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Self-avoiding walks near an excluded line

Carlo Vanderzande

Departement WNIF, Limburgs Universitair Centrum, 3610 Diepenbeek, Belgium

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Abstract. The problem of a SAW starting next to an excluded line, say the negative x axis, is studied. In two dimensions, using arguments based on conformal invariance and scaling, it is shown that the moments of the displacement along the x axis after N steps, x_N, grow like

$$\langle x_N^{2k+1}\rangle \sim N^{(2k+1)\nu}.$$

The argument can, however, be simplified and extended also to the case of three dimensions.

In an interesting recent paper, Considine and Redner (1989) discuss the repulsion of a self-avoiding walk (SAW) from an excluded line. This problem is defined as follows (see figure 1). On a lattice one has one half-line, say the negative x axis, from which any SAW is excluded. One then starts SAWs one lattice spacing away along the axis of the half line. Considine and Redner (1989) calculate the odd moments $\langle x_N^{2k+1}\rangle$ of the distance travelled along the x axis after N steps, x_N. From an exact enumeration of the SAWs with up to 24 steps, they conclude that in two dimensions, asymptotically,

$$\langle x_N^{2k+1}\rangle \sim N^{(2k+1)\nu} \tag{1}$$

where ν is the usual correlation length exponent for SAWs (which in two dimensions equals 3/4). In the present paper we will prove the result (1), using known results from conformal invariance (Cardy 1987), and show that (1) also holds in three dimensions.

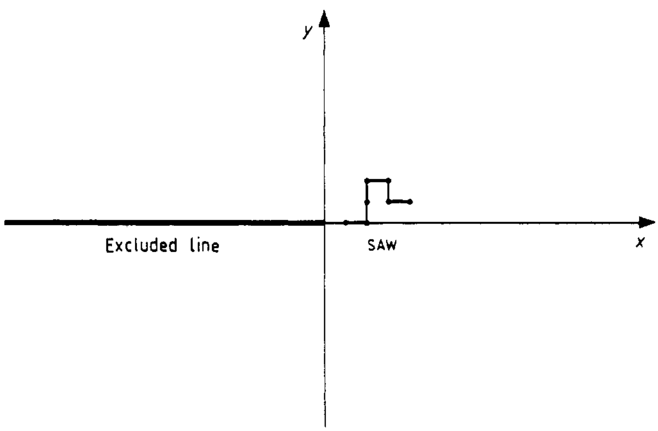

Figure 1. The self-avoiding walk (SAW) near an excluded line.

The most important realisation for the proof in two dimensions is that the plane with an excluded half line (figure 1) can be obtained from a conformal mapping of the half plane (figure 2(a)). Let us denote any point in the half plane by polar coordinates r and θ ($-\pi/2 \leq \theta \leq \pi/2$), and let us denote $z = r\exp(\mathrm{i}\theta)$. The conformal map

$$w = z^{\phi/\pi} \tag{2}$$

maps the half plane on to a wedge with an opening angle ϕ (figure 2(b)). The excluded line case corresponds to the limit $\phi \to 2\pi$.

When applying conformal invariance to critical behaviour one works within a continuum theory (Belavin *et al* 1984, Cardy 1987). Any critical two-point correlation function $G(z_1, z_2)$ transforms under a conformal map $z \to w(z)$ in the following way:

$$G(z_1, z_2) = \left|\frac{\mathrm{d}w}{\mathrm{d}z}(z_1)\right|^x \left|\frac{\mathrm{d}w}{\mathrm{d}z}(z_2)\right|^x G(w_1, w_2) \tag{3}$$

where x is the exponent describing the decay of the critical correlation function in the full two-dimensional plane, i.e. $G(z_1, z_2) \sim |z_1 - z_2|^{-2x}$.

Let us consider the correlation function between a point on the surface and a point at coordinates (r, θ), in the half-plane geometry (figure 2(a)). Cardy (1984) showed, using conformal invariance, that this correlation function $G(r, \theta)$ is given by

$$G(r, \theta) \sim r^{-x-x'}(\cos\theta)^{x'-x} \tag{4}$$

where x' is the usual surface critical exponent (Binder 1983). Using the map (2) with $\phi = 2\pi$, one can obtain using (3) and (4) the correlation function $G(\rho, \psi)$ in the geometry with the excluded line. One finds:

$$G(\rho, \psi) \sim \rho^{-x-x'/2}\left(\cos\frac{\psi}{2}\right)^{x'-x}. \tag{5}$$

Let us now be more specific and take the spin-spin correlation function $G_{\sigma\sigma}(\rho, \psi)$ of the O(n)-model, in the $n \to 0$ limit, but not necessarily at the critical point. This correlation function can be related to the SAW (de Gennes 1979). For the SAW near an excluded line, and working again on a lattice, we have

$$G_{\sigma\sigma}(\rho, \psi) = \sum_N C_N(0; \rho, \psi) K^N \tag{6}$$

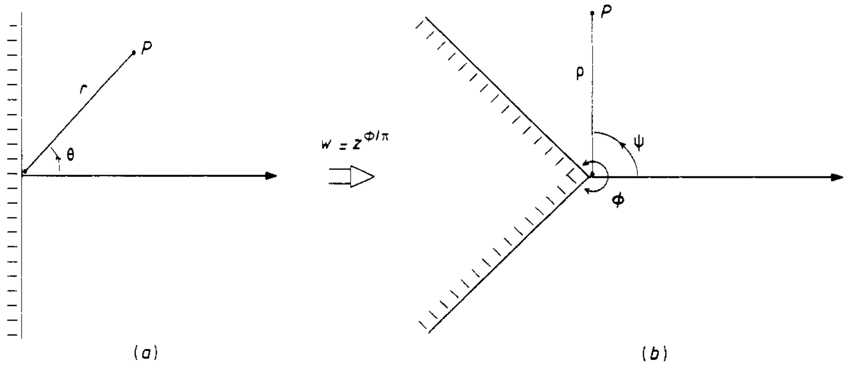

Figure 2. The conformal map $w = z^{\phi/\pi}$ maps the half plane (a) onto a wedge with opening angle ϕ. The point (r, θ) is thus mapped onto (ρ, ψ).

where $C_N(0; \rho, \psi)$ is the number of N-step SAWs going from 0 to the point (ρ, ψ), and K is the $O(n \to 0)$-model coupling constant. All the walks considered in (6) have the same value for x_N, namely $x_N(\rho, \psi) = \rho \cos \psi$.

Furthermore the total number C_N of N-step walks is expected to behave as:

$$C_N = \int \rho \, \mathrm{d}\rho \, \mathrm{d}\psi \, C_N(0; \rho, \psi) \simeq K_c^{-N} N^{\bar{\gamma}-1} \tag{7}$$

where

$$\bar{\gamma} = \nu(2 - x_h - x'_h(\phi = 2\pi)). \tag{8}$$

Here x_h is the exponent describing the decay of the critical spin-spin correlation function in the $O(n \to 0)$ model, and $x'_h(\phi)$ is the exponent describing the decay of the critical spin-spin correlation function for two spins located at the boundary of a wedge of opening angle ϕ (Cardy 1983). For $\phi = \pi$, $x'_h(\phi)$ coincides with the usual surface exponent x'_h already encountered in (4), while for general ϕ, $x'_h(\phi)$ is given by

$$x'_h(\phi) = \frac{\pi}{\phi} x'_h. \tag{9}$$

Also this result was obtained on the basis of conformal invariance (Cardy 1984). In this way, one can rewrite (7) as:

$$C_N \simeq K_c^{-N} N^{\nu(2 - x_h - x'_h/2) - 1}. \tag{10}$$

(Using $x'_h = 5/8$, $x_h = 5/48$, $\nu = 3/4$, one gets $C_N \simeq K_c^{-N} N^{3/16}$, a result which can be verified numerically.)

Now, from (6) one finds:

$$\begin{aligned}
&\int \rho \, \mathrm{d}\rho \, \mathrm{d}\psi \, (\rho \cos \psi)^{2k+1} G_{\sigma\sigma}(\rho, \psi) \\
&\qquad = \sum_N \int \rho \, \mathrm{d}\rho \, \mathrm{d}\psi \, x_N(\rho, \psi)^{2k+1} C_N(0; \rho, \psi) K^N \\
&\qquad = \sum_N \langle x_N^{2k+1} \rangle C_N K^N
\end{aligned} \tag{11}$$

where $\langle x_N^{2k+1} \rangle$ is the average of x_N^{2k+1} over all N-step SAWs. If one assumes:

$$\langle x_N^{2k+1} \rangle \sim N^{z_k} \tag{12}$$

we get, using (10) that for $K \to K_c$ the sum on the RHS of (11) diverges as:

$$\sum_N \langle x_N^{2k+1} \rangle C_N K^N \sim |K_c - K|^{-\nu(2 - x_h - x'_h/2) + z_k}. \tag{13}$$

On the other hand, we assume, using (5) that for $K \to K_c$, $G_{\sigma\sigma}(\rho, \psi)$ will have the scaling behaviour

$$G_{\sigma\sigma}(\rho, \psi) = \rho^{-x_h - x'_h/2} \left(\cos \frac{\psi}{2} \right)^{x'_h - x_h} F(\rho/\xi) \tag{14}$$

where F is a scaling function, $F(z) \to$ constant when $z \to 0$ and $F(z) \to 0$ when $z \to \infty$ and $\xi \sim |K - K_c|^{-\nu}$. Inserting (14) into the LHS of (11), and changing variables shows that the integral on the LHS of (6) diverges as:

$$\int \rho \, \mathrm{d}\rho \, \mathrm{d}\psi \, (\rho \cos \psi)^{2k+1} G_{\sigma\sigma}(\rho, \psi) \sim |K_c - K|^{-\nu(2 + 2k + 1 - x_h - x'_h/2)}. \tag{15}$$

Comparing exponents in (13) and (15) gives our final result $z_k = (2k+1)\nu$ thus proving (1).

Can the result (1) be extended to the problem of a SAW near an excluded line in three dimensions? Here, one loses the conformal invariance which allowed us to give the precise form of $G(\rho, \psi)$ (equation (5)) and equation (8) for $\bar{\gamma}$.

However, using some general scaling assumptions, suggested by the results in two dimensions, one can show that (1) should also hold in three dimensions.

Indeed, let ψ be the angle between the line to a point and the excluded line. From symmetry, one expects the correlation function G between this point and a point near the end of the excluded line to depend only on ψ and the distance ρ from the end of the excluded line to the point. From scaling one expects that near criticality, similarly to (14),

$$G(\rho, \psi) \sim \rho^{-x-\bar{x}} f(\cos\psi) F(\rho/\xi) \tag{16}$$

where $\bar{x}$ is some unknown exponent and f some unknown function. On the other hand, the number of SAWs of N steps which never trespass the excluded line, C_N, will behave as

$$C_N \sim \mu^N N^{\bar{\gamma}-1}. \tag{17}$$

Once more $\bar{\gamma}$ is unknown. But if we take for $G(\rho, \psi)$ the spin-spin correlation function of the O($n \to 0$)-model, and we integrate it over all space, and relate it to the sum over all N of (17) one can obtain the relation

$$\nu(3 - x - \bar{x}) = \bar{\gamma}. \tag{18}$$

We can now repeat the argument in two dimensions and show that also in three dimensions:

$$z_k = (2k+1)\nu. \tag{19}$$

In their numerical work, Considine and Redner (1989) find

$$z_k = 2k + z$$

where $z \simeq 0.35 \neq \nu$. However, on the basis of some exact calculations on the problem of a random walk near an excluded line, they suspect that the result $z \neq \nu$ may be an effect of short SAWs. It seems that the above argument shows that this is indeed true, and that also in three dimensions one should have $z = \nu$.

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