{e}^{f/2}/y)$. The effect of this would be to force paths in figure 6 to end at the same height, and thus the constant term in $g(\mathrm{e}^{f/2} y, \mathrm{e}^{f/2}/y)$ is the generating function of the model in figure 2.

Consider equation (40), and in particular the denominator on the right-hand side (this is the kernel examined above). Substituting $y_1 = \mathrm{e}^{f/2} y$ and $y_2 = \mathrm{e}^{f/2}/y$ then gives it as

$$\begin{aligned} \frac{1}{\mathrm{e}^f - T(1+\mathrm{e}^f y^2)(1+\mathrm{e}^f/y^2)} &= \frac{y^2}{\mathrm{e}^f y^2 - T(1+\mathrm{e}^f y^2)(y^2+\mathrm{e}^f)} \\ &= \frac{y^2}{-\mathrm{e}^f T(y^2-\alpha_1)(y^2-\alpha_2)}, \end{aligned} \quad (42)$$

where the roots of the denominator is given by

$$\begin{aligned} \alpha_1 &= \frac{1 - 2T\cosh(f) + \sqrt{4T^2\sinh^2(f) - 4T\cosh(f) + 1}}{2T}, \\ \alpha_2 &= \frac{1 - 2T\cosh(f) - \sqrt{4T^2\sinh^2(f) - 4T\cosh(f) + 1}}{2T}, \end{aligned} \quad (43)$$

and observe that $\alpha_1 \alpha_2 = 1$. Observe that the radical in these roots are equal to $1/g_0(t; f)$ in equation (21), where $g_0(t; f)$ is the generating function of the model of directed paths pulled in the middle determined in section 2, and is related to the generating function of Legendre polynomials.

Hence, equation (40) can be written as

$$g(\mathrm{e}^{f/2} y, \mathrm{e}^{f/2}/y) = \frac{\mathrm{e}^{-f} y^2 (T[g(0,0) + H(\mathrm{e}^{f/2} y) + H(\mathrm{e}^{f/2}/y)] - \mathrm{e}^f)}{T(y^2-\alpha_1)(y^2-\alpha_2)}. \quad (44)$$

Thence, the generating function of the model in figure 2 is obtained by selecting the constant term in the above:

$$G(1;\, f) = \mathrm{CT}[g(\mathrm{e}^{f/2}y, \mathrm{e}^{f/2}/y)]. \tag{45}$$

Now $H(\mathrm{e}^{f/2}y)$ is a power series in y^2—so define $F_0(y) \equiv H(\mathrm{e}^{f/2}y)$ and $F_1(y) = H(\mathrm{e}^{f/2}/y)$. Then the constant term can be determined as follows:

$$\begin{aligned} G(1,\, f) &= \mathrm{CT}\left[\frac{y^2(\mathrm{e}^{-f}T[g(0,0) + F_0(y) + F_1(y)] - 1)}{T(y^2-\alpha_1)(y^2-\alpha_2)}\right] \\ &= \oint_C \left[\frac{y^2(\mathrm{e}^{-f}T[g(0,0) + F_0(y) + F_1(y)] - 1)}{T(y^2-\alpha_1)(y^2-\alpha_2)}\right]\frac{\mathrm{d}y}{y}, \end{aligned} \tag{46}$$

where C is a circle in the (complex) y-plane centred at the origin with a small radius. Observe that $F_0(y)$ is analytic in a small disc about the origin in the y-plane (and for small values of T is an entire function), while $F_1(y)$ is singular at the origin (but is analytic in the y-plane with a small disc excised about the origin). Note in particular as well that $F_0(y) = F_0(-y)$ and that $F_1(y) \sim y^{-2} + O(y^{-4})$.

The constant term can be determined by using the residue theorem and noting that there are simple poles when $y = \pm\sqrt{\alpha_1}$ and $y = \pm\sqrt{\alpha_2}$. The residue of the term in $y(\mathrm{e}^{-f}Tg(0,0) - 1)$ is zero, as is the residue of $y\mathrm{e}^{-f}TF_0(y)$. This leaves only the term in $F_1(y)$. Direct calculation shows that

$$G(1;\, f) = \frac{F_0(\sqrt{\alpha_1}) - F_0(\sqrt{\alpha_2})}{\mathrm{e}^f T(\alpha_1 - \alpha_2)}, \tag{47}$$

where it was noted that $F_1(y) = F_0(1/y)$ and $\alpha_1\alpha_2 = 1$. The function $F_0(y)$ is explicitly given by

$$\begin{aligned} F_0(y) = {} & \frac{\mathrm{e}^f y^2}{T}\left(\frac{1}{4} - \frac{1}{2\pi}E(4T)\right) \\ & + T(\mathrm{e}^f y^2 - 1)\sum_{j=1}^{\infty}\sum_{k=0}^{j-1}\frac{1}{j+1}\binom{2j}{j}\binom{2j+1}{k}(\mathrm{e}^f y^2)^{j-k}T^{2j}. \end{aligned} \tag{48}$$

Further examination of equation (47) shows that

$$G(1;\, f) = \frac{F_0(\sqrt{\alpha_1}) - F_0(\sqrt{1/\alpha_1})}{\mathrm{e}^f T(\alpha_1 - 1/\alpha_1)} = \frac{F_0(\sqrt{\alpha_2}) - F_0(\sqrt{1/\alpha_2})}{\mathrm{e}^f T(\alpha_2 - 1/\alpha_2)}. \tag{49}$$

In other words, $G(1;\, f)$ is invariant under the exchange $\alpha_1 \leftrightarrow \alpha_2$. This in particular proves the claims in theorem 1 and following equation (8). Expanding $G(1;\, f)$ as a power series in T also shows that

$$G(1;\, f) = 1 + \mathrm{e}^f T + (1 + \mathrm{e}^{2f})T^2 + (4\mathrm{e}^f + \mathrm{e}^{3f})T^3 + (4 + 9\mathrm{e}^{2f} + \mathrm{e}^{4f})T^4 + O(T^5). \tag{50}$$

That is, $G(1,\, f)$ is a formal power series in T with coefficients which are polynomials in e^f with non-negative coefficients.

3.5. *Determining* $g(0, 0)$

Next, the generating function $g(0, 0)$ can be determined. While this generating function played a role in our analysis, it disappeared when the constant term was taken, but it is still present as a limit in our result in equation (47).

The starting point is to note that $\lim_{f\to-\infty}[\mathrm{e}^{-f}\alpha_1] = -1$ and $\lim_{f\to-\infty}[\mathrm{e}^{f}\alpha_2] = -1$. In other words, to leading orders $\alpha_1 = -\mathrm{e}^f + \cdots$ and $\alpha_2 = -\mathrm{e}^{-f} + \cdots$, and taking the

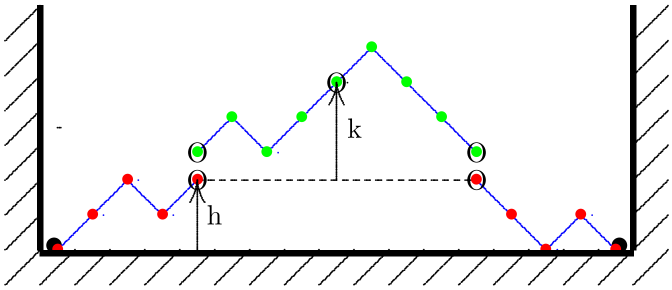

Figure 7. Two pulled Dyck paths with middle vertices at heights h and k can be arranged into a new Dyck path with a middle vertex at height $h + k$ by cutting the first path in its middle vertex, moving the two subpaths apart and then putting the second path in the gap between the two paths with its endpoints coincident with the endpoints of the two subpaths as illustrated.

limit $f \to -\infty$ in equation (47), one obtains (by noting that $e^f \to 0$ (and so $\alpha_1 \to 0$) as $f \to -\infty$),

$$g(0,0) = \frac{F_0(\mathrm{i}\,e^{-f/2})}{-T}. \tag{51}$$

Substitution and evaluation then gives $g(0,0)$ in terms of complete elliptic integrals $E(z)$ (of the second kind) and $K(z)$ (of the first kind):

$$g(0,0) = \frac{E(4T)}{T^2\pi} - \frac{(1-16T^2)K(4T)}{2T^2\pi} - \frac{1}{4T^2}. \tag{52}$$

This in particular shows that the generating function of squared Catalan numbers is

$$\sum_{j=0}^{\infty} \left[\frac{1}{j+1}\binom{2j}{j}\right]^2 T^{2j} = \frac{E(4T)}{T^2\pi} - \frac{(1-16T^2)K(4T)}{2T^2\pi} - \frac{1}{4T^2}, \tag{53}$$

and thence theorem 2 is proven. This result also gives the complete generating function $G(Z; f)$; by consulting equation (41):

$$G(Z; f) = (Z-1)\left(\frac{E(4T)}{T^2\pi} - \frac{(1-16T^2)K(4T)}{2T^2\pi} - \frac{1}{4T^2}\right) + \left[\frac{F_0(\sqrt{\alpha_1}) - F_0(\sqrt{1/\alpha_1})}{e^f T(\alpha_1 - 1/\alpha_1)}\right], \tag{54}$$

with α_1, α_2 and $F_0(y)$ as defined above.

3.6. Discussion

Consider first the model with $Z = 1$ and generating function $G(1; f)$. If the number of Dyck paths with a midpoint at height h and total (even) length n is given by $c_n(h)$, then it follows that the partition function $Z_n(f)$ for paths of length n is

$$Z_n(f) = \sum_{h=0}^{n/2} c_n(h)\, e^{hf}. \tag{55}$$

Paths of lengths n and m can be put together into paths of length $n + m$ by cutting the paths of length n in their midpoint, moving them apart, and then inserting the paths of length m in the resulting gap. This is illustrated in figure 7.

This construction shows that

$$\sum_{h=0}^{k} c_n(h)c_m(k-h) \leqslant c_{n+m}(k). \tag{56}$$

Multiply this by e^k and sum over k. The result is

$$Z_n(f)Z_m(f) \leqslant Z_{n+m}(f). \tag{57}$$

In other words, $Z_n(f)$ is a supermultiplicative function on n for each fixed f. Since $Z_n(f) \leqslant \max\{2^n, 2^n\, e^{fn}\}$ for all finite values of f, this implies that the limiting free energy of the model exists and is given by

$$\mathcal{F}(f) = \lim_{n\to\infty} \frac{1}{n} \log Z_n(f) \tag{58}$$

by a theorem on subadditive functions [18].

The generating function $G(1; f)$ is related to the partition function by

$$G(1; f) = \sum_{n=0}^{\infty} Z_{2n}(f)T^n, \tag{59}$$

where the sum is over all paths of even length and $t^2 = T$, where t is conjugate to the length of the path. The root test for convergence of this series then show, by using equation (58), that the radius of convergence of $G(1; f)$, given by $t_c(f)$, is related to the limiting free energy by

$$\mathcal{F}(f) = -(1/2) \log T_c(f) = -\log t_c(f), \tag{60}$$

where $T_c(f)$ is the radius of convergence of $G(1; f)$ in the T-plane. Observe, in particular, that by existence of the limit in equation (58), that the thermodynamic limit in this model is well defined and that information about it can be obtained by examining the singularities in the generating function $G(1; f)$.

The generating function $G(1; f)$ is a power series in T with coefficients which are polynomials in e^f with positive integer coefficients. Thus, $G(1; f)$ is a non-decreasing function of real f and $T > 0$. Observe that if $G(1; 0)$ is absolutely convergent, then so is $G(1; -|f|)$.

There are several sources of singularities in the generating function $G(Z; f)$. Both the complete elliptic integrals are singular when $T = 1/4$ while there are branch point singularities in α_1 and α_2. Next, the series in $F_0(y)$ (see equation (48)) is divergent if $|T|$ is large, and so one must determine its radius of convergence.

The radius of convergence of $G(1; f)$ in the T-plane can be determined as follows if $f \leqslant 0$: the number of paths with north-east and south-east steps from the origin in the square lattice of even length $2j$ with (both) endpoints in the X-axis is given by $\binom{4j}{2j}$. Thus, it follows that

$$G(1; -|f|) \leqslant G(1; 0) \leqslant \sum_{j=0}^{\infty} \binom{4j}{2j} T^{2j}. \tag{61}$$

On the other hand, if $f \to -\infty$, then the midpoint of the path is also constrained to lie in the X-axis. Thus,

$$\sum_{j=0}^{\infty} \left[\frac{1}{j+1}\binom{2j}{j}\right]^2 T^{2j} = G(1; -\infty) \leqslant G(1; -|f|). \tag{62}$$

Using Stirling's approximation for the binomial factors in the last two sets of inequalities show that the radius of convergence $G(1, -|f|)$ in the T-plane is $T_c = 1/4$.

Examination of $G(Z; f)$ for $f \leqslant 0$ (see equation (54)) and arbitrary Z shows a singularity due to the elliptic integral at $T_c = 1/4$, and one concludes that for all $f \leqslant 0$ the generating function $G(Z; f)$ has a radius of convergence $T_c = 1/4$. (This is in particular true since it can be shown directly that terms in equation (48) containing the infinite series on the one hand, and the terms containing the elliptic integrals on the other hand, are generally not equal for $f \leqslant 0$).

Consider next the case that $f > 0$: instead of considering the function $F_0(y)$ to determine the radius of convergence, observe first that $G(1; f)$ is given explicitly in terms of the number of ballot paths[2] by

$$G(1; f) = \sum_{j=0}^{\infty} \left(\sum_{h=0}^{\lfloor j/2 \rfloor} \left[\frac{2h+1+\delta_j}{j+1} \binom{j+1}{\lfloor j/2 \rfloor - h} \right]^2 \mathrm{e}^{(2h+\delta_j)f} \right) T^j, \tag{63}$$

where the parity term $\delta_j = 0$ if j is even and $\delta_j = 1$ if j is odd (that is, $\delta_j = j - 2\lfloor j/2 \rfloor$).

The maximum rate of exponential growth of the terms in the summations over h in equation (63) can be determined by putting $h = \lfloor \epsilon j \rfloor$ (where $\epsilon \in (0, 1/2)$) in the binomial factors $\binom{j+1}{\lfloor j/2 \rfloor - h}$ and using Stirling's approximation for the factorials. This shows in particular that

$$\max_{\epsilon \in [0,1)} \left\{ \lim_{j \to \infty} \left(\left[\frac{2\lfloor \epsilon j \rfloor + 1}{j+1} \binom{j+1}{\lfloor j/2 \rfloor - \lfloor \epsilon j \rfloor} \right]^2 \mathrm{e}^{(2\lfloor \epsilon j \rfloor) f} \right)^{1/j} \right\} = (1+\mathrm{e}^f)(1+\mathrm{e}^{-f}), \tag{64}$$

where the maximum is found if $\epsilon = [\tanh(f/2)]/2 \in (0, 1/2)$ as required. Thus, by the root test it follows that the radius of convergence of $G(1; f)$ in the above is

$$T_0 = \begin{cases} 4, & \text{if } f \leqslant 0; \\ \dfrac{1}{(1+\mathrm{e}^f)(1+\mathrm{e}^{-f})}, & \text{if } f > 0. \end{cases} \tag{65}$$

Thus, the limiting free energy per edge in this model, if one puts the edge generating variables $s = t$ so that $T = t^2$, is given by

$$\mathcal{F}(f) = \begin{cases} \log 2, & \text{if } f < 0; \\ \log[2\cosh(f/2)], & \text{if } f \geqslant 0. \end{cases} \tag{66}$$

This shows that the force–extension curve (obtained by taking the derivative of $\mathcal{F}(f)$ to f) is given by $\langle h \rangle = [\tanh(f/2)]/2$ if $f > 0$ and $\langle h \rangle = 0$ for $f \leqslant 0$, as claimed in the introduction. This proves a phase transition in this model at $f = 0$ to a ballistic phase for $f > 0$, this concludes the proofs of the claims made in the introduction.

Next, examine the generating function $G(1; f)$ as given in terms of the roots α_1, α_2 and the function $F_0(y)$ as defined in equation (48). Since $G(1; f)$ is given both by equation (49) and by equation (63), one expects that

$$\frac{F_0(\sqrt{\alpha_1}) - F_0(\sqrt{1/\alpha_1})}{\mathrm{e}^f T(\alpha_1 - 1/\alpha_1)} = \sum_{j=0}^{\infty} \left(\sum_{h=0}^{\lfloor j/2 \rfloor} \left[\frac{2h+1+\delta_j}{j+1} \binom{j+1}{\lfloor j/2 \rfloor - h} \right]^2 \mathrm{e}^{(2h+\delta_j)f} \right) T^j, \tag{67}$$

where $\delta_j = j - 2\lfloor j/2 \rfloor$ is a parity term. This identity is true within the radius of convergence of the series on the left-hand and right-hand sides in the T-plane for given fixed finite real values of f. Above it was shown that the radius of convergence of the right-hand side is given by T_0 in equation (65).

To determine the radius of convergence of the left-hand side of equation (67), consider the factors $\binom{2j+1}{k}(\mathrm{e}^f y^2)^{j-k}$ in the definition of F_0 in equation (48) (for $k \in [0, j-1]$). Putting

[2] This approach was suggested by an anonymous referee.

$k = \lfloor \epsilon j \rfloor$ for $\epsilon \in [0, 1)$ and approximating the factorials using Stirling's approximation and maximizing with respect to ϵ shows that the maximum rate of exponential growth in the summation over k is achieved when $\epsilon = 2/(1 + e^f y^2)$ in the limit $j \to \infty$. Observe that this value of ϵ is in $[0, 1)$ when $e^f y^2 > 1$, and substituting this shows that the maximum rate of exponential growth of the terms $\binom{2j+1}{k}(e^f y^2)^{j-k}$ in equation (48) in the $j \to \infty$ limit is

$$\max_{\epsilon\in[0,1)} \left\{ \lim_{j\to\infty} \left[\binom{2j+1}{\lfloor \epsilon j \rfloor} (e^f y^2)^{j-\lfloor \epsilon j \rfloor} \right]^{1/j} \right\} = \begin{cases} 4, & \text{if } e^f y^2 \leqslant 1; \\ \dfrac{e^f y^2}{(1 + e^f y^2)^2}, & \text{if } e^f y^2 > 1. \end{cases} \tag{68}$$

This result shows that the radius of convergence of $F_0(y)$ in the T-plane (by using the root test) is determined by the implicit equations for T:

$$T^2 = \begin{cases} \dfrac{1}{16}, & \text{if } 0 \leqslant e^f y^2 \leqslant 1; \\ \dfrac{1}{4(1 + e^f y^2)(1 + e^{-f} y^{-2})}, & \text{if } e^f y^2 > 1. \end{cases} \tag{69}$$

In view of equations (49) and (54) one has either $y^2 = \alpha_1$ or $y^2 = \alpha_2$ with these given in equation (43). Substitution for α_1 and α_2 and solving for T gives the radius of convergence of the terms $F_0(\sqrt{\alpha_1})$ and $F_0(\sqrt{1/\alpha_1})$. Let T_1 be these radii; then direct calculation shows that

$$T_1 = \begin{cases} \dfrac{1}{4}, & \text{if } f \leqslant 0; \\ \dfrac{e^f}{2(1 + e^{2f})}, & \text{if } f > 0. \end{cases} \tag{70}$$

There are further singularities in $F_0(\sqrt{\alpha_1})$ and $F_0(\sqrt{1/\alpha_1})$ due to branch points in α_1 and α_2. These branch points are located in the T-plane at the solutions of $4T^2 \sinh^2(f) - 4T \cosh(f) + 1 = 0$ and gives the critical points

$$T_\pm = \frac{e^f}{(1 \pm e^f)^2}. \tag{71}$$

Lastly, singular behaviour may also occur if $\alpha_1 = \alpha_2$; solving for T shows that this critical point is at $T = T_\pm$. Observe the relationship

$$\frac{1}{T_1} = \frac{1}{T_+} + \frac{1}{T_-} \quad \text{for } f \geqslant 0, \tag{72}$$

relating T_1 and $T_\pm$.

Taken together, the radius of convergence of the generating function $(F_0(\sqrt{\alpha_1}) - F_0(\sqrt{1/\alpha_1}))/(e^f T(\alpha_1 - 1/\alpha_1))$ is at the minimum of T_1 and $T\pm$, and one can verify that this is at $T = T_1$. Observe in particular that $T_1 < T_0$ when $f > 0$, so that the radius of convergence of the left-hand side of equation (67) is strictly less than the radius of convergence of the series on the right-hand side in the T-plane. In view of equations (58) and (60) the conclusion is that the critical point in this model is given by T_0 and that the singularity in $F_0(\sqrt{\alpha_1})$ at T_1 for $f \geqslant 0$ is unphysical.

One may check the above results numerically. In table 1, I give numerical results obtained by summing the first 1000 terms in each series for the left-hand side and right-hand side of equation (67) with $f = 2$ and for values of T in $[0, T_1]$. These results agree to many digits, and only on approach to T_1 does one see a deterioration in the quality of the estimates obtained from the left-hand side as the singular point in $F_0(\sqrt{\alpha_1})$ is approached. For values of $T > T_1$ one may still attempt to compute both sides, for example, if $T = 1.1T_1$, then the left-hand

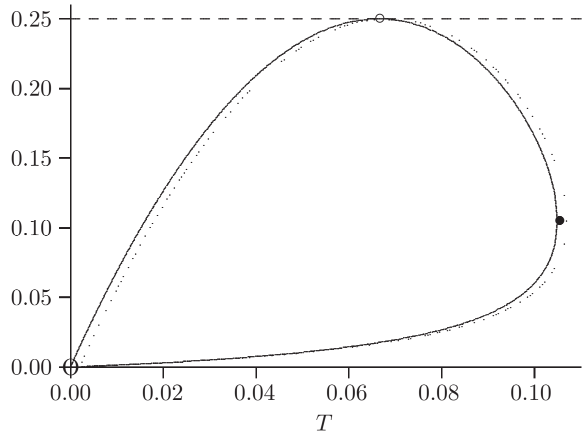

Figure 8. A plot of $\alpha_1 e^f T^2(1+\alpha_2 e^{-f})^2$ (the top curve) and $\alpha_2 e^f T^2(1+\alpha_1 e^{-f})^2$ (the bottom curve) for $f = 2$ against T. The maximum in the top curve is achieved when $T = T_1 = e^2/(2(1+e^4)) = 0.066\,450\,55\ldots$ (see equation (70)). This curve increases to touch its maximum 1/4 exactly at this point, and the function $F_0(\sqrt{\alpha_1})$ has the radius of convergence $T = T_1$. For values of $T > T_1$ the identity in equation (67) breaks down, even though its right-hand side is still convergent while $T < T_0 = (1+e^2)(1+e^{-2})$.

Table 1. Numerical estimates of the lhs and rhs of equation (67).

T	$0.5T_1$	$0.75T_1$	$0.8T_1$	$0.85T_1$	$0.9T_1$	$0.95T_1$	$0.975T_1$	T_1
lhs	1.328 61	1.596 74	1.665 05	1.740 04	1.822 86	1.914 61	1.959 43	–
rhs	1.328 61	1.596 74	1.665 05	1.740 04	1.822 86	1.915 18	1.965 25	2.018 36

side gives $1.831\,93\ldots$ while the right-hand side converges to $2.267\,92\ldots$. In other words, the identity in equation (67) breaks down when $T \in (T_1, T_0)$.

An alternative approach to the above is to note that the root test for convergence shows that $F_0(\sqrt{\alpha_1})$ and $F_0(\sqrt{1/\alpha_1})$ in equation (48) are convergent when $\alpha_1 e^f T^2(1+\alpha_2 e^{-f})^2 < 1/4$ and $\alpha_2 e^f T^2(1+\alpha_1 e^{-f})^2 < 1/4$ respectively. The maximum in the curve $\alpha_1 e^f T^2(1+\alpha_2 e^{-f})^2$ is given by $T = T_1$ at which point it has the value 1/4. Since $F_0(\sqrt{\alpha_1})$ is divergent if $\alpha_1 e^f T^2(1+\alpha_2 e^{-f})^2 > 1/4$ this is a singular point in the T-plane. The curve $\alpha_1 e^f T^2(1+\alpha_2 e^{-f})^2$ decreases for $T \in (T_1, T_0)$ and has another singular point when $T = T_0$ due to the branch point in α_j. This curve is displayed as the top curve in figure 8. The bottom curve in this figure is given by $\alpha_2 e^f T^2(1+\alpha_2 e^{-f})^2$ and is increasing for $T \in [0, T_0]$ and has a singular point for $T = T_0$ due to the branch point in α_j. These results show in particular that $F_0(\sqrt{\alpha_1})$ has a radius of convergence given by $T = T_1$ while $F_0(\sqrt{1/\alpha_1})$ has the radius of convergence given by $T = T_0$.

4. Conclusions

In this paper, I considered two models of directed paths with fixed endpoints pulled by an external force from its middle vertex. These models differ from those in [1] in that the position of the applied force is fixed, rather than averaged over the length of the path.

I computed the generating functions in the first instance of a directed path fixed at its ends and pulled at its middle vertex using a constant term formulation as an example of the method, and then considered a Dyck path with fixed endpoints pulled at its middle vertex. The generating functions of these models are in principle known, and can be computed directly from the expressions in equation (4.156) in [19] or equation (2.1) in [21], or using ballots paths, and in those cases evaluate to series over generalized hypergeometric functions about which apparently little is known. The approach in this paper expressed the generating function of the directed path models in terms of the generating function of Legendre polynomials, and the Dyck path model as a function of complete elliptic integrals and a series over the algebraic roots of a quartic.

The generating function of the Dyck path pulled at its middle vertex was found to have a radius of convergence at an unexpected value of the edge generating variable T, and the reason for this remains unclear—in this context, the identity in equation (67) breaks down at the radius of convergence of the left-hand side, which is not equal to the radius of convergence of the right-hand side. This result indicates that some caution is needed when limiting free energies are determined by considering the radius of convergence of a generating function.

The limiting free energies and force–extension relations in both models were also extracted from generating functions, and in each case were expressed as the logarithms of hyperbolic cosines of the applied forces. The resulting force–extension relations are the expected sigmoid shapes (given in these models partly by the hyperbolic tangent function) also seen for example in [1, 26]. In addition, proofs for the combinatorial identities in equation 4 and theorem 2 were obtained.

The method in this paper is a demonstration that the generating functions of paths pulled at a middle vertex can be obtained by considering two independent paths, and then selecting a constant term. This general approach can be extended to other paths models, including other variations on the point where the force is applied, and even to interacting models of directed paths, or to more general models of interacting directed and partially directed paths. In many of these cases a direct approach may not be otherwise possible. In general, such further generalization to path models pulled at a middle vertex, pose questions of significant difficulty. Determining the generating functions in interacting versions of these models are ongoing and should produce insight into the phase diagram and phase behaviours of adsorbing polymers subject to externally applied forces.

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Appendix. Solving a functional equation

In this section I consider a functional equation of the type

$$H(y) - H(1/y) = (y - 1/y)Y_2(y), \tag{A.1}$$

where $H(y)$ is a power series in y and $Y_2(y)$ is a Laurent series in y given by

$$Y_2(y) = \sum_{j=0}^{\infty} \frac{1}{j+1} \binom{2j}{j} (y + 1/y)^{2j+1} T^{2j+1}. \tag{A.2}$$

The goal is to solve for $H(y)$.

Proceed by noting that for arbitrary fixed N,

$$(y + 1/y)^N = \sum_{k=0}^{N} \binom{N}{k} y^{N-2k}. \tag{A.3}$$

Putting $N = 2j + 1$ and substituting this into equation (A.2) gives the series

$$Y_2(y) = \sum_{j=0}^{\infty}\sum_{k=0}^{2j+1} \frac{1}{j+1}\binom{2j}{j}\binom{2j+1}{k} y^{2j+1-2k}T^{2j+1}. \tag{A.4}$$

Since $H(y)$ is a power series, it follows that $H(y) - H(1/y)$ is a Laurent series without a constant term (it cancels in the subtraction). In other words, one is interested in the positive powers of y in the series for $(y-1/y)Y_2(y)$ in equation (A.4). This will truncate the summation over k at some maximum value.

Next, split the series in equation (A.4) into two parts (over $(y - 1/y)$) to obtain

$$(y - 1/y)Y_2(y) = \sum_{j=0}^{\infty}\sum_{k=0}^{2j+1} \frac{1}{j+1}\binom{2j}{j}\binom{2j+1}{k} y^{2j+2-2k}T^{2j+1} - \sum_{j=0}^{\infty}\sum_{k=0}^{2j+1} \frac{1}{j+1}\binom{2j}{j}\binom{2j+1}{k} y^{2j-2k}T^{2j+1}. \tag{A.5}$$

Observe that positive powers of y are isolated by truncating the first series at $k = j$ and the second series at $k = j - 1$. In these circumstances, the first series is equal to its $k = j$ term plus y^2 times the second series. In other words, $H(y)$ is given, up to an unknown term $f(T)$ independent of y, by

$$H(y) - f(T) = y^2\sum_{j=0}^{\infty} \frac{1}{j+1}\binom{2j}{j}\binom{2j+1}{j} T^{2j+1} + (y^2-1)\sum_{j=1}^{\infty}\sum_{k=0}^{j-1} \frac{1}{j+1}\binom{2j}{j}\binom{2j+1}{k} y^{2j-2k}T^{2j+1}. \tag{A.6}$$

The first series evaluates to a complete elliptic integral of the second kind $E(z)$ defined by

$$E(z) = \int_0^1 \frac{\sqrt{1-z^2x^2}}{\sqrt{1-x^2}}\,\mathrm{d}x, \tag{A.7}$$

so that

$$H(y) = f(T) + \frac{y^2}{T}\left(\frac{1}{4} - \frac{1}{2\pi}E(4T)\right) + T(y^2-1)\sum_{j=1}^{\infty}\sum_{k=0}^{j-1} \frac{1}{j+1}\binom{2j}{j}\binom{2j+1}{k} y^{2j-2k}T^{2j}. \tag{A.8}$$

This completes the proof of equation (33).

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