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Random walks exterior to a rectangle

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Abstract. We show how to simulate random walks terminating on the periphery of a rectangle, both in the continuum and on a square lattice. The method is error-free in principle except for a negligible bias arising from the rejection of very long walks. The average machine time would be O[1] step in the modified procedure. This method may be useful in exploring the distinction between the continuum and the lattice in diffusion-limited aggregation.

1. Introduction

The simulation of random walks on a lattice can be time consuming; therefore it is advisable to make big jumps if this can be done with the correct probabilities. For example, in Monte Carlo simulations of DLA cluster growth [1, 2] a particle must diffuse in from infinity until it touches the cluster. Much of the walk takes place well outside the cluster, and it is desirable to accomplish this part by fast techniques independent of the cluster shape.

In the continuum, an excellent procedure in two dimensions is to surround the cluster with a circle. Since the space outside the circle is free of obstacles, the probability that a walk starting at $\boldsymbol{r}$ from the centre will first enter the circle at $\boldsymbol{R}$ ($r > R$ = radius of circle) is given by the electrostatic formula for charge induced on a circular conductor by a point charge:

$$P_r(\boldsymbol{R})\,\mathrm{d}\phi = \frac{r^2 - R^2}{r^2 - 2rR\cos\phi + R^2}\frac{\mathrm{d}\phi}{2\pi} \tag{1.1}$$

where $\phi = \measuredangle(\boldsymbol{r}, \boldsymbol{R})$. In this way no computer time is wasted on diffusion outside the circle. An alternative procedure [3] is to draw a large empty circle around the starting point, choose a point on the periphery at random, and start again from there until one either hits the cluster or reaches a cut-off distance $r_{\max}$. In the latter case the walk is rejected. Since the circle can be made larger when the walk gets further from the cluster, the computing time is only logarithmic in $r_{\max}$ whereas the bias due to the rejection falls off as $1/r_{\max}^2 \ln r_{\max}$.

For a square lattice in two dimensions, the circle method does not yield quite the correct probabilities, since it really describes an off-lattice walk. Meakin [4] has partially remedied this by switching to an on-lattice walk when close to the cluster.

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His claim that this yields results indistinguishable from true on-lattice diffusion is very likely correct, but it may still be of interest to have an efficient procedure that is rigorously equivalent to on-lattice diffusion. Such a procedure would be based on squares rather than circles. Ball and Brady [5] have introduced an algorithm based on squares, but with some use of continuum probabilities.

Martin and the author are developing [6] an algorithm that rigorously simulates on-lattice diffusion with little sacrifice in computer time. Here we attack only the problem of how to simulate the part of the walk well outside the cluster. Assuming that the whole cluster lies inside a given rectangle, we must answer two mathematical questions.

(i) What is the probability distribution of the first entry point on the perimeter of the rectangle for a particle diffusing from infinity?

(ii) What is the distribution of re-entry points after the particle has exited from the rectangle at a given point?

Our method is to break the walk into segments each restricted to a half-plane. The notation for this is presented in § 2. In § 3 these segments are studied for the continuum version; the walk is then a series of transforms on a function of one variable. This function is subjected to the Laplace transform, and the problem of diffusion from infinity (equivalent to the charge distribution on an isolated conducting rectangle) reduces to the solution of a linear integral equation in the Laplace transform variable.

In § 4 the same method is applied to the lattice. The Green function on the half-plane is expressed in momentum space; one integration is carried out, and the other is deformed in the complex plane. The quantity $z = e^{ik}$ thus becomes real and is the argument of a generating function that replaces the Laplace transform of the preceding section. The walk from infinity then reduces to an integral equation only slightly more complicated than before.

Section 5 treats the re-entry problem on the lattice. The aim is to reduce it to a fast Monte Carlo procedure. Most walks re-enter immediately on the exit side of the rectangle; these can be treated by standard Green functions previously calculated [7]. Those that do not can be treated as a series of steps through z space; the essential point is that all the kernels turn out to be positive definite so that the final probabilities are simulated perfectly by a Monte Carlo procedure based on elementary functions.

Unfortunately the average number of Monte Carlo steps is infinite because of rare walks that go far from the rectangle. However, one may stipulate that the particle is lost if it goes too far; thus a walk may be cancelled whenever $1 - z < \varepsilon \ll 1$. The bias thus introduced is $\sim\varepsilon^2(\ln(1/\varepsilon))^2$, and the average number of Monte Carlo steps is only $\sim\ln(1/\varepsilon)$. Since this in turn applies only to the walks that do not re-enter on the first jump, the bias can easily be made negligible without increasing the computer time beyond O[1].

Section 6 gives conclusions and discusses possible applications.

2. Notation and methodology

Throughout this paper, a capital letter F, G, etc, will denote a probability distribution (not necessarily normalised) over the perimeter of the rectangle. Since such distributions can be added and subtracted, F, G, etc, will be regarded as abstract vectors. Thus the variable that would describe a particular point on the perimeter will be suppressed. If F is written as a function $F(x)$, the argument x stands for an additional parameter on which the distribution depends. If F is a distribution, then $\bar{F}$ denotes its sum or integral over the perimeter; for a normalised distribution $\bar{F} = 1$.

We shall consider a rectangle of sides s (horizontal) and s' (vertical). The vector space of distributions F can be transformed by the group of horizontal and vertical reflections. We denote a reflection about the horizontal (vertical) axis by $\eta(\eta')$. Then

$$\eta^2 = \eta'^2 = 1 \qquad \eta\eta' = \eta'\eta. \tag{2.1}$$

Our method for studying random walks outside the rectangle is as follows. We use cartesian coordinates with the origin at the rectangle's upper right corner. Suppose the particle exits from the top side. Follow its path in the upper half-plane until it hits the x axis. This much of the path is called a *stride*. There are three possibilities.

(1) The first stride ends on the top side of the rectangle.

(2) The first stride ends at $(x, 0)$ on the positive x axis. In this case we follow the particle thereafter in the right half-plane until it hits the y axis; this is the second stride.

(3) The first stride ends at $(-(x+s), 0)$ on the negative x axis beyond the upper left corner of the rectangle. In this case we reflect about the vertical axis (introducing a factor η') and proceed as in case (2).

The second stride can likewise terminate in three ways which are dealt with similarly. The third stride has the same possibilities as the first. We continue until a stride terminates on the rectangle.

If the particle comes from infinity, we regard the first stride as terminating with uniform probability anywhere on the x axis, and proceed from there. In this case it is quickly seen that after any finite number of strides the probability of hitting the rectangle is negligible since the distribution along the axis has infinite normalisation. But after many strides a limiting distribution is reached on the axis, uniform far away from the rectangle and somewhat diminished in its 'shadow'. The *relative* probability of hitting different parts of the rectangle is then non-uniform as it is dominated by the near portion of the axis distribution.

To avoid dealing with infinite quantities, we shall take as our primary object of study the normalised distribution of endpoints (on the rectangle) of walks commencing at $(x, 0)$ or $(0, y)$ on the positive x or y axis. These distributions will be called $F(x)$ and $F'(y)$. The portions (unnormalised) resulting from walks only one stride long will be called $F_1(x)$ and $F'_1(y)$. Then F' is the sum of three terms arising from the three types of termination of the first stride, and is thus a linear combination of F'_1, F and $\eta' F$. Likewise F is a linear combination of F_1, F' and $\eta F'$. Thus F and F' are given by a linear double recursion in which the kernels and sources can be derived from a single stride. Once $F(x)$ and $F'(y)$ are known, the distribution for a particle starting from infinity or from one side of the square can be found in one step.

3. Walks from infinity in a continuum

3.1. Basic equations

In this section we shall study the probability distribution of initial impact on the rectangle by a particle diffusing from infinity through a continuum. This is equivalent to the charge distribution on a charged conducting rectangle alone in two-dimensional space. We take up this case first because it is simpler than the lattice problem but parallel in its solution.

A walk in the upper half-plane starting at $(0, y)$ will terminate on the x axis between x and $x+\mathrm{d}x$ with probability

$$\frac{y}{\pi}\frac{\mathrm{d}x}{x^2+y^2}. \tag{3.1}$$

Hence the recursion for F' is

$$F'(y)=F_1'(y)+\int_0^\infty \tau(y,x)F(x)\,\mathrm{d}x+\int_0^\infty \tau(y,x+s)\eta' F(x)\,\mathrm{d}x \tag{3.2}$$

where $F_1'(y)$ is the distribution (3.1) restricted to the interval $(-s, 0)$—the top side of the rectangle—and

$$\tau(y,x)=\frac{y}{\pi}\frac{1}{x^2+y^2}. \tag{3.3}$$

Likewise

$$F(x)=F_1(x)+\int_0^\infty \tau(x,y)F'(y)\,\mathrm{d}y+\int_0^\infty \tau(x,y+s')\eta F'(y)\,\mathrm{d}y \tag{3.4}$$

where F_1 is obtained from (3.1) by interchanging x and y and restricting to $(-s', 0)$ on the y axis.

It is now useful to introduce Laplace transforms. Let

$$G(\lambda)=\int_0^\infty \mathrm{e}^{-\lambda x}F(x)\,\mathrm{d}x \tag{3.5}$$

$$G'(\mu)=\int_0^\infty \mathrm{e}^{-\mu y}F'(y)\,\mathrm{d}y \tag{3.6}$$

so that $G(\lambda)$ is the unnormalised endpoint distribution for walks whose initial distribution is as $\mathrm{e}^{-\lambda x}\,\mathrm{d}x$ on the x axis, and

$$G_1(\lambda)=\int_0^\infty \mathrm{e}^{-\lambda x}F_1(x)\,\mathrm{d}x \tag{3.7}$$

$$G_1'(\mu)=\int_0^\infty \mathrm{e}^{-\mu y}F_1'(y)\,\mathrm{d}y. \tag{3.8}$$

If we note that (3.3) may be written

$$\tau(y,x)=\frac{1}{\pi}\int_0^\infty \mathrm{e}^{-\lambda x}\sin\lambda y\,\mathrm{d}\lambda \tag{3.9}$$

then (3.2) becomes

$$F'(y)=F_1'(y)+\frac{1}{\pi}\int_0^\infty \sin\lambda y G(\lambda)\,\mathrm{d}\lambda+\frac{1}{\pi}\int_0^\infty \sin\lambda y\,\mathrm{e}^{-\lambda s}\eta' G(\lambda)\,\mathrm{d}\lambda \tag{3.10}$$

and, substituting into (3.6) with the aid of (3.8) and (3.9),

$$G'(\mu)=G_1'(\mu)+\int_0^\infty \tau(\lambda,\mu)(1+\mathrm{e}^{-\lambda s}\eta')G(\lambda)\,\mathrm{d}\lambda. \tag{3.11}$$

Likewise

$$G(\lambda)=G_1(\lambda)+\int_0^\infty \tau(\mu,\lambda)(1+\mathrm{e}^{-\mu s'}\eta)G'(\mu)\,\mathrm{d}\mu. \tag{3.12}$$

At this point we note that in the approach from infinity we shall only use that part of F or G which is symmetric under all reflections. Therefore we can replace $\eta = \eta' = 1$ in these equations, provided we symmetrise the final answer.

It is profitable to study (3.11) and (3.12) on a logarithmic scale.

Setting

$$\alpha = \ln(\lambda s) \qquad \beta = \ln(\mu s) \tag{3.13}$$

and

$$H(\alpha)\,\mathrm{d}\alpha = G(\lambda)\,\mathrm{d}\lambda \qquad H'(\beta)\,\mathrm{d}\beta = G'(\mu)\,\mathrm{d}\mu \tag{3.14}$$

we have (with similar definitions of H_1, H_1')

$$H'(\beta) = H_1'(\beta) + \int_{-\infty}^{\infty} \frac{1}{\pi}\,\mathrm{sech}(\alpha-\beta)\chi(\alpha)H(\alpha)\,\mathrm{d}\alpha \tag{3.15}$$

and

$$H(\alpha) = H_1(\alpha) + \int_{-\infty}^{\infty} \frac{1}{\pi}\,\mathrm{sech}(\alpha-\beta)\chi'(\beta)H'(\beta)\,\mathrm{d}\beta \tag{3.16}$$

where

$$\chi(\alpha) = \tfrac{1}{2}(1 + \mathrm{e}^{-\mathrm{e}^{\alpha}}\eta') \to \tfrac{1}{2}(1 + \mathrm{e}^{-\mathrm{e}^{\alpha}}) \tag{3.17}$$

$$\chi'(\beta) = \tfrac{1}{2}(1 + \mathrm{e}^{-\mathrm{e}^{\beta-\beta_0}}\eta) \to \tfrac{1}{2}(1 + \mathrm{e}^{-\mathrm{e}^{\beta-\beta_0}}) \tag{3.18}$$

and $\beta_0 = \ln(s/s')$.

3.2. *Eigenfunctions and eigenvalues*

Our approach to (3.15) and (3.16) is based on the fact that apart from the factors χ, χ' the kernels are translation invariant. We note that $\sqrt{\chi(\alpha)}H(\alpha)$ satisfies an integral equation with the symmetric kernel

$$\sigma(\alpha_1, \alpha_2) = (\chi(\alpha_1)\chi(\alpha_2))^{1/2}\frac{1}{\pi^2}\int_{-\infty}^{\infty} \chi'(\beta)\,\mathrm{sech}(\alpha_1-\beta)\,\mathrm{sech}(\alpha_2-\beta)\,\mathrm{d}\beta \tag{3.19}$$

where σ depends only on $(\alpha_1 - \alpha_2)$ when both α_1 and $\alpha_2 \to -\infty$, since all the $\chi \to 1$. Therefore the real eigenfunctions of σ must have the form

$$\psi_\omega(\alpha) \simeq \sin(\omega\alpha + \phi_\omega) \qquad \alpha \to -\infty. \tag{3.20}$$

The eigenvalues can be found by studying this same asymptotic region. The basic integral is

$$\int_{-\infty}^{\infty} \frac{1}{\pi}\,\mathrm{sech}(\alpha-\beta)\,\mathrm{e}^{\mathrm{i}\omega\beta}\,\mathrm{d}\beta = \mathrm{sech}\,\tfrac{1}{2}\pi\omega\,\mathrm{e}^{\mathrm{i}\omega\alpha} \tag{3.21}$$

from which it follows that for $\alpha_1 \to -\infty$

$$\begin{aligned}\int_{-\infty}^{\infty} \sigma(\alpha_1, \alpha_2)\psi_\omega(\alpha_2)\,\mathrm{d}\alpha_2 &\simeq \int_{-\infty}^{\infty} \frac{1}{\pi}\,\mathrm{sech}(\alpha_1-\beta)\,\mathrm{d}\beta \\ &\quad\times \int_{-\infty}^{\infty} \frac{1}{\pi}\,\mathrm{sech}(\alpha_2-\beta)\sin(\omega\alpha_2+\phi_\omega)\,\mathrm{d}\alpha_2 \\ &= \int_{-\infty}^{\infty} \frac{1}{\pi}\,\mathrm{sech}(\alpha_1-\beta)\,\mathrm{d}\beta\;\mathrm{sech}\,\tfrac{1}{2}\pi\omega\,\sin(\omega\beta+\phi_\omega) \\ &= \mathrm{sech}^2\,\tfrac{1}{2}\pi\omega\,\sin(\omega\alpha_1+\phi_\omega) \\ &\simeq \mathrm{sech}^2\,\tfrac{1}{2}\pi\omega\psi_\omega(\alpha_1).\end{aligned} \tag{3.22}$$

Since the error can be made as small as desired by taking $\alpha_1 \to -\infty$, the eigenvalue for ψ_ω must be exactly $\operatorname{sech}^2 \frac{1}{2}\pi\omega$.

For $\alpha, \beta \to +\infty$, χ and $\chi' \to \frac{1}{2}$. Therefore ψ_ω in this region has the form $\sin(\hat{\omega}\alpha + \hat{\phi}_\omega)$ where $\frac{1}{4}\operatorname{sech}^2 \frac{1}{2}\pi\hat{\omega} = \operatorname{sech}^2 \frac{1}{2}\pi\omega$, or $\cosh \frac{1}{2}\pi\hat{\omega} = \frac{1}{2}\cosh\frac{1}{2}\pi\omega$. This has a real solution only if $\omega > \omega_c = (2/\pi)\cosh^{-1} 2$. If $\omega < \omega_c$ the asymptotic form of ψ_ω at $\alpha \to \infty$ is $e^{-\hat{\omega}\alpha}$ where $\cos\frac{1}{2}\pi\hat{\omega} = \frac{1}{2}\cosh\frac{1}{2}\pi\omega$. Thus for $\omega < \omega_c$ there is one eigenfunction with a unique ϕ_ω, but for $\omega > \omega_c$ there are two independent eigenfunctions. However, there is no need to complicate the notation so as to show this.

We now wish to express $\sqrt{\chi(\alpha)}H(\alpha)$ as a sum of eigenfunctions ψ_ω of σ. To this end we introduce the weighted transforms

$$\tilde{H}(\omega) = \int_{-\infty}^{\infty} \psi_\omega(\alpha)\sqrt{\chi(\alpha)}H(\alpha)\,\mathrm{d}\alpha \tag{3.23}$$

$$\tilde{H}'(\omega) = \int_{-\infty}^{\infty} \psi'_\omega(\beta)\sqrt{\chi'(\beta)}H'(\beta)\,\mathrm{d}\beta \tag{3.24}$$

and likewise $\tilde{H}_1(\omega)$, $\tilde{H}'_1(\omega)$, where

$$\psi'_\omega(\beta) = \cosh\tfrac{1}{2}\pi\omega\sqrt{\chi'(\beta)} \int_{-\infty}^{\infty} \frac{1}{\pi}\operatorname{sech}(\alpha-\beta)\sqrt{\chi(\alpha)}\psi_\omega(\alpha)\,\mathrm{d}\alpha. \tag{3.25}$$

Then (3.15) and (3.16) become

$$\begin{aligned}\tilde{H}'(\omega) &= \tilde{H}'_1(\omega) + \cosh\tfrac{1}{2}\pi\omega \int\int_{-\infty}^{\infty} \mathrm{d}\alpha_1\,\mathrm{d}\alpha_2\,\sigma(\alpha_1, \alpha_2)\psi_\omega(\alpha_2)\sqrt{\chi(\alpha_1)}H(\alpha_1)\,\mathrm{d}a \\ &= \tilde{H}'_1(\omega) + \operatorname{sech}\tfrac{1}{2}\pi\omega\tilde{H}(\omega)\end{aligned} \tag{3.26}$$

and

$$\tilde{H}(\omega) = H_1(\omega) + \operatorname{sech}\tfrac{1}{2}\pi\omega\tilde{H}'(\omega). \tag{3.27}$$

Therefore

$$\begin{aligned}\tilde{H}(\omega)\tanh^2\tfrac{1}{2}\pi\omega &= \tilde{H}_1(\omega) + \operatorname{sech}\tfrac{1}{2}\pi\omega\tilde{H}'_1(\omega) \\ &= \int_{-\infty}^{\infty} \psi_\omega(\alpha)\sqrt{\chi(\alpha)}H_2(\alpha)\,\mathrm{d}\alpha\end{aligned} \tag{3.28}$$

where

$$H_2(\alpha) = H_1(\alpha) + \frac{1}{\pi}\int_{-\infty}^{\infty} \operatorname{sech}(\alpha-\beta)\chi'(\beta)H'_1(\beta)\,\mathrm{d}\beta. \tag{3.29}$$

Since σ is symmetric in α_1, α_2, its eigenfunctions are orthogonal and (3.23) can be inverted:

$$\sqrt{\chi(\alpha)}H(\alpha) = \int_0^{\infty} \gamma(\omega)\psi_\omega(\alpha)\tilde{H}(\omega)\,\mathrm{d}\omega \tag{3.30}$$

with $\gamma(\omega)$ to be determined at the end of § 3.3. (It is understood that for $\omega > \omega_c$ both eigenfunctions are present.) With (3.28) this gives

$$\sqrt{\chi(\alpha)}H(\alpha) = \int_{-\infty}^{\infty} \xi(\alpha, \alpha')\sqrt{\chi(\alpha')}H_2(\alpha')\,\mathrm{d}\alpha' \tag{3.31}$$

where

$$\xi(\alpha, \alpha') = \int_0^\infty \frac{\psi_\omega(\alpha)\psi_\omega(\alpha')}{\tanh^2 \frac{1}{2}\pi\omega} \gamma(\omega)\, d\omega. \tag{3.32}$$

Thus we have obtained the solution to (3.15) and (3.16) except that we do not have ψ_ω in closed form. However, for the approach from infinity only the region $\omega \to 0$ is important, as we now show.

3.3. Approach from infinity

The first stride produces a distribution uniform on the x axis. The probability of hitting the rectangle on this stride is infinitesimal. Therefore the distribution of final endpoints on the rectangle would be $\int_0^\infty F(x)\, dx$ except that this is infinite since $\bar{F}(x) = 1$ for all x. Therefore we take instead the finite distribution

$$\begin{aligned} F_\infty &= \lim_{\lambda \to 0} \frac{\int_0^\infty e^{-\lambda x} F(x)\, dx}{\int_0^\infty e^{-\lambda x} \bar{F}(x)\, dx} = \lim_{\lambda \to 0} \lambda G(\lambda) \\ &= \lim_{\alpha \to -\infty} H(\alpha). \end{aligned} \tag{3.33}$$

Hence we only need $\xi(\alpha, \alpha')$ as $\alpha \to -\infty$. But then the rapid oscillation of $\psi_\omega(\alpha)$ kills the integral in (3.32) except near $\omega = 0$.

To be explicit, let $h_0(\alpha)$, $h_0'(\beta)$ be defined by the homogeneous equations

$$h_0(\alpha) = \int_{-\infty}^\infty \frac{1}{\pi} \operatorname{sech}(\alpha - \beta) \chi'(\beta) h_0'(\beta)\, d\beta \tag{3.34}$$

$$h_0'(\beta) = \int_{-\infty}^\infty \frac{1}{\pi} \operatorname{sech}(\alpha - \beta) \chi(\alpha) h_0(\alpha)\, d\alpha \tag{3.35}$$

so that $\sqrt{\chi(\alpha) h_0(\alpha)}$ satisfies the eigenvalue equation for $\omega = 0$ (eigenvalue = 1). Thus for $\alpha \to -\infty$ $h_0(\alpha)$ must be linear; we normalise it by

$$\lim_{\alpha \to -\infty} \frac{dh_0}{d\alpha} = -1. \tag{3.36}$$

(Note that h_0 is not a capital; its value at any α is a number, not a distribution.)

Now, for any fixed α very large negative, as $\omega \to 0$, $\psi_\omega(\alpha) \approx \sin \omega\alpha \approx \omega\alpha$ and $d\psi_\omega / d\alpha \approx \omega$. Therefore the normalised relation between h_0 and ψ_ω is

$$-\sqrt{\chi(\alpha)} h_0(\alpha) = \lim_{\omega \to 0} \psi_\omega(\alpha)/\omega \tag{3.37}$$

for all α.

We now write (3.32) in the form

$$\xi(\alpha, \alpha') = \int_0^\infty \frac{\sin(\omega\alpha + \phi_\omega)}{\omega} c(\omega, \alpha, \alpha')\, d\omega \tag{3.38}$$

where

$$c(\omega, \alpha, \alpha') = \frac{\psi_\omega(\alpha)}{\sin(\omega\alpha + \phi_\omega)} \frac{\omega\psi_\omega(\alpha')}{\tanh^2 \frac{1}{2}\pi\omega} \gamma(\omega). \tag{3.39}$$

As $\alpha \to -\infty$, we obtain simply

$$c(\omega, \alpha, \alpha') \to c(\omega, \alpha') = \frac{\omega\psi_\omega(\alpha')}{\tanh^2 \frac{1}{2}\pi\omega}\gamma(\omega). \tag{3.40}$$

Thus

$$\begin{aligned}\xi(-\infty, \alpha') &= \lim_{\alpha\to-\infty}\int_0^\infty \frac{\sin(\omega\alpha+\phi_\omega)}{\omega}c(\omega,\alpha')\,d\omega \\ &= \lim_{|\alpha|\to+\infty}\int_0^\infty -\frac{\sin(\nu-\phi_{\nu/|\alpha|})}{\nu}c\left(\frac{\nu}{|\alpha|},\alpha'\right)d\nu \\ &= \int_0^\infty -\frac{\sin\nu}{\nu}c(0,\alpha')\,d\nu = -\tfrac{1}{2}\pi c(0,\alpha')\end{aligned} \tag{3.41}$$

where by (3.37) and (3.40)

$$c(0, \alpha') = -(4/\pi^2)\sqrt{\chi(\alpha')}h_0(\alpha')\gamma(0). \tag{3.42}$$

Now $\gamma(\omega)$ is the spectral density divided by the normalisation integral. In view of (3.42) we confine ourselves to $\omega < \omega_c$. Temporarily impose a boundary condition $\psi_\omega(-A) = 0$ where A is very large positive. This is equivalent to $\omega A - \phi_\omega = n\pi$ where n is an integer. Therefore the spectral density per unit ω is

$$\rho(\omega) = \frac{1}{\pi}\frac{d}{d\omega}(\omega A - \phi_\omega) = \frac{1}{\pi}(A + O[1]). \tag{3.43}$$

The normalisation integral is

$$\int_{-A}^\infty \psi_\omega(\alpha)^2\,d\alpha = \tfrac{1}{2}A + O[1]. \tag{3.44}$$

Letting $A \to \infty$ we obtain

$$\gamma(\omega) = 2/\pi \tag{3.45}$$

which with (3.41) and (3.42) gives

$$\xi(-\infty, \alpha') = (4/\pi^2)\sqrt{\chi(\alpha')}h_0(\alpha'). \tag{3.46}$$

From (3.31) and (3.33) we now obtain

$$\begin{aligned}F_\infty &= \frac{4}{\pi^2}\int_{-\infty}^\infty \chi(\alpha)h_0(\alpha)H_2(\alpha)\,d\alpha \\ &= \frac{4}{\pi^2}\left(\int_{-\infty}^\infty h_0(\alpha)\chi(\alpha)H_1(\alpha)\,d\alpha + \int_{-\infty}^\infty h_0'(\beta)\chi'(\beta)H_1'(\beta)\,d\beta\right)\end{aligned} \tag{3.47}$$

where we have substituted from (3.30) and used (3.34).

3.4. Explicit probabilities

It only remains to express H_1, H_1' in terms of F_1, F_1'. Let us define a basic distribution $G_0(\lambda)$ which assigns to the interval $(-(u+du), -u)$ on the x axis (i.e. an interval of length du located on the top side a distance u from the right) a probability $e^{-\lambda u}\,du$

(unnormalised). The distribution $F_1'(y)$ assigns to this same interval a probability $(1/\pi)y\,\mathrm{d}u/(u^2+y^2)$, and hence $G_1'(\mu)$ assigns it a probability

$$\begin{aligned}\mathrm{d}u &\int_0^\infty \mathrm{e}^{-\mu y}\frac{1}{\pi}\frac{y}{u^2+y^2}\,\mathrm{d}y\\ &= \mathrm{d}u\int_0^\infty \mathrm{e}^{-\mu y}\frac{1}{\pi}\left(\int_0^\infty \mathrm{e}^{-\lambda u}\sin\lambda y\,\mathrm{d}\lambda\right)\mathrm{d}y\\ &= \mathrm{d}u\int_0^\infty \frac{1}{\pi}\mathrm{e}^{-\lambda u}\frac{\lambda}{\lambda^2+\mu^2}\,\mathrm{d}\lambda \end{aligned}\tag{3.48}$$

which means that

$$G_1'(\mu)=\int_0^\infty \frac{1}{\pi}\frac{\lambda}{\lambda^2+\mu^2}G_0(\lambda)\,\mathrm{d}\lambda. \tag{3.49}$$

Then if as usual $H_0(\alpha)\,\mathrm{d}\alpha = G_0(\lambda)\,\mathrm{d}\lambda$, we have

$$H_1'(\beta)=\int_{-\infty}^\infty \frac{1}{2\pi}\operatorname{sech}(\alpha-\beta)H_0(\alpha)\,\mathrm{d}\alpha \tag{3.50}$$

and with similar definitions

$$H_1(\alpha)=\int_{-\infty}^\infty \frac{1}{2\pi}\operatorname{sech}(\alpha-\beta)H_0'(\beta)\,\mathrm{d}\beta. \tag{3.51}$$

When these are substituted into (3.47) we obtain, by another application of (3.34) and (3.35),

$$\begin{aligned}F_\infty &= \frac{2}{\pi^2}\left(\int_{-\infty}^\infty h_0'(\beta)H_0'(\beta)\,\mathrm{d}\beta+\int_{-\infty}^\infty h_0(\alpha)H_0(\alpha)\,\mathrm{d}\alpha\right)\\ &= \frac{2}{\pi^2}\left(\int_0^\infty h_0'(\ln\mu s)G_0'(\mu)\,\mathrm{d}\mu+\int_0^\infty h_0(\ln\lambda s)G_0(\lambda)\,\mathrm{d}\lambda\right).\end{aligned}\tag{3.52}$$

This is our final result. To recapitulate: first h_0 and h_0' must be obtained by numerical solution of (3.34) and (3.35). (The dimensions of the rectangle enter through χ and χ' given by (3.17) and (3.18).) Then (3.52) says that F_∞ assigns to each interval $\mathrm{d}u$ on the top side, u away from the right corner, a probability $f_\infty(u)\,\mathrm{d}u$ where

$$f_\infty(u)=\frac{2}{\pi^2}\int_0^\infty h_0(\ln\lambda s)\,\mathrm{e}^{-\lambda u}\,\mathrm{d}\lambda \tag{3.53}$$

and to each interval $\mathrm{d}u$ on the right side, u away from the top, a probability $f_\infty'\,\mathrm{d}u$ where

$$f_\infty'(u)=\frac{2}{\pi^2}\int_0^\infty h_0'(\ln\mu s)\,\mathrm{e}^{-\mu u}\,\mathrm{d}\mu. \tag{3.54}$$

The true distribution on the rectangle is $\frac{1}{2}(1+\eta)\frac{1}{2}(1+\eta')F_\infty$, obtained by symmetrising F_∞ with respect to reflections, as explained after (3.12).

4. Walks from infinity on a lattice

4.1. Integrals in momentum space

For the lattice problem we follow the same procedure as in the last section except that integrals over x, y are replaced by sums and the expression in (3.1) and (3.3) is replaced by a lattice Green function which has no simple form. It can be written as a momentum integral:

$$\tau(y,x)=\frac{1}{(2\pi)^2}\int_0^{2\pi}\mathrm{d}k_1\int_0^{2\pi}\mathrm{d}k_2\,\frac{\mathrm{e}^{\mathrm{i}k_1x}[\exp(\mathrm{i}k_2(y-1))-\exp(\mathrm{i}k_2(y+1))]}{4(\sin^2\frac{1}{2}k_1+\sin^2\frac{1}{2}k_2)}$$
$$=\frac{1}{2\pi}\int_0^{2\pi}\mathrm{e}^{\mathrm{i}kx}\,\mathrm{e}^{\mathrm{i}\bar{k}y}\,\mathrm{d}k \tag{4.1}$$

where $k=k_1$, and $\bar{k}$ satisfies

$$\cos\bar{k}+\cos k=2. \tag{4.2}$$

(The integral over k_2 yields a pole at $k_2=\bar{k}$, $|\mathrm{e}^{\mathrm{i}\bar{k}}|<1$.)

Thus (3.2) and (3.4) become

$$F'(y)=F_1'(y)+\sum_{x=1}^{\infty}\frac{F(x)}{2\pi}\int_0^{2\pi}\mathrm{e}^{\mathrm{i}kx}\,\mathrm{e}^{\mathrm{i}\bar{k}y}(1+\eta'\,\mathrm{e}^{\mathrm{i}ks})\,\mathrm{d}k \tag{4.3}$$

and

$$F(x)=F_1(x)+\sum_{y=1}^{\infty}\frac{F'(y)}{2\pi}\int_0^{2\pi}\mathrm{e}^{\mathrm{i}ky}\,\mathrm{e}^{\mathrm{i}\bar{k}x}(1+\eta\,\mathrm{e}^{\mathrm{i}ks'})\,\mathrm{d}k. \tag{4.4}$$

The Laplace transforms must now be replaced by generating functions. Anticipating a later convenience, we define

$$\lambda=(1-z)/\sqrt{z}\qquad\qquad \mu=(1-z')/\sqrt{z'} \tag{4.5}$$

and put

$$G(\lambda)=\sum_1^{\infty}z^xF(x)\qquad\qquad G'(\mu)=\sum_1^{\infty}z'^yF'(y). \tag{4.6}$$

Defining $G_1(\lambda)$, $G_1'(\mu)$ similarly, we have from (4.3), if we set $z=\mathrm{e}^{\mathrm{i}k}$,

$$F'(y)=F_1'(y)+\frac{1}{2\pi}\int_0^{2\pi}G(\lambda)\,\mathrm{e}^{\mathrm{i}\bar{k}y}(1+\eta'\,\mathrm{e}^{\mathrm{i}ks})\,\mathrm{d}k \tag{4.7}$$

and therefore

$$G'(\mu)=G_1'(\mu)+\frac{1}{2\pi}\int_0^{2\pi}G(\lambda)(1+\eta'\,\mathrm{e}^{\mathrm{i}ks})\left(\frac{1}{1-z'\,\mathrm{e}^{-\mathrm{i}\bar{k}}}-1\right)\mathrm{d}k$$
$$=G_1'(\mu)+\frac{1}{2\pi}\oint\frac{\mathrm{d}z}{\mathrm{i}z}G(\lambda)(1+\eta'z^s)\frac{1}{1-z'\bar{z}}$$
$$=G_1'(\mu)+\frac{1}{\pi}\int_{z_0}^{1}\frac{\mathrm{d}z}{z}G(\lambda)(1+\eta'z^s)\,\mathrm{Im}\,\frac{1}{1-z'\bar{z}}. \tag{4.8}$$

Here we have put $z=\mathrm{e}^{\mathrm{i}k}$, $\bar{z}=\mathrm{e}^{\mathrm{i}\bar{k}}$ and shrunk the contour around the branch cut where $\bar{z}$ is discontinuous. The discontinuity arises from the rule that $|\bar{z}|\leqslant 1$. Since (4.2) yields a quadratic in $\bar{z}$ whose two roots are reciprocal, the branch cut occurs in the z plane wherever $|\bar{z}|=1$, and $\bar{z}$ takes complex conjugate values on opposite sides of the cut. Thus the discontinuity in $1/(1-\bar{z}z')$ is 2i times the imaginary part if z' is real. The branch cut in the z plane goes from z_0 to 1 on the real line, where $z_0+z_0^{-1}=6$ or $z_0=3-\sqrt{8}$. (There is another cut from 1 to $1/z_0$; the two should be regarded as distinct since the contour passes between them—this is made clear if a small 'mass' term is added to the denominator of the integral in (4.1).)

We now have, for z on the cut ($|\bar{z}|^2=1$)

$$\begin{aligned}\operatorname{Im}\frac{1}{1-\bar{z}z'}&=\operatorname{Im}\frac{1-\bar{z}^*z'}{1-2z'\operatorname{Re}\bar{z}+z'^2}=\frac{z'\operatorname{Im}\bar{z}}{1-2z'\cos\bar{k}+z'^2}\\&=\frac{\operatorname{Im}\bar{z}}{z'+z'^{-1}-2\cos\bar{k}}=\frac{\operatorname{Im}\bar{z}}{z'+z'^{-1}+2\cos k-4}\\&=\frac{\operatorname{Im}\bar{z}}{z'+z'^{-1}+z+z^{-1}-4}\end{aligned}\tag{4.9}$$

where (4.2) was used to go from $\bar{z}$ to z in the denominator. From (4.5) we recognise the denominator in the last expression as $\lambda^2+\mu^2$. Also, since $z=\mathrm{e}^{ik}$, we can write (4.5) as

$$\lambda=\mathrm{e}^{-ik/2}-\mathrm{e}^{ik/2}=-2\mathrm{i}\sin\tfrac{1}{2}k=2\sin\tfrac{1}{2}\bar{k}\tag{4.10}$$

in view of (4.2). On the branch cut λ is real and therefore $\bar{k}$ is real, giving

$$\operatorname{Im}\bar{z}=\sin\bar{k}=\lambda(1-\tfrac{1}{4}\lambda^2)^{1/2}.\tag{4.11}$$

Also

$$\mathrm{d}z/z=\mathrm{i}\,\mathrm{d}k=\frac{2\mathrm{i}\,\mathrm{d}\sin\frac{1}{2}k}{\cos\frac{1}{2}k}=-\frac{\mathrm{d}\lambda}{(1+\frac{1}{4}\lambda^2)^{1/2}}.\tag{4.12}$$

Thus (4.8) becomes (note that $z=1\to\lambda=0$, $z=z_0\to\lambda=2$)

$$G'(\mu)=G_1'(\mu)+\frac{1}{\pi}\int_0^2\mathrm{d}\lambda\frac{(4-\lambda^2)^{1/2}}{(4+\lambda^2)^{1/2}}G(\lambda)(1+\eta'z^s)\frac{\lambda}{\lambda^2+\mu^2}\tag{4.13}$$

and similarly

$$G(\lambda)=G_1(\lambda)+\frac{1}{\pi}\int_0^2\mathrm{d}\mu\frac{(4-\mu^2)^{1/2}}{(4+\mu^2)^{1/2}}G'(\mu)(1+\eta z'^{s'})\frac{\mu}{\lambda^2+\mu^2}.\tag{4.14}$$

4.2. Results adapted from continuum

Comparing (4.13) with (3.11), we see that the two are identical except for a factor depending only on λ. Therefore equations (3.13)-(3.16) hold *exactly as before* provided we alter (3.17) and (3.18) to be

$$\chi(\alpha)=\tfrac{1}{2}(1+z(\alpha)^s)\left(\frac{4-\lambda^2}{4+\lambda^2}\right)^{1/2}\tag{4.15}$$

$$\chi'(\beta)=\tfrac{1}{2}(1+z'(\beta)^{s'})\left(\frac{4-\mu^2}{4+\mu^2}\right)^{1/2}\tag{4.16}$$

and cut off the integrals in (3.15) and (3.16) at +2 instead of $+\infty$. It is understood that

$$\frac{1-z(\alpha)}{\sqrt{z(\alpha)}}=\frac{\mathrm{e}^\alpha}{s}\qquad\frac{1-z'(\beta)}{\sqrt{z'(\beta)}}=\frac{\mathrm{e}^\beta}{s}.\tag{4.17}$$

The rest of § 3 can be repeated without change, leading to (3.47) with the integrals going from $-\infty$ to +2. However, the derivation of (3.52) must be re-examined.

Again referring to (4.5), we denote by $G_0(\lambda)$ the assignment of relative probability z^u to the point on the top side of the rectangle, u steps from the right corner. To this point $F_1'(y)$ assigns a probability $\tau(y, u)$ given by (4.1), and $G_1'(\mu)$ assigns

$$\sum_1^\infty z'^y \tau(y, u) = \frac{1}{2\pi} \int_0^{2\pi} e^{iku} \left(\frac{1}{1 - z' e^{ik}} - 1 \right) dk$$
$$= \frac{1}{\pi} \int_0^2 d\lambda \left(\frac{4-\lambda^2}{4+\lambda^2} \right)^{1/2} z^u \frac{\lambda}{\lambda^2 + \mu^2} \tag{4.18}$$

by the same steps that led from (4.8) to (4.13).

It follows that

$$G_1'(\mu) = \int_0^2 \frac{1}{\pi} \frac{\lambda}{\lambda^2+\mu^2} \left(\frac{4-\lambda^2}{4+\lambda^2} \right)^{1/2} G_0(\lambda)\, d\lambda \tag{4.19}$$

and with a similar definition of $G_0'(\mu)$

$$G_1(\lambda) = \int_0^2 \frac{1}{\pi} \frac{\mu}{\lambda^2+\mu^2} \left(\frac{4-\mu^2}{4+\mu^2} \right)^{1/2} G_0'(\mu)\, d\mu. \tag{4.20}$$

Thus

$$F_\infty = \frac{1}{\pi^2} \left[\int_0^2 h_0'(\ln \mu s) G_0'(\mu) \left(\frac{4-\mu^2}{4+\mu^2} \right)^{1/2} d\mu + \int_0^2 h_0(\ln \lambda s) G_0(\lambda) \left(\frac{4-\lambda^2}{4+\lambda^2} \right)^{1/2} d\lambda \right] \tag{4.21}$$

where h_0, h_0' are still determined by (3.34) and (3.35), but with χ, χ' given by (4.15) and (4.16). Equations (3.53) and (3.54) are replaced by

$$f_\infty(u) = \frac{2}{\pi^2} \int_0^2 h_0(\ln \lambda s) z^u \left(\frac{4-\lambda^2}{4+\lambda^2} \right)^{1/2} d\lambda \tag{4.22}$$

and

$$f_\infty'(u) = \frac{2}{\pi^2} \int_0^2 h_0'(\ln \mu s) z'^u \left(\frac{4-\mu^2}{4+\mu^2} \right)^{1/2} d\mu \tag{4.23}$$

with (4.5) assumed as usual. There is no longer a factor du in the probability. F_∞ must be symmetrised as before.

5. Re-entry on a lattice

5.1. Monte Carlo procedure

We now take up the re-entry problem. The particle has just exited from a specified point on the perimeter, and we want its re-entry distribution.

We first study an auxiliary problem: how will the endpoints be distributed on the rectangle if the starting points are distributed on the positive x axis in proportion to z^x, where z is a given positive real number < 1? Obviously the endpoint distribution is given, apart from normalisation, by $G(\lambda)$ as in (4.5) and (4.6). $G(\lambda)$ is determined by (4.13) and (4.14).

The method of eigenfunctions does not appear useful here, as we would need to know all the eigenfunctions and not just the limit when $\omega \to 0$. We take our departure instead from the fact that (if $\eta = \eta' = 1$) all the factors in (4.13) and (4.14) are positive definite and so these equations can be converted into a Monte Carlo prescription.

Actually we must not set $\eta = \eta' = 1$ since the starting distribution is not symmetrised. However, this presents no obstacle, as we shall see. First, let us describe how to proceed without the factors η and η'.

We wish the first step to be a selection of μ. Therefore we use (4.20) to write (4.14) (with $\eta = 1$) as

$$G(\lambda) = \frac{1}{\pi}\int_0^2 [G_0'(\mu) + G'(\mu)(1+z'^{s'})]\left(\frac{4-\mu^2}{4+\mu^2}\right)^{1/2}\frac{\mu\,\mathrm{d}\mu}{\lambda^2+\mu^2} \tag{5.1}$$

where the definitions (4.5) and (4.6) still hold. To make this a prescription for choosing μ, we must normalise the quantity in square brackets. Since $G_0'(\mu)$ assigns probabilities z'^u $(u = 0, 1, \ldots, s')$, its normalisation is

$$\bar{G}_0'(\mu) = \sum_0^{s'} z'^u = \frac{1 - z'^{s'-1}}{1 - z'}. \tag{5.2}$$

Likewise

$$\bar{G}'(\mu) = \sum_1^{\infty} z'^y \bar{F}'(y) = \sum_1^{\infty} z'^y = \frac{z'}{1-z'}. \tag{5.3}$$

Therefore,

$$\begin{aligned}\bar{G}_0'(\mu) + \bar{G}'(\mu)(1+z'^{s'}) &= \frac{1 - z'^{s'+1} + z'(1+z'^{s'})}{1-z'}\\ &= \frac{1+z'}{1-z'} = \frac{(4+\mu^2)^{1/2}}{\mu}.\end{aligned} \tag{5.4}$$

We can now write (5.1) as

$$G(\lambda) = \frac{1}{\pi}\int_0^2 P'(\mu)(4-\mu^2)^{1/2}\frac{\mathrm{d}\mu}{\lambda^2+\mu^2} \tag{5.5}$$

where $P'(\mu)$ is the normalised probability distribution over the rectangle, proportional to $G_0'(\mu) + (1+z'^{s'})G'(\mu)$. Hence the first step is to select μ between 0 and 2 with a probability measure proportional to $(4-\mu^2)^{1/2}\,\mathrm{d}\mu/(\lambda^2+\mu^2)$. This can be done quickly by picking $\tan^{-1}(\mu/\lambda)$ uniformly between 0 and $\frac{1}{2}\pi$, rejecting $\mu > 2$, and applying a rejection factor $(1-\frac{1}{4}\mu^2)^{1/2}$ otherwise.

Once μ is selected, we must proceed so as to realise the distribution $P'(\mu)$. This is easily done as follows. Let us refer to our starting position, in which the particle was distributed as z^x over the positive x axis, as 'horizontal stride position'. Likewise in 'vertical stride position' it is distributed as z'^y on the positive y axis. From the horizontal stride position we select μ as above. Then we toss a biased coin whose probability of heads is $z'/(1+z')$, the ratio of (5.3) to (5.4). If it lands heads, we go into vertical stride position with the selected μ. If it is tails, we choose a random number r between 0 and 1. If $r < z'^{s'+1}$, we enter vertical stride position also. If $r > z'^{s'+1}$, we enter the rectangle on the right side, u steps from the top, where u is the largest integer such that $r < z'^u$. (This realises $G_0'(\mu)$.)

From the vertical stride position we proceed similarly: select λ with measure $(4-\lambda^2)^{1/2}\,\mathrm{d}\lambda/(\lambda^2+\mu^2)$ between 0 and 2, throw a biased coin with probability $z/(1+z)$ of heads (always using (4.5)); if heads, go into horizontal stride position with new λ; if tails, choose r; if $r < z^{s+1}$, go into horizontal stride position also; otherwise re-enter top side of rectangle u steps from right where u is largest integer with $r < z^u$.

This procedure would always end up on the top or right side of the rectangle, because we have left out the factors η, η'. However, they are easily included. The factor η should have entered whenever we went into vertical stride position after a throw of tails. Call this an η event. Likewise, an η' event takes place whenever we go into horizontal stride position after a throw of tails. Since the reflections commute, we have only to count these events. At the end of the walk, we reflect about the horizontal axis if there were an odd number of η events, and also about the vertical axis if there were an odd number of η' events. In this way the endpoints are distributed all over the rectangle.

We now return to the original problem: suppose the walk begins with an exit from the top side, u steps from the right. (Other sides are handled similarly.) We assume we have really exited so that the walk begins at $(-u, 1)$. Then the probability that the first stride ends at $(x, 0)$ is $g_1(x+u)$ where

$$g_1(x) = \tau(1, x) = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{\mathrm{i}k|x|}\,\mathrm{e}^{\mathrm{i}\bar{k}}\,\mathrm{d}k \tag{5.6}$$

in accordance with (4.1). (We can take $x \to |x|$ since τ is even in x.) Shrinking the contour in the z plane down to the branch cut and using $z = \mathrm{e}^{\mathrm{i}k}$, $\bar{z} = \mathrm{e}^{\mathrm{i}\bar{k}}$ as in § 4, this becomes

$$\begin{aligned} g_1(x) &= \frac{1}{\pi}\int_{z_0}^{1} \frac{\mathrm{d}z}{z}\, z^{|x|}\, \mathrm{Im}\,\bar{z} \\ &= \frac{1}{\pi}\int_0^2 z^{|x|}\left(\frac{4-\lambda^2}{4+\lambda^2}\right)^{1/2} \lambda\,\mathrm{d}\lambda \end{aligned} \tag{5.7}$$

in view of (4.11) and (4.12). Again all factors are positive definite, and so we interpret (5.7) as the first step in a Monte Carlo procedure.

The normalisation of $z^{|x|}$ is

$$\sum_{-\infty}^{\infty} z^{|x|} = \frac{1+z}{1-z} = \frac{(4+\lambda^2)^{1/2}}{\lambda} \tag{5.8}$$

and therefore the correct probability measure for λ is proportional to $(4-\lambda^2)^{1/2}\,\mathrm{d}\lambda$, between 0 and 2. The first step is to choose λ with this measure.

Once λ is selected, the probability distribution is $z^{|x|}$ on the x axis; therefore we need only slightly modify the procedure used when coming from vertical stride position. We flip the same biased coin as before (heads $z/(1+z)$ of the time). We also pick r uniformly from 0 to 1. If the coin is heads, we enter horizontal stride position if $r < z^u$; otherwise we re-enter the rectangle v steps to the right of our exit point, where v is the smallest integer such that $r > z^v$. If the coin is tails, we enter horizontal stride position (an η' event) if $r < z^{s-u+1}$; otherwise we re-enter the rectangle v steps to the left of our exit, where now v is the largest integer such that $r < z^v$. (Note that v can be zero only if the coin turns up tails; that is why the coin must be biased.)

5.2. *Cut-off for long walks*

This completes the description of the Monte Carlo procedure, but we must now ask how soon it terminates. The probability of immediate termination is small when z or $z' \to 1$, i.e. when λ or $\mu \to 0$. In terms of $\alpha = \ln \lambda s$ or $\beta = \ln \mu s$, as in § 3, this means that walks for which α becomes large negative can be long. Since in this region

$\chi(\alpha) \simeq \chi'(\beta) \simeq 1$, we can drop the distinction between α and β and say that the walk occurs in α space with a step $\Delta\alpha$ distributed as sech $\Delta\alpha$.

Now an unbiased random walk in one dimension has an infinite average length before returning to the origin. This means that some rare very long walks will dominate the computer time; these correspond to the walks in position space that go far from the rectangle. It is necessary to eliminate these walks by putting a cut-off on λ, say by rejecting any walk for which we generate a $\lambda < \lambda_0$ where $\lambda_0 s \ll 1$ is a fixed number. We must now estimate both the bias thereby introduced and the average number of strides to a walk, as a function of λ_0.

We may form an idea of the bias by remembering the electrostatic analogy. The charge distribution induced on the rectangle by a far-off charge may be expanded in multipoles, where the monopole term is independent of the position of the inducing charge. To reject the walk is to replace it by a new walk from infinity, so that the monopole term is retained and the others discarded. The leading error is from the dipole term which is of relative order s/x, x being the distance. Thus we should expect that rejecting the walk at $\lambda = \lambda_0$ would cause an error

$$\sim\left(\sum_1^\infty z^x s/x\right)\left(\sum_1^\infty z^x\right)^{-1} = \frac{1-z}{z} s \ln\frac{1}{1-z} \approx \lambda_0 s \ln\frac{1}{\lambda_0}.$$

This estimate is confirmed by studying the Monte Carlo process. Starting in horizontal stride position, the dipole term is dominated by walks that end in one stride, since afterward the particle tends to forget which side it came from. After μ is chosen, the probability of entering the rectangle immediately is $\frac{1}{2}(1 - z'^{s'+1}) \approx \frac{1}{2}(1 - e^{-\mu s'})$, and so the total fraction of walks that end in one stride is roughly

$$\begin{aligned}
&\left(\int_0^\infty \frac{d\mu}{\lambda_0^2+\mu^2}\tfrac{1}{2}(1-e^{-\mu s'})\right)\left(\int_0^\infty \frac{d\mu}{\lambda_0^2+\mu^2}\right)^{-1}\\
&\qquad = \frac{\lambda_0}{2\pi}\int_0^\infty \frac{d\mu}{\lambda_0^2+\mu^2}(1-e^{-\mu s'})\\
&\qquad = \frac{1}{2\pi}\int_0^\infty \frac{\sin(\lambda_0 s' w)\, dw}{w(w+1)}\\
&\qquad = \frac{1}{2\pi}\lambda_0 s'\left(\ln\frac{1}{\lambda_0 s'} + O[1]\right)
\end{aligned} \tag{5.9}$$

confirming the previous estimate, if s and s' are of the same order. The factor $1/2\pi$ represents rationalised units, and the term in $\ln s'$ is a non-dipole contribution. (We have used (3.9) with changed variables.)

For a more detailed estimate, we resolve into eigenspaces of η, η'. The space with η, $\eta' = 1$ should contain principally a quadrupole correction

$$\left(\sim\sum_1^\infty z^x (s/x)^2\right)\left(\sum_1^\infty z^s\right)^{-1} \approx (\lambda_0 s)^2 \ln(1/\lambda_0)$$

and indeed we find that the result of replacing $H(\alpha)$ by $H(-\infty)$ is, according to (3.32), mainly the omission of a double pole at $\omega = 2i$, which should contribute in proportion to $d/d\omega|_{\omega=2i}\, e^{i\omega|\alpha|}$ or to $|\alpha|\, e^{-2|\alpha|} = (\lambda_0 s)^2 \ln(1/\lambda_0 s)$. The space with $\eta = 1$, $\eta' = -1$ contributes mainly the term $(1/2\pi)\lambda_0 s' \ln(1/\lambda_0 s')$ noted above. For $\eta = -1$, the first stride contribution involves only differences between z'^u and $z'^{s'-u}$, so that it has an extra factor $\sim 1 - z'^s \sim 1 - e^{-\mu s'}$ which gives an extra factor $\lambda_0 s'$ to the last line of (5.9);

the passage to vertical stride involves a factor $1+\eta z^{s'}=1-z'^{s}$ which multiplies all subsequent corrections.

Thus the main errors are $O[(\lambda_0 s)^2 \ln(1/\lambda_0 s)]$ from the symmetric sector, and $(1/2\pi)\lambda_0 s' \ln(1/\lambda_0 s)$ from $\eta'=-1$. But the antisymmetric sectors are already reduced by the time the walk gets to λ_0, by a similar dipole factor. That is, the particle can forget which side is which as easily on the way out as on the way in. Therefore the dominant error is really about

$$\left(\frac{1}{2\pi}\lambda_0 s' \ln\frac{1}{\lambda_0 s'}\right)^2 \tag{5.10}$$

which is still larger than the quadrupole term. (We are assuming that s and s' are of the same order.)

To study the average number of strides, we may regard (5.5) as describing a walk in α (or β) space for which (when $\lambda s \ll 1$, $\mu s' \ll 1$) the kernel is proportional to $\operatorname{sech}(\alpha-\beta)$. The mean square length of a step is

$$\left(\int_{-\infty}^{\infty}\Delta^2 \operatorname{sech}\Delta\, d\Delta\right)\left(\int_{-\infty}^{\infty}\operatorname{sech}\Delta\, d\Delta\right)^{-1}=(\tfrac{1}{2}\pi)^2. \tag{5.11}$$

Therefore if we start at $\lambda s \sim 1$, the cut-off is n steps away where

$$n \simeq \frac{2}{\pi}\ln\frac{1}{\lambda_0 s}. \tag{5.12}$$

In a one-dimensional random walk of fixed-length steps between two walls n steps apart, the average number of steps between impacts is exactly n. Here the steps are not uniform, but the asymptotic behaviour must be the same. Therefore a walk will contain $O[n]$ strides on the average, once it reaches $\lambda \sim 1/s$.

However, the first choice of λ is distributed quasiuniformly from 0 to 2. Thus one usually starts with $\lambda s \gg 1$, so that the probability of survival after each stride is $\zeta=\frac{1}{2}(1+z^s)\simeq\frac{1}{2}(1+e^{-\lambda s})\simeq\frac{1}{2}$. For a walk with kernel $(\zeta/\pi)\operatorname{sech}(\alpha-\beta)$, the probability of arrival from α to β after any number of steps is

$$\sum_1^{\infty}\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(i\omega(\alpha-\beta))(\zeta \operatorname{sech}\tfrac{1}{2}\pi\omega)^n\, d\omega$$

$$=\frac{2}{\pi}\frac{\zeta}{(1-\zeta^2)^{1/2}}\frac{\sinh[(2-\kappa)(\alpha-\beta)]}{\sinh 2(\alpha-\beta)} \tag{5.13}$$

where $\cos\frac{1}{2}\pi\kappa=\zeta$. Thus for $\zeta=\frac{1}{2}$ the probability is

$$\frac{2}{\pi\sqrt{3}}\frac{\sinh\frac{4}{3}(\alpha-\beta)}{\sinh 2(\alpha-\beta)}\simeq\frac{2}{\pi\sqrt{3}}c^{-2(\alpha-\beta)/3} \tag{5.14}$$

if $\alpha-\beta$ is large. So the average number of strides in a walk starting from $\lambda s \gg 1$ is of the order

$$n\exp(-\tfrac{2}{3}\ln\lambda s)\sim(\lambda s)^{-2/3}\ln(1/\lambda_0 s). \tag{5.15}$$

The preceding calculation holds only near the corner. If we must shoot for the corner from u steps away there is an additional factor z^u on the first step of the Monte

Carlo procedure. Say that $u \gg 1$; then for $\lambda \gtrsim 1/u$ this factor makes the likelihood of escape very small. The average number of steps for all λ is then of order

$$m(u) \sim \ln \frac{1}{\lambda_0 s} \int_0^2 (\lambda s)^{-2/3} \mathrm{e}^{-\lambda u} \, \mathrm{d}\lambda$$

$$\sim \frac{1}{s} \left(\frac{s}{u}\right)^{1/3} \ln \frac{1}{\lambda_0 s}. \tag{5.16}$$

This quantity should be averaged over u, with a weighting factor representing the distribution of exits. For large s it seems reasonable that this distribution is given by some function $w(u/s)$ and that the overall number of strides per exterior walk is

$$\bar{m} = \int_0^1 m(\nu s) w(\nu) \, \mathrm{d}\nu \sim \frac{1}{s} \ln \frac{1}{\lambda_0 s} \tag{5.17}$$

always neglecting factors O[1].

The bias introduced by the cut-off must also be multiplied by the frequency with which the cut-off is applied. Starting from $\lambda s \sim 1$, the probability of reaching a wall n steps away before returning to the origin is O[$1/n$]. Therefore the average error is given by replacing O[n] by O[$1/n$] in (5.17) and multiplying by (5.10). This yields (if $s \sim s'$)

$$\frac{1}{s} \left(\ln \frac{1}{\lambda_0 s} \right)^{-1} \left(\lambda_0 s \ln \frac{1}{\lambda_0 s} \right)^2 = \lambda_0^2 s \ln \frac{1}{\lambda_0 s}. \tag{5.18}$$

The implication of (5.17) is that if s is large we can set $\lambda_0 \sim (1/s)\, \mathrm{e}^{-s}$ and still have $\bar{m} \sim 1$ so that long walks will not dominate the computer time. Then (5.18) says that the average error per walk is $\lambda_0^2 s^2$ which is e^{-2s}. If $s = 100$, $\mathrm{e}^{2s} \sim 10^{46}$ so that the bias due to the cut-off is equivalent to a gross misplacement of one in every 10^{46} particles. To perceive this bias above statistical noise one would need a sample of clusters containing 10^{92} particles.

We conclude that the problem of long walks need not worry us.

6. Conclusions

We have given solutions of a rather different kind for the two problems studied. For the approach to infinity the selection of entry point is made in the standard manner according to a probability distribution. This distribution is given by (3.52) once the functions $h_0(\alpha)$, $h_0'(\beta)$ are determined. They in turn are defined by the non-trivial equations (3.33) and (3.34). These equations must be solved numerically, perhaps by iteration. However, there is plenty of time to do this since it only has to be done once for each size rectangle. In simulating DLA one might, for example, multiply either s or s' by three whenever the cluster breaks out of the rectangle. Then to make a cluster of 10^6 points one would not need more than about twelve rectangles. So the time spent on a very accurate calculation of h_0, h_0' would be unimportant.

For the re-entry problem we do not calculate the probability distribution. Instead we introduce an auxiliary Monte Carlo process which has the same final probabilities as those desired. This process is much faster than the original random walk because it goes a whole stride at a time, but still requires only elementary functions at each stride.

The simulated probabilities are exact except for the neglect of very long walks. But the discussion in § 5 makes it clear that the resulting bias can be made small without much cost in machine time. Thus the only significant errors will be those due to the implementation of the procedure: finite statistics, machine rounding, and interpolation and truncation errors in the solution of (3.34) and (3.35).

Since for a large rectangle most re-entries take place in just one stride, it appears that in the simulation of DLA the computing time spent on walks outside the containing rectangle will be a negligible fraction of the whole.

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References

[1] Witten T A and Sander L M 1981 *Phys. Rev. Lett.* **47** 1400
[2] Meakin P 1983 *Phys. Rev.* A **27** 604, 1495
[3] Meakin P 1985 *J. Phys. A: Math. Gen.* **18** L661
[4] Meakin P 1986 *Phys. Rev.* A **33** 3371
[5] Ball R C and Brady R M 1985 *J. Phys. A: Math. Gen.* **18** 869
[6] Friedberg R and Martin O 1987 *University of Illinois preprint* I11-87/3/50
[7] Friedberg R and Martin O 1987 *J. Phys. A: Math. Gen.* **20** 5095