The random walk winding number problem: convergence to a diffusion process with excluded area

1987 J. Phys. A: Math. Gen. 20 5949

(http://iopscience.iop.org/0305-4470/20/17/028)

J. Phys. A: Math. Gen. **20** (1987) 5949-5960. Printed in the UK

The random walk winding number problem: convergence to a diffusion process with excluded area

Mitchell A Berger

Department of Applied Mathematics, University of St Andrews, Fife, KY16 9SS, UK

Received 10 April 1987, in final form 29 June 1987

Abstract. The winding number of a random walk in the plane is the net angle through which the walker encircles the origin. This paper discusses the moments and asymptotic form of the winding number distribution for walks of constant step size l. We show that the root mean square winding number θ_{rms} grows logarithmically with the number of steps N as $N \to \infty$, in contrast with the $N^{1/2}$ growth of the radial distribution. The corresponding diffusion process, however, has infinite θ_{rms}, and does not provide a good approximation for the random walk distribution. Instead, a diffusion process considered recently by Rudnick and Hu, where the area surrounding the origin has been removed out to a radius R, provides the correct asymptotic distribution. We find that the optimum radius for convergence of the finite step and diffusion distributions is precisely $R = e^{-2}l$.

1. Introduction

A particle starts out at the origin in the plane and takes random steps of constant size l. The first step defines the angle $\theta = 0$. How many times does the particle wind about the origin in its travels? This question was first raised by Lévy (1940). The net angle θ traversed at step N will be called the winding number of the walk. Because we distinguish circling about the origin once from no circling, we do not identify $\theta = 2\pi$ with $\theta = 0$; thus $\theta \in (-\infty, \infty)$ (the walk can be pictured as taking place on a Riemann surface covering the plane). The winding number problem has attracted attention recently because of its applications to solar physics (Berger 1987), and polymer physics (Rudnick and Hu 1987). Magnetic field lines in the solar atmosphere can become entangled due to the random motions of their endpoints in the solar photosphere. The relative motion of any two endpoints will have a winding number; as this number increases, the two overlying field lines become more and more braided. Similarly, winding numbers can help describe the random entanglement of two polymer filaments.

The radial development of a random walk can be closely approximated as a diffusion process (e.g. Chandrasekhar (1943) reprinted in Wax (1954)). Suppose a function $\rho_d(r, \phi, t)$ (where $\phi \in (0, 2\pi)$) diffuses away from the origin according to

$$\partial\rho_d/\partial t = D\nabla^2\rho_d.$$

(In this paper quantities related to a diffusion problem will have the subscript d; the corresponding random walk quantities will not be subscripted.) To relate the radial distribution $h_d(r, t) = \int_0^{2\pi} \rho_d \, d\phi$ to the radial distribution $h(r, N)$ for a walk with step size l, one must relate t to N. To this end, one introduces a dimensionless time variable $\tau = 4Dt/l^2$. With the scaling $\tau = N$, the second moments of the radial distributions are equivalent ($\overline{r^2} = \overline{r_d^2} = Nl^2$). Furthermore, the radial distributions converge for large N:

$$h(r, N) \approx h_d(r, \tau = N) = \frac{2}{N} e^{-r^2/N}. \tag{1}$$

This behaviour of the radial random walk suggests that the evolution of winding number may also be described by diffusion. Spitzer (1958) considered a diffusion problem in the plane with initial point $(r, \theta) = (l, 0)$. He showed that the asymptotic distribution $f_d(\theta)$ of winding number was a Cauchy function, i.e.

$$f_d(\theta) \approx \frac{1}{\pi\lambda}\left[1 + \left(\frac{\theta}{\lambda}\right)^2\right]^{-1} \qquad \lambda = \tfrac{1}{2}\log\tau. \tag{2}$$

Other properties of the winding number diffusion problem have been explored by Pitman and Yor (1984), Lyons and McKean (1984) and Berger and Roberts (1988).

Recently, Berger and Roberts (1988) have re-examined the actual random walk problem. They found that the standard eigenfunction method (Roberts and Ursell 1960) for finding random walk distributions fails for winding numbers, because the evolution of winding number is not a commutative process. Also, they conducted a numerical simulation involving 2×10^4 particles taking 10^5 random steps. Significant discrepancies appeared between $f(\theta, N)$ for the simulation and $f_d(\theta, N)$ given by the diffusion distribution. Also, the root mean square winding number θ_{rms} is infinite for the diffusion distribution (Lévy 1940), whereas θ_{rms} for the simulation grew roughly as $\log N$.

Rudnick and Hu (1987) have independently explored a different approach to the winding number problem. Particles which get very close to the origin can move rapidly in θ, which is why the diffusion process yields infinite θ_{rms} (and infinite higher moments in θ). Put another way, the operator $\nabla^2 = r^{-1}\partial_r(r\partial_r) + r^{-2}\partial_\phi^2$ has only a coordinate singularity at the origin. However, for $\theta \in (-\infty, \infty)$, $\nabla^2 = r^{-1}\partial_r(r\partial_r) + r^{-2}\partial_\theta^2$ has a more serious singularity which leads to infinite moments for $f_d(\theta)$. To remove this difficulty, Rudnick and Hu instead considered diffusion with a boundary placed at a radius R, preventing access to the singularity at the origin (Belisle (1986) has independently considered this problem). They showed that θ_{rms} grew logarithmically. Furthermore, a numerical random walk on a square lattice yielded results similar to those for bounded diffusion. Given a reflecting wall at R (see equation (11) below), the asymptotic distribution was found to be a sech function (Hu 1986), i.e. $f(\theta) \sim 1/\cosh(\theta/\lambda)$, where $\lambda \sim \log\tau$.

In the present paper, we explore the relationship between the finite step-size winding number problem and the bounded diffusion process. First, the mean square winding numbers (second moments) $\overline{\theta^2}(N)$ and $\overline{\theta_d^2}(\tau)$ are calculated in § 2. Just as comparison of second moments for the radial distributions determines the scaling $\tau = N$, we can compare second moments of winding number to find the most natural radius R for the reflecting boundary. This radius turns out to have the rather interesting value $R = e^{-2}l$. Section 3 gives equations for the evolution of higher polynomial moments of θ, $\overline{\theta^{2k}}(N)$, where only the radial random walk distribution need be known. These equations are solved in terms of radial Green functions. The correspondence of the random walk with the bounded diffusion process is then established. For the special radius $R = e^{-2}l$ all moments for the two processes converge, in the sense that the fractional error decreases with N as $\log^{-2} N$:

$$\frac{\overline{\theta^{2k}}(N) - \overline{\theta_d^{2k}}(\tau = N)}{\overline{\theta^{2k}}(N)} \sim (\log N)^{-2}.$$

For other values of R, the convergence is slower, with the fractional error decreasing as $4(\log^{-1} N)\log(e^2 R)$. The results of Berger and Roberts' (1988) numerical simulation are shown to be consistent with the finite step winding number distribution converging to the sech function.

2. The mean square winding number

2.1. Random walk

We will choose units such that the step size $l = 1$. Let $\rho(r, \theta, N)$ be the probability distribution at step N, where $0 < r < \infty$, $-\infty < \theta < \infty$. Integrating over θ gives $h(r, N) \equiv \int_{-\infty}^{\infty} \rho(r, \theta, N)\,\mathrm{d}\theta$, and integrating over r gives $f(\theta, N) \equiv \int_0^{\infty} \rho(r, \theta, N)\,\mathrm{d}\theta$. The radial distribution function $h(r, N)$ is described by the classical two-dimensional random walk problem, and quickly converges to the corresponding diffusion distribution (equation (1)). (The precise distribution in the plane centres on the initial point $(r, \theta) = (1, 0)$ rather than the origin, implying that a term of order N^{-2} should be added to $h(r, N)$. We will ignore terms to this order when considering the large-N behaviour of $f(\theta, N)$.) Averages over the entire distribution will be denoted by an overbar, and averages restricted to radius r by brackets, e.g.

$$\langle\theta^2\rangle(r, N) \equiv \int_{-\infty}^{\infty} \theta^2 \rho(r, \theta, N)\,\mathrm{d}\theta \tag{3a}$$

$$\overline{\theta^2}(N) \equiv \int_0^{\infty} \langle\theta^2\rangle(r, N) r\,\mathrm{d}r. \tag{3b}$$

In figure 1, the three independent variables (r, θ, ϕ) describe the position (r, θ) of a point P_{N+1} reached at step $N+1$ and the direction ϕ backwards to the point P_N at step N. The step between P_N and P_{N+1} can also be described by the independent

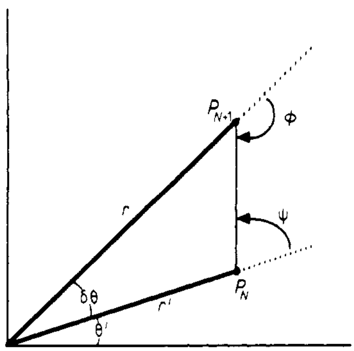

Figure 1. The geometry of the Nth step between P_N and P_{N+1}. The angle at step $N+1$ is $\theta = \theta' + \delta\theta$.

variables (r', θ', ψ), which give the position of P_N and the forward orientation of the step. Let $\delta\theta \equiv \theta - \theta'$. Then

$$r' = (1 + r^2 + 2r \cos\phi)^{1/2} \tag{4a}$$

$$\delta\theta = -\operatorname{sign}(\phi) \cot^{-1} \frac{r + \cos\phi}{\sin|\phi|} \tag{4b}$$

$$= +\operatorname{sign}(\psi) \cot^{-1} \frac{r' + \cos\psi}{\sin|\psi|}. \tag{4c}$$

(Here $-\pi \leqslant \phi, \psi \leqslant \pi$, and $0 \leqslant \cot^{-1} x \leqslant \pi$.) These transformations relate $\rho(r, \theta, N+1)$ to $\rho(r', \theta', N)$. To obtain $\rho(r, \theta, N+1)$, we integrate $\rho(r', \theta', N)$ over all possible previous positions at step N. A particle reaching (r, θ) at step $N+1$ must have come from a point lying on a unit circle centred at (r, θ); this circle is parametrised by ϕ and described by equations (4*a*) and (4*b*). Thus

$$\rho(r, \theta, N+1) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \rho(r', \theta', N)\, d\phi. \tag{5}$$

The mean square winding number defined in equation (3*b*) can be determined knowing only the radial distribution. From equation (5) and $\theta = \theta' + \delta\theta$ the mean square winding number at step $N+1$ is

$$\overline{\theta^2}(N+1) = \int_0^\infty \int_{-\infty}^{\infty} \theta^2 \rho(r, \theta, N+1)\, d\theta\, r\, dr$$
$$= \frac{1}{2\pi} \int_0^\infty \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} [\theta'^2 + 2\theta'\delta\theta + (\delta\theta)^2] \rho(r', \theta', N)\, d\phi\, d\theta\, r\, dr.$$

We must transform the integral to the coordinate set (r', θ', ψ); the Jacobian is just r'/r, so that

$$\overline{\theta^2}(N+1) = \frac{1}{2\pi} \int_0^\infty \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} [\theta'^2 + 2\theta'\delta\theta + (\delta\theta)^2] \rho(r', \theta', N)\, d\psi\, d\theta'\, r'\, dr'. \tag{6}$$

The cross term $2\theta'\delta\theta$ drops out because $\rho(r', \theta', N)$ is even in θ' (also because $\delta\theta$ is even in ψ). Consequently

$$\overline{\theta^2}(N+1) - \overline{\theta^2}(N) = \int_0^\infty \langle \delta\theta^2 \rangle(r') h(r', N) r'\, dr' \tag{7}$$

where

$$\langle \delta\theta^2 \rangle(r') = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left(\cot^{-1} \frac{r' + \cos\psi}{\sin|\psi|} \right)^2 d\psi. \tag{8}$$

The integration of equation (7) is performed in appendix 1. The result is, to first order in N^{-1},

$$\overline{\theta^2}(N+1) - \overline{\theta^2}(N) = \frac{1}{2N} (\log N) + \frac{a}{N} \tag{9}$$

where $a = (4 - \gamma)/2 \approx 1.712$ (γ = Euler's constant = 0.5772...). Summing over N' from $N' = 1$ to $N' = N$ yields

$$\overline{\theta^2}(N) = \tfrac{1}{4} (\log N)^2 + a \log N + b + O\left(\frac{\log N}{N} \right). \tag{10}$$

The neglected order N^{-2} terms determine the constant b; these terms arise in the exact expression for $h(r, N)$, in the integration of (7), and in the sum (rather than integration) over N. The values of $\overline{\theta^2}(N)$ and $\theta_{\rm rms}$ obtained in the numerical simulation of Berger and Roberts (1988) are consistent with these theoretical predictions, to within statistical error. The $\overline{\theta^2}$ for the simulation started off slightly low compared to the first terms of equation (10) (6% low at $N=10$); and reached within $1\sigma = 1.4\%$ (see below) near $N=1000$. The value of b suggested by the data is small in magnitude: $b \approx -0.4 \pm 0.2$.

(For M particles in a simulation the mean square statistical error is

$$\sigma^2(\overline{\theta^2}) = \frac{1}{M}\overline{(\theta^2 - \overline{\theta^2})^2}$$

$$= \frac{1}{M}(\overline{\theta^4} - (\overline{\theta^2})^2).$$

For the sech distribution $\overline{\theta^4} = 5(\overline{\theta^2})^2$ (this was true to within a few per cent for the simulation); thus $\sigma^2(\overline{\theta^2}) = 4/M(\overline{\theta^2})^2$. In the numerical simulation $M = 2\times 10^4$, yielding a 1σ error of 1.4%.)

2.2. *Diffusion*

We wish to relate the finite step-size random walk to a diffusion process where the area around the origin has been blocked off out to a radius R. The distribution $\rho_{\rm d}(r, \theta, t)$ for the diffusion process satisfies

$$\frac{\partial}{\partial \tau}\rho_{\rm d}(r, \theta, \tau) = \tfrac{1}{4}\nabla^2 \rho_{\rm d}(r, \theta, \tau) \tag{11}$$

and has boundary condition $\partial_r|_{r=R}\rho_{\rm d}(r, \theta, \tau) = 0$. Let the initial position at $\tau = 0$ be $(r, \theta) = (R, 0)$. Equation (11) can be integrated to find the evolution of the mean square winding number $\overline{\theta^2_{\rm d}}(\tau)$ and higher moments. Let $h_{\rm d}(r, \tau) = \int_{-\infty}^{\infty} \rho_{\rm d}(r, \theta, \tau)\, {\rm d}\theta$ be the radial distribution analogous to $h(r, N)$. Multiply equation (11) by θ^2 and integrate over r and θ:

$$\frac{\partial}{\partial \tau}\overline{\theta^2_{\rm d}}(\tau) = \frac{1}{4}\int_R^{\infty}\int_{-\infty}^{\infty} \theta^2 \left[\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right] \rho_{\rm d}(r, \theta, \tau)\, {\rm d}\theta\, r\, {\rm d}r.$$

The radial operator integrates to zero and the θ term can be integrated twice by parts, leaving

$$\frac{\partial}{\partial \tau}\overline{\theta^2_{\rm d}}(\tau) = \int_R^{\infty}\left(\frac{1}{2r^2}\right) h_{\rm d}(r, \tau) r\, {\rm d}r. \tag{12}$$

For small R^2/τ the radial distribution $h_{\rm d}(r, \tau)$ is given by equation (1) with N replaced by τ. The right-hand side of equation (12) yields the first exponential integral of R^2/τ (see equation (A1.3)-(A1.5))

$$\frac{\partial}{\partial \tau}\overline{\theta^2_{\rm d}}(\tau) = \frac{1}{2\tau}E_1\left(\frac{R^2}{\tau}\right) \approx \frac{1}{2\tau}\ln\left(\frac{\tau}{R^2}\right) - \frac{\gamma}{2\tau} \tag{13}$$

(plus terms second order in R^2/τ). Comparing equations (9) and (13) shows that the second moments of the finite step and diffusion problems will coincide (down to first order in $\log N$) for $R = e^{-2}$. For different values of R, $\overline{\theta^2}(N) - \overline{\theta^2_{\rm d}}(\tau = N) \approx \log(e^2 R)\log N$.

3. Correspondence with the diffusion problem

3.1. Random walk

Equations analogous to (7) can be found for higher-order moments of the winding number distribution:

$$\begin{aligned}\overline{\theta^{2k}}(N+1)-\overline{\theta^{2k}}(N) &= \overline{(\theta+\delta\theta)^{2k}}(N)-\overline{\theta^{2k}}(N)\\ &= \sum_{m=1}^{k}\binom{2k}{2m}\overline{\theta^{2(k-m)}(\delta\theta)^{2m}}(N) \qquad (14)\\ &= \sum_{m=1}^{k}\binom{2k}{2m}\int_0^\infty \langle\theta^{2(k-m)}\rangle(r', N)\langle(\delta\theta)^{2m}\rangle(r')r'\,\mathrm{d}r'.\end{aligned}$$

Unfortunately, except for $\overline{\theta^2}(N)$, these expressions cannot be evaluated without a knowledge of how lower moments (the functions $\langle\theta^{2(k-m)}\rangle(r')$) vary with r'. To find these functions, we first expand equation (5) as a Taylor series in $\delta\theta(r,\phi)$ and $\delta r(r,\phi)$. Averages over angle ϕ will be denoted by brackets as in (8). All odd powers of $\delta\theta$ vanish upon averaging:

$$\rho(r,\theta,N+1)-\rho(r,\theta,N)=\left[\langle\delta r\rangle\partial_r+\frac{1}{2!}(\langle\delta r^2\rangle\partial_r^2+\langle\delta\theta^2\rangle\partial_\theta^2)+\ldots\right]\rho(r,\theta,N). \qquad (15)$$

It is straightforward to show that for large r this expansion yields the diffusion equation (11) with $N=\tau$. The correspondence with this equation breaks down near the origin, however. Our task will be to resolve this difficulty.

First consider $\langle\theta^2\rangle(r,N)$. Rewrite (15) as

$$\rho(r,\theta,N+1)-\rho(r,\theta,N)=[\mathscr{R}_0+(\mathscr{R}_2+\tfrac{1}{2}\langle\delta\theta^2\rangle)\partial_\theta^2\ldots]\rho(r,\theta,N) \qquad (16)$$

where

$$\begin{aligned}\mathscr{R}_0&=\langle\delta r\rangle\partial_r+\frac{1}{2!}\langle\delta r^2\rangle\partial_r^2+\ldots\\ \mathscr{R}_2&=\frac{3}{3!}\langle\delta r\rangle\langle\delta\theta^2\rangle\partial_r+\frac{6}{4!}\langle\delta r^2\rangle\langle\delta\theta^2\rangle\partial_r^2+\ldots.\end{aligned} \qquad (17)$$

We multiply equation (16) by θ^2 and integrate over θ, integrating by parts to remove the ∂_θ derivatives. The result is, by equation (3a),

$$\langle\theta^2\rangle(r,N+1)-\langle\theta^2\rangle(r,N)=\mathscr{R}_0[\langle\theta^2\rangle(r,N)]+(\langle\delta\theta^2\rangle+2\mathscr{R}_2)h(r,N). \qquad (18)$$

Equation (18) has a simple physical interpretation as a radial diffusion with a source term. The radial operator $\mathscr{R}_0$ is simply the evolution operator for an ordinary axisymmetric random walk in the plane. In other words (neglecting the initial step to $(r,\theta)=(1,0)$) the radial distribution for the finite-step random walk $h(r,N)$ evolves according to $h(r,N+1)-h(r,N)=\mathscr{R}_0h(r,N)$. As particles move about the plane, they carry with them the winding number already obtained in previous travels. The function $\langle\theta^2\rangle(r,N)$ increases because of the source term $(\langle\delta\theta^2\rangle+2\mathscr{R}_2)h(r,N)$, but also diffuses because of the random walk operator $\mathscr{R}_0$. The operator $\mathscr{R}_2$ corrects for an effect which becomes important only for particles that reach $r\approx N$. All such particles must travel almost entirely in a radial direction. Consequently the mean $\delta\theta^2$ they see at previous steps must be smaller than $\langle\delta\theta^2\rangle$, i.e. $\langle\delta\theta^2\rangle$ alone does not give the correct source term for these particles. However, the term involving $\mathscr{R}_2$ is proportional to $\partial_r h(r, N)$, of order N^{-2}, and will be neglected in our calculations.

The solution to (18) is

$$\langle\theta^2\rangle(r, N) = \sum_1^{N-1} \int_0^\infty G(r, N, r_1, N_1)\langle\delta\theta^2\rangle(r_1)h(r_1, N_1)r_1\,\mathrm{d}r_1 \tag{19}$$

where $G(r, N, r_1, N_1)$ is the Green function for $\mathscr{R}_0$. Recall that the standard finite step random walk in radius quickly converges to the corresponding diffusion problem. Just as we have approximated $h(r, N)$ by the diffusion distribution of equation (1), we will approximate $G(r, N, r_1, N_1)$ by

$$\begin{aligned} G(r, N, r_1, N_1) &= \frac{2}{N-N_1}\int_{-\pi}^{\pi} \exp\left(-\frac{r^2+r_1^2-2rr_1\cos\mu}{N-N_1}\right)\frac{\mathrm{d}\mu}{2\pi} \\ &= \frac{2}{N-N_1}\exp\left(-\frac{r^2+r_1^2}{N-N_1}\right)I_0\left(\frac{2rr_1}{N-N_1}\right). \end{aligned} \tag{20}$$

(An evaluation point on the circle at (r, N) is affected by sources distributed over the entire circle at (r_1, N_1). Thus we must integrate over the relative (ordinary) angle μ between source point and evaluation point.) Equation (19) may be checked against equation (7) by integrating over r. Since

$$\int_0^\infty G(r, N, r_1, N_1)r\,\mathrm{d}r = 1$$

one obtains the expected result

$$\overline{\theta^2}(N) = \sum_1^{N-1}\int_0^\infty \langle\delta\theta^2\rangle(r_1)h(r_1, N_1)r_1\,\mathrm{d}r_1. \tag{21}$$

Higher-order moments can be found in a similar manner. The fourth moment is, with $G_{12} \equiv G(r_1, N_1; r_2, N_2)$, etc,

$$\overline{\theta^4}(N) = 6\sum_1^{N-1}\sum_1^{N_1-1}\int_0^\infty\int_0^\infty G_{12}h_2\langle\delta\theta^2\rangle_1\langle\delta\theta^2\rangle_2 r_2\,\mathrm{d}r_2\, r_1\,\mathrm{d}r_1 + \sum_1^{N-1}\int_0^\infty h_1\langle\delta\theta^4\rangle_1 r_1\,\mathrm{d}r_1. \tag{22}$$

This may be compared with equation (14) for $k=2$. As shown in appendix 2, the $\langle\delta\theta^4\rangle_1$ integral grows as $\log N$ whereas $\overline{\theta^4}(N)$ as a whole grows as $\log^4 N$. In general, for all higher moments the leading term in equation (14) (involving $\langle\delta\theta^2\rangle$) dominates the $\langle\delta\theta^4\rangle$ term by a factor of $\log^3 N$, and dominates all other terms by higher powers of $\log N$.

3.2. Diffusion

The general moment equation analogous to equation (12) is

$$\frac{\partial}{\partial\tau}\overline{\theta_{\mathrm{d}}^{2k}}(\tau) = \frac{2k(2k-1)}{2}\int_R^\infty\left(\frac{1}{2r^2}\right)\langle\theta_{\mathrm{d}}^{2k-2}\rangle(r, \tau)r\,\mathrm{d}r. \tag{23}$$

To simplify the analysis of the bounded diffusion process, we approximate the radial distribution function and the Green functions by ignoring the boundary; thus we employ equation (1) for the radial function and equation (20) for the Green function. The error is second order in τ^{-1} (an extension of the arguments given in appendix 2 shows that the resulting fractional error in $\overline{\theta_d^{2k}}(\tau)$ is of order $\log^{-2} \tau$). Thus, in analogy with equations (21) and (22) we write

$$\overline{\theta_d^2}(\tau) = \int_1^\tau \int_0^\infty S(r_1) h_d(r_1, \tau_1) r_1 \, dr_1 \, d\tau_1 \tag{24}$$

$$\overline{\theta_d^4}(\tau) = 6 \int_1^\tau \int_1^{\tau_1} \int_0^\infty \int_0^\infty G_{12} h_{d2} S_1 S_2 r_2 \, dr_2 \, r_1 \, dr_1 \, d\tau_2 \, d\tau_1 \tag{25}$$

where $\langle \delta\theta^2 \rangle(r)$ has been replaced by the source function

$$S(r) = \begin{cases} 0 & \text{if } r < e^{-2} \\ 1/2r^2 & \text{if } r \geqslant e^{-2}. \end{cases} \tag{26}$$

The functions $\langle \delta\theta^2 \rangle(r)$, $S(r)$, and their difference $\varepsilon(r) \equiv \langle \delta\theta^2 \rangle(r) - S(r)$ are plotted in figure 2.

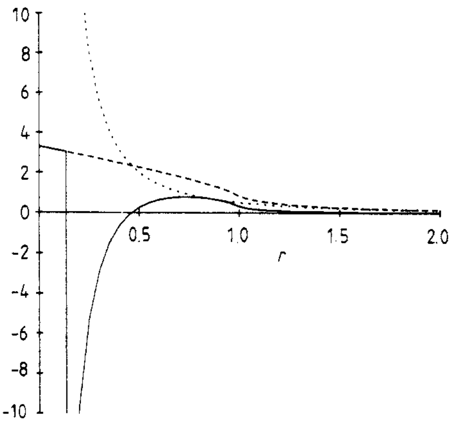

Figure 2. The source functions $\langle \delta\theta^2 \rangle(r)$ (broken curve, equation (8)), $S(r)$ (dotted curve, equation (26)), and their difference $\varepsilon(r)$ (full curve).

3.3. Comparison of random walk and diffusion moments

The discrepancy in fourth moments between the random walk and bounded diffusion is (after approximating the sums in equation (22) by integrals)

$$\overline{\theta^4}(N) - \overline{\theta_d^4}(N) = 6 \int G_{12} h_2 (\varepsilon_1 S_2 + \varepsilon_2 S_1 + \varepsilon_1 \varepsilon_2) r_2 \, dr_2 \, r_1 \, dr_1 \, dN_2 \, dN_1 + O(\log^2 N). \tag{27}$$

Appendix 2 shows that this entire expression is of order $\log^2 N$ (compared to $\log^4 N$ for the entire fourth moment); in general for all moments the discrepancy is small by two powers of log N. In other words, the fractional error $(\overline{\theta^{2k}}(N) - \overline{\theta_d^{2k}}(N))/\overline{\theta^{2k}}(N)$ decreases as $(\log N)^{-2}$. One could also say that the quantities $(\overline{\theta^{2k}})^{1/2k}$ and $(\overline{\theta_d^{2k}})^{1/2k}$ converge.

The data from Berger and Roberts' (1988) random walk simulation are consistent with these results. For the sech function, $\overline{\theta^4} = 5(\overline{\theta^2})^2$, and $\overline{\theta^6} = 61(\overline{\theta^2})^3$. The 1σ statistical error for $\overline{\theta^4}$ was about 5%; deviations between the numerical values of $\overline{\theta^4}$ and the sech predictions became comparable to this percentage near $N = 50$, and were always below 10%. Deviations for the sixth moment were also never clearly greater than statistical error ($1\sigma = 19\%$).

Figure 3 shows how the numerical random walk distribution compares with the bounded diffusion distribution. The diffusion distribution is asymptotically (Hu 1986)

$$f(\theta, \tau) = \frac{1}{2\theta_{\rm rms}}\left(\cosh\frac{\pi\theta}{2\theta_{\rm rms}}\right)^{-1}. \tag{28}$$

We let

$$\theta_{\rm rms} = (\tfrac{1}{4}\log^2 N + a\log N)^{1/2} \tag{29}$$

as in equation (10). Even for N as small as 10 the distributions are close, except at small θ. The Cauchy distribution (equation (2)) is also shown. Figure 4 displays the cumulative distribution

$$P(\theta, N) \equiv 2\int_{|\theta|}^{\infty} f(\theta', N)\,\mathrm{d}\theta'. \tag{30}$$

The function $P(\theta, N)$ gives the probability that the magnitude of the winding number is at least $|\theta|$. For the Cauchy function

$$P(\theta, N) = 1 - \frac{2}{\pi}\tan^{-1}\frac{2\theta}{\log N}$$

and for the sech function

$$P(\theta, N) = 1 - \frac{2}{\pi}\tan^{-1}\sinh\frac{\pi\theta}{2\theta_{\rm rms}}.$$

Here the similarities between the simulation and the sech prediction become quite striking.

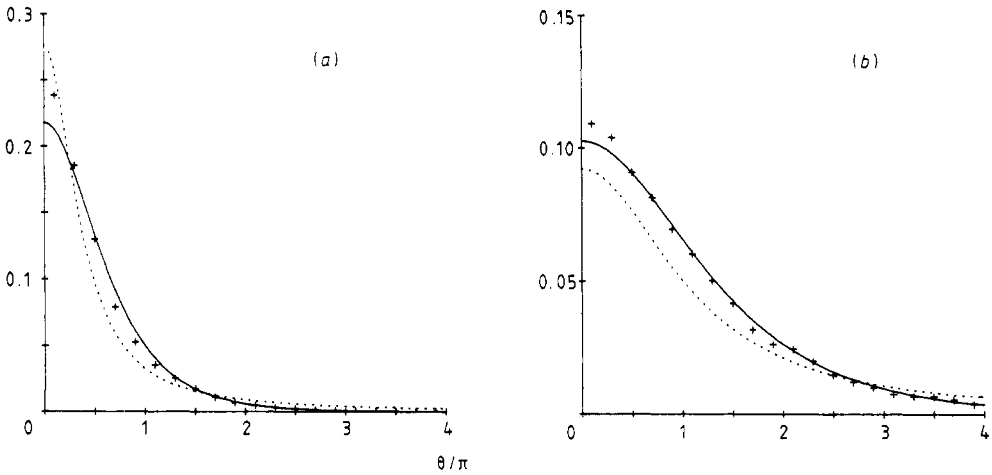

Figure 3. The numerical winding number distribution of 20 000 particles (Berger and Roberts 1987) compared with the bounded diffusion prediction (equations (28) and (29)). The numerical results are given as individual points representing bins of size $\Delta\theta = \pi/5$. The dotted curve shows the Cauchy distribution of equation (2), with $\tau = N$. (*a*) $N = 10$; (*b*) $N = 1000$.

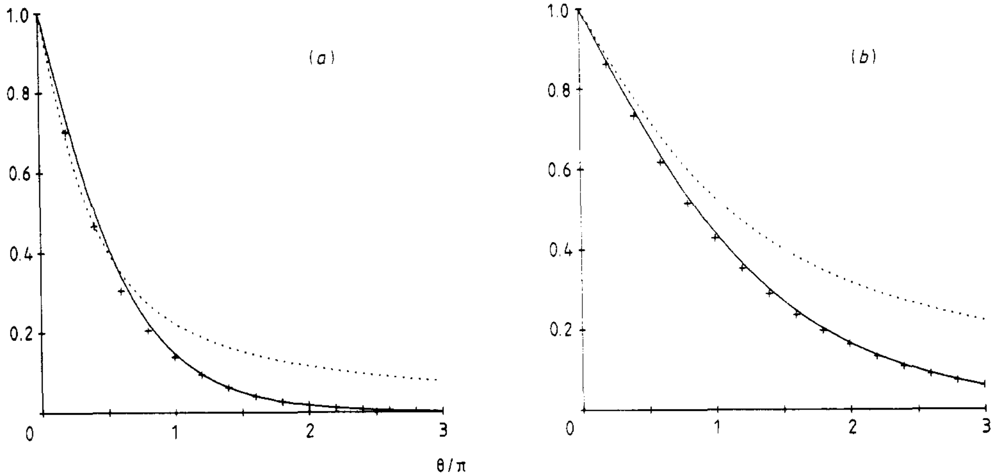

Figure 4. The cumulative probability functions $P(\theta, N)$ (equation (30)) for the simulation are compared to $P(\theta, N)$ for the bounded diffusion problem (full curve), and for the Cauchy distribution (dotted curve). (*a*) $N=10$; (*b*) $N=1000$.

Appendix 1. Calculation of $\overline{\theta^2}(N+1)-\overline{\theta^2}(N)$

We wish to evaluate equation (7) to leading order in N^{-1}. First choose some radius r_0 such that $1<r_0<N^{1/2}$, and separate the radial integration into two parts, $0\leqslant r'<r_0$, and $r'>r_0$. In the exterior region we can expand $\langle\delta\theta^2\rangle(r')$ as a Taylor series in powers of r'^{-1}. From equation (8) and some calculation,

$$\langle\delta\theta^2\rangle(r')=\frac{1}{2r'^2}+\frac{1}{8r'^4}+\frac{1}{18r'^6}\cdots. \tag{A1.1}$$

Now employ equation (1) for $h(r', N)$, and transform to the variable $t=r'^2/r_0^2$:

$$\int_{r_0}^{\infty}\langle\delta\theta^2\rangle(r')h(r', N)r'\,\mathrm{d}r'=\frac{1}{N}\int_1^{\infty}\mathrm{e}^{-r_0^2t/N}\left(\frac{1}{2t}+\frac{1}{8r_0^2t^2}+\ldots\right)\mathrm{d}t+\mathrm{O}(N^{-2}). \tag{A1.2}$$

The exponential integral (e.g. Gradshteyn and Ryzhik 1980) is defined by

$$E_n(z)\equiv\int_1^{\infty}\mathrm{e}^{-zt}t^{-n}\,\mathrm{d}t \tag{A1.3}$$

and satisfies

$$E_n(z)=\frac{1}{n-1}[\mathrm{e}^{-z}-zE_{n-1}(z)] \tag{A1.4}$$

$$E_1(z)=-\left[\gamma+\log z+\sum_{k=1}^{\infty}\frac{(-z)^k}{kk!}\right]. \tag{A1.5}$$

Thus

$$\int_{r_0}^{\infty}\langle\delta\theta^2\rangle(r')h(r', N)r'\,\mathrm{d}r'=\frac{1}{N}\left[\frac{E_1(z)}{2}+\frac{E_2(z)}{8r_0^2}+\ldots\right]+\mathrm{O}(N^{-2}) \tag{A1.6}$$

$$=\frac{1}{\mathrm{N}}\left[\frac{\log N-\gamma}{2}-\log r_0+\frac{1}{8r_0^2}+\mathrm{O}(r_0^{-4})\right]+\mathrm{O}(N^{-2}). \tag{A1.7}$$

In the interior region we expand $h(r', N) \approx 2N^{-1} + O(N^{-2})$ rather than $\langle \delta\theta^2 \rangle(r')$:

$$\int_0^{r_0} \langle \delta\theta^2 \rangle(r') h(r', N) r' \, dr' = \frac{2}{N} \int_0^{r_0} \frac{1}{\pi} \int_0^{\pi} (\delta\theta)^2 \, d\psi \, r' \, dr' + O(N^{-2}) \tag{A1.8}$$

(averaging over angle ψ need only be over $[0, \pi]$, as $\delta\theta$ is even in ψ). We will transform the integration variables from (r', ψ) to $(\psi, \delta\theta)$. Let

$$\begin{aligned} \mu &= (\cot \delta\theta - \cot \psi) \delta\theta^2 (1 + \cot^2 \delta\theta) \\ \psi_0 &= \cot^{-1}(r_0 + \cos \psi)/\sin \psi. \end{aligned} \tag{A1.9}$$

Then

$$\frac{2}{\pi N} \int_0^{r_0} \int_0^{\pi} \delta\theta^2 \, d\psi \, r \, dr = \frac{2}{\pi N} \int_0^{\pi} \sin^2 \psi \int_{\psi_0}^{\psi} \mu \, d\delta\theta \, d\psi. \tag{A1.10}$$

We wish to extract that part of the integral which is independent of ψ_0 (all other terms must cancel with terms in the external integration, leaving an answer independent of r_0). Thus, let

$$\int_{\psi_0}^{\psi} \mu \, d\delta\theta = \int_0^{\psi} (\mu - \cot \delta\theta) \, d\delta\theta - \int_0^{\psi_0} (\mu - \cot \delta\theta) \, d\delta\theta + \int_{\psi_0}^{\psi} \cot \delta\theta \, d\delta\theta \tag{A1.11}$$

(the function $\mu - \cot \delta\theta$ is well behaved at $\delta\theta = 0$). The first term of (A1.11), when introduced into (A1.10), integrates to $2N^{-1}$. The second and third terms can be evaluated to give $(\log r_0 - r_0^{-2}/8 + \ldots)N^{-1}$. Thus equations (A1.7) and (A1.10) combine to give

$$\overline{\theta^2}(N+1) - \overline{\theta^2}(N) = \frac{\log N - \gamma}{2N} + \frac{2}{N} + O(N^{-2}). \tag{A1.12}$$

Appendix 2. Errors in the moment approximations

First we show that the $\langle \delta\theta^4 \rangle$ term in (22) is only first order in $\log N$. To see this, divide the radial integral into two ranges, say $0 \leq r_1 \leq 3$, and $3 \leq r_1 \leq \infty$. In the first range $h_1 \approx 2/N_1$ and in the second range $\langle \delta\theta^4 \rangle_1 \approx 3/8r_1^4$. The second range integrates to $\frac{1}{24}N_1^{-1} + O(N_1^{-2})$. If we let $\alpha = \int_0^3 \langle \delta\theta^4 \rangle_1 r_1 \, dr_1$ then

$$\begin{aligned} \sum_1^{N-1} \int_0^{\infty} h_1 \langle \delta\theta^4 \rangle_1 r_1 \, dr_1 &\approx (2\alpha + \tfrac{1}{24}) \sum_1^{N-1} \frac{1}{N_1} \\ &\approx (2\alpha + \tfrac{1}{24}) \log N. \end{aligned} \tag{A2.1}$$

We now show that the first term in (22) can be evaluated to a good approximation using $S(r)$ as the source function rather than $\langle \delta\theta^2 \rangle(r)$. The deviation is given by equation (27). First consider the $S_1\varepsilon_2$ part. The Bessel function

$$I_0\left(\frac{2r_1r_2}{N_1 - N_2}\right)$$

found in G_{12} will be expanded in a Taylor series, using

$$I_0(z) = \sum_{m=0}^{\infty} \frac{(z/2)^{2m}}{(m!)^2}. \tag{A2.2}$$

Replace the integration variables N_1, N_2, r_1, r_2 by N_2, $\tilde{N} \equiv N_1 - N_2$, $x_1 \equiv r_1^2$, and $x_2 \equiv r_2^2$. The $S_1 \varepsilon_2$ integral becomes

$$\sum_{m=0}^{\infty} \frac{3}{(m!)^2} \int_1^{N-1} \frac{\mathrm{d}N_2}{N_2} \int_1^{N-N_2} \frac{\mathrm{d}\tilde{N}}{\tilde{N}} \int_{R^2/\tilde{N}}^{\infty} \frac{\mathrm{d}x_1}{x_1} \left(\frac{x_1}{\tilde{N}}\right)^m \mathrm{e}^{-x_1/\tilde{N}} \int_0^{\infty} \mathrm{d}x_2\, \varepsilon_2 \left(\frac{x_2}{\tilde{N}}\right)^m \mathrm{e}^{-x_2(1/\tilde{N}+1/N_2)}.$$

The $m = 0$ term simplifies as follows: the integration over x_1 yields the first exponential integral

$$E_1\left(\frac{R^2}{\tilde{N}}\right) = \log \frac{\tilde{N}}{R^2} - \gamma + \frac{R^2}{\tilde{N}} + \mathrm{O}\left(\frac{R^2}{\tilde{N}}\right)^2$$
$$\approx \log \tilde{N} + (4 - \gamma) \tag{A2.3}$$

(for $R = e^{-2}$). Meanwhile, recall that $R = e^{-2}$ was chosen so that equations (9) and (13) would have identical right-hand sides to first order in N^{-1} (for $N = \tau$). This implies, from the definition of $\varepsilon(r)$ below equation (26), that

$$\int_0^{\infty} \varepsilon(r)\, \mathrm{e}^{-r^2/N} r\, \mathrm{d}r = \mathrm{O}(N^{-1}). \tag{A2.4}$$

Thus the x_2 integral gives

$$c\left(\frac{1}{\tilde{N}} + \frac{1}{N_2}\right) + \mathrm{O}\left(\frac{1}{\tilde{N}} + \frac{1}{N_2}\right)^2$$

for some constant c. The $m = 0$ term is then approximately

$$3c \int_1^{N-1} \frac{\mathrm{d}N_2}{N_2} \int_1^{N-N_2} \frac{\mathrm{d}\tilde{N}}{\tilde{N}} (\log \tilde{N} + 4 - \gamma)\left(\frac{1}{\tilde{N}} + \frac{1}{N_2}\right)$$
$$< 3c \int_1^{N} \frac{\mathrm{d}N_2}{N_2} \int_1^{N} \frac{\mathrm{d}\tilde{N}}{\tilde{N}} (\log \tilde{N} + 4 - \gamma)\left(\frac{1}{\tilde{N}} + \frac{1}{N_2}\right)$$
$$= \tfrac{3}{2} c \log^2 N + \mathrm{O}(\log N). \tag{A2.5}$$

The sum of the higher m terms can be estimated with similar methods; the result is first order in $\log N$. The $S_2 \varepsilon_1$ part of equation (27) also yields a $\log^2 N$ growth, while the $\varepsilon_1 \varepsilon_2$ part is zeroth order in $\log N$. Since the total fourth moment goes as $\log^4 N$, this proves that the fractional error between the random walk and diffusion moments is of order $\log^{-2} N$. A similar but more detailed calculation leads to an identical result for all higher moments.

References

Berger M A 1987 *Preprint*

Berger M A and Roberts P H 1988 *Adv. Appl. Prob.* to be published

Belisle C 1986 *Preprint*

Chandrasekhar S 1943 *Rev. Mod. Phys.* **15** 1-89

Gradshteyn I S and Ryzhik I M 1980 *Tables of Integrals, Series and Products* (New York: Academic) pp xxxii, 927

Hu Y 1986 private communication

Lévy P 1940 *Am. J. Math.* **62** 487-550

Lyons T J and McKean H P 1984 *Adv. Math.* **51** 212-25

Pitman J W and Yor M 1984 *Bull. Am. Math. Soc.* **10** 109-11

Roberts P H and Ursell H D 1960 *Phil. Trans. R. Soc.* A **252** 317-56

Rudnick J and Hu Y 1987 *J. Phys. A: Math. Gen.* **20** 4419-36

Spitzer F 1958 *Am. Math. Soc. Trans.* **87** 187-97

Wax N 1954 *Selected Papers on Noise and Stochastic Processes* (New York: Dover)