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Two-dimensional self-avoiding walks

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A weighted random walk is considered on regular two-dimensional lattices. The weight 1 corresponds to the free random walk and the weight 0 to the walk performed in the combinatorial solution of the Ising model. It is argued that the walk with weight $\frac{1}{2}$ might have the same connective constant as the self-avoiding walk. This is shown for the honeycomb lattice. For the square lattice the connective constant is in good agreement with recent estimates. For the triangular lattice, where the construction of the walk is not unique, a "natural" choice results in fair agreement with these estimates.

Subject to some plausible arguments Nienhuis[1] recently analytically calculated the connective constant and some critical exponents and conjectured another for the problem of the self-avoiding walk (SAW) on the honeycomb lattice. His results for the exponents have also been obtained by Dotsenko and Fateev[2] by finding the conformal algebra for the $O(n)$ model. Nienhuis's results prompted Guttmann[3] to extend and reexamine available data[4] pertaining to the square- and triangular-lattice SAW problem, thereby obtaining new estimates of the connective constant for these lattices. These new estimates make the old conjecture by Guttmann and Sykes[5] that the sum of the connective constants of the SAW on the honeycomb lattice (μ_H) and on the triangular lattice (μ_T) equals 6 exactly unlikely. In this paper we report on the construction of a restricted random walk on the three regular two-dimensional (2D) lattices, the generating function of which turns out to have the same radius of convergence (inverse connective constant) for the honeycomb lattice as that obtained by Nienhuis.[1] Actually Nienhuis[1] studied $O(n)$ classical spin models and obtained $\mu_H(n)=(2+\sqrt{2-n})^{1/2}$ for $-2\leq n\leq 2$, where $n=1$ corresponds to the Ising model and $n=0$ to the SAW problem. The restricted walk we are considering is actually also connected to the Ising model in the respect that we assign weights to the walk, the weight 0 corresponding to an Ising walk and the weight 1 corresponding to a free random walk. The weight $\frac{1}{2}$ is what we assign to the restricted walk. Except for recovering the Nienhuis value $\mu_H=(2+\sqrt{2})^{1/2}$ for the honeycomb lattice we obtain $\mu_S=2.637\,866\,464\ldots$ for the square lattice and $\mu_T=4.149\,080\,321\ldots$ for the triangular lattice.

We now describe the restricted walk, but in order to do so we first define what is meant by an Ising walk. The combinational solution of the 2D Ising model due to Kac and Ward[6,7] solves the problem of finding all Euler cycles of given length in the lattice graph by performing a walk on the lattice. We illustrate our reasoning with the square lattice. Let us say we start out from some point on the lattice with a step to the right. If the next step is in the same direction its weight is one, if instead a left turn is made its weight is α, and if a right turn is made its weight is α^{-1}, where $\alpha=e^{i\pi/4}$. Immediate backsteps are forbidden. If written in matrix form we obtain

$$M_S=\begin{pmatrix}1 & 0 & \alpha & \alpha^{-1}\\ 0 & 1 & \alpha^{-1} & \alpha\\ \alpha^{-1} & \alpha & 1 & 0\\ \alpha & \alpha^{-1} & 0 & 1\end{pmatrix} .$$

If this matrix is iterated n times, this gives us the number of walks of length $n+1$. For example, the element in the first row and first column in the iterated matrix gives the number of walks of length $n+1$ which start with a step to the right and end with a step to the right, weighted according to the prescription. Concentrating on this element $a_{11}^{(n+1)}$ it is easy to prove that the same result is obtained by, instead of using the weight $\alpha^{\pm 1}$, putting $a_{12}^{(n)}=0$. That is, no walks which turn back are allowed, which leads to the following recurrence relations:

$$\begin{aligned} a_{11}^{(n+1)}&=a_{11}^{(n)}+2a_{13}^{(n)} ,\\ a_{12}^{(n+1)}&=w(a_{12}^{(n)}+2a_{13}^{(n)}) ,\\ a_{13}^{(n+1)}&=a_{11}^{(n)}+a_{12}^{(n)}+a_{13}^{(n)} ,\end{aligned} \tag{1}$$

with $w=0$. Here we have used the symmetry $a_{14}^{(n)}=a_{13}^{(n)}$. This gives us immediately (for $w=0$) $a_{11}^{(n+1)}/a_{11}^{(n)}\rightarrow\sqrt{2}+1$ for $n\rightarrow\infty$, which is the inverse critical radius for the 2D square Ising model, i.e., $\tanh(J/kT_c)=(\sqrt{2}+1)^{-1}$. This defines what we will call the Ising walk. For $w=1$, which corresponds to a free random walk, we obtain, of course, $a_{11}^{(n+1)}/a_{11}^{(n)}\rightarrow 3$ for $n\rightarrow\infty$. The Ising walk, which does not allow any backturns, could be said to be obtained by putting the weight zero on every backturning edge on the free random walk, which in its turn has the weight one on each such edge. The restricted random walk we now define by assigning instead the weight $\frac{1}{2}$ to a backturning edge. If several backturns are followed by each other the first is given the weight $\frac{1}{2}$, the second the weight $(\frac{1}{2})^2$, and the kth the weight $(\frac{1}{2})^k$. This recipe has the consequence (for all lattices treated here and not only for the square lattice) that the first crossover of the SAW is correctly accounted for. This is illustrated in Fig. 1. Therefore, we might hope that the series so constructed has the same radius of convergence as the SAW series, although the exponent is not the same.

We begin by showing that this is actually so for the honeycomb lattice, the only one for which the connective constant is exactly known. We first derive the Ising walk. The matrix M_H describing this walk has its first row given[7] by $(0\ 0\ \alpha\ 0\ 0\ \alpha^{-1})$ where $\alpha=e^{i\pi/6}$. It is defined with respect to the axes given in Fig. 2, so the row index running from 1 to 6 corresponds to ϕ, $\bar{\phi}$, ξ, $\bar{\xi}$, η, $\bar{\eta}$ in this order, and the same for the column indices. For example, the third element in the first row means that if we start out with

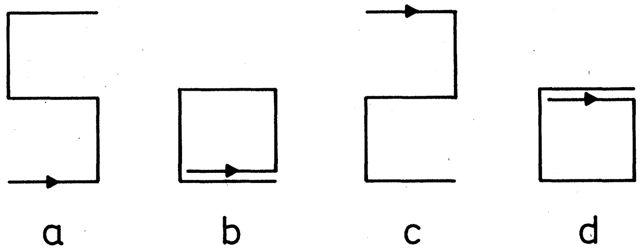

FIG. 1. There are on the square lattice 21 walks per lattice site of length 5 starting and ending with a step to the right. Of these, two are not self-avoiding, those marked b and d in the figure. The recipe gives these, as well as the walks denoted a anc c, weight $\frac{1}{2}$, thereby giving in total $17+4(\frac{1}{2})=19$ restricted random walks, which agrees with the number of SAW's.

a step in the ϕ direction and then make a step in the ξ direction the weight caused by this change of direction is α. Iterating the matrix M_H n times gives the number of weighted walks of length $n+1$. Concentrating on the element $(M)^n_{\phi,\phi}$ we get for this element $2,6,18,\ldots$ for $n=2,4,6,\ldots$. (The free random walk corresponds, of course, to $\alpha=1$, resulting in the ϕ,ϕ element being 2,6,22 for $n=2,4,6$.) The important thing about iterating the matrix M is that the $\phi,\bar{\phi}$ element is zero in all orders and it is easily proven that the same sequence is obtained for the ϕ,ϕ element by putting the weight zero on backturning edges and putting $\alpha\equiv 1$. That is, the recurrence relations are the following:

$$
\begin{aligned}
a_{11}^{(n+1)} &= 2a_{13}^{(n)} \ , \\
a_{12}^{(n+1)} &= 2wa_{14}^{(n)} \ , \\
a_{13}^{(n+1)} &= a_{11}^{(n)} + a_{14}^{(n)} \ , \\
a_{14}^{(n+1)} &= a_{12}^{(n)} + a_{13}^{(n)} \ ,
\end{aligned}
\tag{2}
$$

with $w=0$. (The symmetry $a_{13}^{(n)}=a_{16}^{(n)}$ and $a_{14}^{(n)}=a_{15}^{(n)}$ has been used.) The recurrence relation gives $a_{1j}^{(n+1)}/a_{1j}^{(n)} \rightarrow \sqrt{3}$ for $n\rightarrow\infty$. This is the Ising walk for the honeycomb lattice. Now the restricted random walk puts the weight $\frac{1}{2}$ on each backturning edge, that is, each edge in the $\bar{\phi}$ direction if the walk starts in the ϕ direction. Due to its connectivity the honeycomb lattice has no two successive edges in the same direction, so in this case we do not have to treat an infinite recurrence relation, so the relation is simply given by Eq. (2) with $w=\frac{1}{2}$. This gives[8] $\mu_H=(2+\sqrt{2})^{1/2}$. That is, our restricted-random-walk series has the same connective constant as the SAW series.

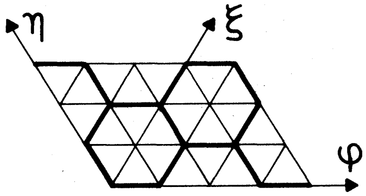

FIG. 2. The system of axes with respect to which the walk matrices M_H and M_T are defined. A bar above the axis symbol means reversed direction, e.g., $\bar{\phi}$ means the negative ϕ direction.

Now we proceed to the square lattice. The Ising walk has already been defined. We now have to deal with an infinite recurrence relation. The recurrence relations for $a_{11}^{(n)}$ and $a_{13}^{(n)}$ are unchanged from Eq. (1). For $a_{12}^{(n)}$ we have a situation where the weight of the nth step depends not only on the last preceding step but on all the preceding steps. The recurrence relations will now be

$$a_{11}^{(n+1)} = a_{11}^{(n)} + 2a_{13}^{(n)} \ , \tag{3a}$$

$$a_{12}^{(n+1)} = 2^{-\mathscr{S}_1} a_{12}^{(3)} + \sum_{k=3}^{n} 2^{-\mathscr{S}_2} 2a_{13}^{(k)} \ , \tag{3b}$$

$$a_{13}^{(n+1)} = a_{11}^{(n)} + a_{12}^{(n)} + a_{13}^{(n)} \ , \tag{3c}$$

where $\mathscr{S}_1=\sum_{i=2}^{n-1} i$ and $\mathscr{S}_2=\sum_{i=1}^{n-k+1} i$.

The relation for a_{12} can be derived as follows. Consider a walk starting with a right step and ending with a left step. Starting with the last step and tracing the walk backwards, we have the possibility that the walk consists of the maximum possible number of left steps, i.e., $n-1$ for a walk of length $n+1$. This gives rise to the first term in the relation for $a_{12}^{(n+1)}$. Otherwise, we have the possibility that the walk after $n+1-k$ left steps counted from the end of the walk, where k ranges from 3 to n, is interrupted by an up or down step. This gives rise to the second term in the relation for $a_{12}^{(n+1)}$. This relation can be simplified by performing the sums in the exponents, resulting in

$$a_{12}^{(n+1)} = 2^{-(n+1)(n-2)/2} + \sum_{k=3}^{n} 2^{-(n-k)(n-k+3)/2} a_{13}^{(k)} \ . \tag{3b$'$}$$

If we define the generating functions

$$g(x) = \sum_{n=3} a_{11}^{(n)} x^n, \quad f(x) = \sum_{n=3} a_{12}^{(n)} x^n \ ,$$

and

$$h(x) = \sum_{n=3} a_{13}^{(n)} x^n \ ,$$

Eq. (3) can be rewritten

$$[g(x)-3x^3]/x = g(x) + 2h(x) \ , \tag{4a}$$

$$[f(x)-x^3]/x = u_0(x) + [u_0(x)/x^2+1]h(x) \ , \tag{4b}$$

$$[h(x)-2x^3]/x = g(x) + f(x) + h(x) \ , \tag{4c}$$

where

$$u_0(x) = \sum_{n=3} 2^{-(n+1)(n-2)/2} x^n \ .$$

The derivation of Eq. (4b) is a little tricky, so we describe it in more detail. Multiply the left-hand member of Eq. (3b$'$) with x^n and sum from $n=3$ to infinity. This gives trivially ($a_{12}^{(3)}=1$) the left-hand member of Eq. (4b). Performing the same summation on the right-hand member of

Eq. (3b′) gives

$$\sum_{n=3} 2^{-(n+1)(n-2)/2}x^n+\sum_{n=3}\left[\sum_{k=3}^{n} 2^{-(n-k)(n-k+3)/2}a_{13}^{(k)}\right]x^n=u_0(x)+\sum_{k=3}\left[\sum_{n=k} 2^{-(n-k)(n-k+3)/2}x^{n-k}\right]a_{13}^{(k)}x^k$$

$$=u_0(x)+\sum_{k=3}\left[\sum_{s=0} 2^{-s(s+3)/2}x^s\right]a_{13}^{(k)}x^k=u_0(x)+[u_0(x)/x^2+1]h(x) \ ,$$

i.e., the right-hand member of Eq. (4b). Solving the system of Eqs. (4a)–(4c), we get

$$g(x)=\frac{3x^3+x^4-x^5-x^3u_0(x)}{1-2x-2x^2+x^3-(1-x)u_0(x)} \ . \tag{5}$$

The inverse of the smallest positive root of the denominator will give us the connective constant μ_S of the restricted random walk. We find $\mu_S=2.637\,866\,464\,58\ldots$.

We now proceed to discuss the restricted random walk on the triangular lattice. As usual, we start with the Ising walk. The matrix M_T describing this walk has its first row given by[7] $(1\ 0\ \alpha\ \alpha^{-2}\ \alpha^2\ \alpha^{-1})$, where $\alpha=e^{i\pi/6}$ and is defined with respect to the same axes as for the honeycomb lattice (see Fig. 2). (The free random walk is, of course, given by $\alpha=1$.) Just as was the case for the other lattices, the effect on the ϕ,ϕ element of iterating this matrix is the same as putting the weight zero on edges turning back into the left half plane and putting $\alpha=1$, i.e., implying the following recurrence relations:

$$a_{11}^{(n+1)}=a_{11}^{(n)}+2a_{13}^{(n)}+2a_{14}^{(n)} \ , \tag{6a}$$

$$a_{12}^{(n+1)}=w(a_{12}^{(n)}+2a_{13}^{(n)}+2a_{14}^{(n)}) \ , \tag{6b}$$

$$a_{13}^{(n+1)}=a_{11}^{(n)}+a_{12}^{(n)}+2a_{13}^{(n)}+a_{14}^{(n)} \ , \tag{6c}$$

$$a_{14}^{(n+1)}=a_{11}^{(n)}+a_{12}^{(n)}+a_{13}^{(n)}+w2a_{14}^{(n)} \ , \tag{6d}$$

with $w=0$. (The symmetry $a_{13}^{(n)}=a_{16}^{(n)}$ and $a_{14}^{(n)}=a_{15}^{(n)}$ has been used.) Note that in contrast to what was the case for the honeycomb and square lattices it is now not enough to put $a_{12}^{(n)}=0$, because walks entering the left half plane can be constructed from repeated steps in the η and $\bar{\xi}$ directions solely. This recurrence relation is simply solved for $w=0$ giving $a_{1j}^{(n+1)}/a_{1j}^{(n)}\to\sqrt{3}+2$ for $n\to\infty$ $(j=1,2,3,4)$ in agreement with $1/\tanh(J/kT_c)=\sqrt{3}+2$ for the critical temperature for the Ising model on the triangular lattice. The fact that w shows up in both Eqs. (6b) and (6d) makes the treatment of the restricted random walk more complicated. First, consider the assignment of weights to backturning edges. For the $\bar{\phi}$ direction this should be unchanged. For the η and $\bar{\xi}$ directions each step means half a step projected on the $\bar{\phi}$ axis. A prescription which leaves the assignment of weights to steps along the $\bar{\phi}$ axis unchanged, still gives all weights in powers of two, and gives the same total weight to a backturning walk from A to B, irrespective of the specific route taken (as long as it consists of steps in the $\bar{\phi}$, η, and $\bar{\xi}$ directions) is, if l is the number of backsteps, and a step in the η or $\bar{\xi}$ directions counts as half a backstep, that the total weight of such a sequence of l consecutive backsteps, $w(l)$, is given by the product of the first $2l$ factors in the product $1\times\frac{1}{2}\times\frac{1}{2}\times\frac{1}{2}\times\frac{1}{4}\times\frac{1}{4}\times\frac{1}{4}\times\frac{1}{4}\times\frac{1}{8}\ldots$. If we write $2l-1=4n+k$, where $k=2l-1 \pmod 4$, it is easily shown that

$$w(l)=2^{-(n+1)(2n+k)} \ . \tag{7}$$

A treatment similar to that performed for the square lattice gives, for the generating function $f(x)=\sum_{n=4}a_{11}^{(n)}x^n$,

$$f(x)=\frac{x^2+2x^3-2x^4-2x^5+4x^2u_4+2x^3(2u_2+u_3-u_1-2u_4)+4x^4(u_2-u_1-u_4)+8x^3(u_2u_3-u_1u_4)}{1-3x-4x^2+2x^3+2x^4-2x(u_1+2u_4+u_3)+2x^2(u_1+2u_4-u_3-2u_2)+4x^3(u_1+u_4-u_2)-8x^2(u_2u_3-u_1u_4)} \ , \tag{8}$$

where

$$u_i(x)=\sum_{s=2} t_i(s)x^s \ ,$$

$$t_i(s)=\sum_{t=0}^{s-2}\binom{s-2}{t}2^{s-2-t}w^{(i)}(s,t) \ ,$$

$$w^{(1)}(s,t)=w_2+w_{3/2},\quad w^{(2)}(s,t)=w_{3/2} \ ,$$

$$w^{(3)}(s,t)=w_{3/2}+w_1,\quad w^{(4)}(s,t)=w_1 \ ,$$

and

$$w_\alpha=w[\alpha+t+(s-2-t)/2] \ .$$

We find the connective constant μ_T of the triangular lattice for the restricted random walk to be $\mu_T=4.149\,080\,321\,44\ldots$.

In summary, we have defined a restricted random walk on the regular 2D lattices. The construction of this walk is based on the observation that if the weight zero is assigned to all backturning edges we recover the Ising walk, which by construction is self-avoiding, and the connective constant of which is a lower bound to the connective constant of the SAW. If instead the weight one is assigned to the backturning edges, the free random walk is obtained, the connective constant of which, of course, is an upper bound to that of the SAW. By the choice of one-half for the weight, we find that the restricted random walk correctly reproduces the SAW when the first crossing of walks happens. Furthermore, for the honeycomb lattice the two walks have the same connective constant, $\mu_H=(2+\sqrt{2})^{1/2}$.

This recipe for the random restricted walk has been applied to the square and triangular lattices for which no exact results are known. We obtain $\mu_S=2.637\,866\,4\ldots$, which is in good agreement with Guttmann's Padé-approximant estimate 2.6380 ± 0.0003.[3] For the triangular lattice the obtained value $\mu_T=4.149\,080\,3\ldots$ is very close to, but not within one standard deviation of, Guttmann's Padé-approximant estimate 4.1507 ± 0.0004.[3] (These estimates are subject to the assumption that the exponent $\gamma=\frac{43}{32}$ and that the correction-to-scaling exponent equals 1.) At this point we would like to quote Guttmann, who, after having performed an analysis of the Padé approximants to the logarithmic derivative of the SAW series, finds indications of "a higher value of γ for both the square and honeycomb lattices, though the triangular lattice does not conform to this observation" ($\gamma > \frac{4}{3}$). That is, one possible explanation of the discrepancy between our value for μ_T and Guttmann's estimate is that his error bars are too small; another is the recipe for the restricted random walk on the triangular lattice. We had to extend the recipe for this lattice in order to deal with backsteps along the η and $\bar{\xi}$ directions. The extension made seems natural, but the choice is certainly not unique. (A third possibility is, of course, that the walk treated here and the SAW do not have the same connective constant on the triangular lattice.)

For the connective constant we get, for the honeycomb lattice, a quartic equation, the same as Guttmann's Eq. (5.3), but for the other lattices we get transcendental equations. The fact that we get a quartic equation for the honeycomb lattice is due to its low coordination number. This low coordination number in turn appears to be the reason why Nienhuis's model was solvable on that lattice only.[3] The results obtained are certainly intriguing, and it is hoped that the observations reported here will stimulate research to clarify if the restricted random walk defined here and the SAW have the same connective constant.

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