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LETTER TO THE EDITOR

Exact enumeration of parallel walks on directed lattices

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Abstract. Mutually avoiding pairs of parallel walks on a number of d-dimensional lattices are mapped onto undirected random walks which return to the origin on a projected $(d-1)$-dimensional lattice. Generating functions for the number of such pairs of a given length are thus expressed in terms of standard Green's functions. Directed lattices considered include the directed hypercubic and body-centred hypercubic. The generating function for a directed triangular lattice is also obtained. This work is a generalization of known results for the square lattice.

Consider a crystal lattice in d dimensions with nearest-neighbour bonds which are directed so as to have a positive component along some chosen axis. Figure 1 shows the directed square lattice where the chosen axis is labelled t. In this letter, the generating function for the number of pairs of directed walks which start at the origin and meet again for the first time at distance s in the direction of the chosen axis is expressed in terms of that for undirected random walks on a lattice in d-1 dimensions. Figure 1 shows such a pair meeting at distance $t=s=9$. It may be noted that the directedness constraint makes the walks self-avoiding and the further condition to be imposed is mutual avoidance except at the initial site and the final site visited.

The walk configurations we enumerate are described by Fisher (1984) as reunions of vicious drunks and he solved this problem for an arbitrary number of walkers on the directed square lattice. In Fisher's context the directed walks are the spacetime trajectories of one-dimensional walkers.

Each pair of walks forms a polygon of perimeter p, equal to the sum of the walk lengths, and the enumeration problem is therefore isomorphic to the counting of a subset of the undirected polygons on the chosen d-dimensional lattice. In the case of the hypercubic lattice the subset is known as the staircase polygons. The name derives from the case $d=2$ where each walk is in the form of a staircase (see figure 1). The hypercubic case has recently been solved by Guttmann and Prellberg (1993). The present work gives an alternative derivation of their results and provides an extension to other lattices. In particular we obtain explicit results for the triangular lattice and the body-centred hypercubic lattice.

In the case of the hypercubic and body-centred hypercubic lattices, both members of the walk pair have the same number of steps and the corresponding polygon perimeter $p=2s$ (in figure 1 the polygon has 18 sides). However, for the triangular lattice there are polygons which correspond to walk pairs of different lengths and a two variable generating function is obtained which determines the counts as a function of p and s.

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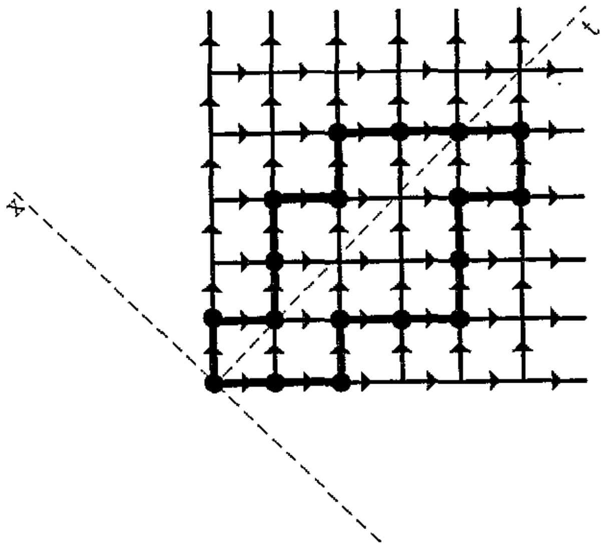

Figure 1. A directed walk pair on the square lattice meeting for the first time after $t=s=9$ steps. The projected walks and the difference walk, referred to in the text, take place along the x-axis and in the figure the projected walks end at $x=-1$. Ignoring the directing gives a staircase polygon of perimeter 18.

For the hypercubic and body-centred hypercubic lattices let $R(u)$ be the generating function for R_s the number of pairs of s-step directed walks which make a reunion for the first time on the last step (R_s is the coefficient u^s in the expansion of $R(u)$). Firstly we note that equation (5) of Guttmann and Prellberg (1993) extends to both types of lattice in the form

$$R(u)=\tfrac{1}{2}(1-ku-Z(u)^{-1}) \tag{1}$$

where $Z(u)$ is the generating function for the number of ordered pairs of directed s-step walks which start at the origin and end at the same lattice point with no other constraint, in particular they may intersect any number of times. The coefficient k is the number of choices for a given walker at each step (d for the d-dimensional hypercubic lattice and 2^{d-1} for the body-centred hypercubic lattice). The origin of equation (1) becomes clear when written in the equivalent form

$$Z(u)=1+(ku+2R(u))Z(u). \tag{1a}$$

The first term on the right counts the zero length walks. All other pairs counted by $Z(u)$ are generated recursively by following any ordered pair of walks having one or more steps, meeting for the first time on the last step, with any pair generated by $Z(u)$ (including the zero length pair). The k pairs of length 1 are generated by ku and the remaining ordered pairs by $2R(u)$. The factor 2 is included since $R(u)$ counts unordered pairs. It will be argued that $Z(u)$ is the generating function for the number of undirected single walks of length $2s$ which return to the origin on a lattice of dimension d-1.

(a) *Body-centred hypercubic lattice.* The result is most easily seen for the body-centred hypercubic lattice for which the single step vectors are

$$B=\{j_1e_1+j_2e_2+\cdots+j_{d-1}e_{d-1}+e_d|j_n=\pm1, n=1,\ldots,d-1\} \tag{2}$$

where $\{e_1, e_2, \ldots, e_d\}$ is the standard orthonormal basis with e_i parallel to the ith Cartesian axis. Projecting these vectors onto a plane perpendicular to the symmetry direction e_d is equivalent to subtracting e_d from each vector and the resulting projected vectors are the possible step vectors of a walk on the undirected body-centred hypercubic lattice in d-1 dimensions. There is thus a bijection between the ordered pairs of parallel s-step directed walks contributing to $Z(u)$ and the $2s$-step undirected walks which return to the origin on the d-1 dimensional lattice. The mapping is obtained by reversing the steps of the second walk on the directed lattice. We conclude that

$$Z_{\mathrm{bchc}}(d, u) = G_{\mathrm{bchc}}(d-1, u) \tag{3}$$

where the coefficient of u^s in $G_{\mathrm{bchc}}(d-1, u)$ is the number of walks which return to the origin in $2s$-steps on the undirected body-centred hypercubic lattice in d-1 dimensions. For $d=2$ the directed lattice is the square lattice of figure 1 with e_1 parallel to the x-axis and e_2 parallel to the t-axis. The projected walks in this case are along the x-axis and we obtain the result for the directed square lattice in terms of the generating function for undirected one-dimensional random walks which return to the origin (Feller 1967).

$$Z_{\mathrm{sq}}(u) = Z_{\mathrm{bchc}}(2, u) = G_{\mathrm{chain}}(u) = (1-4u)^{-1/2} \tag{4}$$

which gives

$$R_{\mathrm{sq}}(u) = [1-2u-(1-4u)^{1/2}]/2 \tag{4a}$$

$$= u^2 + 2u^3 + 5u^4 + 14u^5 + 42u^6 + \cdots \tag{4b}$$

in agreement with Guttmann and Prellberg equation (9). For $d=3$ and 4, $G_{\mathrm{bchc}}(d-1, u)$ is the generating function for returns to the origin on the undirected square and body-centred cubic lattices respectively (which arise in the context of Green's functions for solid state physics). These may be expressed in terms of the complete elliptic integral $K(m)$ (Montroll and Weiss 1965, Joyce 1971) defined by

$$K(m) = \int_0^{\pi/2} (1 - m \sin^2\theta)^{-1/2}\, \mathrm{d}\theta \tag{5}$$

thus

$$Z_{\mathrm{bcc}}(u) = Z_{\mathrm{bchc}}(3, u) = G_{\mathrm{sq}}(u) = (2/\pi)K(16u) \tag{6}$$

$$R_{\mathrm{bcc}}(u) = 10u^2 + 88u^3 + 938u^4 + 11032u^5 + 137784u^6 + \cdots \tag{6a}$$

$$Z_{\mathrm{bchc}}(4, u) = G_{\mathrm{bcc}}(u) = [(2/\pi)K(\tfrac{1}{2} - \tfrac{1}{2}(1-64u)^{1/2})]^2 \tag{7}$$

$$R_{\mathrm{bchc}}(u) = 76u^2 + 2528u^3 + 102860u^4 + 4652576u^5 + 224702112u^6 + \cdots \tag{7a}$$

(b) *Hypercubic lattice.* Walks on the directed hypercubic lattice have the single step vectors $\boldsymbol{B} = \{e_1, e_2, \ldots, e_d\}$ and the symmetry direction is $\boldsymbol{e} = e_1 + e_2 + \cdots + e_d$. Let f_i be the projection of e_i on to a plane perpendicular to $\boldsymbol{e}$. The f_i are the step vectors for walks on a cyclically directed hypertriangular lattice in d-1 dimensions. This lattice has directed cycles but no preferred direction and for $d=3$ has been considered by Blease (1977) in the context of percolation theory. Projection alone is therefore not sufficient to reduce the problem to one of counting undirected walks and we further resort to the idea of Fisher (1984) of considering the difference walk.

The basic idea is simply illustrated by the case of the directed square lattice (figure 1). Let x_1 and x_2 be the coordinates of the two walkers perpendicular to $\boldsymbol{e}$ (the coordinates relative to the x-axis in figure 1), the difference walker is a one-dimensional walker with coordinate $x=x_2-x_1$. At each time step the value of x either increases by 2, decreases by 2 or stays the same (in one of two ways) if the two walkers move parallel to one another. In the latter case the difference walker will be said to hop. Whenever the two walkers meet up the difference walker is at $x=0$, so that to determine Z we must count difference walks which start at and return to the origin and visit only points with even x coordinate. If we give weight u to each step of the difference walk and ignore the hops then the generating function for difference walks is $G_{\text{chain}}(u^2)$ where G_{chain} is defined above. To allow for the hops we must include a factor $1/(1-2u)$ for each site visited by the difference walk and we obtain

$$Z_{\text{sq}}(u)=G_{\text{chain}}(u^2/(1-2u)^2)/(1-2u)=(1-4u)^{-1/2} \tag{8}$$

as before. The additional factor of $1/(1-2u)$ allows for there being $s+1$ sites in a walk of s steps.

For the general hypercubic lattice the possible steps for the difference walker are $\boldsymbol{D}=\{\boldsymbol{f}_i-\boldsymbol{f}_j|i,j=1,\ldots,d\}$. The steps in which the walkers move parallel to one another give zero displacement for the difference walker and there are therefore d zero vectors in $\boldsymbol{D}$ for which the difference walker hops. Now imagine that the vectors $\boldsymbol{B}$ are located at the origin then the ends of these vectors are at the vertices of a $(d-1)$-dimensional regular simplex (hypertriangle). There are two oppositely directed non-zero vectors in $\boldsymbol{D}$ corresponding to each of the $\frac{1}{2}d(d-1)$ edges of this simplex and these are the nearest neighbour vectors of a $(d-1)$-dimensional hypertriangular lattice of coordination number $d(d-1)$. The difference walker therefore moves on this undirected hypertriangular lattice. The generating function for the number of ordered walk pairs on the directed hypercubic lattice which start at the origin and meet up on the last step is therefore

$$Z_{\text{hc}}(d,u)=G_{\text{ht}}(d-1,u/(1-du))/(1-du). \tag{9}$$

Here $G_{\text{ht}}(d-1,x)$ is the generating function for random walks on the undirected hypertriangular lattice which return to the origin on the last step but may visit the origin any number of times. A walk of s steps is weighted with x^s.

Although the objective of reducing the problem to one of counting undirected walks has been achieved, a further simplification is possible. Consider the $(d-1)$-dimensional hyperdiamond lattice which has two sublattices A and B. Each A site has d neighbouring B sites which are reached by the vectors $\{\boldsymbol{f}_1,\boldsymbol{f}_2,\ldots,\boldsymbol{f}_d\}$, above and each B site has d neighbouring A sites reached by the vectors $\{-\boldsymbol{f}_1,-\boldsymbol{f}_2,\ldots,-\boldsymbol{f}_d\}$. This undirected lattice has coordination number d. Suppose that the origin is on the A sublattice then after an even number of steps a walker will still be on the same sublattice. In particular the walks which return to the origin have an even number of steps $s=2t$ and each such walk may be considered as a sequence of 2-step moves on the A sublattice. Since each 2-step move uses one step vector from the A sublattice and one from the B sublattice the possible two step moves are $(\boldsymbol{f}_i-\boldsymbol{f}_j|i,j=1,\ldots,d\}$ which are exactly the same as for the difference walker above. Hence the number of t-step difference walks which return to the origin is equal to the number of $2t$-step walks which return to the origin on the $(d-1)$-dimensional hyperdiamond lattice, since they are both equal to the numbers of walks with hops on the hypertriangular lattice. We conclude that

$$Z_{\mathrm{hc}}(d,u)=G_{\mathrm{hd}}(d-1,u). \tag{10}$$

For $d=3$ and 4 the $(d-1)$-dimensional hyperdiamond lattice is the honeycomb lattice and the standard diamond lattice respectively. For the honeycomb lattice the Green's function $G_{\mathrm{hon}}(u)$ can be expressed in terms of the elliptic integral $K(m)$ (Horiguchi 1972) which together with (10) yields

$$Z_{\mathrm{cubic}}(u)=G_{\mathrm{hon}}(u)=(1-u^{1/2})^{-3/2}(1+3u^{1/2})^{-1/2}(2/\pi)K(m) \tag{11}$$

where

$$m=16u^{3/2}(1-u^{1/2})^{-3}(1+3u^{1/2})^{-1}. \tag{12}$$

Similarly the diamond lattice Green's function can be expressed as a product of two elliptic integrals (Iwata 1969, Joyce 1973). Hence, from (10) the generating function for walk pairs on the 4-dimensional hypercubic lattice is

$$Z_{\mathrm{hc}}(4,u)=G_{\mathrm{dia}}(u)=(2/\pi)^2K(m_+)K(m_-) \tag{13}$$

where

$$m_\pm=\tfrac{1}{2}\pm 8u(1-4u)^{1/2}-\tfrac{1}{2}(1-8u)(1-16u)^{1/2}. \tag{14}$$

The result for $d=4$ is the same as that obtained by Guttmann and Prellberg (1993) but for $d=3$ their result may be written

$$Z_{\mathrm{cubic}}(u)=(1-9u)^{-1/2}(1-u)^{-1/2}(2/\pi)[K(m_+)K(m_-)]^{1/2} \tag{15}$$

where

$$1-2m_+=(1-u)^{-1/2}(1-9u)^{-3/2}(1+18u-27u^2) \tag{16}$$

and

$$1-2m_-=(1-u)^{-3/2}(1-9u)^{-1/2}(1-6u-3u^2). \tag{17}$$

This is not obviously the same as (11) but may be shown to be so (Joyce and Essam 1993). Equation (9) also yields results (11) and (13) by using the G functions for the triangular (Horiguchi 1972) and face centred cubic lattices (Iwata 1969, Joyce 1972) respectively.

(c) *Hyperdiamond lattice.* A generalization of the directed honeycomb lattice to d dimensions may be obtained by expanding the directed hypercubic lattice along its symmetry axis $\boldsymbol{e}$ via the duplication of each layer of atoms perpendicular to this direction and the insertion of additional connecting bonds directed parallel to $\boldsymbol{e}$. For $d=3$ this gives the diamond lattice. The generating function for walk pairs on this hyperdiamond lattice is

$$R_{\mathrm{hd}}(d,u)=R_{\mathrm{hc}}(d,u^2)/u. \tag{18}$$

For the directed honeycomb lattice ($d=2$) the explicit formula (4*a*) for the square lattice yields

$$\begin{aligned}R_{\mathrm{hon}}(u)=R_{\mathrm{sq}}(u^2)/u&=[1-2u^2-(1-4u^2)^{1/2}]/(2u)\\&=u^3+2u^5+5u^7+14u^9+42u^{11}+\cdots.\end{aligned} \tag{19}$$

(d) *Triangular lattice*. The single step vectors for the triangular lattice are $e=(2,0)$, $e_+=(1,3^{1/2})$ and $e_-=(1,-3^{1/2})$ where e is parallel to the z-axis. Define $R(u,w)$ by

$$R(u,w)=\sum_{s,p} R_{sp}u^s w^0 \tag{20}$$

where R_{sp} is the number of walk pairs which meet at $z=s$ and correspond to a polygon of perimeter p. The extension of equation (1) is

$$R(u,w)=\tfrac{1}{2}(1-2uw^2-u^2w^2-Z(u,w)^{-1}) \tag{21}$$

where again Z is the generating function for ordered pairs of walks which start at the origin and are together on the last step. Z will be determined by the difference walker technique as in the second approach to the square lattice.

It is convenient to write $e_1=e/2$ and split steps in this direction into two so that all steps progress unit distance in the z direction and s then becomes the number of steps (see figure 2(a)). The price to be paid for this is that there are now two types of site, the original sites (A-type, white) and the newly introduced interstitial sites (type-B, black). The steps available to the one-dimensional difference walker depend on the types of site currently occupied by the two directed walkers. If both are on B sites then after the next step both must be on A sites and there is no change in relative position. If one is on A and one is on B then there are three possible next positions: both move to A sites with either an increase or decrease of $\sqrt{3}$ in relative distance, or one moves from A to B and the other from B to A with no change in relative position. Lastly if both are on A sites there are nine next possible next positions. In four of these both stay on A sites and the relative distance either increases or decreases by $2\sqrt{3}$ or stays

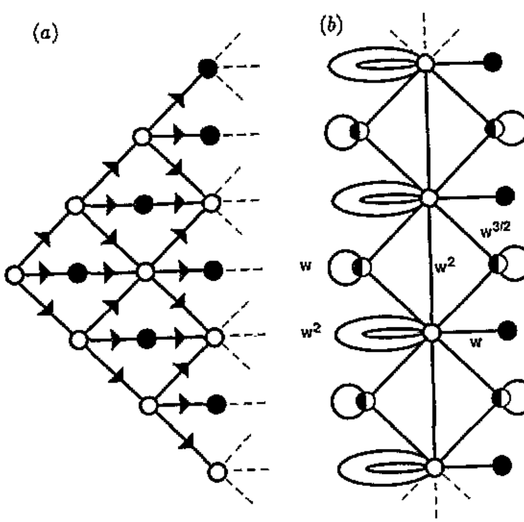

Figure 2. (a) Directed triangular lattice showing the original A-sites (white) and the added interstitial B-sites (black). (b) The one-dimensional lattice on which the difference walker moves. The three types of site correspond to both walkers on A-sites (white), both on B-sites (black) and one walker on each type of site (black and white). Steps may be made in both directions along the bonds but the loops attached to the vertices correspond to hops. All steps are given a weight u but a further power of w must be included depending on the type of bond, as shown.

the same in two ways (these are the square lattice moves). Both can move to B sites with no change in relative position. In the four remaining cases one walker moves to an A site and the other to a B site and the relative distance can increase or decrease by $\sqrt{3}$. The possible moves of the relative walker and the weights to be attached to each step are shown in figure 2(b). From this it is clear that the required configurations can be enumerated by renormalizing both the sites and bonds of the simple one-dimensional walker. From (4) we obtain

$$Z(u, w)=v(1-4(xv)^2)^{-1/2} \tag{22}$$

where

$$x=w^2u+2w^3u^2/(1-wu) \tag{23}$$

$$v=[1-2w^2u-w^2u^2-4w^3u^2/(1-wu)]^{-1}. \tag{24}$$

This yields the explicit formula

$$Z(u, w)=(1+uw)^{-1}(1-2uw-4uw^2+w^2u^2)^{-1/2}. \tag{25}$$

Combining this with (21) and expanding we obtain

$$R(u, w)=2u^2w^3+(u^2+2u^3)w^4+(4u^3+2u^4)w^5+(2u^3+9u^4+2u^5)w^6 + (12u^4+16u^5+2u^6)w^7+\cdots. \tag{26}$$

The generating function for the polygons grouped by perimeter has the expansion

$$R(1, w)=2w^3+3w^4+6w^5+13w^6+30w^7+72w^8+178w^9+450w^{10}+1158w^{11} +3023w^{12}+\cdots. \tag{27}$$

A generalization of these results to a directed hypertriangular lattice is clearly possible using the difference walker technique but the result would be quite complex and will not be attempted here.

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References

Blease J 1977 *J. Phys. C: Solid State Phys.* **10** 917–24
Feller W 1967 *An introduction to probability theory, 3rd edition* Vol 1 (New York: John Wiley)
Fisher M E 1984 *J. Stat. Phys.* **34** 665–729
Horiguchi T 1972 *J. Math. Phys.* **13** 1411–9
Guttmann A J and Prellberg T 1993 *Phys. Rev.* A **47** 2233
Iwata G 1969 *Natl. Sci. Rep.* Ochanomizu University, Tokyo **20** 13–8
Joyce G S 1971 *J. Phys. C: Solid State Phys.* **4** L53–6
Joyce G S 1973 *Phil. Trans. Roy. Soc. Lond.* **273** 583–610
Joyce G S and Essam J W 1993 *J. Phys. A: Math. Gen.* to be submitted
Montroll G W and Weiss G H 1965 *J. Math. Phys.* **6** 167–81