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An exactly solvable self-avoiding walks model

In-mook Kim†, Agnes S Kim‡ and Sungwoon Kim§

† Department of Physics, Korea University, Seoul, Korea
‡ Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA and (present address) Department of Mechanical Engineering, University of California, Berkeley, CA 94720, USA
§ Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA and (present address) Department of Mathematics, Korea University, Seoul, Korea

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Abstract. A self-avoiding walks model is studied in which the walker is, in addition to the usual self-avoiding condition, restricted not to make any turn which will put the walker in a direction rotated more than Φ_{max} from any of the directions previously taken. Here, $\Phi_{max} < \Phi_R$ where $\Phi_R = 2\pi -$ (the smallest exterior angle of the unit cell of the lattice under consideration).

The generating function for the square lattice is obtained, and various properties such as the number of N-step walks, the total number of steps to given directions and the mean-square end-to-end distance are evaluated analytically. The model exhibits characteristics reminiscent of one-dimensional self-avoiding walks in all directions, while retaining the anisotropic effect of the direction of the first step.

1. Introduction

The mathematical problems of calculating the exact analytical properties of the self-avoiding walks (SAW) are formidable. In efforts to circumvent the difficulties, a number of modified SAW models have been actively investigated. Most notable examples are the spiral SAW (SSAW) and the directed SAW (DSAW).

In SSAW, turns to specific directions are prohibited, in addition to the usual self-avoiding condition. The model has been solved for the square lattice ([1-7]) and for the triangular lattice ([8-12]). Due to the very nature of the model, the walker cannot double back and the resulting walks are very compact. The model exhibits different critical behaviour in square and triangular lattices.

In DSAW, steps to specific directions are prohibited. The two-choice and three-choice DSAW in square and triangular lattices and the four-choice DSAW in the triangular lattice have been solved analytically ([13-16]). The most obvious shortcoming of the model is that the walker cannot reach certain quarters of the plane. The five-choice DSAW in the triangular lattice, in which the walker may reach any quarter of the plane, has not been solved analytically. DSAW exhibit mixed behaviour, displaying characteristics reminiscent of one-dimensional self-avoiding walks in certain directions and random-walk-like characteristics in other directions.

In this paper a model is studied in which all self-avoiding steps are allowed except turns which will put the walker in a direction rotated by an angle greater than $\pm\Phi_{max}$ from any of the directions previously taken (see figure 1). The Φ_{max} is the maximum angle of rotation, measured from any of the directions taken previously, the walker

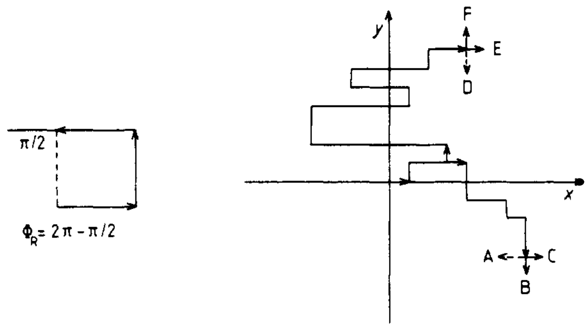

Figure 1. In the square lattice, $\Phi_R = \frac{3}{2}\pi$. With the restriction $\Phi_{max} < \Phi_R$, the maximum angle of rotation the walker may take in the square lattice is $\Phi_{max} = \pi$. The walks leading to A and D are not permissible in the model since the last steps are rotated by more than Φ_{max} from the directions previously taken, while the walks to B, C, E and F are permissible.

may take in the lattice under the consideration, not violating the restriction $\Phi_{max} < \Phi_R$. Here, $\Phi_R = 2\pi -$ (the smallest exterior angle of the unit cell of the lattice under consideration). In the expression, 2π represents the total exterior angle of the unit cell. For the square lattice $\Phi_R = \frac{3}{2}\pi$ and $\Phi_{max} = \pi$. The model is amenable to exact analytic treatment. In the following section, the generating function for the square lattice is obtained, and various properties such as the number of N-step walks, the total number of steps to given directions and the mean square end-to-end distance are evaluated. In this model, the walker may reach any quarter of the plane, and exhibits the characteristics of a one-dimensional self-avoiding walk in all directions. A similar model has been considered previously, but for a very limited set of paths ([17]).

2. The exact solutions for the square lattice

The generating function for the walks in the square lattice may be obtained from other generating functions of simpler walks:

$$G_1(x_+) = \frac{1}{1 - x_+} \tag{1a}$$

$$G_1(x_+, x_-) = \frac{1 - x_+ x_-}{(1 - x_+)(1 - x_-)} \tag{1b}$$

$$G_2(x_+, y_+) = \frac{1}{1 - (x_+ + y_+)} \tag{1c}$$

$$G_3(x_+ | y_+, y_-) = \frac{G_1(y_+, y_-)}{1 - x_+ G_1(y_+, y_-)}. \tag{1d}$$

$G_1(x_+)$ is the generating function of one-dimensional SAW restricted to the x_+ direction, while in $G_1(x_+, x_-)$ both the x_+ and x_- directions are permitted. $G_1(x_+, x_-)$ is symmetric in x_+ and x_-. $G_2(x_+, y_+)$ is the generating function of the two-choice DSAW in the square lattice in which the walker is restricted only to take either the x_+ or the y_+ direction. The function is symmetric in x_+ and y_+. $G_3(x_+ | y_+, y_-)$ is the generating function of the three-choice DSAW in the square lattice in which the walker is restricted to take steps only in the y_+, y_- and x_+ directions. The function is symmetric with respect to y_+ and y_-.

In this model, for the symmetry reasons, it is sufficient to consider only the walks which start out in the x_+ direction. In the following, all the properties obtained are only for the walks started out in the x_+ direction. Let us suppose the walker takes the y_+ direction after the initial steps in the x_+ direction. Up to this point, the walks are represented by $x_+G_1(x_+)y_+$. After these steps, if the walker never takes any step in the y_- direction, the walks become three-choice DSAW permitted to take steps in the x_+, x_- and y_+ directions and the walks are represented by $x_+G_1(x_+)y_+G_3(y_+|x_+, x_-)$.

On the other hand, if the walker is to take any steps in the y_- direction it must take steps in the x_+ direction first before the y_- steps. After the first y_- steps, the walker may take steps in the y_+, y_- and x_+ directions. The walks would be three-choice DSAW in the y_+, y_- and x_+ directions, minus all the walks not having any steps in the y_- direction. The walks are represented by $x_+G_1(x_+)y_+G_1(y_+)x_+(G_3(x_+|y_+, y_-) - G_2(x_-, y_+))$.

From the symmetry consideration, we get similar forms for the walks turned to the y_- direction after the initial steps in the x_+ direction by simply exchanging y_+ and y_-. Therefore, the generating function for the walks started out in the x_+ direction in the square lattice is given by

$$\begin{aligned} G(x_+|x_-|y_+, y_-) &= [G_1(x_+) - 1] + x_+G_1(x_+)[y_+G_3(y_+|x_+, x_-) \\ &\quad + y_+G_1(y_+)x_+(G_3(x_+|y_+, y_-) - G_2(x_+, y_+))] \\ &\quad + x_+G_1(x_+)[y_+G_3(y_-|x_+, x_-) \\ &\quad + y_-G_1(y_-)x_+(G_3(x_+|y_-, y_+) - G_2(x_+, y_-))]. \end{aligned} \tag{2}$$

The generating function is symmetric in y_+ and y_-.

To obtain the total number of N-step walks a_N, we evaluate the contour integral

$$a_N = \frac{1}{2\pi i}\oint \frac{dz}{z^{N+1}}[G(x_+|x_-|y_+, y_-)]_{x_+=x_-=y_+=y_-=z} \tag{3}$$

along a small circle around the origin. The integral reduces to

$$a_N = \frac{1}{2\pi i}\oint \frac{dz}{z^{N+1}} \frac{z(1-z)}{(1-2z)(1-2z-z^2)}. \tag{4}$$

It is only necessary to evaluate the residues at $z = \frac{1}{2}$ and $-1 \pm \sqrt{2}$. The result is

$$a_N = \tfrac{1}{2}(1+\sqrt{2})^{N+1} + \tfrac{1}{2}(1-\sqrt{2})^{N+1} - 2^N. \tag{5}$$

Similarly, the total number of steps in the x_+, x_-, y_+ and y_- directions in the ensemble of the N-step walks may be obtained by evaluating

$$b_N^{(X_+)} = \frac{1}{2\pi i}\oint \frac{dz}{z^{N+1}}\left(x_+ \frac{\partial}{\partial x_+} G(x_+|x_-|y_+, y_-)\right)_{x_+=x_-=y_+=y_-=z} \tag{6}$$

and similar integrals. The results are:

$$\begin{aligned} b_N^{(x_+)} &= \tfrac{1}{8}(1+\sqrt{2})^{N+1}[\sqrt{2}\,N + (6-2\sqrt{2})] \\ &\quad + \tfrac{1}{8}(1-\sqrt{2})^{N+1}[-\sqrt{2}\,N + (6+2\sqrt{2})] - 2^{N-1}(N+1) - \tfrac{1}{2} \end{aligned} \tag{7a}$$

$$b_N^{(x_-)} = \tfrac{1}{8}(1+\sqrt{2})^{N+1}[(2-\sqrt{2})N - \sqrt{2}] + \tfrac{1}{8}(1-\sqrt{2})^{N+1}[(2+\sqrt{2})N + \sqrt{2}] + \tfrac{1}{2} \tag{7b}$$

$$\begin{aligned} b_N^{(y_+)} = b_N^{(y_-)} &= \tfrac{1}{16}(1+\sqrt{2})^{N+1}[2N - (6-3\sqrt{2})] \\ &\quad + \tfrac{1}{16}(1-\sqrt{2})^{N+1}[2N - (6+3\sqrt{2})] - 2^{N-2}(N-1). \end{aligned} \tag{7c}$$

The average number of the steps in given directions may be obtained by dividing them by a_N. We list only the asymptotic expressions as $N \to \infty$:

$$\langle x_+\rangle \sim \tfrac{1}{4}[1+(\sqrt{2}-1)]N \tag{8a}$$

$$\langle x_-\rangle \sim \tfrac{1}{4}[1-(\sqrt{2}-1)]N \tag{8b}$$

$$\langle y_+\rangle = \langle y_-\rangle \sim \tfrac{1}{4}N. \tag{8c}$$

Both $\langle x_+\rangle$ and $\langle x_-\rangle$ are proportional to N, but there are more x_+ steps than x_- steps due to the fact that the walks started out in the x_+ direction.

To obtain the mean-square end-to-end distance, we need

$$C_N = \frac{1}{2\pi i}\oint \frac{dz}{z^{N+1}}\left\{\left[\left(x_+\frac{\partial}{\partial x_+}\right)^2 - 2\left(x_+\frac{\partial}{\partial x_+}\right)\left(x_-\frac{\partial}{\partial x_-}\right) + \left(x_-\frac{\partial}{\partial x_-}\right)^2 + \left(y_+\frac{\partial}{\partial y_+}\right)^2 - 2\left(y_+\frac{\partial}{\partial y_+}\right)\left(y_-\frac{\partial}{\partial y_-}\right) + \left(y_-\frac{\partial}{\partial y_-}\right)^2\right] G(x_+|x_-|y_+,y_-)\right\}_{x_+=x_-=y_+=y_-=z} \tag{9}$$

$$= c_N^{(x_+^2)} - 2c_N^{(x_+x_-)} + c_N^{(x_-^2)} + c^{(y_+^2)} - 2c_N^{(y_+y_-)} + c_N^{(y_-^2)}. \tag{10}$$

The calculations are straightforward, but they are long and tedious. To save any repetition of the calculation by others, we give the entire results:

$$c_N^{(x_+^2)} = \tfrac{1}{64}(1+\sqrt{2})^{N+1}[(-4+6\sqrt{2})N^2+(38-10\sqrt{2})N+(10+3\sqrt{2})] + \tfrac{1}{64}(1-\sqrt{2})^{N+1}[(-4-6\sqrt{2})N^2+(38+10\sqrt{2})N+(10-3\sqrt{2})] - 2^{N-2}N(N+3) - \tfrac{1}{2}(N+1) \tag{11a}$$

$$c_N^{(x_-^2)} = \tfrac{1}{64}(1+\sqrt{2})^{N+1}[(4-2\sqrt{2})N^2-(2-2\sqrt{2})N-(6+5\sqrt{2})] + \tfrac{1}{64}(1-\sqrt{2})^{N+1}[(4+2\sqrt{2})N^2-(2+2\sqrt{2})N-(6-5\sqrt{2})] + \tfrac{1}{2}(N+1) \tag{11b}$$

$$c_N^{(x_+x_-)} = \tfrac{1}{64}(1+\sqrt{2})^{N+1}[(4-2\sqrt{2})N^2+(6-6\sqrt{2})N+(2-\sqrt{2})] + \tfrac{1}{64}(1-\sqrt{2})^{N+1}[(4+2\sqrt{2})N^2+(6+6\sqrt{2})N+(2+\sqrt{2})] \tag{11c}$$

$$c_N^{(y_+^2)} = c_N^{(y_-^2)} = \tfrac{1}{64}(1+\sqrt{2})^{N+1}[(6-2\sqrt{2})N^2-(18-13\sqrt{2})N-4\sqrt{2}] + \tfrac{1}{64}(1-\sqrt{2})^{N+1}[(6+2\sqrt{2})N^2-(18+13\sqrt{2})N+4\sqrt{2}] - 2^{N-3}N(N-1) + \tfrac{1}{4} \tag{11d}$$

$$c_N^{(y_+y_-)} = \tfrac{1}{64}(1+\sqrt{2})^{N+1}[(-2+2\sqrt{2})N^2-(6-\sqrt{2})N+(4+2\sqrt{2})] + \tfrac{1}{64}(1-\sqrt{2})^{N+1}[(-2-2\sqrt{2})N^2-(6+\sqrt{2})N+(4-2\sqrt{2})] - \tfrac{1}{4}. \tag{11e}$$

The averages are again obtained by dividing them by a_N. We list only the asymptotic expressions as $N \to \infty$:

$$\langle R_x^2\rangle = (c_N^{(x_+^2)} - 2c_N^{(x_+x_-)} + c_N^{(x_-^2)})/a_N \sim \tfrac{1}{4}(\sqrt{2}-1)N^2 \tag{12a}$$

$$\langle R_y^2\rangle = (c_N^{(y_+^2)} - 2c_N^{(y_+y_-)} + c_N^{(y_-^2)})/a_N \sim \tfrac{1}{4}[1-(\sqrt{2}-1)]N^2 \tag{12b}$$

$$\langle R^2\rangle = c_N/a_N \sim \tfrac{1}{4}N^2. \tag{12c}$$

Both $\langle R_x^2\rangle$ and $\langle R_y^2\rangle$ are proportional to N^2. It is seen that the model exhibits characteristics of one-dimensional self-avoiding walks in all directions, while the anisotropy created by the direction taken in the first step persists (see equations (8)).

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