

Directed paths in a wedge

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Abstract

Models of directed paths have been used extensively in the scientific literature to model linear polymers. In this paper, we examine a directed path model of a linear polymer in a confining geometry (a wedge). We are particularly interested in c_n , the number of directed lattice paths of length n steps which take steps in the North–East and South–East directions and are confined in the wedge $Y = \pm X/p$, where p is an integer. We examine the case $p = 2$ in detail and show that the generating function satisfies a functional equation with quartic kernel. We give a formal solution by using the kernel method, show that this model is not D -finite and determine asymptotics to leading order for c_n . In particular, the number of paths of length n in the wedge $Y = \pm X/2$ is given by

$$c_n = [0.67874\dots] \times 2^n + (4/3^{3/4})^{n+o(n)}$$

where the constant $0.67874\dots$ can be determined to arbitrary accuracy with little computational effort.

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1. Introduction

Lattice paths and lattice walks (such as the self-avoiding walk or undirected lattice trails) have long been used as models of conformational entropy in linear polymers [10, 11]. Perhaps the most famous of these models is the self-avoiding walk [17, 23]. The most fundamental quantity in this model is w_n , the number of self-avoiding walks of length n steps from the origin in the hyper-cubic lattice. It is known that $w_n = \mu^{n+o(n)}$, where μ is the growth constant of the self-avoiding walk, and that the limit $\lim_{n \rightarrow \infty} w_n^{1/n} = \mu$ exists [13]. The self-avoiding

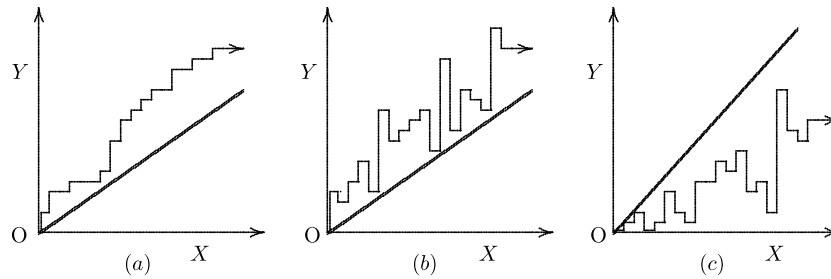


Figure 1. (a) A directed path in the wedge formed by the Y -axis and the line $Y = rX$. (b) A partially directed path in the wedge formed by the Y -axis and the line $Y = rX$. (c) A partially directed path in a wedge formed by a line $Y = rX$ and the X -axis.

walk is a non-Markovian model, and it is generally very difficult to extract its properties by rigorous, or even numerical, means.

Directed paths, in particular models in two dimensions, are generally recurrent models which can often be solved exactly by a renewal type argument. A particular example is the Dyck path which renews itself each time it visits the line $Y = X$ in the square lattice. This property relies on a translational invariance in the model, which can be used directly to solve for the generating function as a root of a quadratic polynomial (see, for example, [9]). This general observation holds for other models, including a model of directed paths above the line $Y = 2X$ [12] and partially directed lattice paths including bar-graph paths [4, 5, 26–28] and other related models such as Motzkin paths [6].

Confining a lattice path to a wedge in the square lattice introduces complexities which often makes the model harder to solve. These models are directed versions of the self-avoiding walk confined in a wedge [14], which in turn is a model of a linear polymer in a confined geometry. A Dyck path is a simple model of a directed path confined in a wedge. In figure 1(a), a more generic directed path in a wedge formed by the Y -axis and the line $Y = rX$ is illustrated (where $r \geq 0$). This model can be solved exactly for $r \in \{0, 1, 2, 3\}$, but no explicit solutions are known for other values of r although the radius of convergence of the generating function is known explicitly for all $r \geq 0$ (see, for example, [7, 8, 16, 18, 20, 21]).

Generally models of the type in figure 1(a) pose challenging combinatorial questions. If the line $Y = rX$ has a rational slope, then the generating function is a root of a polynomial (it is algebraic), and a recurrence can be determined by a renewal type argument; the path renews itself each time it visits the line $Y = rX$. More generally r is irrational, and in these models there is no translational invariances along the line $Y = rX$ and a recurrence for the number of paths seems out of the question. For more on these models see, for example, [1, 7, 8].

The model in figure 1(a) can be generalized by considering a partially directed path above the line $Y = rX$ as illustrated in figure 1(b). A functional equation for the generating function of these model has been written down for some values of r [19], but generally these models pose significant mathematical problems.

A third variant of these models is illustrated in figure 1(c). In this case, a partially directed path is confined in the wedge formed by the X -axis and the line $Y = rX$. A model of this type was proposed and solved in the case that $r = 1$ in [22]. Models of this type are of directed or partially directed paths interacting with two boundaries. Generalized random walks confined in the quarter plane are similarly examples of models of paths in confining geometries interacting with two boundaries [2, 24, 25].

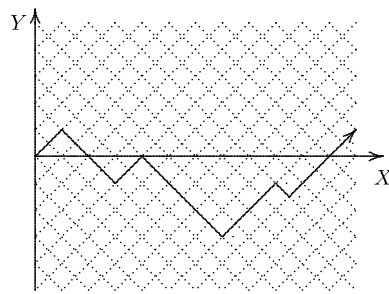


Figure 2. A fully directed path in the square lattice, starting at the origin, and giving steps in the North-East and South-East directions.

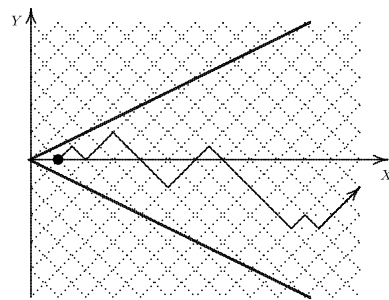


Figure 3. A directed path from the vertex $(2, 0)$ in a symmetric wedge formed by the lines $Y = \pm X/2$.

In this paper, we generalize models of fully directed paths from the origin to a model of paths in a wedge. Consider the directed path in figure 2 in the square lattice which takes steps only in the North-East and South-East directions. The most fundamental quantity in this model is c_n , the number of paths from the origin of length n steps. Obviously, in this model $c_n = 2^n$. This path can be put into a wedge generally as illustrated in figure 3. This is a symmetric wedge (about the X -axis), and is an alternative and more challenging model compared to the cases illustrated in figure 1(a) since the path interacts with two boundaries.

We are primarily interested in a model of directed paths starting from the vertex $(2, 0)$ and confined in the wedge formed by the lines $Y = \pm X/2$. We determine functional equations for the generating function using the kernel method [25], and in particular a variant of this method developed in [3, 22] (the *iterated kernel method*).

The most fundamental quantity in our model is c_n , the number of paths of length n steps and confined in the wedge formed by $Y = \pm X/2$ and starting from the vertex with coordinates $(2, 0)$. We will solve for the generating function of c_n , and our solution will be an alternating series of compositions of a root of a quartic polynomial. This will allow us to determine c_n to high accuracy: in particular, we show that asymptotically,

$$c_n = [0.67874 \dots] \times 2^n + (4/3^{3/4})^{n+o(n)} \quad (1)$$

where the constant 0.67874 can be determined to hundreds of significant digits with minimal computational effort.

In section 2, we define our models and determine functional equations for the generating function. In addition, note that $\lim_{n \rightarrow \infty} c_n^{1/n} = 2$, solve for the generating function using

the kernel method and examine the properties of the roots of the kernel. These results allow us to compute the constant in equation (1) in section 3 by examining the singularities in the generating function. In particular, we show that c_n is to leading order proportional to 2^n ; that is, its increase with n is exponential without a power-law correction. This is in contrast with the number of self-avoiding walks of length n , which is thought to increase to leading order as $An^{-\gamma}\mu^n$, where γ is the entropic exponent and μ is the growth constant (A is a constant). We conclude the paper with some final comments in section 4.

2. Directed paths in a wedge

Let \mathbb{L} be the square lattice of points with integer coordinates in the plane. A directed path in this lattice is a path that takes only North–East (NE) and South–East (SE) steps. If the path consists of n steps (or *edges*), then there are 2^n such paths. One such path is illustrated in figure 2. Let XY be the usual Cartesian coordinate system in figure 2, with the origin at the first vertex of the path. Then the edges in the directed path each have length $\sqrt{2}$.

The directed path in figure 2 is unconstrained by the boundaries of the wedge $Y = \pm X$. This model becomes more interesting if the path is constrained by a narrower wedge $Y = \pm X/p$, where $p \geq 1$ is, in the first instance, an integer. Define the $1/p$ -wedge V_p by

$$V_p = \{(x, y) \in \mathbb{L} \mid \text{where } -x/p \leq y \leq x/p\}. \quad (2)$$

Then V_p is the subset of \mathbb{L} in the first and fourth quadrants bounded by $Y = \pm X/p$. In figure 3, a directed path confined in the wedge V_p is drawn where $p = 2$. This path has its first vertex at the point with coordinates $(2, 0)$. Generally, directed paths in the wedge $Y = \pm X/p$ will have their first vertices at $(p, 0)$.

2.1. Directed paths in the wedge formed by $Y = \pm X/2$

In this section, we determine a functional equation for the generating function G_2 of directed paths giving NE and SE steps from the vertex $(2, 0)$ in the wedge V_2 . Proceed by introducing the edge generating variable t and define

$$G_2(a, b) = \sum_{n, u, v \geq 0} c_n^{(2)}(u, v) a^u b^v t^n \quad (3)$$

where $c_n^{(2)}(u, v)$ is the number of directed paths in the wedge V_2 from the vertex $(2, 0)$ of length n and with the final vertex a vertical distance u from $Y = \lceil X/2 \rceil$ and a vertical distance v from $Y = -\lceil X/2 \rceil$.

Observe that the unit of vertical distance is determined by the fact that the squares in figure 3 have diagonal length 2. For example, a NE step will increase the Y -coordinate of the endpoint by 1, and the distance between the endpoint and $Y = \lceil X/2 \rceil$ may either decrease by 1 if the initial X -coordinate is even, or remain unchanged otherwise.

Consider the examples in figure 4. The vertical distances are measured to the step-functions $Y = \pm \lceil X/2 \rceil$, and in these examples the vertical distances are $u = 11$ and $v = 7$ (figure 4(a)) and $u = 13$ and $v = 7$ (figure 4(b)).

We are fundamentally interested in $c_n^{(2)} = \sum_{u, v \geq 0} c_n^{(2)}(u, v) = G_2(1, 1)$, the number of paths of length n in the wedge V_2 . The generating variables a and b are introduced to account for the vertical distance of the endpoint from the wedge boundaries and to enable us to determine $G_2(1, 1)$.

The examples of paths in figure 4 show that the enumeration of these paths is affected by a parity effect since only the endpoints of paths of length $2 + 4n$ can touch the lines $Y = \pm X/2$,

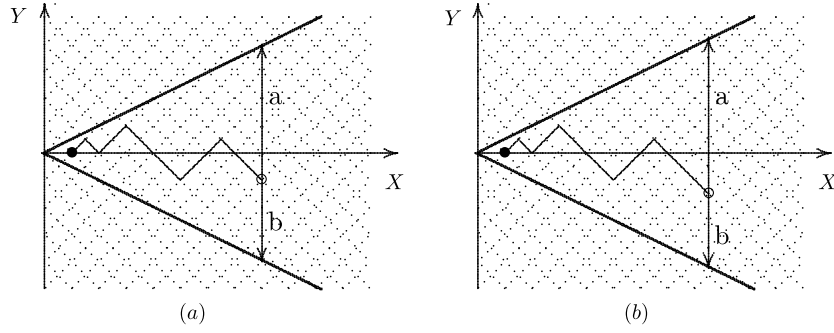


Figure 4. A symmetric wedge formed by the lines $Y = \pm X/2$. The path in (b) is obtained by adding a South-East step to the path in (a).

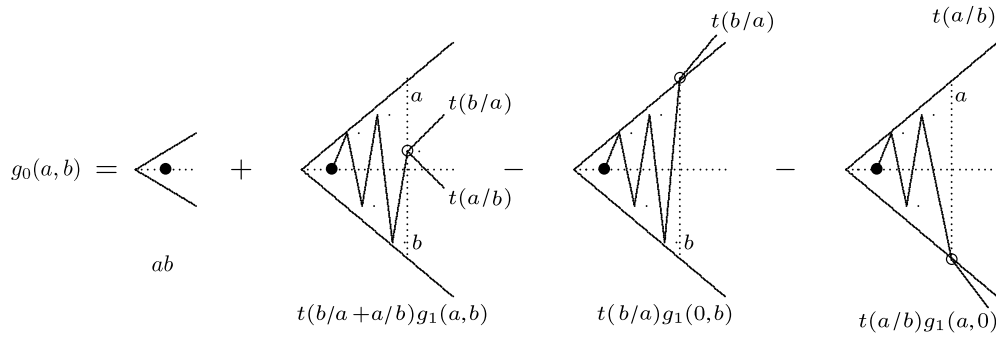


Figure 5. Determining $g_0(a, b)$. Each path generated by $g_0(a, b)$ is either the single vertex at $(2, 0)$ generated by ab , or it is generated by appending a NE -edge onto a path of odd length (this gives the term $(tab)(b/a)g_1(a, b)$), or it is generated by appending a SE -edge onto a path of odd length (giving the term $(tab)(a/b)g_1(a, b)$). Lastly, paths which step outside the wedge must be subtracted: $(tab)(b/a)g_1(0, b)$ if the path steps over the line $Y = X/2$ and $(tab)(a/b)g_1(a, 0)$ if the path steps over the line $Y = -X/2$.

and that paths of odd length are always at least a distance of 1 removed from the step-functions $Y = \pm \lceil X/2 \rceil$.

Let $g_0(a, b)$ be the generating function of paths of even length, and let $g_1(a, b)$ be the generating function of paths of odd length. Then

$$G_2(a, b) = g_0(a, b) + g_1(a, b). \quad (4)$$

Thus, by determining $g_0(a, b)$ and $g_1(a, b)$, we can determine $G_2(a, b)$.

Functional equations for $g_0(a, b)$ and $g_1(a, b)$ can be obtained by arguing as in figures 5 and 6. The basic idea is to create paths counted by $g_1(a, b)$ by appending an edge to paths of even length counted by $g_0(a, b)$, and to create paths counted by $g_0(a, b)$ by appending an edge to paths counted by $g_1(a, b)$. The resulting set of coupled functional equations is

$$\begin{aligned} g_0(a, b) &= ab + t(a/b + b/a)g_1(a, b) - t(a/b)g_1(a, 0) - t(b/a)g_1(0, b), \\ g_1(a, b) &= t(a^2 + b^2)g_0(a, b) - ta^2g_0(a, 0) - tb^2g_0(0, b). \end{aligned} \quad (5)$$

These equations can be iterated to enumerate the directed paths. The numbers for even length paths are given in table 1.

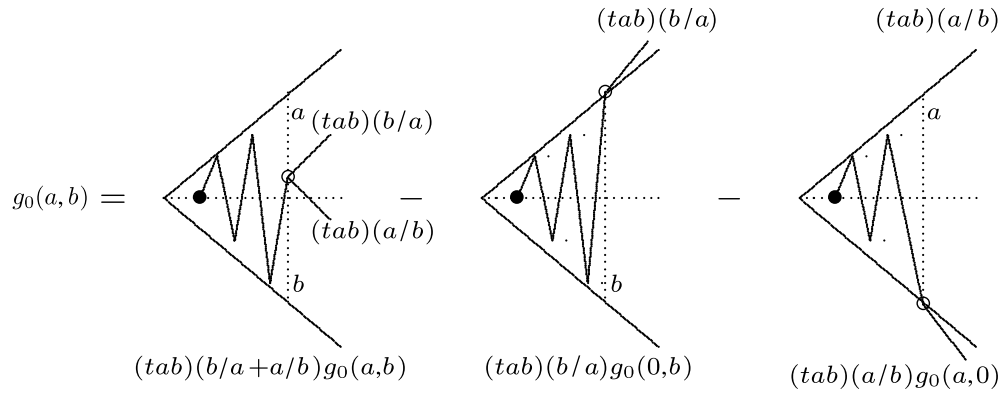


Figure 6. Determining $g_1(a, b)$. Each path generated by $g_1(a, b)$ is obtained by appending a NE -edge or SE -edge onto a path of even length. In this case, the vertical distance to the wedge does not increase by a full step, and thus no new factors of a or b are included, apart from accounting for stepping closer to the top boundary if a NE -edge is added, or stepping closer to the bottom boundary if a SE -edge is added. This generates the term $t(a/b + b/a)g_0(a, b)$ as indicated above. Lastly, paths which step outside the wedge must be subtracted: $t(b/a)g_0(0, b)$ if the path steps over the line $Y = X/2$ and $t(a/b)g_0(a, 0)$ if the path steps over the line $Y = -X/2$.

Table 1. The number of directed paths in V_2 .

n	c_n	n	c_n
0	1	42	2 985 401 474 160
2	4	44	11 941 093 593 120
4	12	46	47 764 374 372 480
6	48	48	191 053 247 884 320
8	180	50	764 212 991 537 280
10	720	52	3 056 816 328 436 200
12	2 820	54	12 227 265 313 744 800
14	11 280	56	48 908 759 609 676 540
16	44 760	58	195 635 038 438 706 160
18	179 040	60	782 537 580 134 560 920
20	713 760	62	3 130 150 320 538 243 680
22	2 855 040	64	12 520 579 171 583 415 840
24	11 403 060	66	50 082 316 686 333 663 360
26	45 612 240	68	200 329 075 631 136 029 040
28	182 321 460	70	801 316 302 524 544 116 160
30	729 285 840	72	3 205 263 549 296 411 867 340
32	2 916 160 800	74	12 821 054 197 185 647 469 360
34	11 664 643 200	76	51 284 202 287 042 290 859 820
36	46 650 808 680	78	205 136 809 148 169 163 439 280
38	186 603 234 720	80	820 547 109 423 871 153 955 280
40	746 350 368 540	82	3 282 188 437 695 484 615 821 120

The number of digits in the c_n in table 1 increases linearly with n , which suggests that c_n grows exponentially. It is in fact possible to prove explicitly that c_n increases proportionally to 2^n , using the techniques in [14]. In addition, since $c_n c_m \leq c_{n+m}$ (concatenate a path of length m with a path of length n by translating the first until its first vertex coincides with the last vertex of the second to see this), c_n is a super-multiplicative function of n , and thus the limit

$$\lim_{n \rightarrow \infty} c_n^{1/n} \quad (6)$$

exists [15] and is equal to 2. Thus, there is a function of n , $C_0 = e^{o(n)}$, such that

$$c_n = C_0 2^n + o(2^n). \quad (7)$$

Examination of the data in table 1 shows that $c_n/2^n$ approaches a constant. Assuming that C_0 is a constant, one may estimate it numerically. Dividing c_n by 2^n and looking at n up to $n = 82$ gives C_0 to five digits, namely

$$C_0 = 0.67874\dots \quad (8)$$

We proceed next by computing C_0 by solving equations (5) by iteration, and by examining the singularities in $g_0(a, b)$.

2.2. Solving equations (5)

In this section, we use the iterated kernel method (see [3, 22]) to find an expression for the generating function $g_0(a, b)$. Simplify the equations by introducing $K = t(a/b + b/a)$ and $L = t(a^2 + b^2)$, and also note that $g_0(a, 0) = g_0(0, a)$, and that $g_1(a, 0) = g_1(0, a)$.

Since paths of odd length generated by $g_1(a, b)$ cannot intersect the boundaries of the wedge, they will be weighted by a factor ab . Hence, one expects $g_1(a, 0) = g_1(0, b) = 0$. Ignoring this last observation for the moment gives the functional equations in slightly simplified form:

$$g_0(a, b) = ab + K g_1(a, b) - t(a/b)g_1(a, 0) - t(b/a)g_1(b, 0), \quad (9)$$

$$g_1(a, b) = L g_0(a, b) - t a^2 g_0(a, 0) - t b^2 g_0(b, 0). \quad (10)$$

Substitute these equations into one another, and write them in kernel form. This gives

$$(1 - KL)g_0(a, b) = ab - t a^2 K g_0(a, 0) - t b^2 K g_0(b, 0) - t(a/b)g_1(a, 0) - t(b/a)g_1(b, 0), \quad (11)$$

$$(1 - KL)g_1(a, b) = Lab - t a^2 g_0(a, 0) - t b^2 g_0(b, 0) - t(a/b)L g_1(a, 0) - t(b/a)L g_1(b, 0). \quad (12)$$

We identify the *kernel* $(1 - KL)$ in these equations. Generally, we say that functional equations are in *kernelized form* if the generating function and its coefficients have been collected on the left-hand side, while all other terms and boundary terms are on the right-hand side. The kernel $(1 - KL)$ may be simplified, and then the quartic polynomial (in a and b)

$$t^2(a^2 + b^2)^2 - ab \quad (13)$$

appears as a factor.

To proceed with, consider this to be a quartic in b with a and t as two parameters. To solve the original functional equations, one must determine the roots of this quartic. Closer examination shows that the four roots of the quartic have the following properties: The first real root is $\beta_0(a)$, which is a power-series in t :

$$\beta_0(a) = a^3 t^2 + 2a^7 t^6 + 9a^{11} t^{10} + 52a^{15} t^{14} + \dots \quad (14)$$

The second real root is $\beta_1(a)$, which is singular at $t = 0$:

$$\beta_1(a) = \frac{a^{1/3}}{t^{2/3}} - \frac{2a^{5/3}t^{2/3}}{3} - \frac{28a^{13/3}t^{10/3}}{81} + \dots \quad (15)$$

while the two remaining roots are a complex conjugate pair:

$$\beta_{\pm}(a) = -\frac{a^{1/3}(1 \mp i\sqrt{3})}{2t^{2/3}} + \frac{a^{5/3}t^{2/3}(1 \pm i\sqrt{3})}{3} - \frac{a^3t^2}{3} + \dots \quad (16)$$

which are also singular at $t = 0$.

Substituting $b = \beta_0(a) \equiv \beta_0$ into the kernelized equations into (11) and (12) produces a system of two linear equations in $g_0(a, 0)$, $g_0(b, 0)$, $g_1(a, 0)$ and $g_1(b, 0)$,

$$K(ta^2g_0(a, 0) + t\beta_0^2g_0(\beta_0, 0)) + (t(a/\beta_0)g_1(a, 0) + t(\beta_0/a)g_1(\beta_0, 0)) = a\beta_0, \quad (17)$$

$$(ta^2g_0(a, 0) + t\beta_0^2g_0(b, 0)) + L(t(a/\beta_0)g_1(a, 0) + t(\beta_0/a)g_1(\beta_0, 0)) = La\beta_0, \quad (18)$$

which may be simplified to give

$$ta^2g_0(a, 0) + t\beta_0^2g_0(\beta_0, 0) = La\beta_0, \quad (19)$$

$$t(a/\beta_0)g_1(a, 0) + t(\beta_0/a)g_1(\beta_0, 0) = 0. \quad (20)$$

It follows from the second of these equations that

$$g_1(\beta_0(a), 0) = -\frac{a^2}{\beta_0^2}g_1(a, 0) \quad (21)$$

and since this generating function cannot be negative, the conclusion is that

$$g_1(a, 0) = 0 \quad (22)$$

identically, as claimed above. The first solution above gives

$$g_0(a, 0) = \frac{L(a, \beta_0)\beta_0}{ta} - \frac{\beta_0^2}{a^2}g_0(\beta_0, 0). \quad (23)$$

Proceed by defining $\beta^{(n)}(a) = (\beta_0 \circ \beta_0 \circ \dots \circ \beta_0)(a)$ to be the composition of β_0 n -times with itself. Define $\beta^{(0)}(a) = a$, then the last equation may be written as

$$g_0(\beta^{(n-1)}, 0) = \frac{L(\beta_0^{(n-1)}, \beta_0^{(n)})\beta_0^{(n)}}{t\beta_0^{(n-1)}} - \left(\frac{\beta_0^{(n)}}{\beta^{(n-1)}}\right)^2 g_0(\beta^{(n)}, 0). \quad (24)$$

This may be iterated to obtain a formal solution for $g_0(a, 0) = g_0(\beta_0^{(0)}, 0)$:

$$g_0(a, 0) = \frac{1}{ta^2} \sum_{n=0}^{\infty} (-1)^n L(\beta_0^{(n)})\beta_0^{(n)}\beta_0^{(n+1)}. \quad (25)$$

Thus, one may solve for the generating function $g_0(a, b)$ from the kernelized equations in (11) and (12):

$$g_0(a, b) = \frac{ab - tK(a^2g_0(a, 0) + b^2g_0(b, 0))}{1 - KL} \quad (26)$$

and the radius of convergence is given by the dominant root of the quartic in equation (13), provided that $g_0(a, 0)$ does not have singularities at the same points.

2.3. More on the roots of $t^2(a^2 + b^2)^2 - ab$

One may check that

$$\beta_0(a) = [2t^2a^3] \sum_{n=0}^{\infty} \binom{4n+1}{n} \frac{(at)^{4n}}{3n+2} \quad (27)$$

as given in equation (14). The radius of convergence of this series is the solution of $|at|^4 = 3^3/4^4$.

Closer examination also shows that $\beta_0(a)$ counts directed paths with first step in the SE-direction, above the line $Y = -X/2$ and with last vertex in the line $Y = -X/2$. The root β_1 is the inverse function of β_0 : direct calculation shows that $\beta_0 \circ \beta_1(a) = \beta_1 \circ \beta_0(a) = a$.

The roots β_+ and β_- are not independent, and one may verify that

$$\beta_+ \left(\frac{ix^3}{8} \right) = -\beta_- \left(\frac{-ix^3}{8} \right) = -\frac{ix}{2t^{2/3}} + \frac{it^{2/3}x^5}{48} + \frac{it^2x^9}{1536} + \frac{7it^{10/3}x^{13}}{165888} + \dots \quad (28)$$

Solving for the roots of the quartic is equivalent to solving the nonlinear system

$$r^2 = (a^2 + b^2), \quad (29)$$

$$t^2r^4 = ab \quad (30)$$

for a and b . There are four solutions, two given by the pairs $(a_1(r), b_1(r))$ and $(-a_1(r), -b_1(r))$, where

$$a_1(r) = \frac{\sqrt{2}r^3t^2}{\sqrt{1 + \sqrt{1 - 4t^4r^4}}} = \frac{r\sqrt{1 - \sqrt{1 - 4t^4r^4}}}{\sqrt{2}}, \quad (31)$$

$$b_1(r) = \frac{r\sqrt{1 + \sqrt{1 - 4t^4r^4}}}{\sqrt{2}} = \frac{\sqrt{2}r^3t^2}{\sqrt{1 - \sqrt{1 - 4t^4r^4}}}, \quad (32)$$

and two more given by the pairs $(b_1(r), a_1(r))$ and $(-b_1(r), -a_1(r))$ (where we interchanged a_1 and b_1). An expression for r^2 is given below in equation (35). One may check as well that

$$a_1(r) = t^2r^3 \left(1 + t^4r^4 \sum_{n=0}^{\infty} \binom{4n+3}{2n} \frac{(tr)^{4n}}{(2n+1)4^{n+1/2}} \right) \quad (33)$$

$$b_1(r) = r \left(1 - t^4r^4 \sum_{n=0}^{\infty} \binom{4n+1}{2n} \frac{(tr)^{4n}}{(2n+2)4^n} \right). \quad (34)$$

The roots of the quartic may be found by inverting a_1 to obtain $r_a(a)$ so that $r_a \circ a_1 = a_1 \circ r_a$ is the identity map. Then $\beta_0(a) = b_1 \circ r_a$. Inverting b_1 to obtain $r_b(b)$ gives a second root by the composition $\beta_1 = a_1 \circ r_b$. In particular, this means for example that $\beta_0 \circ \beta_1 = b_1 \circ (r_a \circ a_1) \circ r_b = b_1 \circ r_b = \text{identity}$ since $a_1^{-1} = r_a$ and $b_1^{-1} = r_b$. This proves the observation above that $\beta_0 \circ \beta_1 = \beta_1 \circ \beta_0$ is the identity map. In other words, the composition of the two real roots of the quartic is the identity.

The other two roots of the quartic are given by the compositions $b_1 \circ r_b$ and $a_1 \circ r_a$. Unfortunately, while explicit expressions for r_a and r_b can be obtained, they are rather lengthy; both r_a^2 and r_b^2 are roots of the quartic $t^4x^4 - c^2x + c^4$ where $c = a$ for r_a and $c = b$ for r_b . This may be examined by iteration to determine the first few terms in r_a^2 . Comparison of the results to the online encyclopedia of integers [29] shows that

$$r_a^2(a) = a^2 \sum_{n=0}^{\infty} \binom{4n}{n} \frac{(at)^{4n}}{3n+1}. \quad (35)$$

The second root of $t^4x^4 - c^2x + c^4$ proposes the ‘unphysical’ series starting with $(a/t^2)^{2/3} + O(a^2)$ for $r_a^2(a)$. The series expression for $r_a^2(a)$ may finally be substituted into $b_1(r)$ to obtain an expression for the root $\beta_0(a)$ of the quartic:

$$\beta_0(a) = \frac{r_a(a)\sqrt{1 + \sqrt{1 - 4t^4r_a^4(a)}}}{\sqrt{2}}. \quad (36)$$

Remarkably, this evaluates to equation (27) and compositions of this with itself will eventually lead to the expression for $g_0(a, 0)$ in equation (25).

In addition, having determined $\beta_0(a)$, one may consider the composition of $a_1(r)$ and $r_a(a)$, which is

$$\frac{r_a(a)\sqrt{1 - \sqrt{1 - 4t^4r_a^4(a)}}}{\sqrt{2}} = a, \quad (37)$$

and which must be the identity map. In other words, by appealing to equation (30) it follows that:

$$a \cdot \beta_0(a) = t^2r_a(a)^4, \quad (38)$$

and from equation (27) one concludes that the identity

$$\left[\sum_{n=0}^{\infty} \binom{4n}{n} \frac{(at)^{4n}}{3n+1} \right]^2 = 2 \sum_{n=0}^{\infty} \binom{4n+1}{n} \frac{(at)^{4n}}{3n+2} \quad (39)$$

should be closely related to the combinatorial properties of directed paths in the wedge V_2 .

3. Determining C_0

In this section, we examine the generating function $g_0(a, b)$ in equation (26) with $a = b = 1$. Singularities in this generating function arise from several possible sources. In the first instance, there are simple poles at the zeros of the kernel $(1 - KL)$ in the denominator. These are located at $t = \pm 1/2$. In order to determine the constant C_0 , we examine the residue of $g_0(1, 1)/t^{n+1}$ at $t = \pm 1/2$.

Put $a = 1$ and $t = 1/2$ in $\beta_0(a)$. Compositions of $\beta_0(a)$ with itself at this point are

$$\begin{aligned} \beta_0^{(0)}(1) &= 1 \\ \beta_0^{(1)}(1) &= 2.955\,977\,425\,220\,847\,7098 \dots \times 10^{-1} \\ \beta_0^{(2)}(1) &= 6.463\,362\,544\,384\,777\,7820 \dots \times 10^{-3} \\ \beta_0^{(3)}(1) &= 6.750\,183\,207\,315\,027\,8963 \dots \times 10^{-8} \\ \beta_0^{(4)}(1) &= 7.689\,297\,945\,739\,216\,5146 \dots \times 10^{-23} \\ \beta_0^{(5)}(1) &= 1.136\,580\,175\,293\,716\,2161 \dots \times 10^{-67} \\ \beta_0^{(6)}(1) &= 3.670\,626\,862\,567\,744\,0729 \dots \times 10^{-202} \end{aligned}$$

where explicitly

$$\beta_0^{(1)}(1) = \beta_0(1) = \frac{5 - \sqrt{33}}{12}(19 + 3\sqrt{33})^{2/3} + \frac{\sqrt{33} - 1}{12}(19 + 3\sqrt{33})^{1/3} - \frac{1}{3},$$

and the other terms are more complicated expressions involving nested radicals which do not simplify to manageable expressions.

Generally, we observe that $\beta_0^{(n)}(1) = \alpha_n$ at $t = 1/2$, and one may check that $\alpha_{n+1} \approx \alpha_n^3/4$. For example, $\alpha_3^3/4 = 7.689\,297\,941 \dots \times 10^{-23} \approx \alpha_4$. This observation follows from the

expansion $\beta_0(a) = a^3 t^2 + O(a^7 t^6)$ so that compositions of β_0 at $t = 1/2$ and $a = 1$ quickly converge to zero. In other words, the recurrence $x_{n+1} = \beta_0(x_n)|_{t=1/2}$ is a fixed point iteration of order 3. This fast convergence allows the accurate numerical estimation of $\beta_0^{(n)}(1)$ at $t = 1/2$.

At $a = b = 1$ the expression of $g_0(1, 1)$ in terms of $g_0(1, 0)$ and $g_0(0, 1)$ is given by

$$g_0(1, 1) = \frac{1 - 2t^2(g_0(1, 0) + g_0(0, 1))}{1 - 4t^2}, \quad (40)$$

where

$$g_0(1, 0) = g_0(0, 1) = \sum_{n=0}^{\infty} (-1)^n L(\beta_0^{(n)}) \beta_0^{(n)} \beta_0^{(n+1)},$$

and where $L(a) = a^2 + \beta_0^2$. Numerical evaluation of the residue at $t = 1/2$ using the calculated values of $\beta_0^{(n)}(1)$ above gives the leading order behaviour of the number of paths of length n

$$c_n = 2^{n-1} \times 0.678\,740\,530\,798\,109\,457\,417\,2327 \dots + \text{parity term} + \dots$$

where the seven values of $\beta_0^{(n)}(1)$ listed above produce C_0 accurately up to at least $O(10^{-401})$ or 400 digits if each is calculated to at least this accuracy by using equations (38) or (27) or by explicitly using the closed-form expression for $\beta_0(a)$ and computing it to high accuracy using a symbolic computations package such as Maple.

To determine the parity effects, we determine the residue at the pole located at $t = -1/2$ by repeating the analysis above. Put $a = 1$ and $t = -1/2$ in $\beta_0(a)$. Compositions of $\beta_0(a)$ with itself at this point give the identical values obtained above for $t = 1/2$. Thus, we conclude that

$$c_n = 2^{n-1} (1 + (-1)^n) \times (0.678\,740\,530\,798\,109\,457\,417\,2327 \dots) + \dots$$

This is not an unexpected result since $g_0(1, 1)$ should only enumerate even length paths; we note that $c_{2n+1} = 0$ in the generating function $g_0(1, 1)$. This result verifies the numerical estimate for C_0 from the data in table 1 in equations (1) and (8). Since n is even, the two contributions to c_n , arising from different poles in $g_0(1, 1)$, may be combined to give

$$c_n = 2^n \times (0.678\,740\,530\,798\,109\,457\,417\,2327 \dots) + \dots$$

for even values of n . This verifies the leading term in the asymptotics claimed in equation (1) for even values of n . We address odd values of n near the end of this section.

Contributions to c_n also arise from singularities in the numerator in equation (26). In particular, there are branch points and possibly other singularities in $g_0(1, 0)$ and $g_0(0, 1)$, and these are due to branch points in β_0 .

The radius of convergence of β_0 can be determined when $a = 1$ by examining equations (35) and (38) with $a = 1$. In particular, $r_1(1)$ in equation (35) is convergent for all $|t| \leq 3^{3/4}/4$; in fact, evaluation shows directly that $r_1(1)$ is convergent for $|t| = 3^{3/4}/4$. Since $3^{3/4}/4 > 1/2$, this proves that the simple poles at $t = \pm 1/2$ are within the radius of convergence of $\beta_0(1)$.

Further examination of $\beta_0(a)$ using a symbolic computations program (Maple 9) shows a complicated expression of nested radicals which explicitly contains factors of the form $\sqrt{81 - 768a^4 t^4}$. This shows that there are branch points at $at = 3^{3/4}\omega/4$ where ω is a fourth root of unity. There may be more branch points on the circle $at = 3^{3/4}/4$, but we did not verify this, and this will not play a crucial role in what follows.

Next, we consider the compositions of β_0 in the alternating sum definition of $g_0(1, 0)$. Since $r_1(t)$ is a positive term power series it follows by the triangle inequality in equation (35) that for (complex) t such that $|t| \leq 3^{3/4}/4$,

$$|r_1^2(1)| \leq \sum_{n=0}^{\infty} \binom{4n}{n} \frac{(3^{3/4}/4)^{4n}}{3n+1} = \frac{4}{3}. \quad (41)$$

Thus, by equation (38)

$$|\beta_0(1)| \leq [3^{3/4}/4]^2(16/9) = \frac{1}{\sqrt{3}}, \quad \text{if } |t| \leq 3^{3/4}/4. \quad (42)$$

Since $\beta_0(a)$ is a power series with positive coefficients in both a and t , $|\beta_0(a)| \leq |\beta_0(1)|$ for any $|t| \leq 3^{3/4}/4$ and $|a| \leq 1$, and by the triangle inequality, $\beta_0(a)$ is a maximum when $t = 3^{3/4}/4$ for a fixed value of a . Thus, for fixed values of $|a| \leq 1$, $\beta_0(a)$ is a maximum on the closed disk $|t| \leq 3^{3/4}/4$ when $t = 3^{3/4}/4$.

The above shows that for $t = 3^{3/4}/4$, $|\beta_0(a)| \leq 1/\sqrt{3}$ for $|a| \leq 1$. Moreover, it follows from equation (27) that $|\beta_0(a)| \leq |a|/\sqrt{3}$ for $|a| \leq 1$ when $t = 3^{3/4}/4$. In other words,

$$|\beta_0(\beta_0(1))| \leq |3^{3/4}/4\sqrt{3}(\sqrt{3} \cdot 3^{3/4}/4)| = \frac{1}{\sqrt{3}^2}. \quad (43)$$

It follows inductively that

$$|\beta_0^{(n)}(1)| \leq \frac{1}{\sqrt{3}^n}. \quad (44)$$

Since the branch points in $\beta_0^{(n)}(1)$ will occur at values of t that $|\beta_0^{(n-1)}(1)| = 3^{3/4}/4$, and $|\beta_0^{(n-1)}(1)| \leq 1/\sqrt{3}^{n-1} < 3^{3/4}/4$ at $a = 1$ and for $n > 2$, this implies that the branch points in $\beta_0^{(n)}(1)$ for $n > 1$ lie outside the circle with radius $|t| = 3^{3/4}/4$, and contributions of these branch points to c_n are dominated by the contributions to c_n which is a result of the branch points in $\beta_0(1)$ itself.

In particular, since the radius of convergence of $\beta_0(a)$ is determined by $|at| = 3^{3/4}/4$ and $|\beta_0^{(n-1)}(1)| \leq 1/\sqrt{3}^{n-1}$, it follows that the radius of convergence of $\beta_0^{(n)}(1)$ in the t -plane is on or outside the circle with radius $|t| = 3^{3/4}\sqrt{3}^{n-1}/4$, for $n > 2$. Thus, the generating function $g_0(a, 0)$ has infinitely many singularities in the t -plane for $a = 1$, and by remark 1 following proposition 9 in [3], $g_0(1, 0)$ cannot be holonomic (or D-finite). Thus, $g_0(1, 1)$, the generating function of even length directed paths in the wedge formed by $Y = \pm X/2$, is not holonomic.

The bound in equation (44) also proves that $g_0(1, 0)$ is an absolutely convergent series on the open disk with radius $|t| = 3\sqrt{3}$ which includes the simple poles of $g_0(1, 1)$ at $t = \pm 1$ and the branch points on the circle $|t| = 3^{3/4}/4$ in its interior. In other words, the asymptotic behaviour of c_n is given by

$$c_n = 2^n \times (0.678\,740\,530\,798\,109\,457\,417\,2327\dots) + \text{corrections}. \quad (45)$$

The corrections are due to the branch points in $\beta_0(1)$ and they grow at the exponential rate $(4/3^{3/4})^{n+o(n)}$. Since $4/3^{3/4} \approx 1.75 < 2$, the effects of the correction terms will disappear fast with increasing n , and $c_n/2^n$ will approach $0.678\,740\,530\,798\,109\,457\,417\,2327\dots$ at an exponential rate with increasing (and even) n . This verifies the sub-leading term in equation (1).

We next turn our attention to odd values of n . Since $g_1(a, 0) = g_1(0, b) = 0$ (see equation (22)), it follows from equation (9) that $g_0(a, b) = ab + Kg_1(a, b)$ with $K = t(a/b + b/a)$. In terms of c_n this implies that $c_{2n} = 2c_{2n-1}$. In other words, the asymptotic expression for c_n for odd values of n is obtained by adding a factor of one half to the expression for c_n in equation (45), and so this expression, with the claimed sub-leading correction, gives the asymptotics for both even and odd values of n . This verifies equation (1) for both even and odd values of n .

4. Narrower wedges

It is possible to consider this problem in the narrower wedge V_p where a and b measure vertical distances to the functions $Y = \pm[X/p]$ and where the path starts at the vertex with coordinates

$(p, 0)$. In this case the paths are counted by a generating function $G_p(a, b) = \sum_{i=0}^{p-1} g_i(a, b)$, where $g_i(a, b)$ generates paths of length $i \bmod p$ and satisfies a set of coupled functional-differential equations:

$$\begin{aligned} g_0 &= ab + t(a/b + b/a)g_{p-1}, \\ g_1 &= t(a^2 + b^2)g_0 - ta^2g_0(a, 0) - tb^2g_0(0, b), \\ g_2 &= t(a/b + b/a)g_1 - ta \left[\frac{\partial g_1}{\partial b} \right]_{b=0} - tb \left[\frac{\partial g_1}{\partial a} \right]_{a=0} \\ g_3 &= t(a/b + b/a)g_2 - ta \left[\frac{\partial g_2}{\partial b} \right]_{b=0} - tb \left[\frac{\partial g_2}{\partial a} \right]_{a=0} \\ &\dots = \dots \\ g_{p-1} &= t(a/b + b/a)g_{p-2} - ta \left[\frac{\partial g_{p-2}}{\partial b} \right]_{b=0} - tb \left[\frac{\partial g_{p-2}}{\partial a} \right]_{a=0}. \end{aligned} \quad (46)$$

Putting $p = 2$ in the above recovers the functional equations in equation (5), if the fact that $g_1(a, 0) = g_1(0, b) = 0$ is used.

Put $a = b = 1$, write $G = \sum_{i=0}^{p-1} g_i$ and rewrite the boundary terms $\Delta g_0(a, 0) = 0$, $\Delta g_1(a, 0) = g_1(a, 0)$ and $\Delta g_i(a, 0) = \left[\frac{\partial g_i}{\partial b} \right]_{b=0}$ for $i = 2, 3, \dots, p-1$ and similarly for $\Delta g_i(0, b)$. Summing the above functional equations then gives

$$G = 1 + 2tG - \sum_{i=0}^{p-1} (\Delta g_i(1, 0) + \Delta g_i(0, 1)). \quad (48)$$

The boundary terms $\sum_{i=0}^{p-1} (\Delta g_i(1, 0) + \Delta g_i(0, 1))$ represent the generating function of paths starting at the point $(p, 0)$ and ending within one step of the lines $Y = \pm X/p$. Such paths of length $2pn$ must contain almost (within a constant) $(p+1)n$ North-East steps. The number of these paths grows at the exponential rate $\lambda^{2p} = ((2p)^{2p}/(p-1)^{p-1}(p+1)^{p+1})^n$. Hence the generating function of these paths is convergent inside the circle of radius $1/\lambda$. One can show that this is strictly greater than $1/2$, thus all the boundary generating functions $\Delta g_i(1, 0)$ and $\Delta g_i(0, 1)$ of paths ending near the boundary of the wedge are convergent on the disk with radius strictly greater than $1/2$.

Thus, rearranging equation (48) to get

$$G = \frac{1 - \sum_{i=0}^{p-1} (\Delta g_i(1, 0) + \Delta g_i(0, 1))}{1 - 2t} \quad (49)$$

the dominant singularity in G is at $t = 1/2$ and is a simple pole. The sub-dominant singularities give terms growing to exponential order $\lambda^{n+o(n)}$ where

$$\lambda = ((2p/(p-1))^{(p-1)/2p} (p+1)^{(p+1)/2p})^n. \quad (50)$$

In other words,

$$c_n^{(p)} = A_p 2^n + \lambda^{n+o(n)}. \quad (51)$$

Putting $p = 2$ produces the leading order term and the order of the next term obtained in equation (45).

5. Conclusions

The main results in this paper are given by equations (1) and (26). We have shown that the model of fully directed paths in the wedge V_2 with starting vertex $(2, 0)$ in figure 3 can be solved formally using the iterated kernel method. This model is the second in a sequence

of models in the wedge V_p with starting vertices $(p, 0)$, for $p \in \{1, 2, 3, \dots\}$. Functional equations for $p > 2$ are given in section 2.4 (when $p = 1$ the model is trivial, and $c_n = 2^n$). We proved that the number of fully directed paths of length n in V_2 increases exponentially at the rate $C_0 2^n$, plus sub-dominant terms which are also exponentials. In addition, we showed that C_0 (the coefficient of the leading order term) can be determined easily to high accuracy.

In the more general wedge V_p it may be shown (using the techniques in [14]) that the number of paths of length n is $c_n^{(p)} = C_0^{(p)} 2^n + \text{lesser terms}$. In this event $C_0^{(p)}$ is known for $p = 1$ ($C_0^{(1)} = 1$) and to high accuracy for $p = 2$ ($C_0^{(2)} = 0.678\,740\dots$). No estimates exist for other values of p , but one should be able to determine these by examining the kernel of the functional equation for the models with $p \geq 3$.

The ‘physical’ root $\beta_0(a)$ of the quartic kernel (see equation (27)) counts directed paths from $(2, 0)$ (see figure 3) above the line $Y = -X/2$ and with last vertex in the line $Y = -X/2$. By reversing the horizontal direction, this is also equal to the number of paths from the origin above the line $Y = X/2$ and with last vertex in the line $Y = X/2$. The generating function in equation (25) is an alternating series of products of compositions of $\beta_0(a)$, suggesting that that $g_0(a, 0)$ is ‘constructed’ by an inclusion–exclusion process of directed paths above the lines $Y = -X/2$ and $Y = X/2$.

These observations suggest that a combinatorial explanation for the generating function $g_0(a, b)$ in equation (26) might be possible in terms of paths ‘bouncing off’ the boundaries of the wedge V_2 ; this is similar to an observation made for partially directed paths confined to a wedge [22]. While we have not been able to find such an explanation, we note that this poses an interesting open question. An explicit explanation along these lines might give clues about the nature of the generating function of models in more general wedges, including the models of directed paths in the wedges V_p for $p > 2$ formed by the lines $Y = \pm X/p$, and also in the half-wedges formed by the X -axis and the lines $Y = X/p$. Such models in half-wedges (or even models in more general asymmetric wedges) will be more difficult to solve, since the symmetric nature of V_2 played a key role in writing down equation (26) and then determining C_0 by examining the singularities in equation (40).

Finally, our models in the wedge V_p map to the well-known problem of random walks with given step-sets in the quarter plane (the first quadrant). These have been studied, for example, in [2, 3, 24]. The models in this paper correspond to models with starting vertex (p, p) and step set $\{(1 - p, p + 1), (p + 1, 1 - p)\}$. For $p = 2$, this produces the generalized knight’s walk model with step set $(-1, 3)$ and $(3, -1)$ [22]. The corresponding functional equation (in the quarter plane) for the generating function in this model has kernel

$$K(a, b) = ab - (a^4 + b^4) \quad (52)$$

as opposed to our equation (13). Analysing the functional equation by examining the roots of this quartic is equivalent to the manipulations in section 2.3. Indeed, the (physical) root of this kernel is given by

$$\beta'_0(a) = \sum_{m=0}^{\infty} \binom{4m}{m} \frac{a^{4m-1}}{3m+1}, \quad (53)$$

and its relation to the roots of the kernel in equation (13) is given in equations (35) and (39), with $t = 1$.

The knight’s walk problem itself (with step set $\{(-1, 2), (2, -1)\}$ and starting vertex $(1, 1)$) was studied in [3], where it was shown that its generating function is not holonomic (or D -finite). This model corresponds to the choice $p = 3$ (but with starting vertex $(2, 0)$ —observe that starting vertex $(3, 0)$ gives a model which has the same generating function).

In general, for arbitrary and rational values of p , the wedge problem maps to a class of quarter plane models. Unfortunately, there appears to be no inherent (mathematical) advantage in formulating the models in either a wedge or a quarter plane version, though parity effects may simplify in one or the other. Kernels of the functional equations in these models will be polynomials of high degree which makes these models difficult to solve explicitly in either formulation. We note that the models of paths in wedges with an irrational value of p are well defined, but they have no natural counterpart in the quarter plane.

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