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Forces in square lattice directed paths in a wedge

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Abstract

A square lattice directed path confined to a wedge with vertex angle α exerts an entropic force F_α on the wedge. We show that this is a repulsive force of magnitude

$$F_\alpha = \begin{cases} \left[\dfrac{1+\cot^2\alpha}{(1+\cot\alpha)^2}\right]\log(\cot\alpha), & \text{if } 0 \leqslant \alpha < \pi/4, \\ 0, & \text{if } \pi/4 \leqslant \alpha \leqslant \pi/2. \end{cases}$$

This force is determined by examining the combinatorial properties of the directed path and by determining the exact entropic contribution to the free energy in the limit as the path length goes to infinite.

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1. Introduction

Linear polymers, and even single linear polymer chains, have rich physical and thermodynamic properties that are the consequences of a phase diagram that includes a wide variety of phases, critical points and critical lines. The phases of a linear polymer are the result of the enthalpic and entropic contributions to its free energy, and the conformational degrees of freedom of the polymer makes, in particular, a large entropic contribution to its free energy. These contributions cannot be ignored and may in some cases make a dominant contribution that determines the properties of the polymer.

Lattice paths, and in particular directed lattice paths and more general objects such as the self-avoiding walk, have traditionally been proposed as an appropriate model for linear polymers [5–7, 16]. Self-avoiding walk models of polymers in confined geometries have also received considerable attention in the literature [9, 14, 15], and the connection of these models to conformal field theories enabled the prediction of exact values for some critical exponents [4, 12]. Directed versions of these models have also been considered (see, for example, [1, 3, 5]).

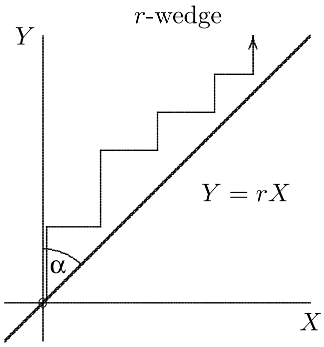

Figure 1. A fully directed path in a wedge formed by the Y-axis and the line $Y = rX$. The angle α is related to r by $\cot\alpha = r$. The path exerts a repulsive entropic force on the lines bounding the wedge if the angle has a rational tangent. If the tangent is not rational, then the line never visits points in the line, but may come arbitrarily close.

In this paper, we are interested in one of the simplest models of a linear polymer in a constrained geometry: a fully directed path confined to a wedge in the square lattice. The polymer should exercise a force on the walls of the wedge [2], and we calculate the force in this model explicitly.

A fully directed path from the origin with steps only in the north (N) and east (E) directions is the simplest directed model of a two-dimensional polymer. By introducing a line $Y = rX$ in the square lattice with a directed path, and excluding steps that would take a path below this line, a model of a directed path confined to a wedge with vertex at the origin is defined by the Y-axis and the line $Y = rX$. The wedge angle α is related to r by $\cot\alpha = r$, see figure 1, and we call the wedge an r-wedge.

Let $c_n^{(r)}$ be the number of directed paths in an r-wedge of length n and which steps from the origin. In this paper we are interested in the generating function $g_r = \sum_{n=0}^{\infty} c_n^{(r)} t^n$, where we surpress the argument t by putting $g_r = g_r(t)$. In some cases g_r is exactly known. For example, if $r = 1$, then it is not hard to demonstrate that

$$g_1 = \frac{1 - 2t - \sqrt{1 - 4t^2}}{2t(2t - 1)} \tag{1}$$

and it is trivial to see that if $r = 0$, then $g_0 = 1/(1 - 2t)$.

In this paper we show that the radius of convergence of the generating function g_r is given by

$$t_r = \begin{cases} \dfrac{1}{2}, & \text{if } 0 \leqslant r \leqslant 1, \\ \dfrac{r^{r/(1+r)}}{1+r}, & \text{if } r > 1, \end{cases} \tag{2}$$

and both the cases, $r = 0$ or $r = 1$, have critical value of t equal to $1/2$. The expression for t_r is of particular interest since the free energy per vertex of the (infinite length) path can be computed from t_r. One finds that

$$\mathcal{F}_r = -\log t_r = \log(1 + r) - \frac{r \log r}{1 + r} \tag{3}$$

explicitly as a function of r. The derivative of the $\mathcal{F}_r$ gives the entropic 'spring' force of the path as the wedge is squeezed by increasing r. In particular, it would be of interest to express $\mathcal{F}_r$ as a function of α, and to examine the force as a function of α.

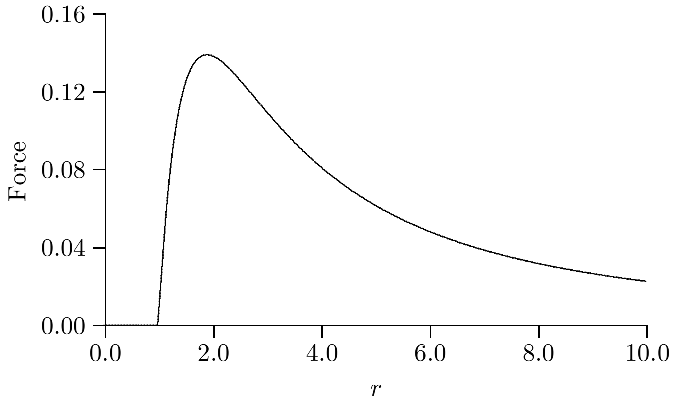

Figure 2. The magnitude of the entropic force on line $Y = rX$ in the vertical direction.

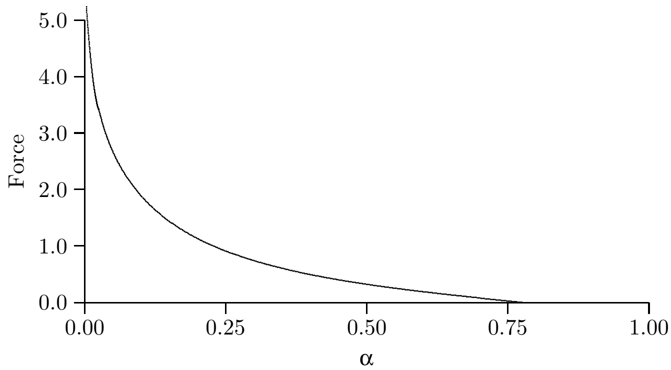

Figure 3. The magnitude of the force as a function of the wedge angle α.

We show that in this model, the magnitude of the repulsive force is given as a function of r by

$$F_r = \begin{cases} 0, & \text{if } 0 \leqslant r < 1, \\ \dfrac{\log r}{(1+r)^2}, & \text{if } r \geqslant 1. \end{cases} \tag{4}$$

F_r is maximum when $r = 2.093\,49\ldots$. This value is obtained by solving for the maximum in F_r using Maple 9; the solution is $\log r = 1/2 + W(1/\sqrt{4e})$ where W is the Lambert-W function. This value of r corresponds to the angle $\alpha = 0.445\,624\,612\ldots$, and note that $\pi/7 = 0.448\,798\,950\ldots$. Thus, the force (in the r-direction) is nearly a maximum if $\alpha = \pi/7$ (see figure 2).

In terms of the wedge angle the force becomes

$$F_\alpha = \begin{cases} \left[\dfrac{1+\cot^2\alpha}{(1+\cot\alpha)^2}\right]\log(\cot\alpha), & \text{if } 0 \leqslant \alpha < \pi/4, \\ 0, & \text{if } \alpha \geqslant \pi/4. \end{cases} \tag{5}$$

In other words, the repulsive force decreases with increasing wedge angle until it reaches zero strength at $\alpha = \pi/4$. Thereafter, the path exerts no force on the line (see figure 3).

Since these forces are conservative, one may compute the work performed as a function of the wedge angle. Direct integration of (5) or (4) shows that the amount of work is $\sqrt{2}$ units to close the angle from any angle larger than $\pi/4$ to zero.

These results are in contrast to a model of self-avoiding walks in a wedge. Let $c_n^{(\alpha)}$ be the number of self-avoiding walks from the origin of length n, and confined to the wedge in the square lattice with vertex angle α, and bounded by the Y-axis and the line $Y = [\cot(\alpha)]X$. Then it is known for any angle $\alpha \in (0, 2\pi]$ that

$$\lim_{n\to\infty} \left[c_n^{(\alpha)}\right]^{1/n} = \mu_2, \tag{6}$$

and where $\mu_2 = 2.6381\ldots$ is the growth constant of self-avoiding walks in the square lattice [8, 13, 14]. Thus, the free energy is independent of α, and there is no net entropic force acting on the wedge as it is closed in the limit of very long walks. This implies that the wedge can be forced to arbitrarily small values of the angle α (in fact, one may take $\alpha \to 0^+$) without performing any work.

In section 2 we briefly review Dyck paths. In section 3 we extend our results to paths in an r-wedge by applying a basic result from recursive iterations to our model, and we show that the radius of convergence in this model is indeed given by equation (2). The paper is concluded by some final comments in section 4.

2. Dyck paths

A Dyck path is a fully directed path from the origin in a 1-wedge and is constrained to have its final vertex in the main diagonal $Y = X$ (see figure 4). Dyck paths are enumerated by Catalan numbers; if C_{2n} is the number of Dyck paths of length $2n$ from the origin to the point (n, n) on the main diagonal, then

$$C_{2n} = \frac{1}{n+1}\binom{2n}{n}. \tag{7}$$

The generating function of Dyck paths is known to be

$$g_1(t) = \frac{1-\sqrt{1-4t^2}}{2t^2} = \frac{2}{1+\sqrt{1-4t^2}}. \tag{8}$$

The generating function of Dyck paths can be determined from a functional recursion for $g_1(t)$: consider figure 4, and note that every Dyck path is either the empty path (a single vertex at the origin), or is composed of a Dyck path returning for the first time to a vertex v in the main diagonal and which is then followed by an arbitrary Dyck path. The first part of this path is a Dyck path, but with endpoints in the superdiagonal $Y = X + 1$, and with two extra edges appended to its endpoints to join it to the origin and to the vertex at v. This is generated by $t^2 g_1(t)$, and is also known as an excursion or as a primitive Dyck path. In terms of $g_1(t)$, this shows that

$$g_1(t) = 1 + [t^2 g_1(t)] \cdot g_1(t) = 1 + [t g_1(t)]^2 \tag{9}$$

and by solving this quadratic for $g_1(t)$, equation (8) is obtained; for more details and numerous references to other results and sources, see [10].

3. q/p-Dyck paths

A functional recurrence can be found for the generating function of directed paths from the origin above or on the line $Y = (q/p)X$, and with endpoint with coordinates of the type

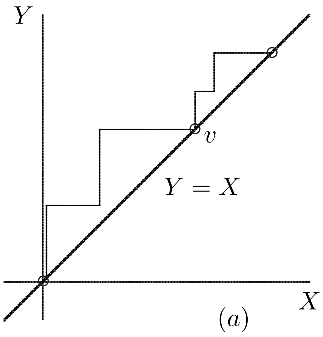

Figure 4. A Dyck path. Such a path has a first return (v) to the main diagonal. Thereafter it may be either empty, or it may continue as an arbitrary Dyck path.

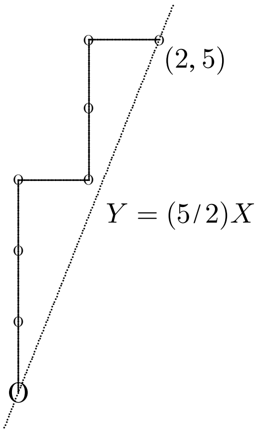

Figure 5. An example of a q/p-Dyck path. In this case a 5/2-Dyck path is illustrated, and its length is a multiple of 7.

(Np, Nq). An example of such a path is in figure 5, where $p = 2$, $q = 5$ and $N = 1$. Observe that the length of such a path is always a multiple of $(p+q)$, and that the fraction of horizontal edges is $p/(p+q)$. These paths are called q/p-Dyck paths.

Define the number $E_{q/p}$ of q/p-Dyck paths of length $(p+q)$. Thus, paths counted by $E_{q/p}$ are q/p-Dyck paths from the origin and ending in the vertex with coordinates (p, q). These paths are all those q/p-Dyck paths of minimal positive length. The path in figure 5 is a 5/2-Dyck path of length $(2+5) = 7$, and is counted by $E_{5/2}$.

Consider the sequence (p_n, q_n) of pairs of positive and relative prime integers, and suppose that

$$\lim_{n\to\infty} \frac{q_n}{p_n} = r \tag{10}$$

where r is a non-negative real number. Then one is interested in the number E_{q_n/p_n}. The following theorem can be found in [11].

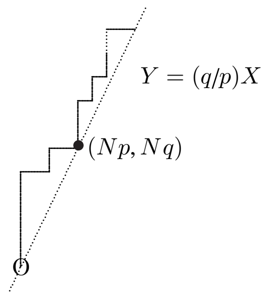

Figure 6. A q/p-Dyck path has a first return • to the line $Y = (q/p)X$, and may continue after this return as an arbitrary q/p-Dyck path. The path between the origin and the first return is a p/q-excursion or a primitive path. Every p/q-Dyck path is either the path composed of one vertex, or is a q/p-excursion followed by an arbitrary q/p-Dyck path. This observation gives a functional recurrence for the generating function $g_{q/p}(t)$ of q/p-Dyck paths.

Theorem 3.1. *Suppose that (p_n, q_n) are pairs of positive and relative prime integers, and that the ratios $q_n/p_n \to r$, where r is a non-negative real number. Then the sequence $\langle E_{q_n/p_n}^{1/(p_n+q_n)} \rangle$ has a limit, and moreover,*

$$\lim_{n\to\infty} E_{q_n/p_n}^{1/(p_n+q_n)} = \frac{1+r}{r^{r/(1+r)}}.$$

4. A recurrence for $g_{q/p}$

Fix (p, q) relative prime to one another, and consider q/p-Dyck paths. We call a q/p-Dyck path with only two vertices in the line $Y = (q/p)X$ a q/p-excursion.

Observe that each q/p-Dyck path has a first return to the line $Y = (q/p)X$, and after that, it either terminates, or it continues as an arbitrary q/p-Dyck path. This can be understood by considering, for example, figure 6. On its first return to the line $Y = (q/p)X$ the path may continue until it terminates in a final vertex. The initial part of the path, until the first return, is a q/p-excursion. This observation shows that each q/p-Dyck path is either the empty path, or is a q/p-excursion followed by an arbitrary q/p-Dyck path. In other words, if the generating function of q/p-Dyck paths is $g_{q/p}$ and $e_{q/p}$ is the generating function of q/p-excursions, then

$$g_{q/p} = 1 + e_{q/p} g_{q/p}. \tag{11}$$

The generating function for excursions is not generally known, but one can show that the recurrence

$$g_{q/p} = 1 + E_{q/p}[t g_{q/p}]^{p+q} \tag{12}$$

generates a subclass of q/p-Dyck paths. On the other hand, the recurrence

$$g_{q/p} = 1 + \binom{p+q}{q} [t g_{q/p}]^{p+q} \tag{13}$$

generates a class of objects that includes all q/p-Dyck paths. Following the arguments in [11], one may instead consider a recurrence of the kind

$$g_{q/p} = 1 + F_{q/p}[t g_{q/p}]^{p+q} \tag{14}$$

where $F_{q/p}$ is a constant and is bounded by

$$E_{q/p} \leqslant F_{q/p} \leqslant \binom{p+q}{q}. \tag{15}$$

Consider therefore the recurrence in equation (14). The radius of convergence $t_{q/p}$ of $g_{q/p}$ may be found from recurrence (14) by considering the following iterations, both derived from it. Fix t and choose $g_{q/p}[0]$ as an initial guess of $g_{q/p}$. Solve for $g_{q/p}$ from equation (14) in two ways to set up the iterative schemes

$$g_{q/p}[N+1] = F_{q/p}[tg_{q/p}[N]]^{p+q} + 1, \qquad \text{for} \quad N = 1, 2, 3, \ldots, \text{ given } g_{q/p}[0], \tag{16}$$

and

$$g_{q/p}[N+1] = \frac{1}{t}[(g_{q/p}[N] - 1)/F_{q/p}]^{1/(p+q)}, \qquad \text{for} \quad N = 1, 2, 3, \ldots, \text{ given } g_{q/p}[0]. \tag{17}$$

These recurrences may be written in simplified fashion by defining the functions

$$f_-(x) = F_{q/p}(xt)^{p+q} + 1, \qquad \text{and} \qquad f_+(x) = \frac{1}{t}\left(\frac{x-1}{F_{q/p}}\right)^{1/(p+q)}, \tag{18}$$

in which case the recurrences are $g_{q/p}[N+1] = f_\pm(g_{q/p}[N])$ for $N = 1, 2, 3, \ldots$ for given $g_{q/p}[0]$ and fixed values of $t \in (0, \infty)$.

Observe that the recurrence $g_{q/p}[N+1] = f_-(g_{q/p}[N])$ generates a power series in t, and we expect it to be convergent if $t < t_{q/p}$, where $t_{q/p}$ is the radius of convergence of the generating function $g_{q/p}$. On the other hand, the recurrence $g_{q/p}[N+1] = f_+(g_{q/p}[N])$ generates a power series in $1/t$, and so it should be convergent for values of $t > t_{q/p}$. When these recurrences are convergent for a given choice of t, then one may suppose that there are fixed points $g^-_{q/p}$ and $g^+_{q/p}$ respectively:

$$g^-_{q/p} = f_-(g^-_{q/p}), \qquad \text{and} \qquad g^+_{q/p} = f_+(g^+_{q/p}). \tag{19}$$

By the fixed-point theorem, the recurrences will converge to fixed points if for both f_- and f_+, it is the case that

$$\left|\frac{\mathrm{d}f_\pm}{\mathrm{d}g}\right|_{g=g^\pm_{q/p}} < 1, \tag{20}$$

and for appropriate choices of the initial guess $g_{q/p}[0]$. This implies certain conditions on the choice of t in the recurrences; in particular, it shows that for f_-,

$$t^{p+q} < \frac{1}{F_{q/p}(p+q)[g^-_{q/p}]^{p+q-1}}, \tag{21}$$

and for f_+,

$$t^{p+q} > \frac{1}{F_{q/p}(p+q)^{p+q}\left[g^+_{q/p} - 1\right]^{p+q-1}}. \tag{22}$$

These bounds on t give critical values for t in each of the two recurrences. We plot a representative critical value for the case $p = 2$ and $q = 3$ in figure 7 against g. Curve B corresponds to the critical value of t in equation (21); for values of t in the region below this curve the recurrence $g_{q/p}[N+1] = f_-(g_{q/p}[N])$ will converge. Curve A corresponds to the critical value of t in equation (22). Values of t above this curve will give convergence in the recurrence $g_{q/p}[N+1] = f_+(g_{q/p}[N])$.

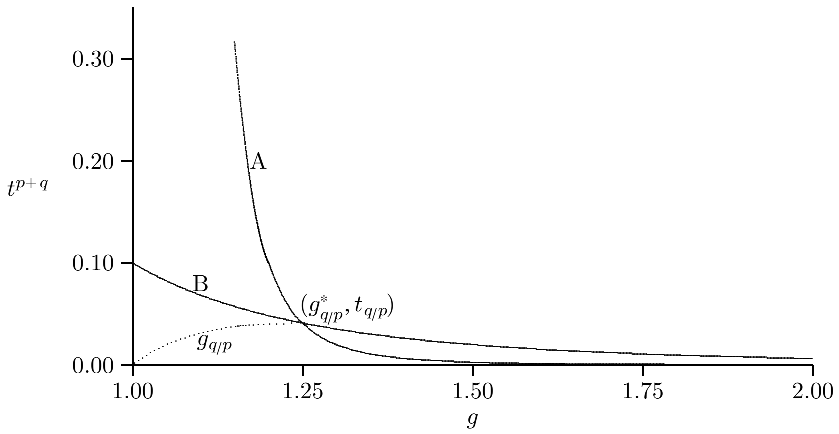

Figure 7. The curves $1/[F_{q/p}(p+q)g^{p+q-1}]$ and $1/[F_{q/p}(p+q)^{p+q}(g-1)^{p+q-1}]$ plotted against g (see equations (21) and (22)) where we chose $p = 2$ and $q = 3$ while $F_{3/2}$ was taken to be equal to 2. The recurrence $g_{N+1} = f_-(g_N)$ is convergent if the value of t^{p+q} is below the curve marked by B; the dotted curve is the numerical solution of the recurrence $g_{N+1} = f_-(g_N)$—with increasing t; this curve converges on the critical point at $(g^*_{q/p}, t_{q/p})$. The recurrence $g_{N+1} = f_+(g_N)$ is convergent in the region above the curve marked by A. If $t = t_{q/p}$, then both recurrences have the same fixed point $g = g^*_{q/p}$; this can be checked by substituting $t_{q/p}$ and $g^*_{q/p}$ into equation (14). Since the recurrence $g_{N+1} = f_-(g_N)$ generates a power series for $g_{p/q}$ in t, and it is divergent if $g = g^*$ and $t > t_{q/p}$, we deduce that the radius of convergence of $g_{p/q}$ is $t_{q/p}$.

The intersection of the two critical curves in figure 7 gives the point (g^*, t^*) as a potential fixed point for the functional recurrence in equation (14). Solving directly for $g^*_{q/p}$ in

$$t_{q/p}^{p+q} = \frac{1}{F_{q/p}(p+q)[g^*_{q/p}]^{p+q-1}} = \frac{1}{F_{q/p}(p+q)^{p+q}[g^*_{q/p}-1]^{p+q-1}} \tag{23}$$

gives the result that

$$g^*_{q/p} = \frac{p+q}{p+q-1}. \tag{24}$$

One may then determine the corresponding value for $t_{q/p}$:

$$t_{q/p}^{p+q} = \frac{(p+q-1)^{p+q-1}}{F_{q/p}(p+q)^{p+q}}. \tag{25}$$

Direct substitution of $(g^*_{q/p}, t_{q/p})$ into the functional recurrence (14) proves that for $t = t_{q/p}$, the fixed point is indeed $g^*_{q/p}$ as given in equation (24). Since $g = g^*_{q/p}$ is the fixed point when t is in the critical curve in equation (21), we conclude that $t_{q/p}$ is the radius of convergencex of $g_{q/p}$.

This gives the following lemma.

Lemma 4.1. *Consider the generating function $g_{q/p}$ of paths generated by the functional recurrence*

$$g_{q/p} = 1 + F_{q/p}[tg_{q/p}]^{p+q}.$$

Then the radius of convergence of $g_{q/p}$ is

$$t_{q/p} = \frac{(p+q-1)^{(p+q-1)/(p+q)}}{F_{q/p}^{1/(p+q)}(p+q)}$$

and moreover, $g^*_{q/p} = g_{q/p}(t_{q/p}) = (p+q)/(p+q-1)$.

The important fact in this lemma is that $g^*_{p/q}$ is independent of $F_{q/p}$, and since $F_{q/p}$ is bounded as in equation (15), there is also a bound on the critical value $t_{q/p}$.

5. Directed paths in an *r*-wedge

The results in the last two sections can now be used to examine directed paths in an r-wedge. Let r be an irrational number and suppose that $\langle (p_n, q_n) \rangle$ is a sequence of positive and relative prime integers such that both $q_n/p_n > r$ and $\lim_{n\to\infty} q_n/p_n = r$.

Let $c_n^{(r)}$ be the number of fully directed paths from the origin confined to the r-wedge of length n, and define the generating function

$$g_r = \sum_{n=0}^{\infty} c_n^{(r)} t^n. \tag{26}$$

Clearly, $g_{q_n/p_n} \leqslant g_r$ since $q_n/p_n > r$. Thus, the radius of convergence of g_r is less than or equal to t_{q_n/p_n}; in other words $t_r \leqslant t_{q_n/p_n}$ for each value of n. Observe that $t_r \geqslant 1/2$ for any r, since the number of directed paths grows as 2^n.

On the other hand, each path counted by $c_n^{(r)}$ has at most $\lceil n/(1+r) \rceil$ horizontal edges. Hence

$$c_n^{(r)} \leqslant \sum_{m=0}^{\lceil \frac{n}{1+r} \rceil} \binom{n}{m}. \tag{27}$$

Take the $1/n$-power of this and let $n \to \infty$. This shows that

$$\lim_{n\to\infty} \left[c_n^{(r)}\right]^{1/n} \leqslant \begin{cases} 2, & \text{if } r \leqslant 1, \\ \dfrac{1+r}{r^{r/(1+r)}}, & \text{if } r > 1. \end{cases} \tag{28}$$

This shows that $t_r \geqslant 1/2$ if $r \in [0, 1]$, and $t_r \geqslant r^{r/(1+r)}/(1+r)$ if $r > 1$. These arguments give the theorem.

Theorem 5.1. *Let $r \geqslant 0$ be a real number. The radius of convergence of the generating function g_r of fully directed paths in an r-wedge is*

$$t_r = \begin{cases} \dfrac{1}{2}, & \text{if } r \leqslant 1, \\ \dfrac{r^{r/1+r}}{1+r}, & \text{if } r > 1. \end{cases}$$

Proof. Observe that t_r is increasing with r. Since $g_1 = \sum_{n\geqslant 0} c_n^{(1)} t^n$ is given in equation (1), one may directly check that $t_1 = 1/2$. Since $t_r \geqslant 1/2$, the result is that $t_r = 1/2$ for all $r \in [0, 1]$.

Let $r > 1$ now be an irrational number and suppose that $\langle (p_n, q_n) \rangle$ is a sequence of positive and relative prime integers such that both $q_n/p_n > r$ and $\lim_{n\to\infty} q_n/p_n = r$. We argued that $t_r \leqslant t_{q_n/p_n}$, and by lemma 4.1,

$$t_r \leqslant t_{q_n/p_n} = \frac{(p_n + q_n - 1)^{(p_n+q_n-1)/(p_n+q_n)}}{F_{q_n/p_n}^{1/(p_n+q_n)} (p_n + q_n)},$$

provided that F_{q_n/p_n} is chosen equal to its lower bound in equation (15).

Take $n \to \infty$, and use the result in theorem 3.1 and in equation (15) to compute the limit of $F_{q_n/p_n}^{1/(p_n+q_n)}$. This gives

$$t_r \leqslant \frac{r^{r/(1+r)}}{1+r}$$

for any irrational $r > 0$. On the other hand, by equation (28) the opposite inequality is also valid if $r > 1$.

These arguments fix the value of t_r if $r > 0$ is irrational. Thus, t_r may be extended to a measurable function defined on real numbers. The result is a continuous and differentiable function. This proves the theorem. □

This theorem proves the claim in equation (2).

6. Conclusions

In this paper we have considered the generating function of fully directed paths in an r-wedge. We were particularly interested in the entropic force of the path on the wedge walls. We determined an explicit formula for the magnitude of the force and plot it in figures 1 and 2. It is interesting to note that the resultant force is zero whenever the wedge angle is larger than $\pi/4$.

Forces in fully directed paths in confined geometries have also been determined by Brak *et al* [2]. The net entropic force of a fully directed path confined to a strip of width w is given by

$$F_w^s = \frac{\pi \tan(\pi/(w+2))}{(w+2)^2} \tag{29}$$

and it falls off as an inverse cube of w as $w \to \infty$: $F_w^s = \pi^2/w^3 + O(w^{-4})$ for large w. In a wedge with wedge angle α, the behaviour of F_α in equation (5) is also of interest as $\alpha \to 0^+$. Examination of our results show that the magnitude of the force diverges logarithmically with α as $\alpha \to 0$:

$$F_\alpha = -\log\alpha + \alpha\log\alpha^2 + O(\alpha^2\log\alpha), \qquad \text{as } \alpha \to 0^+. \tag{30}$$

Similar results have been obtained for Motzkin paths and partially directed paths in a wedge, and results will be presented in a future publication.

Acknowledgment

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