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LETTER TO THE EDITOR

Distribution of the area enclosed by a plane random walk

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Abstract. We derive an exact expression for the distribution function for the (algebraic) area enclosed by a plane closed random walk, using a continuous model from the start. Our result has a different analytical form but is numerically close to an expression for the same quantity of a discrete model, derived by Brereton and Butler.

In a recent paper Brereton and Butler (1987) pointed out that topologically constrained polymers can be roughly represented by random walks which enclose a constant area. This was the motivation for an explicit derivation of the distribution function for the (algebraic) area enclosed by a plane closed random walk of N steps, of equal average length l; see equation (4.12) of Brereton and Butler (1987).

In view of the importance of topological problems in polymer physics we have studied the problem of Brereton and Butler with a different method in which a continuous model is used from the beginning. Our result has a different analytical form but is quantitatively close to the expression derived by these authors.

First, we note that the probability density of a plane random walk has the Wiener integral representation

$$p(\boldsymbol{r}, N) = \int_{\boldsymbol{r}_0,0}^{\boldsymbol{r},N} \exp\left[-\frac{1}{l^2}\int_0^N \left(\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\nu}\right)^2 \mathrm{d}\nu\right] \mathrm{d}(\boldsymbol{r}(\nu)) \tag{1}$$

in an obvious notation (cf Wiegel 1986 and references therein). In the limit $\boldsymbol{r}\to\boldsymbol{r}_0$ in which the end point of the walk approaches the initial position $\boldsymbol{r}_0$ the probability density is

$$\lim_{\boldsymbol{r}\to\boldsymbol{r}_0} p(\boldsymbol{r}, N) = (\pi N l^2)^{-1}. \tag{2}$$

As the constraint that the (algebraic) area which is enclosed by a trajectory $\boldsymbol{r}(\nu)$ equals A can be expressed analytically by

$$A = \frac{1}{2}\int_0^N \left(x\frac{\mathrm{d}y}{\mathrm{d}\nu} - y\frac{\mathrm{d}x}{\mathrm{d}\nu}\right) \mathrm{d}\nu \tag{3}$$

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then the desired distribution function for A is given by the path integral

$$P(A, N) = \pi N l^2 \int_{\boldsymbol{r}_0, 0}^{\boldsymbol{r}_0, N} \delta\left[A - \frac{1}{2}\int_0^N \left(x\frac{\mathrm{d}y}{\mathrm{d}\nu} - y\frac{\mathrm{d}x}{\mathrm{d}\nu}\right)\mathrm{d}\nu\right] \times \exp\left[-\frac{1}{l^2}\int_0^N \left(\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\nu}\right)^2 \mathrm{d}\nu\right] \mathrm{d}(\boldsymbol{r}(\nu)). \tag{4}$$

Of course, the delta function can be represented by a Fourier integral, which gives

$$P(A, N) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \tilde{P}(g, N)\exp(\mathrm{i}gA)\,\mathrm{d}g \tag{5}$$

where

$$\tilde{P}(g, N) = \pi N l^2 \int_{\boldsymbol{r}_0, 0}^{\boldsymbol{r}_0, N} \exp\left(-\int_0^N L\,\mathrm{d}\nu\right)\mathrm{d}(\boldsymbol{r}(\nu)) \tag{6}$$

with

$$L = \frac{1}{l^2}\left(\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\nu}\right)^2 + \tfrac{1}{2}\mathrm{i}g\left(x\frac{\mathrm{d}y}{\mathrm{d}\nu} - y\frac{\mathrm{d}x}{\mathrm{d}\nu}\right). \tag{7}$$

It will be shown shortly that (5) can be evaluated by contour integration in the complex g plane and that the singularities of the function $\tilde{P}(g, N)$ are located on the imaginary g axis. Hence we put $\mathrm{i}g = -\lambda$, treat λ as a real number and write

$$L = \frac{1}{l^2}\left(\frac{\mathrm{d}x}{\mathrm{d}\nu}\right)^2 + \frac{1}{l^2}\left(\frac{\mathrm{d}y}{\mathrm{d}\nu}\right)^2 - \tfrac{1}{2}\lambda\left(x\frac{\mathrm{d}y}{\mathrm{d}\nu} - y\frac{\mathrm{d}x}{\mathrm{d}\nu}\right). \tag{8}$$

The evaluation of the path integral (5) is straightforward as (5) is similar to the path integral for a quantum mechanical particle in a constant magnetic field. To make this letter more self-contained we nevertheless outline the main steps.

The maximum contribution comes from the trajectory which is a solution of the Euler–Lagrange equations

$$\frac{\mathrm{d}^2x}{\mathrm{d}\nu^2} = -\tfrac{1}{2}\lambda l^2\frac{\mathrm{d}y}{\mathrm{d}\nu} \qquad \frac{\mathrm{d}^2y}{\mathrm{d}\nu^2} = \tfrac{1}{2}\lambda l^2\frac{\mathrm{d}x}{\mathrm{d}\nu}. \tag{9}$$

One finds the general solution

$$x(\nu) = A + C\sin(\phi + \omega_0\nu) \tag{10a}$$

$$y(\nu) = B - C\cos(\phi + \omega_0\nu) \tag{10b}$$

where

$$\omega_0 = \tfrac{1}{2}\lambda l^2. \tag{11}$$

The four real constants A, B, C, ϕ follow from the condition that the trajectory passes through $\boldsymbol{r}_0$ for $\nu = 0$ and through $\boldsymbol{r}_1$ for $\nu = N$; later we shall take the limit $\boldsymbol{r}_1 \to \boldsymbol{r}_0$. The shape of the trajectory is part of a circle which has its centre in (A, B) and which has a radius C. This arc is traversed with a uniform value of

$$\left(\frac{\mathrm{d}x}{\mathrm{d}\nu}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}\nu}\right)^2 = \omega_0^2 C^2. \tag{12}$$

A simple geometric consideration shows that the arc length equals $N\omega_0 C$ on the one hand, but

$$2C\sin^{-1}\{[(x_1-x_0)^2+(y_1-y_0)^2]^{1/2}/2C\}$$

on the other hand. Hence by equating these two expressions one finds

$$C=[(x_1-x_0)^2+(y_1-y_2)^2]^{1/2}/2\sin(\tfrac{1}{2}N\omega_0) \tag{13}$$

which in principle determines the trajectory.

Next one substitutes the explicit form of the most likely path back into (8) and integrates over $\mathrm{d}\nu$. This calculation is again remarkably tedious and can be somewhat simplified by the use of geometrical considerations. The result is

$$S=\int_0^N L\,\mathrm{d}\nu=-\frac{\omega_0}{l^2}(x_0y_1-y_0x_1)+\frac{\omega_0}{2l^2}[(x_1-x_0)^2+(y_1-y_0)^2]\cot\mathrm{an}(\tfrac{1}{2}N\omega_0). \tag{14}$$

A standard argument for path integrals with quadratic exponentials now shows that the path integral

$$G(x_1,y_1,N|x_0,y_0)=\int_{r_0,0}^{r_1,N}\exp\left\{-\int_0^N\left[\frac{1}{l^2}\left(\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}\nu}\right)^2-\frac{\lambda}{2}\left(x\frac{\mathrm{d}y}{\mathrm{d}\nu}-y\frac{\mathrm{d}x}{\mathrm{d}\nu}\right)\right]\mathrm{d}\nu\right\}\mathrm{d}(\boldsymbol{r}(\nu)) \tag{15a}$$

must have the form

$$G(x_1,y_1,N|x_0,y_0)$$
$$=f(N)\exp\left(\frac{\omega_0}{l^2}(x_0y_1-y_0x_1)-\frac{\omega_0}{2l^2}[(x_1-x_0)^2+(y_1-y_0)^2]\cot\mathrm{an}(\tfrac{1}{2}N\omega_0)\right) \tag{15b}$$

where $f(N)$ does *not* depend on x_0, y_0, x_1 or y_1.

It also follows from the definition of the path integral that

$$G(x_1,y_1,N|x_0,y_0)=\int_{-\infty}^{\infty}\mathrm{d}x^1\int_{-\infty}^{\infty}\mathrm{d}y^1\,G(x_1,y_1,N-N^1|x^1,y^1)G(x^1,y^1,N^1|x_0,y_0) \tag{16}$$

for all N^1 such that $0<N^1<N$. Upon substitution of (15) one finds that the unknown function $f(N)$ has the property

$$f(N)=\frac{2\pi l^2/\omega_0}{\cot\mathrm{an}(\tfrac{1}{2}N^1\omega_0)+\cot\mathrm{an}[\tfrac{1}{2}(N-N^1)\omega_0]}f(N^1)f(N-N^1). \tag{17}$$

It is easy to verify that the solution of this functional equation is

$$f(N)=\frac{\omega_0}{2\pi l^2}\frac{1}{\sin(\tfrac{1}{2}N\omega_0))}. \tag{18}$$

Substitution of the last equation into (15) gives

$$G(x_1,y_1,N|x_0,y_0)$$
$$=\frac{\omega_0}{2\pi l^2\sin(\tfrac{1}{2}N\omega_0)}\exp\bigg(\frac{\omega_0}{l^2}(x_0y_1-x_1y_0)$$
$$-\frac{\omega_0}{2l^2}[(x_1-x_0)^2+(y_1-y_0)^2]\cot\mathrm{an}(\tfrac{1}{2}N\omega_0)\bigg). \tag{19}$$

Using this result for $x_0 = x_1$, $y_0 = y_1$ and putting $\lambda = -\mathrm{i}g$ again, (6) becomes

$$\tilde{P}(g, N) = \frac{\frac{1}{4}Ngl^2}{\sinh(\frac{1}{4}Ngl^2)}. \tag{20}$$

Note that $\tilde{P}(0, N) = 1$, as it should because the integral of the distribution function for A should be normalised to unity. Substituting the previous equation into (5) one finds that $P(A, N)$ is of the form

$$P(A, N) = \frac{2}{\pi Nl^2} p\left(\frac{4A}{Nl^2}\right) \tag{21}$$

where

$$p(\xi) = \int_{-\infty}^{+\infty} \frac{u}{\sinh u} \exp(\mathrm{i}u\xi)\, \mathrm{d}u. \tag{22}$$

The integrand has singularities at $u = n\pi\mathrm{i}$ with $n = \pm 1, \pm 2, \ldots$. Near $n\pi\mathrm{i}$ one can write $\sinh u \simeq (-1)^n(u - n\pi\mathrm{i})$. For a positive value of ξ the contour of integration can be closed with a semicircle in the positive complex u plane. Hence Cauchy's theorem gives a series for $p(\xi)$ which can be summed to give

$$p(\xi) = \pi/4 \cosh^2(\tfrac{1}{2}\pi\xi). \tag{23}$$

Combination of (21) and (23) gives the final result

$$P(A, N) = \left[2Nl^2 \cosh^2\left(\frac{2\pi A}{Nl^2}\right)\right]^{-1}. \tag{24}$$

This analytical result for the continuous random walk model is remarkably simple. In order to compare with the results of Brereton and Butler (1987) for the discrete model we should consider $P(A, N)$ as a function of A/Nl^2 for large N. Equation (24) starts with the value $\frac{1}{2}$ for $(A/Nl^2) = 0$ and has the asymptotic behaviour $\exp(-4\pi A/Nl^2)$ for $(A/Nl^2) \gg 1$. The results for $P(A, N)$ for the discrete model start with a value of about 0.53 and have the asymptotic behaviour $\exp(-aA/bNl^2)$ with $a \simeq 4.95$ and $b \simeq 0.45$. As $a/b \simeq 10.9$ is fairly close to $4\pi \simeq 12.6$ we conclude that the continuous random walk result (24) is a fair approximation to the distribution of the area enclosed by a discrete random walk.

References

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