Random Walks in Octants, and Related Structures

Heinrich Niederhausen
Florida Atlantic University, Boca Raton
Niederhausen@math.fau.edu

March 18, 2003

Abstract

A diffusion walk in $\mathbb{Z}^2$ is a (random) walk with unit step vectors $\rightarrow$, $\uparrow$, $\leftarrow$, and $\downarrow$. Particles from different sources with opposite charges cancel each other when they meet in the lattice. This cancellation principle is applied to enumerate diffusion walks in shifted half-planes, quadrants, and octants (a 3-D version is also considered). Summing over time we calculate expected numbers of visits and first passage probabilities. Comparing those quantities to analytically obtained expressions leads to interesting identities, many of them involving integrals over products of Chebyshev polynomials of the first and second kind. We also explore what the expected number of visits means when the diffusion in an octant is bijectively mapped onto other combinatorial structures, like pairs of non-intersecting Dyck paths, vicious walkers, bicolored Motzkin paths, staircase polygons in the second octant, and $\{\rightarrow\uparrow\}$-paths confined to the third hexadecant enumerated by left turns.

Keywords: Random walks, lattice path enumeration, first passage.

AMS subject classification: Primary 60J15, Secondary 05A15, 05A19

1 Introduction

There are many applications and therefore many names for random walks in the square integer lattice $\mathbb{Z}^2$ with unit step vectors $\rightarrow$, $\uparrow$, $\leftarrow$, and $\downarrow$; we will call them diffusion walks because of the fruitful physical interpretation of the walkers as particles spreading out from a source and being able to interact with particles coming from other sources. We find this "cancellation principle" of particles of opposite charges a better model for enumeration than the frequently applied "reflection principle". For example, let us start *two* diffusion processes at the same time, one from the source $\oplus$ at the origin, and a negatively charged synchronous diffusion from the source $\ominus$ at the "mirror" location $(-2l, 0)$, where l is a positive integer. The diagrams in Table 1 show the location of the sources and the number of ways a particle can reach a lattice point after $k = 1, 2, 3$ steps. The walks from the (virtual) negative source are counted as negative numbers; they annihilate the walks from the positive source when reaching the boundary line $x = -l$. Thus the boundary is absorbing, and no particle that visits a point to the right of it has ever been to the boundary.

			$x = -l$		$x = 0$	
			■		⋮	
	-1		■		1	
-1	⊖	-1	■	1	⊕	1
	-1		■		1	
			■		⋮	
			■		⋮	
$k = 1$						

				$x = -l$		$x = 0$		
		-1		■		1		
	-2		-2	■	2	⋮	2	
-1	⋯	-4	⋯	0	⋯	4	⋯	1
	-2		-2	■	2	⋮	2	
		-1		■		1		
				■		⋮		
$k = 2$								

	-1		■		1	
-3		-3	■	3	⋮	3
	-9		0		9	
-9	⊖	-8	■	8	⊕	9
	-9		0		9	
-3		-3	■	3	⋮	3
	-1		■		1	
$k = 3$						

Table 1: Diffusion right of $x = -r$

Only eight such sources, four positive and four negative, are needed to keep the diffusion inside a shifted octant, to the right of $x = -l$ and strictly above $y = x - d$ (see Fig. 2). This will explain why the expression for the number of such diffusion walks from the origin to (n, m) in $m + n + 2k$ steps in the second octant (when $l = d = 1$) is so simple,

$$\frac{(n+1)(2+m)(m+3+n)(m+1-n)}{6(n+k+1)}\binom{n+m+2k+2}{n+k}\binom{n+m+2k}{k}\Big/\binom{n+m+k+3}{3}.$$

To show how the complexity increases if the cancellation principle is applied in three dimensions, we solve a generalization of the above problem, the enumeration of 3-D diagonal diffusion with eight step vectors $(\pm1, \pm1, \pm1)$ when the walks stay in the cone $z \geq y \geq x \geq 0$. Instead of 8 we need 48 sources; the formula is given in Subsection 2.3.1, equation (12). A special case of that formula is the number of walks returning to the origin in $2k$ steps,

$$20C_kC_{k+1}C_{k+2}\Big/\left(\binom{k+5}{3}\binom{k+4}{3}\right) \qquad (1)$$

where C_k stands for the k-th Catalan numbers.

There are several statistics on walks in octants that lead to combinations of Catalan numbers, like $C_{\lfloor (k+1)/2\rfloor}C_{\lfloor 1+k/2\rfloor}$ in (8), the related C_kC_{k+1} in (10)), and $C_kC_{k+2} - C_{k+1}^2$ in (11). Thus diffusion in an octant is only one of several visualizations of the same (unnamed) underlying combinatorial structure; they all deserve attention, but we will mention only a few in Section 4 on related structures,

- pairs (and triples) of non-intersecting Dyck paths (and three vicious walkers),
- bicolored Motzkin paths,
- staircase polygons in the (augmented) second octant, and
- $\{\rightarrow\uparrow\}$-paths in the (augmented) third hexadecant enumerated by left turns

(omitting Young tableaux [13], and skew Ferrer's diagrams [6]).

The physical approach (diffusion of particles) has a long history; a wealth of results can be found in *Random paths in two and three dimensions* by McCrea and Whipple [23, 1940]. Via the expected number $\mathrm{E}(n,m)$ of visits to (n,m) they found numerous first passage probabilities for random walks in a rectangle by solving the difference equation $\mathrm{E}(n,m) = \frac{1}{4}(\mathrm{E}(n-1,m) + \mathrm{E}(n+1,m) + \mathrm{E}(n,m-1) + \mathrm{E}(n,m+1))$. The cancellation principle provides easy proofs of (hence) easy problems, using the enumeration of diffusion walks (with a given number of steps) in a half-plane as a building block for more restricted regions like quarter planes, octants, infinite strips, cylinders, rectangles and triangles, passing through formulae with increasing complexity. On the other hand, the analytic method of McCrea and Whipple starts for uniqueness sake with the diffusion in a bounded region like a rectangle, thus begins with the highest level of complexity, simplifying when parts of the boundary are removed. In Section 3 we let the two approaches meet, generating interesting identities. Here are a few examples:

$$\begin{aligned} & 4^{-m-l}\binom{m+l-1}{m}\,{}_4F_3\left[\begin{matrix}\frac{m+l+2}{2},\frac{m+l+1}{2},\frac{m+l+1}{2},\frac{m+l}{2};\\ m+l+1,l+1,m+1\end{matrix}\;1\right] \qquad (2)\\ =\; & \frac{l}{\pi(m+l)}\int_0^\pi \cos((m-l)\theta)\cot^{l+m}\left(\frac{\pi+2\theta}{4}\right)d\theta \\ =\; & \frac{1}{2\pi}\int_0^\pi \cot^{m+l}\left(\frac{\pi+2\theta}{4}\right)\left(\cos((m-l)\theta)-\frac{\sin((m-l)\theta)}{\cos\theta}\right)d\theta \\ =\; & \frac{1}{\pi}\int_0^\pi \cos(m\lambda)\left(2-\cos\lambda-\sqrt{(2-\cos\lambda)^2-1}\right)^l d\lambda \end{aligned}$$

(see (21), (22), (23), and (24)), and

$$\begin{aligned} & \sum_{k=0}^{\infty}\binom{2k+m+l}{k}\binom{2k+m+l+1}{k+1+m}\frac{4^{-2k-m-l}l(m+1)}{(k+m+l+1)(2k+m+l)} \\ =\; & \frac{2}{\pi}\int_0^\pi \sin(lx)\sin(x)\left(2-\cos x-\sqrt{(2-\cos x)^2-1}\right)^{m+1}dx \end{aligned}$$

(see (29)) for all integers $m \geq 0$, $l \geq 1$, or

$$\begin{aligned} & 6\sum_{k=0}^{\infty}\frac{4^{-2k-1}}{(k+3)(k+2)}C_{k+1}C_k \\ =\; & \frac{1}{\pi}\int_0^\pi \frac{1-\sin x}{1+\sin x}\left(\frac{1}{3}(1+5\sin(x))+\frac{(1-\sin x)^2(1+4\sin^2 x)}{5(1+\sin x)}\right)dx \end{aligned}$$

(the case $m=0$ in (31)).

We did not derive these identities for the purpose of actual computations. In the process of numerically verifying the formulas, however, one notices that the sums are slowly converging. Only if the number of oscillations in the integrands gets very large, the numerical algorithms for evaluating the integrals can fail to produce a result.

A Few Historical Notes. It is the intention of this paper to show how far the cancellation principle can carry us with just a finite number of sources, and how little effort is required to obtain those beautiful results. However, an *infinite* number of sources is needed if we restrict the diffusion to bands with parallel boundaries, and subsets thereof. Another example requiring infinitely many sources is the $\{\leftarrow, \downarrow, \nearrow\}$-walk in the first quadrant, representing the ballot problem with three candidates where the winner ($\nearrow$) never falls behind the losers ($\leftarrow, \downarrow$) during the counting of the votes (Kreweras [19]). There is a wealth of approaches to the enumeration of walks bounded by hyperplanes, some of them attacking the problem (including all those with binomial results in this paper) from a very general angle [10],[2], or considering different kinds of boundary conditions and step sets [28]. In a recent paper, Bousquet-Mélou (2002) applies the *kernel method* to "Counting Walks in the Quarter Plane" [3]. Of course, these few references cannot even scratch the surface of the mountain of literature that has accumulated on the topic of planar walks; the situation gets worse when we discuss related structures in Section 19. Some references can be found in Janse van Rensburg's book [21], and a few others are interspersed among the results in Section 19. Mohanty's book on "Lattice Path Counting and Applications" [25] is still a valuable resource for a first introduction to that topic.

Acknowledgement This work began with the quest for a simpler proof of a much harder problem, the enumeration of diffusion walks in the second octant, conditioned on the number of visits to the diagonal[1]. For an analytic approach to this question see Janse van Rensburg [21]. I am also indebted to Y. Itoh for drawing my attention to the paper by McCrea and Whipple [23], and for the interpretation of diffusion in an octant as a gamblers' ruin problem. M.E.H. Ismail pointed out the connection to Chebyshev polynomials, which helps to "explain" some of the identities, and A.J. Guttmann showed me how to enumerate polyominoes by gap size. Finally, most of the references have been provided by one of the referees.

2 Restricted Diffusion

If the diffusion has only one source $\oplus$, at the origin, say, and no restrictions, then the number $U_k(n,m)$ of ways a particle can reach the point (n,m) in k steps is

$$U_k(n,m) = \binom{k}{\frac{k+n+m}{2}}\binom{k}{\frac{k+n-m}{2}}. \tag{3}$$

This is of course well-known; for a proof by picture see Fig. 3. No particle can reach (n,m) in k steps if $k+n+m$ is odd, or $|n|+|m|>k$; we must interpret the binomial coefficient $\binom{i}{j}$ as 0 if i or j are fractions or negative integers. Note the four axes of symmetry in diffusion walks: the x-axis, y-axis, and the diagonals $y=\pm x$. Thus

$$U_k(n,m) = U_k(|n|,|m|) = U_k(|m|,|n|).$$

[1] Since the completion of this paper, I have been able to prove by very different and much less elegant methods [26] that the number of such walks from the origin to (n,n) in $2k$ steps making d contacts with the diagonal equals $\frac{\binom{2k+2}{k+n+2}\binom{2k}{k}}{\binom{2k+1}{d+1}2(k+1)^2}\left((n+1)(d-1)\binom{k}{d-1}+\frac{(2k+1-d)(2n+d+2)}{d+1}\left(\binom{k-n}{d}-\binom{k}{d}+n\binom{k}{d-1}\right)\right)$.

Stirling approximation shows that for large k the walk ends at (n,m) after $2k+|n|+|m|$ steps with probability approximately $(\pi k)^{-1}$. Hence the expected number of visits to (n,m) is infinite.

We begin with a review of well known results in the enumeration of diffusion walks restricted to half- and quarter-planes. The pictures we show are not proofs in the strict sense; they are a suggestive "physical interpretation", based on the cancellation principle. However, the answers they suggest can be easily verified by checking the recursion and initial values. Another iteration of the "method of images" or cancellation principle leads from walks in quadrants to octants in Subsection 2.3. A more algebraic than geometric way of applying the cancellation principle is shown in Subsection 2.3.1.

2.1 Half-planes

Suppose l is a positive integer. As a prototype of diffusion restricted to half of the lattice we count the walks strictly to the right of the *l*eft boundary $x=-l$. We start *two* diffusion processes at the same time, one from the source $\oplus$ at the origin, and a synchronous negatively charged diffusion from the source $\ominus$ at the mirror location $(-2l,0)$. The diagrams in Table 1 show the location of the sources and the number of walks after $k=1,2,3$ steps. The walks from the (virtual) negative source are counted as negative numbers; they annihilate the walks from the positive source when reaching the boundary line $x=-l$. Thus the number $H_k^{l|}(n,m)$ of walks in a *H*alf plane to (n,m) from the origin in $k\geq|n|+|m|$ steps strictly to the right of the line $x=-l$ is

$$\begin{aligned} H_k^{l|}(n,m) &= U_k(n,m)-U_k(n+2l,m) \\ &= \binom{k}{\frac{k+n+m}{2}}\binom{k}{\frac{k+n-m}{2}}-\binom{k}{\frac{k+n+m}{2}+l}\binom{k}{\frac{k+n-m}{2}+l}. \end{aligned} \tag{4}$$

The case $l=1$ shows that for $n\geq 0$

$$H_{2k+n+|m|}^{1|}(n,m)=\frac{n+1}{2k+n+|m|+1}\binom{2k+n+|m|+1}{k}\binom{2k+n+|m|+1}{k+|m|}$$

walks reach (n,m) in $2k+n+|m|$ steps staying strictly in the right half plane.

Denote the number of walks to (n,m) strictly left of $x=r$ by $H_k^{|r}(n,m)$. By symmetry, $H_k^{|r}(n,m)=H_k^{r|}(-n,m)$. For more results on two-dimensional random walks in general see Csáki [4]; for diffusion in a quadrant Guy, Krattenthaler and Sagan [15], and for planar walks inside a rectangle [27].

2.2 Quadrants

If we want the diffusion to stay in the shifted first quadrant (a *quadrant walk*) strictly above the bottom line $y=-b$ and right of $x=-l$ we only have to study the scheme in Fig. 1.

One negative source $\mathfrak{H}$ of a virtual walk in the half-plane $x\geq -l$ is needed to cancel along $y=-b$ the same type of half-plane walk from the origin. Let $n>-l$ and $m>-b$. Thus

$$Q_k^{l\llcorner b}(n,m):=H_k^{l|}(n,m)-H_k^{l|}(n,m+2b)$$

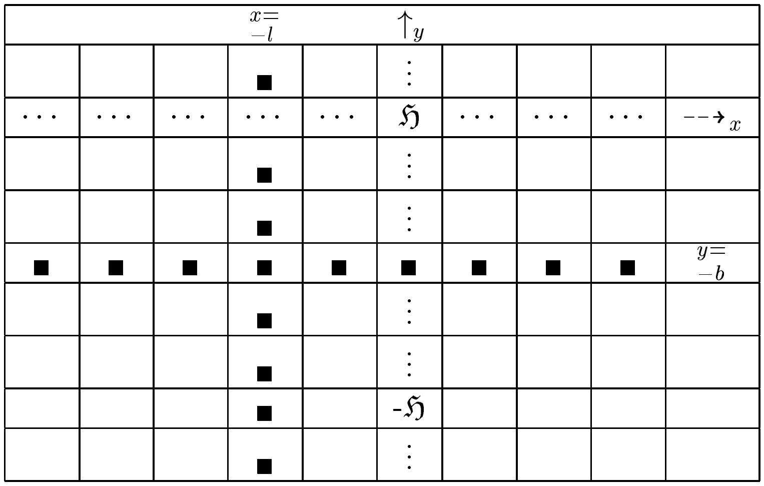

Figure 1: Diffusion in a shifted quadrant

is the number of Quadrant walks from the origin to (n,m) in k steps. Note that $Q_k^{l\llcorner b}(n,m) = Q_k^{b\llcorner l}(-m,-n)$.

The diagram also shows that $Q_k^{l\ulcorner b}(n,m) := H_k^{l|}(n,m) - H_k^{l|}(n,m-2b)$ where $Q^{l\ulcorner b}$ enumerates fourth-quadrant walks strictly right of $x=-l$ and below $y=b$. Note that for $m>0$

$$Q_k^{l\llcorner b}(n,m-b) = H_k^{l|}(n,b-m) - H_k^{l|}(n,-m-b) = Q_k^{l\ulcorner b}(n,b-m)\,.$$

For $l=b=1$ we obtain the number $\frac{(n+1)(m+1)}{(k+n+m+1)(k+n+m+2)}\binom{2k+n+m}{k}\binom{2k+n+m+2}{k+n+1}$ of quadrant walks to $(n,m)\in\mathbb{N}_0^2$ in $2k+n+m$ steps, applying (4)

$$\begin{aligned} & H_{2k+n+m}^{1|}(n,m) - H_{2k+n+m}^{1|}(n,m+2) \\ = \; & \frac{n+1}{2k+n+m+1}\binom{2k+n+m+1}{k}\binom{2k+n+m+1}{k+m} \\ & -\frac{n+1}{2k+n+m+1}\binom{2k+n+m+1}{k-1}\binom{2k+n+m+1}{k+m+1} \\ = \; & \frac{(n+1)(m+1)}{(k+n+m+1)(k+n+m+2)}\binom{2k+n+m}{k}\binom{2k+n+m+2}{k+n+1}. \end{aligned}$$

If $Q_k^{l\lrcorner b}(n,m)$ are the paths staying in the shifted second quadrant strictly above the line $y=-b$ and *left* of $x=l$ then $Q_k^{l\lrcorner b}(n,m) = Q_k^{l\llcorner b}(-n,m)$.

2.3 Octants

Are there any more results on bounded diffusion that are as beautiful and surprisingly simple as the diffusion in a quadrant, where the two positive sources exactly cancel the two negative sources at the right places? The answer is yes, because diffusion has another axis of symmetry that we can utilize, the first diagonal. Thus there is at least one more "nice" case, the diffusion inside an octant. Diffusion walks in an octant may be seen as the difference of two quadrant walks (originating at $\mathfrak{Q}$ and -$\mathfrak{Q}$ on the right side of Fig. 2), or as the sum of an array of alternating unrestricted walks arranged along the corners of an octagon (left side of Fig. 2).

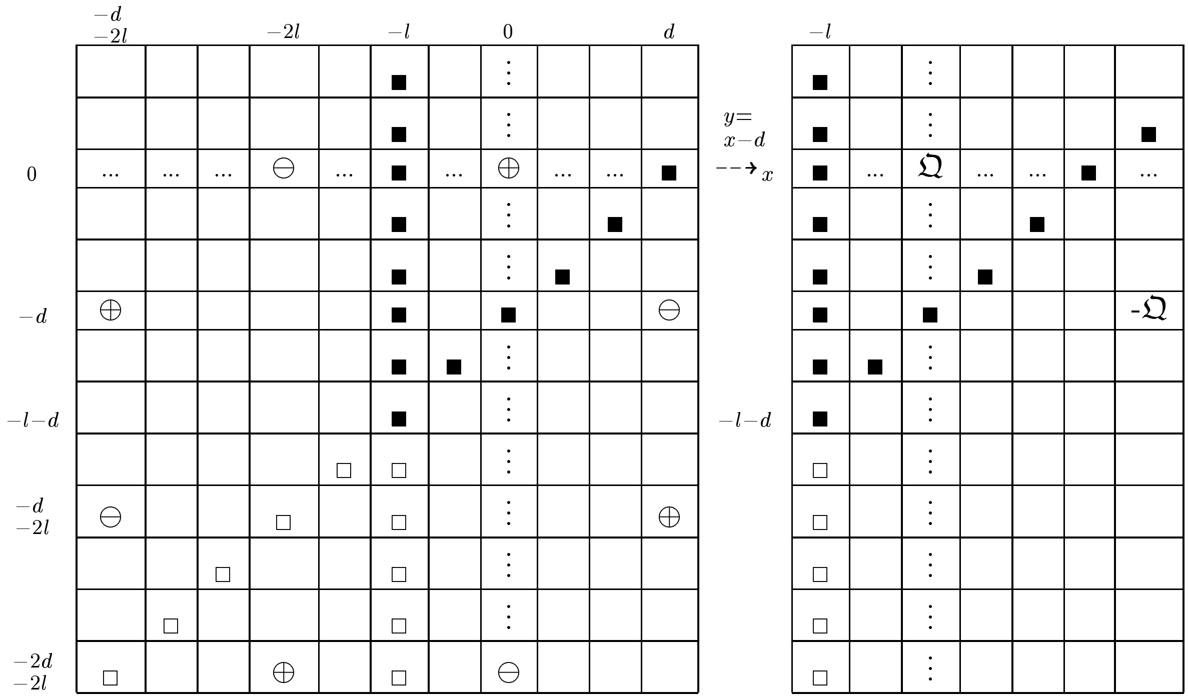

Figure 2: Only 7 virtual sources are needed to keep the diffusion in an octant!

In order to respect the boundary $x = -l$ and enable cancellation along $y = x - d$, the positive $\mathfrak{Q}$ must be $\mathfrak{Q}^{l\llcorner l+d}$, and the negative quadrant source must be $\mathfrak{Q}^{l+d\llcorner l}$.

Let $n > -l$ and $m > n - d$ for two given positive integers l and d. The number of paths from the origin to (n, m) in k steps strictly to the right of $x = -l$ and strictly above $y = x - d$ equals $O_k^{l|\diagup d}(n, m)$

$$\begin{aligned}
&= U_k(n,m) - U_k(n+2l,m) - U_k(n-d,m+d) + U_k(n+d+2l,m+d) \\
&\quad + U_k(n-d,m+d+2l) - U_k(n+d+2l,m+d+2l) \\
&\quad - U_k(n,m+2d+2l) + U_k(n+2l,m+2d+2l) \\
&= H_k^{l|}(n,m) - H_k^{l|}(m+d,n-d) + H_k^{l|}(m+d,n+d+2l) - H_k^{l|}(n,m+2d+2l) \\
&= Q_k^{l\llcorner l+d}(n,m) - Q_k^{l\llcorner l+d}(m+d,n-d).
\end{aligned} \tag{5}$$

If we extend formula (5) for $O_k^{l|\diagup d}(n, m)$ to *all* lattice points (n, m) we note that $O_k^{l|\diagup d}(n-l, m) = -O_k^{l|\diagup d}(-n-l, m)$, and $O_k^{l|\diagup d}(n, m) = -O_k^{l|\diagup d}(m+d, n-d)$.

Remark 1 *Diffusion in the second octant is related to a ruin problem where two players called E.W. and S.N. play, in random order against a bank. Player E.W. has a capital of l dollars, and the bank holds d dollars; player S.N. is of unlimited wealth in this version, and cannot be ruined. In every game the players either win or lose a dollar; the associated diffusion walk takes a step*

to the East, $\rightarrow$*, if E.W. wins, to the West,* $\leftarrow$*, if E.W. loses,*
to the South, $\downarrow$*, if S.N. wins, and to the North,* $\uparrow$*, if S.N. loses.*

Player E.W. is ruined when his capital is down to zero; the same holds for the bank. Thus $O_k^{l|\!\!\diagup d}(1-l,m)$ *is the number of ways gambler E.W. can get ruined in* $k+1$ *games when player S.N. has a gain (or loss) of* m *dollars. The banker can get ruined in* $O_k^{l|\!\!\diagup d}(n,n-d+1)+O_k^{l|\!\!\diagup d}(n-1,n-d)$ *ways in* $k+1$ *games when player S.N. has a loss (or gain) of* n *dollars, and E.W. has a gain (or loss) of* $n-d$ *dollars. Ruin probabilities can be obtained from the first passage probabilities in Subsection 3.3.*

If player S.N. has limited capital a *we must restrict the walk to the right triangle* $-l<x<y-d$, $y<a$. *It needs an infinite array of virtual octant walks to keep the diffusion inside that triangle. A more efficient approach starts with McCrea and Whipple's formula [23] for diffusion restricted to a rectangle, and views the triangle walks as the difference of to rectangular diffusions; see [20] for the corresponding ruin problems.*

For walks in the second octant ($l=d=1$) we drop the superscript $l|\!\!\diagup d$ from the notation. The number of such walks from the origin to (n,m) in $m+n+2k$ steps is for $m\geq n\geq 0$

$$\begin{aligned} O_{n+m+2k}(n,m) \\ &= \left(\binom{n+m+2k}{k}-\binom{n+m+2k}{k-3}\right)\left(\binom{n+m+2k}{n+k}-\binom{n+m+2k}{n+k-1}\right) \\ &\quad+\left(\binom{n+m+2k}{k-2}-\binom{n+m+2k}{k-1}\right)\left(\binom{n+m+2k}{n+k+1}-\binom{n+m+2k}{n+k-2}\right) \\ &= \frac{(n+1)(2+m)(m+3+n)(m+1-n)}{6(n+k+1)\binom{n+m+k+3}{3}}\binom{n+m+2k+2}{n+k}\binom{n+m+2k}{k} \end{aligned} \tag{6}$$

(there is a printing error in the corresponding formula (4.186) in [21]).

The number of paths in the second octant *ending on the* y*-axis* at height $m\geq 0$ in $m+2k$ steps is therefore

$$O_{m+2k}(0,m)=\frac{1}{k+1}\binom{m+3}{3}\binom{m+2k+2}{k}\binom{m+2k}{k}\Big/\binom{m+k+3}{3}. \tag{7}$$

Summing over the end point gives the number of walks in the second octant ending on the y-axis after k steps,

$$\sum_{j=0}^{k/2}\frac{1}{j+1}\binom{k-2j+3}{3}\binom{k+2}{j}\binom{k}{j}\Big/\binom{k-j+3}{3}=C_{\lfloor (k+1)/2\rfloor}C_{\lfloor 1+k/2\rfloor} \tag{8}$$

(sequence A005817 in the *On-Line Encyclopedia of Integer Sequences*), where $C_k=\binom{2k}{k}/(k+1)$ is the k-th Catalan number. To the diagonal, at (n,n), will return

$$O_{2n+2k}(n,n)=\frac{1}{4(n+k+1)}\binom{2n+4}{3}\binom{2n+2k+2}{n+k}\binom{2n+2k}{k}\Big/\binom{2n+k+3}{3} \tag{9}$$

paths after $2n+2k$ steps. This time summing over the end point gives the number of walks in the second octant ending on the diagonal after $2k$ steps,

$$\sum_{j=0}^{k} \frac{1}{4\left(k+1\right)} \binom{2k-2j+4}{3} \binom{2k+2}{k} \binom{2k}{j} / \binom{2k-j+3}{3} = C_k C_{k+1} \tag{10}$$

(sequence A005568). To the origin will return

$$O_{2k}\left(0,0\right) = 12 \frac{(2k)!\,(2k+1)!}{k!^2\,(k+3)!\,(k+2)!} = C_k C_{k+2} - C_{k+1}^2 \tag{11}$$

walks after $2k$ steps. More on the Catalan and other connections in Section 4.

Best suited for numerical experiments with planar walks are spreadsheets, but matrices are also a useful tool for displaying the effect of virtual sources. Start with a finite piece of the double infinite matrix $R = \left(R_{ij}\right)_{i,j\in\mathbb{Z}}$ where $R_{ij} = 1$ if $|i+j| = 1$, and 0 else. This matrix represents the recursion in the sense that $O_{k+1} = RO_k + O_k R$. The initial matrix O_0 has ones and minus ones at the position of the sources. Table 2 shows an example for the case $l = d = 1$.

0	0	0	0	0	−1	**0**	1	0	0	0	0	**0**
0	0	0	0	−3	0	**0**	0	3	0	0	**0**	0
0	0	0	−2	0	−6	**0**	6	0	2	**0**	0	0
0	0	2	0	−5	0	**0**	0	5	**0**	−2	0	0
0	3	0	5	0	−3	**0**	3	**0**	−5	0	−3	0
1	0	6	0	3	0	**0**	**0**	−3	0	−6	0	−1
0	0	0	0	0	0	**0**	0	0	0	0	0	0
−1	0	−6	0	−3	**0**	**0**	0	3	0	6	0	1
0	−3	0	−5	**0**	3	**0**	−3	0	5	0	3	0
0	0	−2	**0**	5	0	**0**	0	−5	0	2	0	0
0	0	**0**	2	0	6	**0**	−6	0	−2	0	0	0
0	**0**	0	0	3	0	**0**	0	−3	0	0	0	0

Table 2: A piece of the matrix O_4, with boldface boundary values

2.3.1 Three dimensional diffusion

The same cancellation principle can be applied to solve 3-D diffusion problems. However, it is much harder to place the sources in space just by geometrical intuition. For example, consider the 3-D diagonal diffusion with eight step vectors $(\pm1, \pm1, \pm1)$, and require that the walks (weakly) stay in the cone $z \geq y \geq x \geq 0$. Denote by $D_k\left(n,m,l\right)$ the number of walks from the origin to (n,m,l) in k steps. If n, m, l, and k are not of the same parity, this number will be zero. Thus the bounding planes to be avoided by the walk are of the form $x = -1$, $y = x-2$, and $z = y-2$. We derive the location of the sources by an algebraic instead of a visual argument.

Let S be the set of sources. If (a, b, c) is a source, then its effect on the boundaries $x = -1$, $y = x - 2$, and $z = y - 2$ must be canceled by the opposite sources at $f(a, b, c) := (-a - 2, b, c)$, $g(a, b, c) := (b + 2, a - 2, c)$, and $h(a, b, c) := (a, c + 2, b - 2)$, respectively. Denote by C the noncommutative group generated by the three reflections f, g, and h. Hence $(a, b, c) \in S$ implies $p(a, b, c) \in S$ for all $p \in C$. In other words, $S = \{p(0, 0, 0) : p \in C\}$. For a better understanding of S and C we temporarily move the origin into the intersection of the three planes, so that $(0, 0, 0) \mapsto (1, 3, 5)$. The three reflections are now $f'(a, b, c) = (-a, b, c)$, $g'(a, b, c) = (b, a, c)$, and $h'(a, b, c) = (a, c, b)$. Correspondingly, C' is the group generated by f', g' and h', and $S' = \{p'(1, 3, 5) : p' \in C'\}$. Note that g' and h' are transpositions on three elements. In cycle notation, $g' = (a, b), (c)$ and $h' = (a), (b, c)$. The third transposition can be obtained as $h'g'h' = (a, c)(b)$. Hence g' and h' generate the group of all 3-permutations, $\mathfrak{S}_3$, which implies that any permutation of $(1, 3, 5)$ is in S'. The reflection f' changes the sign of the first coordinate, $g'f'g'$ the sign of the second, and $h'g'f'g'h'$ the sign of the third. Hence the 48 elements of S' are the permutations of $(\pm 1, \pm 3, \pm 5)$. The group C' is well known as the group generated by the symmetries of the cube (the hyperoctahedral group on signed 3-permutations). Every element p' of C' can be written as a composition of transpositions $(g', h', h'g'h')$ and some sign changes induced by f'. The parity of the number of transpositions in p' is an invariant, and so is the parity of the number of sign changes f'. We call p' even or odd depending on the parity of the number of transpositions plus sign changes. An even (odd) p' can only be written as a composition of an even (odd) number of reflections. Now we return to our set of sources, $S = \{p'(1, 3, 5) - (1, 3, 5) : p' \in C'\}$. A source $s = p'(1, 3, 5) - (1, 3, 5)$ is positive iff p' is even. We have shown the following lemma.

Lemma 2 *Let $P := \{(\pm u, \pm v, \pm w)$, where (u, v, w) is a permutation of $(1, 3, 5)\}$. Then $\{(-1, -3, -5) + (x, y, z) : (x, y, z) \in P\}$ is the set of sources. The sources $(-1, -3, -5) + (x, y, z)$ and $(-1, -3, -5) + \left((-1)^i x, (-1)^j y, (-1)^k z\right)$ have the same sign iff $i + j + k$ is even.*

The 3-D version of Fig.3 would show that unrestricted diagonal diffusion in three dimensions is generated by three independent random walks along the three coordinate axis. The number of unrestricted walks to (n, m, l) in k steps is therefore $U_k(n, m, l) := \binom{k}{(k+n)/2}\binom{k}{(k+m)/2}\binom{k}{(k+l)/2}$. After adding up the 48 unrestricted walks starting at the 48 sources in S with the appropriate signs we arrive at $D_k(n, m, l)$. It follows from the above Lemma that

$$D_k(n, m, l) = \sum_{i=0}^{7} (-1)^{\lfloor i/4 \rfloor + \lfloor i/2 \rfloor + i} \begin{vmatrix} \binom{k}{\frac{k+n+1-(-1)^{\lfloor i/4 \rfloor}}{2}} & \binom{k}{\frac{k+n+1-3(-1)^{\lfloor i/2 \rfloor}}{2}} & \binom{k}{\frac{k+n+1-5(-1)^{i}}{2}} \\ \binom{k}{\frac{k+m+3-(-1)^{\lfloor i/4 \rfloor}}{2}} & \binom{k}{\frac{k+m+3-3(-1)^{\lfloor i/2 \rfloor}}{2}} & \binom{k}{\frac{k+m+3-5(-1)^{i}}{2}} \\ \binom{k}{\frac{k+l+5-(-1)^{\lfloor i/4 \rfloor}}{2}} & \binom{k}{\frac{k+l+5-3(-1)^{\lfloor i/2 \rfloor}}{2}} & \binom{k}{\frac{k+l+5-5(-1)^{i}}{2}} \end{vmatrix}.$$

To shorten the expansion, we define $B_t^i := \binom{k}{(k+i)/2} - \binom{k}{t+(k+i)/2}$ and find $D_k(n, m, l) =$

$$B_1^n \left(B_3^m B_5^l - B_5^{m-2} B_3^{l+2}\right) + B_1^{m+2} \left(B_5^{n-4} B_3^{l+2} - B_3^{n-2} B_5^l\right) + B_1^{l+4} \left(B_3^{n-2} B_5^{m-2} - B_5^{n-4} B_3^m\right) \quad (12)$$

The special case $D_{2k}(0, 0, 0)$ gives formula (1).

We chose the example of an eight-step diagonal diffusion in view of an application to counting watermelons at the end of Section 4.1. The more common “nearest neighbor walks” with six steps $(\pm 1,0,0)$, $(0,\pm 1,0)$, and $(0,0,\pm 1)$ can be enumerated in the same way, with boundaries $x=-1$, $y=x-1$, and $z=y-1$, and corresponding sources at $(a,b,c)-(1,2,3)$, where (a,b,c) is a permutation of $(\pm 1,\pm 2,\pm 3)$. The same approach solves the boundary problem that restricts the walks to the region

$$x>-b,\ y>x-c,\ z>y-d$$

where b, c, and d are positive integers. If the six nearest neighbor steps are reduced to the three unit steps $(1,0,0)$, $(0,1,0)$, and $(0,0,1)$, we obtain the more familiar "ballot problem with three candidates". The condition $x>-b$ is automatic in this case, thus there are only six sources, $(0,0,0)$, $(c,-c,0)$, $(c,d,-c-d)$, $(c+d,0,-c-d)$, $(c+d,-c,-d)$, and $(0,d,-d)$. In terms of trinomial coefficients, the well known number of ballot paths to (n,m,l) is $\binom{l+n+m}{n,m}-\binom{l+n+m}{n-c,m+c}+\binom{l+n+m}{n-c,m-d}-\binom{l+n+m}{n-c-d,m}+\binom{l+n+m}{n-c-d,m+c}-\binom{l+n+m}{n,m-d}$which simplifies to $\frac{(m-n+1)(l+1-m)(l+2-n)}{(l+1)(l+2)(m+1)}\binom{l+n+m}{n,m}$ if $c=d=1$. In this "totally ordered" version of the ballot problem, the winner stays ahead of the second winner, who himself remains ahead of the looser throughout the counting of votes. Even with only three candidates the ballot problem becomes much more difficult if the boundary $z\geq y\geq x$ is replaced by $z\geq\max(x,y)$, which is the version mentioned in the Introduction (see [19],[18], and for the latest proof [3]). Lemma 2 is easily generalized to any dimension d. If we require that the walk stays in the chamber $x_i>x_{i-1}-c_i$ for all $i=1,\dots,d$ (with $x_{-1}=0$, $c_i\geq 1$), then the sources must be placed at $\mathbf{p}-\mathbf{c}$, where $\mathbf{c}=(c_1,c_1+c_2,\dots,c_1+c_2+\dots+c_d)$, and $\mathbf{p}\in P:=\{(\pm u_1,\pm u_2,\dots,\pm u_d)$, where $(u_1,u_2,\dots,u_d)$ is a permutation of the components of $\mathbf{c}\}$. The source is positive if the permutation is even, and negative else. Note that the location of sources is independent of the step set of the walk. Of course, the admissible step sets must be symmetric with respect to all the bounding hyperplanes. The resulting solution to the totally ordered ballot problem was first solved by Frobenius and MacMahon [24]. For general $c_i's$ see [31]. For more on the general problem see [9],[10], and [14].

3 Expected Number of Visits and First Passage

Diffusion is not only a physical concept, modeled in combinatorics by discrete time and a lattice of discrete states, it is also an intensively studied area of probability theory. We compare in this section some probabilistic results on the long term behavior of diffusion to the corresponding expressions obtained from combinatorial enumeration. Most of the identities that are obtained this way seem to be hard to prove by other methods.

Denote by $V_{n,m}$ the random variable that reports the number of visits a random diffusion walk makes to (n,m) before being absorbed at some boundary, thus the expected number of visits to (n,m) equals

$$\mathrm{E}\left[V_{n,m}\right]=\sum_{j\geq 0}\Pr\left(V_{n,m}\geq j\right)=\sum_{k\geq 0}4^{-k}D_k\left(n,m\right) \tag{13}$$

if $D_k(n,m)$ is the number of paths to (n,m) in k steps under the same restrictions. Without any restrictions on the paths, the expectation is infinite. The enumeration results of Section

2 enable us to express the expected number of visits in half planes, quadrants and octants as sums; for half-planes and quadrants they also have been expressed as integrals in a paper by McCrea and Whipple [23] as limiting cases of planar walks in a rectangle. However, those integrals look different from the obvious integrals (16) obtained from the combinatorial sums!

3.1 Half-planes

Denote by $\mathrm{E}_H^{l|}[V_{n,m}]$ the expected number of visits to the point (n,m) of a random diffusion walk in the half-plane $x > -l$. Because of symmetry, $\mathrm{E}_H^{l|}[V_{n,m}] = \mathrm{E}_H^{l|}[V_{n,-m}]$, and the same holds for the first passage probability. All formulae in this subsection will be written for $m \geq 0$; every occurrence of m can be replaced by $|m|$. We find four formulas for $\mathrm{E}_H^{l|}[V_{n,m}]$: (14), (16), (19), and (20). We begin with an expression for $\mathrm{E}_H^{l|}[V_{n,m}]$ derived from (13) and (4)

$$\mathrm{E}_H^{l|}[V_{n,m}] = \sum_{k\geq 0} 4^{-k}\left(U_k(n,m) - U_k(n+2l,m)\right) \tag{14}$$

This sum can be written as an integral using the identities

$$\begin{aligned} \int_0^\pi \cos(mx)(\cos x)^n\,dx &= \begin{cases} \frac{\pi}{2^n}\binom{n}{(n-m)/2} & \text{if } n \geq m \geq 0 \text{ and } n-m \text{ is even} \\ 0 & \text{else} \end{cases} \\ \sum_{n=0}^{\infty}\binom{2n+x}{n}\xi^n &= \frac{2^x}{\sqrt{1-4\xi}}\left(1+\sqrt{1-4\xi}\right)^{-x}. \end{aligned} \tag{15}$$

We get for all integers n

$$\begin{aligned} 4^{-2k-|n|-m}U_{|n|+m+2k}(n,m) &= \frac{\binom{|n|+m+2k}{k}}{2^{|n|+m+2k}\pi}\int_0^\pi \cos\left((m-|n|)x\right)\cos^{|n|+m+2k}(x)\,dx \\ \sum_{k\geq 0}(\xi/4)^{2k+|n|+m}U_{|n|+m+2k}(n,m) &= \frac{1}{\pi}\int_0^\pi \left(\frac{\cos(x)}{1+\sqrt{1-\xi\cos(x)^2}}\right)^{|n|+m}\frac{\cos\left((m-|n|)x\right)}{\sqrt{1-\xi\cos(x)^2}}dx \end{aligned}$$

This expansion converges for $|\xi| < 1$, diverges for $\xi = 1$, but converges for $\xi = -1$. The power series
$\sum_{k\geq 0}(\xi/4)^k\left(U_k(n,m) - U_k(n+2l,m)\right)$
$= \int_0^\pi \frac{\left(\frac{\cos(x)}{1+\sqrt{1-\xi\cos(x)^2}}\right)^{|n|+m}\cos((m-|n|)x) - \left(\frac{\cos(x)}{1+\sqrt{1-\xi\cos(x)^2}}\right)^{n+2l+m}\cos((m-n-2l)x)}{\pi\sqrt{1-\xi\cos(x)^2}}dx$
converges for $\xi = 1$, thus $\mathrm{E}_H^{l|}[V_{n,m}] =$

$$\int_0^\pi \frac{\left(\cot\left(\frac{\pi+2x}{4}\right)^{|n|+m}\cos\left((m-|n|)x\right) - \cot\left(\frac{\pi+2x}{4}\right)^{n+2l+m}\cos\left((m-n-2l)x\right)\right)}{\pi\sin(x)}dx \tag{16}$$

for $n \geq -l$.

Remark 3 *From $U_k(n,m) = U_k(m,n)$ follows*
$\mathrm{E}_H^{l|}[V_{n,m}] = \sum_{k\geq 0} 4^{-k}(U_k(n,m) - U_k(n+2l,m)) = \sum_{k\geq 0} 4^{-k}(U_k(m,n) - U_k(m,n+2l))$.

McCrea and Whipple [23] determined $\mathrm{E}_H^{l}[V_{n,m}]$ from the recursion

$$\mathrm{E}_H^{l|}[V_{n,m}] = \frac{1}{4}\left(\mathrm{E}_H^{l|}[V_{n-1,m}] + \mathrm{E}_H^{l|}[V_{n+1,m}] + \mathrm{E}_H^{l|}[V_{n,m-1}] + \mathrm{E}_H^{l|}[V_{n,m+1}]\right) \tag{17}$$

when $(n,m) \neq (0,0)$, $n > -l$, and (because all walks start at the origin)

$$\mathrm{E}_H^{l|}[V_{0,0}] = 1 + \frac{1}{4}\left(\mathrm{E}_H^{l|}[V_{-1,0}] + \mathrm{E}_H^{l|}[V_{1,0}] + \mathrm{E}_H^{l|}[V_{0,-1}] + \mathrm{E}_H^{l|}[V_{0,1}]\right). \tag{18}$$

The recursion has a unique solution if the paths are restricted to the inside of a rectangle. Removing all but one side of the rectangle by limit processes, McCrea and Whipple found $\mathrm{E}_H^{l|}[V_{n,m}] =$

$$\frac{2}{\pi}\int_0^\pi \frac{\cos(\lambda m)\left(e^{-|n|\mu} - e^{-(n+2l)\mu}\right)}{\sinh(\mu)}d\lambda = \begin{cases} \frac{4}{\pi}\int_0^\pi \frac{\cos(\lambda m)e^{-l\mu}\sinh((n+l)\mu)}{\sinh(\mu)}d\lambda & \text{if } -l \leq n \leq 0 \\ \frac{4}{\pi}\int_0^\pi \frac{\cos(\lambda m)e^{-(n+l)\mu}\sinh(l\mu)}{\sinh(\mu)}d\lambda & \text{if } n \geq 0 \end{cases} \tag{19}$$

where $2 = \cos(\lambda) + \cosh(\mu)$. Denote by $\mathcal{T}_k$ and $\mathcal{U}_k$ the Chebyshev polynomials of the first and second kind, respectively, of degree k, i.e., $\mathcal{T}_k(x) = \cos(k\lambda)$ and $\mathcal{U}_{k-1}(x) = \sin(k\lambda)/\sin(\lambda)$ if $x = \cos(\lambda)$. It is easy to check that we can write (19) in this notation as

$$\mathrm{E}_H^{l|}[V_{n,m}] = \begin{cases} \frac{4}{\pi}\int_{-1}^1 \mathcal{T}_m(x)\,\mathcal{U}_{n+l-1}(2-x)\,\frac{e^{-l\mu}dx}{(1-x^2)^{1/2}} & \text{if } -l \leq n \leq 0 \\ \frac{4}{\pi}\int_{-1}^1 \mathcal{T}_m(x)\,\mathcal{U}_{l-1}(2-x)\,\frac{e^{-(n+l)\mu}dx}{(1-x^2)^{1/2}} & \text{if } n \geq 0 \end{cases} \tag{20}$$

Note that $e^\mu = e^{\operatorname{arccosh}(2-\cos(\lambda))} = \sqrt{(2-x)^2 - 1} + 2 - x$.

Remark 4 *Denote by $\mathrm{E}_H^{|r}[V_{n,m}]$ the expected number of visits at (n,m) of walks to the left of $x = r$. From $\mathrm{E}_H^{|r}[V_{n,m}] = \mathrm{E}_H^{r|}[V_{-n,m}]$ follows $\mathrm{E}_H^{|r}[V_{n,m}] =$*

$$\frac{2}{\pi}\int_0^\pi \frac{\cos(\lambda m)\left(e^{-|n|\mu} - e^{(n-2r)\mu}\right)}{\sinh(\mu)}d\lambda = \begin{cases} \frac{4}{\pi}\int_0^\pi \frac{\cos(\lambda m)e^{-r\mu}\sinh((r-n)\mu)}{\sinh(\mu)}d\lambda & \textit{if } 0 \leq n \leq r \\ \frac{4}{\pi}\int_0^\pi \frac{\cos(\lambda m)e^{(n-r)\mu}\sinh(r\mu)}{\sinh(\mu)}d\lambda & \textit{if } n \leq 0 \end{cases}.$$

3.1.1 First Passage

As before in this subsection about half-planes we assume that $m \geq 0$ and $l \geq 1$. A particle makes its "first passage" to the boundary point $(-l,m)$ at time k if it stayed away from $x = -l$ and reached $(1-l,m)$ at time $k-1$. By formula (5) there are

$$H_{k-1}^{l|}(1-l,m) = U_{k-1}(1-l,m) - U_{k-1}(1+l,m)$$

ways for the first passage at time k, and the probability of first passage (summed over time) at height $m \geq 0$ is $P_H^{l|}(-l,m) = \mathrm{E}_H^{l|}[V_{1-l,m}]$. We begin with a direct determination, using only formula (5), and find $P_H^{l|}(-l,m)$

$$\begin{aligned} &= \sum_{k \geq m+l} 4^{-k} H_{k-1}^{l|}(1-l,m) = \sum_{k=0}^{\infty} 4^{-2k-m-l} \binom{2k+m+l}{k} \binom{2k+m+l}{k+l} \frac{l}{2k+m+l} \\ &= 4^{-m-l} \binom{m+l-1}{m} {}_4F_3 \left[\begin{matrix} 1+\frac{m+l}{2}, \frac{1}{2}+\frac{m+l}{2}, \frac{1}{2}+\frac{m+l}{2}, \frac{m+l}{2}; \\ m+l+1, 1+l, 1+m \end{matrix} 1 \right]. \end{aligned} \tag{21}$$

Applying (15) together with the identity

$$\sum_{n=0}^{\infty} \binom{2n+x}{n} \frac{1}{2n+x} \xi^n = \frac{2^x}{x\left(1+\sqrt{1-4\xi}\right)^x},$$

we obtain $P_H^{l}(-l,m) =$

$$\begin{aligned} &\sum_{k=0}^{\infty} 4^{-2k-m-l} \binom{2k+m+l}{k} \frac{l}{2k+m+l} \frac{2^{2k+m+l}}{\pi} \int_0^{\pi} \cos\left((m-l)\theta\right) (\cos\theta)^{2k+m+l} \, d\theta \\ = &\frac{l}{\pi(m+l)} \int_0^{\pi} \cos\left((m-l)\theta\right) \left(\frac{\cos\theta}{1+\sin\theta}\right)^{m+l} d\theta. \end{aligned}$$

Hence

$$P_H^{l|}(-l,m) = \frac{l}{\pi(m+l)} \int_0^{\pi} \cos\left((m-l)\theta\right) \cot^{m+l}\left(\frac{\pi+2\theta}{4}\right) d\theta. \tag{22}$$

for all integers $m \geq 0$. With $x = \cos\theta$ and $dx/d\theta = -\sin\theta$ we get

$$P_H^{l|}(-l,m) = \frac{l}{\pi(m+l)} \int_{-1}^{1} \frac{\mathcal{T}_{|m-l|}(x)\left(1-\sqrt{1-x^2}\right)^{m+l}}{x\sqrt{1-x^2}} dx.$$

The next formula follows from (16), $P_H^{l|}(-l,m) =$

$$\begin{aligned} &\frac{1}{4\pi} \int_0^{\pi} \frac{\left(\cot^{l-1+m}\left(\frac{\pi+2\theta}{4}\right)\cos\left((m-l+1)\theta\right) - \cot^{1+l+m}\left(\frac{\pi+2\theta}{4}\right)\cos\left((m-1-l)\theta\right)\right)}{\sin\theta} d\theta \\ = &\frac{1}{2\pi} \int_0^{\pi} \cot^{m+l}\left(\frac{\pi+2\theta}{4}\right) \left(\cos\left((m-l)\theta\right) - \frac{\sin\left((m-l)\theta\right)}{\cos\theta}\right) d\theta. \end{aligned} \tag{23}$$

Finally, we know from (19) or [23] that $P_H^{l|}(-l,m) =$

$$\frac{1}{\pi} \int_0^{\pi} \cos(\lambda m) e^{-l\mu} d\lambda = \frac{1}{\pi} \int_{-1}^{1} \frac{\mathcal{T}_{|m|}(x)}{\left(\sqrt{(2-x)^2-1}+2-x\right)^l} \frac{dx}{\sqrt{1-x^2}}. \tag{24}$$

Thus (21), (22), (23), and (24) are the combinatorial/probabilistic reason for the identities (2).

3.2 Quadrants

We saw that the number $Q_k^{l\llcorner b}(n,m)$ of planar walks in the quadrant $-l<x$, $-b<y$ can be written in terms of half-plane walks as $Q_k^{l\llcorner b}(n,m)=H_k^{l|}(n,m)-H_k^{l|}(n,m+2b)$. Hence

$$\mathrm{E}_Q^{l\llcorner b}[V_{n,m}]=\mathrm{E}_H^{l|}[V_{n,m}]-\mathrm{E}_H^{l|}[V_{n,m+2b}]$$

can be calculated from any of the formulas for $\mathrm{E}_H^{l|}[V_{n,m}]$. In the following proposition we apply (19) because of an interesting and useful overlap in the domain of the two expressions for $\mathrm{E}_Q^{l\llcorner b}[V_{n,m}]$ (being identical for $-|m|\le n\le |m|$).

Proposition 5 *Let* $2=\cos(\lambda)+\cosh(\mu)$, $x=\cos\lambda$, *thus* $e^{\mu}=\sqrt{(2-x)^2-1}+2-x$. *For* $n>-l$, *and* $m>-b$ *holds* $\mathrm{E}_Q^{l\llcorner b}[V_{n,m}]$

$$=\begin{cases}\frac{8}{\pi}\int_0^{\pi}\frac{\sin(b\lambda)\sin((m+b)\lambda)\sinh((n+l)\mu)}{\sinh\mu}d\lambda=\frac{4}{\pi}\int_{-1}^{1}\frac{\left(\mathcal{T}_{|m|}-\mathcal{T}_{m+2b}\right)(x)\mathcal{U}_{n+l-1}(2-x)}{e^{l\mu}(1-x^2)^{1/2}}dx & \text{if } n\le |m|\\ \frac{8}{\pi}\int_0^{\pi}\frac{\sin(b\lambda)\sin((m+b)\lambda)\sinh(l\mu)}{e^{(n+l)\mu}\sinh\mu}d\lambda=\frac{4}{\pi}\int_{-1}^{1}\frac{\left(\mathcal{T}_{|m|}-\mathcal{T}_{m+2b}\right)(x)\mathcal{U}_{l-1}(2-x)}{e^{(n+l)\mu}(1-x^2)^{1/2}}dx & \text{if } n\ge -|m|\end{cases}$$

Proof. Formula (19) implies

$$\mathrm{E}_Q^{l\llcorner b}[V_{n,m}]=\begin{cases}\frac{8}{\pi}\int_0^{\pi}\frac{\sin(b\lambda)\sin((m+b)\lambda)\sinh((n+l)\mu)e^{-l\mu}}{\sinh\mu}d\lambda & \text{if } n\le 0\\ \frac{8}{\pi}\int_0^{\pi}\frac{\sin(b\lambda)\sin((m+b)\lambda)\sinh(l\mu)e^{-(n+l)\mu}}{\sinh\mu}d\lambda & \text{if } n\ge 0\end{cases}$$

(see also [23]). The two integrals do not only agree for $n=0$; if $m>-b$; they are the same for all $-|m|\le n\le|m|$, as shown in Proposition 7 below. ■

Lemma 6 *Let* $\cos\lambda+\cosh\mu=2$.

$$\int_0^{\pi}\frac{\cos(m\lambda)\sinh(n\mu)}{\sinh\mu}d\lambda=0 \text{ for } |n|\le|m|$$

Proof. (By M.E.H. Ismail) Let $0\le n\le m$, $x=\cos\lambda$, and $z=\cos(i\mu)=\cosh(\mu)$, thus $z=2-x$. Denote by $\mathcal{T}_k$ and $\mathcal{U}_k$ the Chebyshev polynomials of the first and second kind, respectively, of degree k,

$$\mathcal{T}_k(x)=\cos(k\lambda)\ \text{ and } \mathcal{U}_{k-1}(z)=\frac{\sin(ki\mu)}{\sin(i\mu)}=\frac{\sinh(k\mu)}{\sinh(\mu)}.$$

From $dx/d\lambda=-\sin\lambda$ follows

$$\int_0^{\pi}\frac{\cos(m\lambda)\sinh(n\mu)}{\sinh\mu}d\lambda=\int_{-1}^{1}\frac{T_m(x)\,U_{n-1}(z)}{\sin\lambda}dx=\int_{-1}^{1}\frac{T_m(x)\,U_{n-1}(2-x)}{\sqrt{1-x^2}}dx$$

The Chebyshev polynomials are orthogonal on $[-1,1]$ with respect to $(1-x^2)^{-1/2}$, and $U_{n-1}(2-x)$ is of degree less than m, hence the integral is zero. The integral vanishes for all $0\le n\le|m|$ because it is even in m, and it is odd in n. ■

Proposition 7 *For* $\max\{-|m|, -|m+2b|\} \le n \le \min\{|m|, |m+2b|\}$

$$\int_0^\pi \frac{\sin(\lambda b)\sin(\lambda(m+b))\sinh((n+l)\mu)e^{-l\mu}}{\sinh\mu}d\lambda = \int_0^\pi \frac{\sin(\lambda b)\sin(\lambda(m+b))\sinh(l\mu)e^{-(n+l)\mu}}{\sinh\mu}d\lambda$$

Proof. From $-|m| \le n \le |m|$ follows $\int_0^\pi (\cos(m\lambda)\sinh(n\mu)/\sinh\mu)\,d\lambda = 0$, and in the same way $\int_0^\pi (\cos(|m+2b|\lambda)\sinh(n\mu)/\sinh\mu)\,d\lambda = 0$. Hence

$$0 = \int_0^\pi \frac{(\cos(m\lambda) - \cos((m+2b)\lambda))\sinh(n\mu)}{\sinh\mu}d\lambda = 2\int_0^\pi \frac{\sin(\lambda b)\sin(\lambda(m+b))\sinh(n\mu)}{\sinh\mu}d\lambda$$

and $\int_0^\pi (\sin(\lambda b)\sin(\lambda(m+b))e^{n\mu}/\sinh\mu)\,d\lambda = \int_0^\pi (\sin(\lambda b)\sin(\lambda(m+b))e^{-n\mu}/\sinh\mu)\,d\lambda$. Subtract
$\int_0^\pi \left(\sin(\lambda b)\sin(\lambda(m+b))e^{-(n+2l)\mu}/\sinh\mu\right)d\lambda$ from both sides and get

$$\int_0^\pi \frac{\sin(\lambda b)\sin(\lambda(m+b))\left(e^{n\mu} - e^{-(n+2l)\mu}\right)}{\sinh\mu}d\lambda = \int_0^\pi \frac{\sin(\lambda b)\sin(\lambda(m+b))\left(e^{-n\mu} - e^{-(n+2l)\mu}\right)}{\sinh\mu}d\lambda.$$

■

3.2.1 First passage

The first passage probability $P_Q^{l\llcorner b}(-l,m)$ to the boundary $x=-l$ at height $m > -b$ equals $P_H^{l|}(-l,m) - P_H^{l|}(-l,m+2b) =$

$$\frac{1}{2\pi}\int_0^\pi \left(\cot^{l+|m|}\left(\frac{\pi+2\lambda}{4}\right)\left(\cos((|m|-l)\lambda) - \frac{\sin((|m|-l)\lambda)}{\cos\lambda}\right)\right. \tag{25}$$
$$\left. - \cot^{l+m+2b}\left(\frac{\pi+2\lambda}{4}\right)\left(\cos((m+2b-l)\lambda) - \frac{\sin((m+2b-l)\lambda)}{\cos\lambda}\right)\right)d\lambda$$
$$= \frac{2}{\pi}\int_0^\pi \sin(\lambda b)\sin(\lambda(m+b))\left(2-\cos\lambda - \sqrt{(2-\cos\lambda)^2-1}\right)^l d\lambda \tag{26}$$
$$= \frac{l}{\pi}\int_0^\pi \left(\frac{\cos((|m|-l)\lambda)}{\left(\frac{1+\sin\lambda}{\cos\lambda}\right)^{|m|+l}(|m|+l)} - \frac{\cos((m+2b-l)\lambda)}{\left(\frac{1+\sin\lambda}{\cos\lambda}\right)^{m+2b+l}(m+2b+l)}\right)d\lambda. \tag{27}$$

using (23), (24), and (22) (remember that $\cot\left(\frac{\pi+2\lambda}{4}\right) = \frac{\cos\lambda}{1+\sin\lambda}$). Note that $P_Q^{l\llcorner b}(n,-b) = P_Q^{b\llcorner l}(-b,n)$. Written as sums, $P_Q^{l\llcorner b}(-l,m) = P_H^l(-l,m) - P_H^l(-l,m+2b) =$

$$= \sum_{k=0}^{b-1} 4^{-2k-m-l}\binom{2k+m+l}{k+m+l}\binom{2k+m+l}{k+m}\frac{l}{2k+m+l} \tag{28}$$
$$+\sum_{k=b}^{\infty}\frac{4^{-2k-m-l}l}{2k+m+l}\left(\binom{2k+m+l}{k}\binom{2k+m+l}{k+m} - \binom{2k+m+l}{k-b}\binom{2k+m+l}{k+b+m}\right)$$

For example, if $b = 1$ we get $P_Q^{l\llcorner 1}(-l, m) =$

$$
\begin{aligned}
&\sum_{k=0}^{\infty} \binom{2k+m+l}{k} \binom{2k+m+l+1}{k+1+m} \frac{4^{-2k-m-l} l\,(m+1)}{(k+m+l+1)\,(2k+m+l)} \\
= \;& \frac{2}{\pi} \int_0^{\pi} \sin(lx) \sin(x) \left(2 - \cos x - \sqrt{(2-\cos x)^2 - 1}\right)^{m+1} dx. \qquad (29)
\end{aligned}
$$

If $l = b = 1$ we find the following five expressions for the first passage probability in the first quadrant to the y-axis at height $m \geq 0$,

from (28): $P_Q^{1\llcorner 1}(-1, m) = \sum_{k=0}^{\infty} 4^{-2k-m-1} \frac{(m+1)}{(k+m+1)(k+1)} \binom{2k+m}{k} \binom{2k+m+2}{k}$,

from (29): $= \frac{2}{\pi} \int_0^{\pi} \sin^2(\lambda) \left(2 - \cos\lambda - \sqrt{(2-\cos\lambda)^2 - 1}\right)^{m+1} d\lambda$,

from (26): $= \frac{2}{\pi} \int_0^{\pi} \sin(\lambda) \sin(\lambda(m+1)) \left(2 - \cos\lambda - \sqrt{(2-\cos\lambda)^2 - 1}\right) d\lambda$,

from (27): $= \frac{l}{\pi} \int_0^{\pi} \left(\frac{\cos\lambda}{1+\sin\lambda}\right)^{m+1} \left(\frac{\cos(\lambda(m-1))}{m+1} - \frac{\left(\frac{\cos\lambda}{1+\sin\lambda}\right)^2 \cos(\lambda(m+1))}{m+3}\right) d\lambda$,

from (25): $= \frac{1}{\pi} \int_0^{\pi} \left(\frac{\cos\lambda}{1+\sin\lambda}\right)^{m} \cos(m\lambda) \sin(\lambda) \frac{1+\cos^2\lambda}{(1+\sin\lambda)^2} dx$.

3.3 Shifted Octants

The number $O_k^{l|\!\!/ d}(n, m)$ of planar walks in the shifted octant $-l < x$, $y > x - d$ can be written in terms of quadrant walks as $O_k^{l|\!\!/ d}(n, m) = Q_k^{l\llcorner l+d}(n, m) - Q_k^{l+d\llcorner l}(n-d, m+d) = Q_k^{l\llcorner l+d}(n, m) - Q_k^{l\llcorner l+d}(m+d, n-d)$. Hence

$$
\mathrm{E}_O^{l|\!\!/ d}[V_{n,m}] = \mathrm{E}_Q^{l\llcorner l+d}[V_{n,m}] - \mathrm{E}_Q^{l+d\llcorner l}[V_{n-d,m+d}] = \mathrm{E}_Q^{l\llcorner l+d}[V_{n,m}] - \mathrm{E}_Q^{l\llcorner l+d}[V_{m+d,n-d}] \qquad (30)
$$

for $-l - d < n - d < m$. We can calculate the probability $P_O^{l|\!\!/ d}(-l, m)$ of first passage to the line $x = -l$ from the first passage probabilities in shifted quadrants. This is not the case for the first passage to the diagonal line $y = x - d$, thus we need to know $\mathrm{E}_O^{l|\!\!/ d}[V_{n,m}]$. Formula (30) shows that any of the expressions for $\mathrm{E}_Q^{l\llcorner b}[V_{n,m}]$ can be used to find $\mathrm{E}_O^{l|\!\!/ d}[V_{n,m}]$. An example is worked out in the following proposition.

Proposition 8 *Let* $\cos\lambda + \cosh\mu = 2$, $x = \cos\lambda$, *thus* $e^{\mu} = \sqrt{(2-x)^2 - 1} + 2 - x$. *For* $-l - d < n - d < m$ *holds* $\mathrm{E}_O^{l|\!\!/ d}[V_{n,m}]$

$$
= \begin{cases}
\frac{8}{\pi} \int_0^{\pi} \frac{\left(\sin(\lambda(l+d)) - \sin(\lambda l) e^{-d\mu}\right) \sin(\lambda(m+l+d)) \sinh((n+l)\mu)}{e^{l\mu} \sinh\mu} d\lambda & \text{if } n \leq |m| \\
\frac{8}{\pi} \int_0^{\pi} \frac{\sin(\lambda(m+l+d)) \left(\sin(\lambda(l+d)) \sinh(l\mu) e^{-n\mu} - \sin(\lambda l) \sinh((n+l)\mu) e^{-d\mu}\right)}{e^{l\mu} \sinh\mu} d\lambda & \text{if } n \geq -|m|
\end{cases}
$$

$$
= \begin{cases}
\frac{4}{\pi} \int_{-1}^{1} \left(\frac{\left(\mathcal{T}_{|m|} - \mathcal{T}_{m+2(l+d)}\right)(x)}{e^{l\mu}} - \frac{\left(\mathcal{T}_{|m+d|} - \mathcal{T}_{m+d+2l}\right)(x)}{e^{(l+d)\mu}}\right) \frac{\mathcal{U}_{n+l-1}(2-x)}{(1-x^2)^{1/2}} dx & \text{if } n \leq |m| \\
\frac{4}{\pi} \int_{-1}^{1} \left(\frac{\left(\mathcal{T}_{|m|} - \mathcal{T}_{m+2(l+d)}\right) \mathcal{U}_{l-1}(2-x)}{e^{(n+l)\mu}} - \frac{\left(\mathcal{T}_{|m+d|} - \mathcal{T}_{m+d+2l}\right)(x) \mathcal{U}_{n+l-1}(2-x)}{e^{(l+d)\mu}}\right) \frac{dx}{\sqrt{1-x^2}} & \text{if } n \geq -|m|
\end{cases}
$$

The proof is a straight forward application of Proposition 5 to $\mathrm{E}_O^{l|\!\diagup d}[V_{n,m}] = \mathrm{E}_Q^{l\llcorner l+d}[V_{n,m}] - \mathrm{E}_Q^{l+d\llcorner l}[V_{n-d,m+d}]$, noting that $n-d \leq |m+d|$ inside the shifted octant $-l-d < n-d < m$. A different looking formula for $\mathrm{E}_O^{l|\!\diagup d}[V_{n,m}]$ can be derived in the same way if we write $\mathrm{E}_O^{l|\!\diagup d}[V_{n,m}] = \mathrm{E}_Q^{l\llcorner l+d}[V_{n,m}] - \mathrm{E}_Q^{l\llcorner l+d}[V_{m+d,n-d}]$.

3.3.1 First passage to $x = -l$

The probability $P_O^{l|\!\diagup d}(-l,m)$ of first passage strictly inside the shifted octant $x > -l$, $y > x-d$ to the vertical boundary $x = -l$ can be obtained in different variations from (25) - (28) because

$$P_O^{l|\!\diagup d}(-l,m) = \frac{1}{4}\mathrm{E}_O^{l|\!\diagup d}[V_{1-l,m}] = P_Q^{l\llcorner l+d}(-l,m) - P_Q^{l+d\llcorner l}(-l-d,m+d)$$

If $d = l = 1$, we write P_O instead of $P_O^{1|\!\diagup 1}$, and we get from (7) that $P_O(-1,m) =$

$$\begin{aligned}
& 4^{-m-1}\binom{m+3}{3}\sum_{k=0}^{\infty}\frac{4^{-2k}}{k+1}\binom{m+2k+2}{k}\binom{m+2k}{k}\Big/\binom{m+k+3}{3} \qquad (31)\\
= & \frac{1}{\pi}\int_0^{\pi}\cos((m-1)x)\left(\frac{\cos x}{1+\sin x}\right)^{m+1}\left(\frac{1}{m+1}-\left(\frac{\cos x}{1+\sin x}\right)^2\frac{2}{m+3}\right)dx\\
& -\frac{1}{\pi}\int_0^{\pi}\left(\frac{\cos x}{1+\sin x}\right)^{m+5}\left(\frac{\cos((m+3)x)-2\cos((m+1)x)}{m+5}\right)dx.
\end{aligned}$$

For some numerical examples see Table 3.

3.3.2 First passage to $y = x - d$

Let $n > 1-l$. There are two ways to get to the boundary point $(n, n-d)$, from above at $(n, n-d+1)$ and from the left at $(n-1, n-d)$. Thus $P_O^{l|\!\diagup d}(n,n-d) = \frac{1}{4}\mathrm{E}_O^{l|\!\diagup d}[V_{n,n-d+1}] + \frac{1}{4}\mathrm{E}_O^{l|\!\diagup d}[V_{n-1,n-d}]$. We apply Proposition 8, noting that $n \geq -|n-d+1|$ and $n-1 \geq -|n-d|$ for all n. Hence $P_O^{l|\!\diagup d}(n,n-d) =$

$$\begin{aligned}
& \frac{2}{\pi}\int_0^{\pi} e^{-l\mu}\left[\sin(\lambda(l+d))\sinh(l\mu)e^{-n\mu}(\sin(\lambda(n+1+l))+e^{\mu}\sin(\lambda(n+l)))\right.\\
& \left.-\sin(\lambda l)e^{-d\mu}(\sinh((n+l)\mu)\sin(\lambda(n+1+l))+\sinh((n+l-1)\mu)\sin(\lambda(n+l)))\right]\frac{d\lambda}{\sinh\mu}.
\end{aligned}$$

In terms of Chebyshev polynomials, $P_O^{l|\!\diagup d}(n,n-d)$

$$\begin{aligned}
= & \frac{1}{\pi}\int_{-1}^{1}\left[\frac{\left(\mathcal{T}_{|n-d+1|}-\mathcal{T}_{n+1+2l+d}+e^{\mu}\left(\mathcal{T}_{|n-d|}-\mathcal{T}_{n+2l+d}\right)\right)\mathcal{U}_{l-1}(2-x)}{e^{(l+n)\mu}}\right.\\
& \left.-\frac{\left(\mathcal{T}_{|n+1|}-\mathcal{T}_{n+1+2l}\right)(x)\,\mathcal{U}_{n+l-1}(2-x)+\left(\mathcal{T}_{|n|}-\mathcal{T}_{n+2l}\right)(x)\,\mathcal{U}_{n+l-2}(2-x)}{e^{(l+d)\mu}}\right]\frac{dx}{\sqrt{1-x^2}}
\end{aligned}$$

Again, $\cos\lambda + \cosh\mu = 2$, $x = \cos\lambda$, thus $e^{\mu} = \sqrt{(2-x)^2 - 1} + 2 - x$.

For $n = 1 - l$, the boundary point $(1-l, 1-l-d)$ below the corner of the shifted octant can only be reached from above. Hence $P_O^{l\swarrow d}(1-l, 1-l-d) = \frac{1}{4}\mathrm{E}_O^{l\swarrow d}[V_{1-l,2-l-d}] = P_O^{l\swarrow d}(-l, 2-l-d)$, the probability of passage to the vertical boundary $x = -l$.

If the walk is restricted to the second octant ($l = b = 1$), first passage below the diagonal to $(n, n-1)$ happens with probability

$$\begin{aligned} P_O(n, n-1) &= \sum_{k=0}^{\infty} \left(4^{-2k-2(n-1)-1} O_{2(n-1)+2k}(n-1, n-1) + 4^{-2k-2n-1} O_{2n+2k}(n, n)\right) \qquad (32) \\ &= \sum_{k=0}^{\infty} \frac{4^{-2k-2n}(n+1)\binom{2n+2k}{n+k-1}\binom{2n+2k-2}{k}}{3(n+k)\binom{2n+k+2}{4}} \left((n+1)(n(2n+1) + 2k(n+1)) + k\right) \\ &= \frac{2}{\pi}\int_0^{\pi} e^{-\mu}\Big[\sin(2\lambda) e^{-n\mu}\left(\sin(\lambda(n+2)) + e^{\mu}\sin(\lambda(n+1))\right) \\ &\quad - \frac{\sin(\lambda) e^{-\mu}}{\sinh\mu}\left(\sinh((n+1)\mu)\sin(\lambda(n+2)) + \sinh(n\mu)\sin(\lambda(n+1))\right)\Big]\, d\lambda. \end{aligned}$$

$j =$	0	1	2	3	4	5	6	7	8	20
$P_O(-1, j) =$	.27005	.08018	.02658	.00991	.00416	.00194	$.0^3 99$	$.0^3 54$	$.0^3 32$	$.0^6 6$
$P_O(j+1, j) =$	.29414	.02935	.00691	.00229	.00093	.00044	$.0^3 23$	$.0^3 13$	$.0^4 7$	$.0^6 15$

Table 3: Some examples of first passage proabilities in the second octant

4 Related structures

Certain subsets of the diffusion walks in an octant can be visualized by structures that may look quite different. We list non-crossing pairs of Dyck paths, bicolored Motzkin paths, staircase polygons in the second octant, and $\{\rightarrow\uparrow\}$-paths enumerated by left turns. Of course, other aspects of such structures may not be efficiently represented by diffusion walks. A thorough discussion of these and other structures and their applications can be found in *The Statistical Mechanics of Interacting Walks, Polygons, Animals and Vesicles*, by Janse van Rensburg [21].

4.1 Pairs of Non-crossing Dyck paths

The diagonal diffusion, with step set $\{\nearrow, \swarrow, \searrow, \nwarrow\}$, is easily mapped onto the ordinary diffusion by the matrix $\frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$. The matrix maps the diagonal steps $\nearrow, \swarrow, \searrow, \nwarrow$ onto $\uparrow, \downarrow, \rightarrow, \leftarrow$ (in this order). If we draw two independent random walks with steps ± 1 on the integers, a vertical walk V along the y-axis (marked by $\vdots$ in Fig. 3) and a horizontal walk H along the x-axis ($\cdots$), then *the diagonal diffusion (•) is the vector sum of the two integer walks*, i.e., if H and V are at the positions $(h_k, 0)$ and $(0, v_k)$ at time k, then (h_k, v_k) is the position of the diagonal diffusion walk (this proves formula (3)).

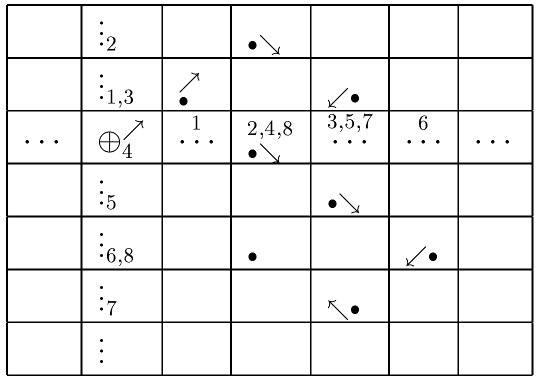

Figure 3: Diagonal diffusion generated by two perpendicular integer walks. The subscripts and superscripts indicate the position at step k of the vertical and horizontal walks, respectively.

If we restrict the one-dimensional walks to nonnegative integers and require that the i-th term v_i in the vertical walk is not larger than the i-th term h_i in the horizontal walk (making them dependent!), i.e., $h_i \geq v_i \geq 0$ for all i, then the diagonal diffusion stays in the first octant as in Fig. 4. Note that these restricted one-dimensional walks along the axes become Dyck paths (i.e., weakly above the x-axis) if we replace the steps $1, -1$ by $\nearrow$ and $\searrow$, respectively. In the pair P_H, P_V of paths we write the horizontal walk (P_H) first ; if the Dyck pair P_H, P_V ends at (k, h), (k, v) the diagonal diffusion ends at (h, v) after k steps (k, h and v are of the same parity). The image under $\frac{1}{2}\left(\begin{smallmatrix} 1 & -1 \\ 1 & 1 \end{smallmatrix}\right)$ (ordinary diffusion) of the diagonal diffusion stays in the second octant.

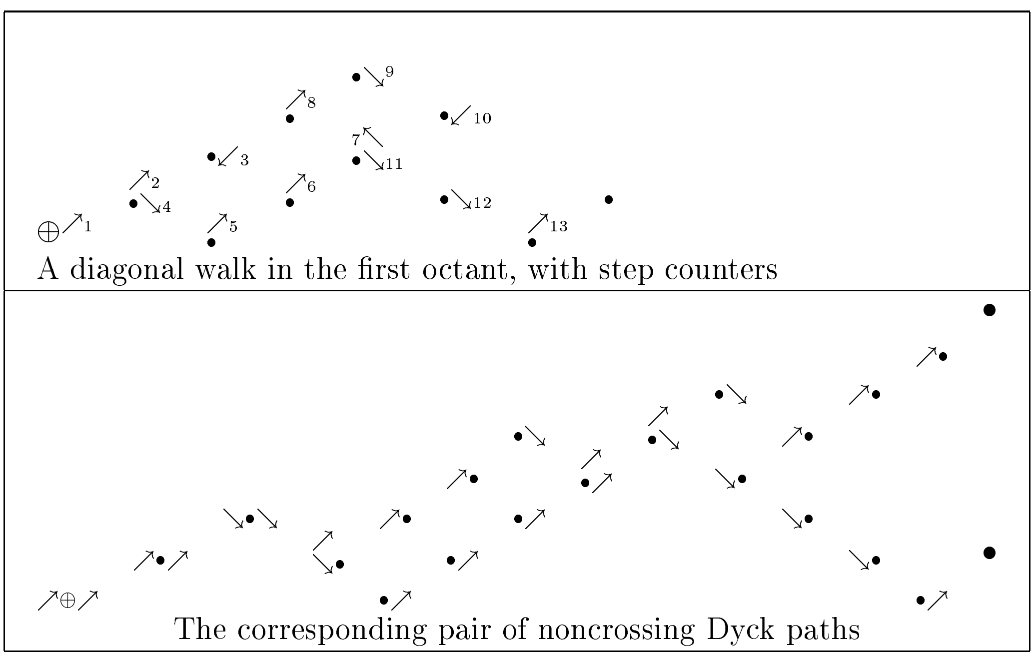

Figure 4: The correspondence between diagonal diffusion and Dyck pairs

Hence the number of pairs of noncrossing Dyck paths from the origin to $(k, h), (k, v)$ equals the number of diagonal diffusion walks to (h,v) in k steps staying in the first octant, which in turn equals the number of ordinary diffusion walks in the second octant reaching $\frac{1}{2}\binom{1\ -1}{1\ \ 1}\binom{h}{v}$ $= ((h-v)/2, (h+v)/2)$ after k steps,

$$O_k\left((h-v)/2,(h+v)/2\right) = \frac{(2+h-v)(4+h+v)(h+3)(v+1)}{12(k-v+2)}\binom{k+2}{\frac{k-v}{2}}\binom{k}{\frac{h+k}{2}}\Big/\binom{\frac{h+k}{2}+3}{3}$$

(see (6)). The pairs that end at a common point are equivalent to staircase polygons (parallel polyominoes); we discuss them in Subsection 4.3 in more detail.

It follows from the bijection between pairs of noncrossing Dyck paths and diffusion walks that

- the expected number of pairs of noncrossing paths P_H, P_V where the bottom path P_V falls below the x-axis for the first time when the top path P_H is at height h, equals $4P_O(h/2, (h-2)/2)$ (see (32)).

- the number of noncrossing Dyck pairs ending on the line $x = 2k$ with the bottom path on the x-axis equals $C_k C_{k+1}$ (see (10)).

Remark 9 *There is also a connection between* single *Dyck paths and "short" walks in an octant. If any diffusion walk reaches the point (n,m) in the first quadrant in $n+m$ steps, all steps must be either $\rightarrow$ or $\uparrow$. The number of $\{\rightarrow\uparrow\}$-paths reaching (n,m) in $n+m$ steps* while staying in the second octant *is*

$$O_{n+m}(n,m) = \frac{m+1-n}{n+m+1}\binom{n+m+1}{n}.$$

Mapping $\rightarrow$ to $\searrow$, and $\uparrow$ to $\nearrow$ shows that this is also the number of (single) Dyck paths to $(n+m, m-n)$. If $m = n$, the Dyck paths end on their boundary, the x-axis, and their number is $C_n = \binom{2n}{n}/(n+1)$, the n-th Catalan number. These results are familiar from the classical ballot problem (with two candidates), first solved in 1887 by André [1].

Mapping diffusion walks to pairs of noncrossing Dyck paths goes back at least to Feller [8]. The method can be extended to n-tuples of Dyck paths. We only want to discuss triples. For this purpose we consider 3-D diagonal diffusion as in Subsection 2.3.1, generated by three independent random walks with steps ± 1 on the integers, a vertical walk V along the y-axis, a horizontal walk H along the x-axis as before, and an additional up-down walk U along the z-axis. We map the walks H, V, U into a triple P_H, P_V, P_U of Dyck paths ($1 \mapsto \nearrow$ and $-1 \mapsto \searrow$), requiring that $v_i \geq 0$, $h_i \geq 0$, and $u_i \geq 0$ for all i. Formula (12) tells us how many diagonal diffusion walks reach (n,m,l) in k steps, restricted to lattice points (h_i, v_i, u_i), where $0 \leq h_i \leq v_i \leq u_i$ for all $i = 0, \ldots, k$ (and $h_0 = v_0 = u_0 = 0$, $h_k = n$, $v_k = m$, $u_k = l$). This number, $D_k(n,m,l)$, is therefore the same as the number of noncrossing Dyck triples from $(0,0)$ to (k,n), (k,m), and (k,l). Suppose we separate the triples by shifting the top path upwards two units, and then the upper pair again upwards two units, resulting in an unchanged bottom path from $(0,0)$ to (k,n), a shifted middle path from $(0,2)$ to $(k, m+2)$, and a shifted top

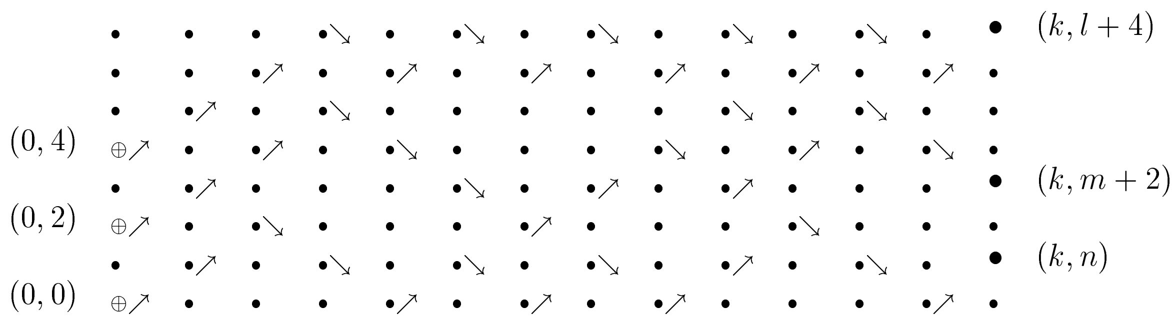

Figure 5: Three vicious walkers

path from $(0,4)$ to $(k,l+4)$. The three paths never occupy the same lattice point; the particles moving along those paths are called *vicious walkers* (Fig. 5).

If $n=m=l=0$ such a configuration of nontouching Dyck paths is called a *watermelon* with three ribs. Note that k must be even in this case, $k=2r$, say. Thus $D_{2r}(0,0,0)=\binom{6}{3}C_rC_{r+1}C_{r+2}/\left(\binom{r+5}{3}\binom{r+4}{3}\right)$ (see (1)) is the number of water melons. The number of watermelons with many ribs can be found by restricting the diagonal diffusion walk in many dimensions to the appropriate cone ([9],[14]). For more on this topic and additional references see [17]. The determinant enumerating several non-intersecting lattice paths (now called the Lindström-Gessel-Viennot formula) goes back to the work of Lindström [22], and Gessel and Viennot [12], [11].

4.2 Bicolored Motzkin paths

A Motzkin path has step set $\{\nearrow, \searrow, \longrightarrow\}$ and stays weakly above the x-axis. Map the step vectors of the diffusion walks onto $\{\nearrow, \searrow, \longrightarrow, \dashrightarrow\}$ according to Table 4.

Diffusion:	$\longrightarrow$	$\longleftarrow$	$\uparrow$	$\downarrow$
Bicolored Motzkin:	$\circ\nearrow$	$\bullet\searrow$	$\bullet\longrightarrow$	$\circ\longrightarrow$
color:	white	black	black	white

Table 4: The bijection

Diffusion in the right half plane is in one-to-one correspondence to bicolored Motzkin paths. We say that the Motzkin path has excess m if it ends with m more black $\longrightarrow$-steps than white $\dashrightarrow$-steps. Diffusion in the first quadrant is bijectively mapped onto bicolored Motzkin paths that reach any point in the first octant with at least as many black $\longrightarrow$-steps as white $\dashrightarrow$-steps, i.e., the excess is never negative along the path. The diffusion will stay in the second octant iff the corresponding bicolored Motzkin paths reach any point in the first octant with a total number of white steps ($\nearrow$ or $\dashrightarrow$) not exceeding the total number of black steps ($\searrow$ or $\longrightarrow$). We call them saturated. Let $m \geq n$. The number $O_k(n,m)$ of octant walks to (n,m) in k steps (see ((6))) equals the number of saturated Motzkin paths to (k,n) with excess m.

First passage through the x-axis at height m of the diffusion walk corresponds to the saturated path with excess m, crossing through the x-axis for the first time. First passage of the

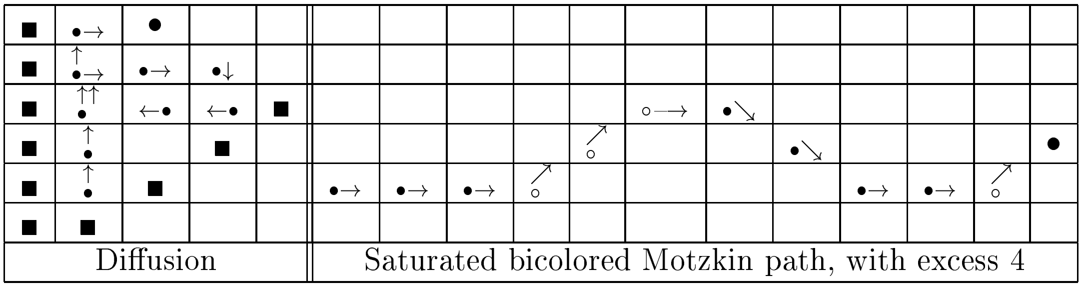

Figure 6: Diffusion in octant $\longleftrightarrow$ bicolored Motzkin

diffusion walk through the diagonal to $(n, n-1)$ corresponds to the bicolored Motzkin path of height n and excess $n-1$, having for the first time more white than black steps. See (31) and (32) for the first passage probabilities. Expression in terms of Catalan numbers are obtained if we enumerate all saturated paths ending at $(k, 0)$ with any excess (see (8)), and if we count all saturated paths ending on the line $x = 2k$ with an equal number of black and white steps (see (10)). For recent work on Motzkin paths see [30] and [29].

4.3 Staircase polygons in the augmented second octant

A staircase polygon (parallelogram polyomino) is a polygon bounded by two $\{\rightarrow\uparrow\}$-paths (staircases) that have only the beginning and the endpoint in common. Because staircase polygons are considered invariant under vertical and horizontal shifts, we can assume that the pair of bounding paths starts at the origin.

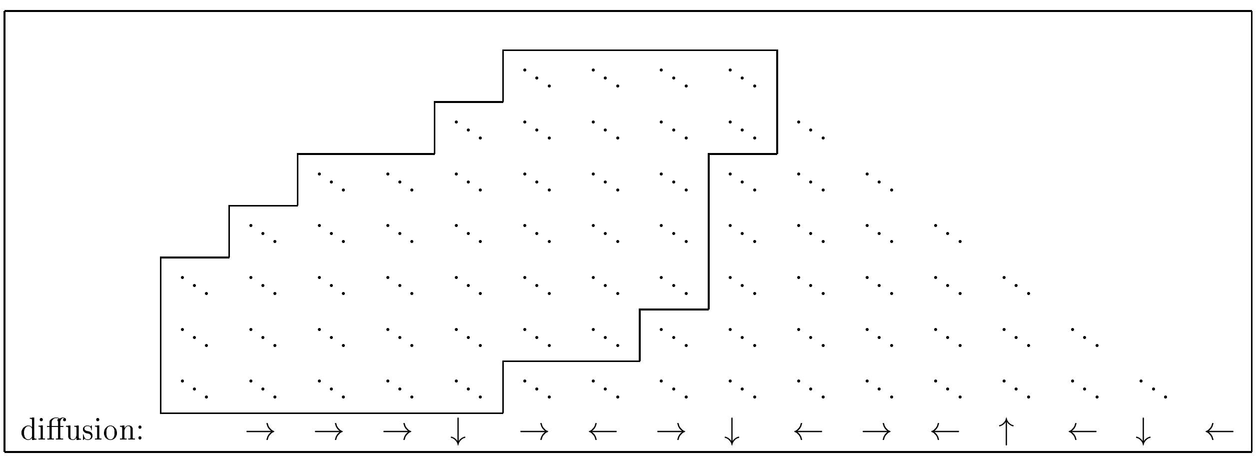

Figure 7: Staircase polygons and dotted diagonal gaps

If we look at a staircase polygon from the Northeast, we see (diagonal) gaps between the paths. We map the polygon into a diffusion according to the change of gaps. An increase (decrease) in gap width is mapped to a $\rightarrow$-step ($\leftarrow$-step). If the gap is just shifted to the right (diagonally shifted upwards) we map it onto a $\downarrow$-step ($\uparrow$-step). Thus a staircase polygon corresponds to a $\{\rightarrow\uparrow\leftarrow\downarrow\}$-planar walk (see also [7],[21]). Among the first k steps let l_k be the number of $\leftarrow$-steps, and r_k the number of $\rightarrow$-steps. Because there cannot be less (expanding) $\rightarrow$-steps than (shrinking) $\leftarrow$-steps in any beginning part of the walk, we find $r_k \geq l_k$; the path stays in the right half-plane $x \geq 0$, and returns to the x-axis at the end. The vertical steps do not change the gap width of the polygon; there can be any number (u_k up, and d_k down) of them, at any location. Vice versa, any diffusion walk in the right half plane ending at $(0, j)$ after k steps can be mapped onto a staircase polygon with lower left corner $(0,0)$ and upper right corner $(n+1, m+1)$ where $j = m - n$ and $k = m + n$. We can thus use equation (4) to find the number of all staircase polygons from $(0,0)$ to (n, m),

$$\binom{n+m-2}{n-1}\binom{n+m-2}{m-1} - \binom{n+m-2}{m}\binom{n+m-1}{n}$$

a Narayana number. The enumeration by gap width allows for much deeper results than the above application (see [5]). A bijection between staircase polygons and bicolored Motzkin paths is described in [21]; for an approach via skew Ferrer's diagrams see [6].

We say that a staircase polygon stays in the augmented second octant if it stays weakly above $y = x - 1$. Any staircase polygon is bounded by two $\{\rightarrow\uparrow\}$-paths, starting with a lower left corner $\llcorner$ at $(0,0)$,and ending with an upper right corner $\urcorner$ at $(n+1, m+1)$, say. If we remove those two corners from a staircase polygon in the augmented second octant, then shift both paths so that they start at the origin and end at (n, m), and turn the shifted pair downwards by $45°$, we obtain a pair of non-crossing Dyck paths from the origin to the common endpoint $(n+m, m-n)$. We enumerated such pairs in Section 4.1; if we denote by $S(n, m)$ the number of staircase polygons to (n, m) in the augmented second octant, we find for $m \geq n$

$$S(n+1, m+1) = O_{m+n}(0, m-n) = 6\frac{(m+n)!\,(m+n+2)!}{n!\,(n+1)!\,(m+2)!\,(m+3)!}\binom{m-n+3}{3}$$

(or use formula (7)). Some special cases of staircase polygons in the augmented second octant:

- If $m = n$ the polygon ends at $(n+1, n+1)$, and by (11) there are

  $$6\frac{(2n)!\,(2n+2)!}{n!\,(n+1)!\,(n+2)!\,(n+3)!} = C_n C_{n+2} - C_{n+1}^2$$

  such staircase polygons.

- From $O_{(n+k)+k}(0, n) = S(k+1, n+k+1)$ follows that the expected number of polygons ending n vertical steps above the diagonal equals $4P_O(-1, n)$ (see (31)).

- The number of polygons ending on the line $n + m = k$ for given integer $k \geq 2$ equals $C_{\lfloor (k-1)/2 \rfloor} C_{\lfloor k/2 \rfloor}$ (see (8)).

- The number of polygons ending on the diagonal at (n, n) equals $O_{2n-2}(0,0) = C_{n-1}C_{n+1} - C_n^2$ (see (11)).

4.4 $\{\rightarrow\uparrow\}$-paths in the augmented third hexadecant enumerated by left turns

Denote by $[u, v]$ the discrete interval $u \leq x \leq v$, where $x \in \mathbb{Z}$, and by $\binom{[u,v]}{k}$ set set of all k-element subsets $[u, v]$. Several interesting combinatorial problems can be bijectively mapped to $\binom{[u,v]}{k} \times \binom{[p,q]}{l}$ (or subsets thereof) for certain choices of the parameters. The following examples are connected with diffusion walks in the second octant.

Lemma 10 *Let n_p, n_q and m be nonnegative integers. There exists a bijection between $\binom{[0,m+n_p-1]}{m} \times \binom{[0,m+n_q-1]}{m}$ and*

1. *pairs p, q of $\{\rightarrow\uparrow\}$-paths, starting at the origin and ending at the point (n_p, m) and (n_q, m), respectively.*
2. *$\{\rightarrow\uparrow\}$-paths, starting at the origin and ending at $(m + n_p, m + n_q)$, taking m left turns ($\underset{\rightarrow}{}\overset{\uparrow}{\circ}$).*
3. *$\{\rightarrow\uparrow\}$-paths, starting at the origin and ending at $(m + n_p, m + n_q)$, taking m right turns ($\underset{\uparrow}{\circ}\rightarrow$).*

Proof. Consecutively label the $m+n_p$ steps of the path p with the numbers $0, \ldots, m+n_p-1$. Let x_i be the label of the i-th vertical step, thus $0 \leq x_1 < \cdots < x_m \leq m + n_p - 1$, and $\{x_i : i \in [1, m]\} \in \binom{[0,m+n_p-1]}{m}$. In the same way, the labels $\{y_i : i \in [1, m]\}$ of the m vertical steps in the path q are elements of $\binom{[0,m+n_q-1]}{m}$. Vice versa, the m-subsets of $[0, m + n_p - 1]$ and $[0, m + n_q - 1]$ correspond to a unique pair of paths p, q.

If we interpret the sequence $(x_i + 1, y_i)$, $i = 1, \ldots, m$ as the sequence of left turn coordinates we obtain a unique lattice path from the origin to $(m + n_p, m + n_q)$ with m left turns; vice versa, the left turn sequence of any such path defines a unique element from $\binom{[0,m+n_p-1]}{m} \times \binom{[0,m+n_q-1]}{m}$.
■

Corollary 11 *There exists a bijection between $\binom{[0,m+n]}{m+1} \times \binom{[1,m+n+1]}{m+1}$ and*

1. *pairs of $\{\rightarrow\uparrow\}$-paths, both starting at the origin and ending at the common point $(n, m + 1)$.*
2. *pairs u, b of $\{\rightarrow\uparrow\}$-paths, both starting at the origin and ending at the common point $(n + 1, m + 1)$ such that u ends and b begins with a horizontal step (in the case of nonintersecting pairs, u would be the upper and b the bottom path).*
3. *diagonal diffusion walks from $(0, 0)$ to $(n - m - 1, n - m - 1)$ in $n + m + 1$ steps, weakly staying inside the rectangle $-m - 1 \leq x \leq n$ and $-m - 1 \leq y \leq n$.*
4. *$\{\rightarrow\uparrow\}$-paths, starting at the origin and ending at $(m + n + 1, m + n + 1)$, taking $m + 1$ right turns ($\underset{\uparrow}{\circ}\rightarrow$).*
5. *$\{\rightarrow\uparrow\}$-paths, starting at the origin and ending at $(m + n + 1, m + n + 1)$, taking $m + 1$ left turns ($\underset{\rightarrow}{}\overset{\uparrow}{\circ}$).*

Proof. For the terminology we refer to the proof of Lemma 10. Take any pair u', b' of $\{\to\uparrow\}$-paths from the origin to the common endpoint $(n, m+1)$. By Lemma 10 such pairs can be bijectively mapped onto $\binom{[0,m+n]}{m+1} \times \binom{[0,m+n]}{m+1}$. Make b' into the "$b$ottom" path b by inserting a $\to$ step at the beginning of b, and u' into the $u$pper path u by appending a $\to$ step at the end of u (the paths may still intersect; they end at $(n+1, m+1)$). The vertical label subsets are now in $\binom{[0,m+n]}{m+1} \times \binom{[1,m+n+1]}{m+1}$, which shows parts 1 and 2. For part 3, interpret u' as the vertical, and b' as the horizontal walk defining a diagonal diffusion as in Fig. 3. The horizontal (vertical) walk moves $m+1$ steps to the left (downwards) and n steps to the right (upwards), which defines the boundary for the resulting diagonal diffusion. Parts 4 and 5 follow directly from Lemma 10 ■

In a staircase polygon to $(n+1, m+1)$ the upper and bottom paths make a pair u, b as in the above bijection, with the additional condition of no common points except at the beginning and end. The $m+1$ positions x_i and y_i of the vertical steps in the sequence of all steps determine the whole pair u, b. Note that $x_1 = 0$, $x_{m+1} \leq m+n$ and $y_1 \geq 1$, $y_{m+1} = m+n+1$ in every such staircase polygon. Therefore we disregard x_1 and y_{m+1}, and consider only $\{x_{i+1} \mid 1 \leq i \leq m\} \in \binom{[1,m+n]}{m}$ and $\{y_i \mid 1 \leq i \leq m\} \in \binom{[1,m+n]}{m}$. When the bottom path takes the i-th vertical step, it has taken $y_i - i + 1$ horizontal steps; the i-th vertical step leads from the vertex $(y_i - i + 1, i - 1)$ to the vertex $(y_i - i + 1, i)$, for $i = 1, \ldots, m+1$. Exchange x with y and the same holds for the upper path u. The pair u, b is nontouching; when the bottom path b moves upwards, to $(y_i - i + 1, i)$, it must stay below the upper path, hence $x_{i+1} - (i+1) + 1 < y_i - i + 1$, i.e.,

$$x_{i+1} \leq y_i \tag{33}$$

for all $i = 1, \ldots, m$. This condition (together with $x_1 = 0$ and $y_{m+1} = m+n+1$) characterizes the staircase polygons. We now map them bijectively onto lattice paths enumerated by left turns in the augmented third hexadecant, where $x - 1 \leq y \leq 2x$. Instead of creating $m+1$ turns at (x_i, y_i) as described in the proof of Lemma 10, we place only m left turns at $(x_{i+1}, y_i - 1)_{i=1,\ldots,m}$ $\in \binom{[1,m+n]}{m} \times \binom{[0,m+n-1]}{m}$, because x_1 and y_{m+1} are fixed in any staircase polygon. The image path runs from $(0,0)$ to $(n+m, n+m)$ and stays weakly above $y = x-1$ because this condition holds at the end point and at all left turns, $y_i - 1 \geq x_{i+1} - 1$ (see (33)).

We said in the previous subsection that a staircase polygon to $(n+1, m+1)$ is in the augmented second octant iff the bottom path b stays weakly above $y = x - 1$. To keep b weakly above $y = x - 1$ we need $i - 1 \geq y_i - i$, i.e., $y_i + 1 \leq 2i$ for $i = 1, \ldots, m+1$. In the corresponding lattice path the sequence (s_i, t_i) of left turns must satisfy the condition $i \geq 1 + t_i/2$ for $i = 1, \ldots, m$.

The condition $i \geq t_{i+1}/2$ is equivalent to the restriction that every point (v, w) on the path is reached with at least $w/2$ left turns; equivalently, the path stays weakly below $y = 2x$. From $x - 1 \leq y \leq 2x$ for all points (x, y) on the path follows that the path stays in the augmented third hexadecant. Denote by $h(v, w; i)$ the number of $\{\to, \uparrow\}$-paths from the origin to (v, w) in the augmented third hexadecant with i left turns. We have shown that $h(n+m, n+m; m) = S(n+1, m+1) = O_{m+n}(0, m-n) = 6\frac{(m+n)!(m+n+2)!}{n!(n+1)!(m+2)!(m+3)!}\binom{m-n+3}{3}$ for all $m \geq n$. It is also easy to verify that $h(i, 2i; i) = C_i$, the i-th Catalan number. From $h(k, k; k-n) = O_k(0, k-2n)$

and (8) follows that $C_{\lfloor(k+1)/2\rfloor}C_{\lfloor 1+k/2\rfloor}$ ordinary $\{\rightarrow\uparrow\}$-paths stay in the augmented third hexadecant and end at (k,k) (independent of the number of left turns).

References

[1] André, D. (1887). Solution directe du problème résolu par M. Bertrand, *C. R. Acad. Sci. Paris*, **105**, 436-437.

[2] Biane, P. (1992). Minuscule weights and random walks on lattices, in *Quantum probability & related topics*, (Ed.: L. Accardi), World Sci. Publishing, River Edge, NJ, 51–65.

[3] Bousquet-Mélou, M. (2002). Counting walks in the quarter plane, *Trends in Mathematics*, 49-67, Birkhäuser, Basel.

[4] Csáki, E. (1997). Some results for two-dimensional random walk. *Advances in Combinatorial Methods and Applications to Probability and Statistics* (Ed.: N. Balakrishnan), 115-124, Boston, Birkhäuser.

[5] Conway,A., Delest, M., and Guttmann,A.J. (1997). The number of three-choice polygons. *Math. Comput. Modelling*, **26**, 51-58.

[6] Delest, M.-P. and Fedou, J.M. (1993). Enumeration of skew Ferrer's diagrams, Discrete Math., **112**, 65-79.

[7] Delest, M. and Viennot, G. (1984). Algebraic languages and polyominoes enumeration. *Theor. Comput. Sc.* **34**, 169-206.

[8] Feller, W. (1968). *An Introduction to Probability Theory and its Application.* Wiley, New York.

[9] Fisher, M.E. (1984). Walks, walls, wetting and melting, *J. Stat. Phys.* **34**, 667-729.

[10] Gessel, I.M. and Zeilberger, D. (1992). Random walk in a Weyl chamber, *Proc. Amer. Math. Soc.* **115**, 27-31.

[11] Gessel, I.M. and Viennot, X.G. (1989). Determinants, paths, and plane partitions, preprint, available at http://www.cs.brandeis.edu/~ira

[12] Gessel, I.M. and Viennot, G. (1985). Binomial determinants, paths, and hook length formulae. *Adv. in Math.* 58, 300–321.

[13] Gouyou-Beauchamps, D. (1986). Chemins sous-diagonaux et tableau de Young, in *Combinatoire Enumerative* (Montreal 1985), Lect. Notes Math. **1234**, 112-125.

[14] Grabiner, D.J. (2002). Random walk in an alcove of an affine Weyl group, and noncolliding random walks on an interval, *J. Combin. Theory Ser. A*, **97**, 285-306.

[15] Guy, R.K., Krattenthaler, C. and Sagan, B.E. (1992). Lattice paths, reflections, and dimension changing bijections. *Ars Combinatoria*, **34**, 3-15.

[16] Krattenthaler, C. (2002). Watermelon configurations with wall interaction: exact and asymptotic results. To appear in *J. of Statistical Planning and Inference.*

[17] Krattenthaler, C., Guttmann, A.J. and Viennot, X. G. (2000). Vicious walkers, friendly walkers and Young tableaux II: with a wall, *J. Phys. A: Math. Gen.* **33**, 8835-8866.

[18] Kreweras, G. and Niederhausen, H. (1981). Solution of an enumerative problem connected with lattice paths. *Europ. J. of Combinatorics* **2**, 55-60.

[19] Kreweras, G. (1965). Sur une classe de problèmes liés au treillis des partitions d'entiers, *Cahiers du B.U.R.O.* **6**, 5-105.

[20] Itoh, Y. and Maehara, H. (1998). A variation to the ruin problem. *Mathematica Japonica* **47**, 97-102.

[21] Janse van Rensburg, E.J. (2000). *The Statistical Mechanics of Interacting Walks, Polygons, Animals and Vesicles.* Oxford University Press, Oxford, UK.

[22] Lindström, B. (1973). On the vector representations of induced matroids, *Bull. London Math. Soc.* **5**, 85-90.

[23] McCrea, W.H. and Whipple, F.J.W. (1940). Random paths in two and three dimensions. *Proc. Royal Soc. Edinburgh* **60**, 281-298.

[24] MacMahon, P.A. (1916). *Combinatorial Analysis.* Reprinted by Chelsea, 1960.

[25] Mohanty, S.G. (1979). *Lattice Path Counting and Applications.* Academic Press, New York.

[26] Niederhausen, H. (2003). Enumeration of diffusion walks in the first octant by their number of contacts with the diagonal. Submitted to the *Electronic J. Combin.*

[27] Niederhausen, H. (1998). Planar random walks inside a rectangle, *Congr. Numerantium*, **132**, 125-144.

[28] Niederhausen, H. (2002). Planar walks with recursive initial conditions, *J. of Statistical Planning and Inference*, **101**, 229-253.

[29] Pergola, E., Pinzani, R., Rinaldi, S., and Sulanke, R. A. (2002). A bijective approach to the area of generalized Motzkin paths. *Adv. in Appl. Math.* **28**, 580–591.

[30] Sulanke, R. A. (2001). Bijective recurrences for Motzkin paths, Adv. in Appl. Math. **27**, 627–640.

[31] Zeilberger, D. (1983). Andre's reflection proof generalized to the many-candidate ballot problem, *Discrete Math.*, **44**, 325-326