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The winding angle distribution of an ordinary random walk

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Abstract. The winding angle about a selected point of a random walk quantifies what is perhaps the simplest manifestation of entanglement, a phenomenon of great importance in the study of polymers. The distribution of winding angles is studied here for ordinary or non-self-avoiding walks. New results highlight the crucial influence of the exclusion of a finite region about the selected point on the winding angle distribution. The results of this analysis are compared with simulations of random walks on a lattice; the agreement between the two is very good. There are, however, small and as yet unexplained discrepancies.

1. Introduction

A two-dimensional random walker that starts out in the vicinity of some point on a plane will, in the course of its wanderings, tend to follow a path that wraps around that point. By the same token, a long-chain polymer that grows in the vicinity of a long straight rod will, in all likelihood, end up wrapped around the rod. This latter process represents what may be the simplest manifestation of the phenomenon of entanglement. One measures the extent of the wrapping in both cases via the *winding angle*, which is just the angle about the rod or reference point that is swept out by the growing polymer or random walker. How this quantity is defined for a random walk in a plane is illustrated in figure 1.

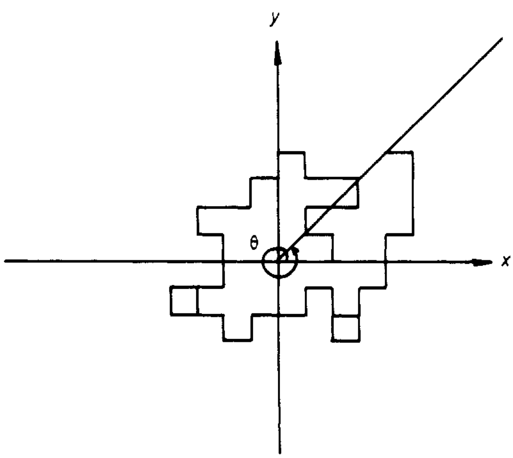

Figure 1. A typical path of a random walk on a square lattice. The winding angle is measured with respect to the direction of the first step. In this figure the first step is in the x direction and the winding angle $\theta \simeq 7.07$ rad.

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In this paper we present some new results pertaining to the distribution of winding angles of unrestricted random walks in a plane. These results generalise straightforwardly to the case of a random walker in d dimensions whose path wraps around a $(d-2)$-dimensional 'rod'. They are not directly applicable in unmodified form to a polymer in the vicinity of a rod in three dimensions, because the statistics of a long-chain polymer are those of a *self-avoiding* rather than the unrestricted random walk. In the light of current knowledge about polymer statistics it is, however, reasonable to expect the distribution of winding angles for a chain polymer in $4-\varepsilon$ dimensions to approach, as $\varepsilon \to 0$, the winding angle distribution for unrestricted walks (Ma 1976). An ε expansion ought to yield the appropriate corrections to the unrestricted walk distribution when ε is small. There is, in addition, a case in which we expect our results to apply directly to polymers in a physical dimensionality. At the θ point, where attractive interactions between monomeric units are on the threshold of having sufficient strength to cause polymeric collapse, a chain polymer in three dimensions has essentially the same statistics as an unrestricted random walk. Our results should be exact at this multicritical point, subject to 'marginal' corrections (de Gennes 1975).

The winding angle distribution for unrestricted random walks was first studied by Spitzer (1958) (see also Pitman and Yor 1986) some years ago. He analysed random walks in the continuum—or diffusion equation—limit and derived an expression for the winding angle distribution of an N-step walk, $P_N(\theta)$, whose form is equivalent to the following:

$$P_N(\theta) = \frac{1}{\pi} \frac{c \ln(N)}{(c \ln(N))^2 + \theta^2} \qquad N \gg 1 \tag{1.1}$$

where the quantity c is a constant. This Lorentzian-like or Cauchy distribution has two noteworthy features. First, its width grows as $\ln(N)$, i.e. quite slowly with the number of steps in the walk. This kind of behaviour is reasonable. As N grows the walker tends to get further and further away from the origin and the increment in the winding angle with each step ought to get smaller and smaller on average as N increases. Second, (1.1) predicts an *infinite* second moment for $P_N(\theta)$:

$$\begin{aligned} \bar{\theta}^2 &= \int P_N(\theta)\theta^2 \, \mathrm{d}\theta \\ &= \int_{-\infty}^{\infty} \frac{c \ln(N)\theta^2}{(c \ln(N))^2 + \theta^2} \, \mathrm{d}\theta = \infty. \end{aligned} \tag{1.2}$$

The second property mentioned above is obviously very troubling. By construction, the winding angle of a walk with a finite number of steps cannot have an infinite second moment. An absolute upper bound is

$$\bar{\theta}^2 < cN^2 \tag{1.3}$$

where c is a constant. This latter feature of Spitzer's formula appears to signal a breakdown of the diffusion equation approach. In particular, while (1.1) implies

$$\overline{|\theta|^\nu} = \int_{-\infty}^{\infty} P_N(\theta)|\theta|^\nu \, \mathrm{d}\theta \propto (\ln N)^\nu \tag{1.4}$$

for $-1 < \nu < 1$, it is natural to ask, in the light of the above, whether higher moments for real random walks will scale in the same way or whether they increase qualitatively more rapidly with N.

A more recent investigation of the winding angle distribution, by Fisher *et al* (1984), brings numerical methods to bear on the problem for self-avoiding walks in a plane. Fisher *et al* find in this case that the second moment of θ scales as follows with N:

$$\overline{\theta^2} \propto (\ln N)^{-1}. \tag{1.5}$$

They also find that the following relation between $\overline{\theta^2}$ and $\overline{\theta^4}$ holds to a good approximation:

$$\overline{\theta^4} = 3\overline{\theta^2} \tag{1.6}$$

which is consistent with a Gaussian form for $P_N(\theta)$. This points to what appears to be a striking contrast between unrestricted and self-avoiding walks.

One can see later (appendix 2) that the divergence of the second moment in Spitzer's formula arises from the fact that in Spitzer's treatment of the continuous approximation the walker is allowed to approach the reference point arbitrarily closely. However, in the case of the lattice walker if the origin is interstitial the walker cannot get any closer to it than the nearest vertex, while if the origin is on a vertex the walker must not be allowed to step on it or it would be impossible to define winding angles unambiguously. On the other hand, the rod around which a growing polymer wraps itself presents a physical barrier that keeps the polymer away from a one-dimensional region passing through the origin. The exclusion of a finite region about the origin is thus mathematically well motivated for random walks on a lattice and is a consequence of physical considerations in the case of a polymer grown in the vicinity of a rod.

The work described in the remainder of this paper is a new investigation of the winding angle problem for unrestricted random walks in a plane. The focus of this investigation is the behaviour of the distribution function $P_N(\theta)$ in the large θ wings and on the consequences of this behaviour on the way in which the higher-order moments of $P_N(\theta)$ scale with $\ln(N)$. Our most important result has to do with the effect on $P_N(\theta)$ of not allowing the walker to enter a region of finite extent surrounding the reference point about which the winding angle is measured. When this restriction is imposed the winding angle distribution takes on a form for large θ that differs qualitatively from (1.1). We find for $P_N(\theta)$ in that regime

$$P_N(\theta) \propto \exp(-2\pi|\theta|\ln N) \qquad \theta, N \gg 1. \tag{1.7}$$

Note that the exponent in (1.7) is independent of the size of the region excluded. Formula (1.1) is recovered as the size shrinks to zero, but only as a singular limit. All positive moments of $P_N(\theta)$ are thus finite. In particular

$$\langle\theta^2\rangle \propto (\ln N)^2 \tag{1.8}$$

and, in general,

$$\overline{\theta^{2m}} \propto (\ln N)^{2m} \tag{1.9}$$

for all positive integer m.

Our analytical results are supplemented by simulations. We obtain numerically winding angle distributions for a random walk on a two-dimensional square lattice and three-dimensional cubic lattice that are consistent with the results of our analysis.

The remainder of this paper is organised as follows. In § 2 we obtain the winding angle distribution for unrestricted random walks in the continuum approximation. We concentrate on the effects on the distribution that follow from the exclusion of a finite region about the origin. In § 3 we obtain numerical winding angle distributions using both exact enumeration and Monte Carlo methods. Section 4 contains concluding remarks. Certain important details in the calculations described in § 2 are relegated to appendices 1 and 3. In appendix 2 we recover Spitzer's form for the winding angle distribution as a limit of a more general formula. This limit is achieved when the size of the excluded region goes to zero.

2. Theory

Random walks are conveniently studied with the use of generating functions (de Gennes 1979). Let $C_N(\boldsymbol{x}', \boldsymbol{x})$ represent the number of N-step random walks—of any type—that start at the point $\boldsymbol{x}'$ and end up at $\boldsymbol{x}$. The generating function $G(\boldsymbol{x}', \boldsymbol{x}, z)$ is given by

$$G(\boldsymbol{x}', \boldsymbol{x}, z) = \sum_{N=0}^{\infty} C_N(\boldsymbol{x}', \boldsymbol{x}) z^N. \tag{2.1}$$

This means that if we are given an expression for $G(\boldsymbol{x}', \boldsymbol{x}, z)$ we can, in principle, extract $C_N(\boldsymbol{x}', \boldsymbol{x})$; it is the coefficient of z^N in the power series expansion of $G(\boldsymbol{x}', \boldsymbol{x}, z)$.

When the walk is unrestricted and on a lattice, the generating function can be shown to satisfy the following equation:

$$\frac{1}{z} G(\boldsymbol{x}', \boldsymbol{x}, z) - \sum_{n=1}^{(z^*)^{-1}} G(\boldsymbol{x}', \boldsymbol{x} + \boldsymbol{l}_n, z) = \frac{1}{z} \delta_{\boldsymbol{x}', \boldsymbol{x}}. \tag{2.2}$$

In (2.2) $\boldsymbol{l}_n$ is the displacement vector that connects the lattice point $\boldsymbol{x}$ to one of its $(z^*)^{-1}$ nearest neighbours. The walker is understood to take steps only along links connecting nearest-neighbour sites. We now assume that the generating function has a sufficiently smooth variation with $\boldsymbol{x}$ and $\boldsymbol{x}'$ that we can approximate it by a continuous function of those variables. Taylor-expanding $G(\boldsymbol{x}', \boldsymbol{x} + \boldsymbol{l}_n, z)$ with respect to the $\boldsymbol{l}_n$ and retaining terms of up to second order only we obtain the following equation for the generating function of the continuous variables $\boldsymbol{x}$ and $\boldsymbol{x}'$:

$$\frac{1}{z} G(\boldsymbol{x}', \boldsymbol{x}, z) - \frac{1}{z^*} G(\boldsymbol{x}', \boldsymbol{x}, z) - l'^2 \nabla^2 G(\boldsymbol{x}', \boldsymbol{x}, z) = \frac{1}{z} \delta(\boldsymbol{x} - \boldsymbol{x}'). \tag{2.3}$$

We have assumed that the lattice possesses reflection symmetry. The quantity l'^2 is equal to the square of the magnitude of a characteristic $\boldsymbol{l}_n$ times a number of order unity. In other words, it is the order of the square of the distance covered in a single step in the random walk. If $z \simeq z^*$ then we can write

$$\frac{1}{z} - \frac{1}{z^*} \simeq \frac{1}{z^{*2}} (z^* - z) \equiv \frac{r}{z^*} \tag{2.4}$$

and (2.3) becomes

$$\begin{aligned} rG(\boldsymbol{x}', \boldsymbol{x}, z) - z^* l'^2 \nabla^2 G(\boldsymbol{x}', \boldsymbol{x}, z) &= \frac{z^*}{z} \delta(\boldsymbol{x} - \boldsymbol{x}') \\ &\simeq \delta(\boldsymbol{x} - \boldsymbol{x}') \end{aligned}$$

or

$$\kappa^2 G(\boldsymbol{x}', \boldsymbol{x}, z) - \nabla^2 G(\boldsymbol{x}', \boldsymbol{x}, z) = \alpha \delta(\boldsymbol{x} - \boldsymbol{x}') \tag{2.5}$$

where $\kappa^2 = r/(z^* l'^2)$ and $\alpha = 1/(z^* l'^2)$. This approximation for the equation governing the generating function represents the continuum or *diffusion equation* limit for random walk statistics.

In the case of the two-dimensional random walk we can transform to cylindrical coordinates ($x = \rho \cos \theta$, $y = \rho \sin \theta$), and (2.5) becomes

$$\left(\frac{1}{\rho}\frac{\partial}{\partial \rho}\rho\frac{\partial}{\partial \rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial \theta^2}\right)G(\rho', \theta', \rho, \theta, z)-\kappa^2 G=-\alpha\frac{1}{\rho}\delta(\rho-\rho')\delta(\theta-\theta'). \tag{2.6}$$

The angles θ and θ' are commonly understood to be defined modulo 2π. If, however, we do not allow the random walker to enter a region around the origin we can take both θ and θ' to go from $-\infty$ to ∞. The only proviso in this is that the walker must also be prohibited from taking any steps that both span the excluded region and pass directly over the origin. It is this new generating function that yields the winding angle distribution.

We take θ', the angle at which the walker starts, to be equal to zero. Then we Fourier transform (2.6) with respect to θ to obtain

$$\left(\frac{\partial^2}{\partial \rho^2}+\frac{1}{\rho}\frac{\partial}{\partial \rho}\right)G(\rho', \rho, \nu, z)-\left(\kappa^2+\frac{\nu^2}{\rho^2}\right)G(\rho', \rho, \nu, z)=-\frac{\alpha}{\rho}\delta(\rho-\rho'). \tag{2.7}$$

The Fourier transformed generating function $G(\rho, \rho', \nu, z)$ is given by

$$G(\rho, \rho', \nu, z)=\frac{1}{2\pi}\int_{-\infty}^{\infty} G(\rho', 0, \rho, \theta, z)\, \mathrm{e}^{-\mathrm{i}\nu\theta}\, \mathrm{d}\theta. \tag{2.8}$$

It is worthwhile noting the very important difference between the Fourier transform (2.8) that is appropriate for the generating function that we are now considering and the Fourier transform appropriate to the commonly studied generating function. In the latter case, in which angles are defined modulo 2π, the continuous variable ν is replaced by the variable n, which can take on integer values only. The quantity that we are now studying is a non-trivial extension of the familiar generating function.

We can, nevertheless, treat it in much the same way as we would the standard generating function for random walks. For instance, the requirement that the walker never enters a region around the origin can be enforced by placing an absorbing wall at the perimeter of that region (Feller 1968). This kind of barrier causes the generating function to vanish there. To take advantage of cylindrical symmetry we exclude the region $\rho < R$. This means that the generating function vanishes when ρ or ρ' is equal to or less than R. The solution to (2.7), subject to these boundary conditions and a constant difference, is

$$G(\rho', \rho, \nu, z)=K_\nu(\kappa\rho_>)\left(\frac{I_\nu(\kappa\rho_<)K_\nu(\kappa R)-I_\nu(\kappa R)K_\nu(\kappa\rho_<)}{K_\nu(\kappa R)}\right) \tag{2.9}$$

where $\rho_<$ is the smaller, and $\rho_>$ is the larger, of ρ and ρ'. The functions $K_\nu(x)$ and $I_\nu(x)$ are modified Bessel functions of νth order.

We are now in a position to extract the winding angle distribution. To do this we reconstruct the generating function $G(\rho', 0, \rho, \theta, z)$, integrate over all possible values of ρ, the distance from the origin to the point at which the walker ends up, and then extract the coefficient of z^N in the power series expansion of this result. According to (2.8) and (2.9)

$$G(\rho', 0, \rho, \theta, z) = \int_{-\infty}^{\infty} G(\rho', \rho, \nu, z)\, \mathrm{e}^{\mathrm{i}\nu\theta}\, \mathrm{d}\nu$$
$$= \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\nu\theta}\, K_\nu(\kappa\rho_>)\left(\frac{I_\nu(\kappa\rho_<)K_\nu(\kappa R) - I_\nu(\kappa R)K_\nu(\kappa\rho_<)}{K_\nu(\kappa R)}\right) \mathrm{d}\nu. \tag{2.10}$$

As noted above we integrate this function over all values of ρ to obtain the winding angle distribution $P(\theta, z)$. More specifically,

$$P(\theta, z) = \int_R^{\infty} G(\rho', 0, \rho, \theta, z)\rho\, \mathrm{d}\rho. \tag{2.11}$$

Note that the winding angle distribution depends on ρ', the random walker's initial distance from the origin. This dependence will not be strong if the walk consists of enough steps. It will thus be neglected.

We can write

$$\int_R^{\infty} G(\rho', 0, \rho, \theta, z)\rho\, \mathrm{d}\rho = \int_R^{\rho'} G(\rho', 0, \rho, \theta, z)\rho\, \mathrm{d}\rho + \int_{\rho'}^{\infty} G(\rho', 0, \rho, \theta, z)\rho\, \mathrm{d}\rho. \tag{2.12}$$

If ρ' is not too large the first term on the left-hand side of (2.12) can be neglected as compared to the second. Doing this and using (2.10) we have

$$P(\theta, z) \propto \int_{\rho'}^{\infty} \left[\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\nu\theta}\, K_\nu(\kappa\rho)\left(\frac{I_\nu(\kappa\rho')K_\nu(\kappa R) - I_\nu(\kappa R)K_\nu(\kappa\rho')}{K_\nu(\kappa R)}\right) \mathrm{d}\nu\right]\rho\, \mathrm{d}\rho. \tag{2.13}$$

It turns out to be sufficient to replace the lower limit in the integral over ρ by 0. This integral then yields the multiplicative factor

$$\int_0^{\infty} K_\nu(\kappa\rho_>)\rho_>\, \mathrm{d}\rho_> = \frac{1}{\kappa^2}\int_0^{\infty} K_\nu(x)x\, \mathrm{d}x = \frac{1}{\kappa^2}\int_0^{\infty} \frac{\cosh(\nu t)}{(\cosh(t))^2}\, \mathrm{d}t. \tag{2.14}$$

A table of integrals (Abramowitz and Stegun 1964) was used to obtain the final equality in (2.14). Note that when $\nu > 2$ the integrals in (2.14) are not convergent and the lower limit cannot be replaced by 0.

The problem of extracting the coefficient of z^N in the power series expansion of the function $P(\theta, z)$ is reviewed in appendix 1. Here we simply note the result of the analysis that is carried out there. We find in appendix 1 that the winding angle distribution for an N-step walk, $P_N(\theta)$, is proportional to the integral of the term in square brackets in (2.13) with κ replaced by $N^{-1/2}$. That is,

$$P_N(\theta) \propto \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\nu\theta}\, C(\nu)\left(\frac{I_\nu(\rho' N^{-1/2})K_\nu(RN^{-1/2}) - I_\nu(RN^{-1/2})K_\nu(\rho' N^{-1/2})}{K_\nu(RN^{-1/2})}\right) \mathrm{d}\nu \tag{2.15}$$

where

$$C(\nu) = \frac{1}{K^2}\int_{\rho_< K}^{\infty} K_\nu(x)x\, \mathrm{d}x \underset{\nu<2}{=} C' \int_0^{\infty} \frac{\cosh(\nu t)}{(\cosh(t))^2}\, \mathrm{d}t \tag{2.16}$$

with C' a constant.

When the size of the excluded region goes to zero (2.15) is replaced by

$$P_N(\theta) \propto \int_{-\infty}^{\infty} e^{i\nu\theta}\, C(\nu) I_{|\nu|}(\rho' N^{-1/2})\, d\nu. \tag{2.17}$$

This is the limit considered by Spitzer (1958). The properties of $P_N(\theta)$ as given by the right-hand side of (2.17) are very different in important respects from the properties of the winding angle distribution as given by (2.15). We now discuss the latter.

We will concentrate on two predictions for the winding angle distribution. The first is for the behaviour of moments of the distribution. Recall that the Lorentzian distribution obtained by Spitzer—a distribution that follows directly from (2.17) as is shown in appendix 2—possesses second- and higher-order moments that are infinite. This is not a feature of the winding angle distribution as given by (2.15). The second property of $P_N(\theta)$ that will be discussed is its decay for large θ. What we find is that the decay of $P_N(\theta)$ for large θ is fundamentally different when there is an excluded region than when there is not.

As a prelude to a detailed discussion of the moments of $P_N(\theta)$ we note the following connection between the moments of an arbitrary distribution, $f(\theta)$, and the properties of its Fourier transform $\phi(\nu)$, where

$$f(\theta) = \int_{-\infty}^{\infty} \phi(\nu)\, e^{i\nu\theta}\, d\nu. \tag{2.18}$$

If $f(\theta)$ is real and an even function of θ ($f(-\theta) = f(\theta)$) then $\phi(\nu)$ will also be real and an even function of ν. Using $\theta^n e^{i\nu\theta} = i^{-n} (d^n/d\nu^n) e^{i\nu\theta}$ we have

$$\begin{aligned}
\int_{-\infty}^{\infty} \theta^n f(\theta)\, d\theta &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi(\nu)\theta^n e^{i\nu\theta}\, d\nu\, d\theta \\
&= 2\pi(-1)^m \frac{d^{2m}}{d\nu^{2m}}\phi(\nu)\Big|_{\nu=0} && \text{when } n = 2m \\
&= 0 && \text{otherwise.}
\end{aligned} \tag{2.19}$$

In (2.19) $\phi(\nu)$ has been assumed to be sufficiently well behaved at $\nu = \pm\infty$ that integrations by parts can be carried out. The moment structure of $P_N(\theta)$ is thus controlled by the small-ν behaviour of the term in large round brackets in (2.15).

That the winding angle distribution $P_N(\theta)$ is even in θ is manifestly obvious—at least for the kind of 'non-chiral' walks that we are considering here. We thus expect a Taylor expansion in ν of the term in large round brackets in (2.15):

$$\frac{I_\nu(\rho' N^{-1/2}) K_\nu(RN^{-1/2}) - I_\nu(RN^{-1/2}) K_\nu(\rho' N^{-1/2})}{K_\nu(RN^{-1/2})} \tag{2.20}$$

to consist of even powers only. We now establish this.

First, we make use of the connection between the two kinds of modified Bessel functions, I_ν and K_ν (Abramowitz and Stegun 1964):

$$K_\nu(x) = \frac{\pi}{2} \frac{I_{-\nu}(x) - I_\nu(x)}{\sin(\nu\pi)}. \tag{2.21}$$

If the power series expansion in ν of $I_\nu(x)$ consists entirely of integer powers of ν then the corresponding expansion of $K_\nu(x)$ will consist of even powers only. Consider, now, the following integral representation of $I_\nu(x)$ (Abramowitz and Stegun 1964):

$$I_\nu(x) = \frac{1}{\pi}\int_0^\pi \exp(x\cos\theta)\cos(\nu\theta)\,\mathrm{d}\theta - \frac{\sin(\nu\pi)}{\pi}\int_0^\infty \exp(-x\cosh(t)-\nu t)\,\mathrm{d}t. \tag{2.22}$$

According to (2.22) such an expansion indeed exists. In fact, combining (2.21) and (2.22) we obtain the following integral representation for $K_\nu(x)$:

$$K_\nu(x) = \int_0^\infty \exp(-x\cosh(t))\cosh(\nu t)\,\mathrm{d}t. \tag{2.23}$$

It is evident from this last result that the Taylor expansion in ν of the modified Bessel function $K_\nu(x)$ will consist of even powers only.

Applying (2.21) to the numerator of (2.20) we obtain the following result:

$$\begin{aligned} I_\nu(\rho' N^{-1/2})K_\nu(RN^{-1/2}) &- I_\nu(RN^{-1/2})K_\nu(\rho' N^{-1/2}) \\ &= \frac{\pi}{2}\frac{1}{\sin(\nu\pi)}(I_\nu(\rho' N^{-1/2})I_{-\nu}(RN^{-1/2}) - I_\nu(RN^{-1/2})I_{-\nu}(\rho' N^{-1/2})). \end{aligned} \tag{2.24}$$

The numerator and the denominator of the right-hand side of (2.24) are both analytic functions of ν consisting of odd powers only. Thus the numerator of (2.20) will, when expanded in powers of ν, generate a series consisting of even powers only.

The dominant dependence of $P_N(\theta)$ on the parameter ν will be through one of the modified Bessel functions. Since

$$I_\nu(x) \sim (\tfrac{1}{2}x)^\nu/\Gamma(\nu+1) \tag{2.25}$$

as $x \to 0$, a limit that is approached in (2.20) as $N \to \infty$, we have for small ν

$$\begin{aligned} &\frac{1}{\sin(\nu\pi)}(I_\nu(\rho' N^{-1/2})I_{-\nu}(RN^{-1/2}) - I_\nu(RN^{-1/2})I_{-\nu}(\rho' N^{-1/2})) \\ &\quad \to \frac{1}{\nu\pi}((\rho' N^{-1/2})^\nu (RN^{-1/2})^{-\nu} - (RN^{-1/2})^\nu(\rho' N^{-1/2})^{-\nu}) \\ &\quad = \frac{1}{\nu\pi}\left[\left(\frac{\rho'}{R}\right)^\nu - \left(\frac{\rho'}{R}\right)^{-\nu}\right]. \end{aligned} \tag{2.26}$$

Since $\rho' \simeq R$ there is no special N dependence of the low-order coefficients in the power series expansion of (2.26). However

$$\begin{aligned} K_\nu(RN^{-1/2}) &\to \tfrac{1}{2}\pi\left(\frac{(\frac{1}{2}RN^{1/2})^{-\nu} - (\frac{1}{2}RN^{1/2})^\nu}{\sin(\nu\pi)}\right) \\ &= \frac{-\pi}{\sin(\nu\pi)}\sinh[\nu\ln(\tfrac{1}{2}RN^{-1/2})] \\ &= \frac{\pi}{\sin(\nu\pi)}\sinh\{\nu[\tfrac{1}{2}\ln(N) - \ln(\tfrac{1}{2}R)]\} \end{aligned} \tag{2.27}$$

as $N \to \infty$ and $\nu \to 0$. The behaviour of the moments of θ will thus be determined by the expansion in ν of the modified Bessel function $K_\nu(RN^{-1/2})$ in the denominator of (2.15). When N is sufficiently large we can neglect $\ln(R)$ as compared to $\ln(N)$ in (2.27). We then have

$$[K_\nu(RN^{-1/2})]^{-1} \simeq \pi\left(\tfrac{1}{2}\ln(N) + \frac{\nu^2}{48}[\ln(N)]^3\right)^{-1}$$

$$\simeq 2\pi\left([\ln(N)]^{-1} - \frac{\nu^2}{24}\ln(N)\right). \tag{2.28}$$

The mean square of θ, $\langle\theta^2\rangle$, is equal to the ratio of the second to the zeroth moment of $P_N(\theta)$. Recalling (2.15) and (2.19) we see that this ratio is just the negative of the ratio of the second derivative with respect to ν of the function

$$C(\nu)\left(\frac{I_\nu(\rho' N^{-1/2})K_\nu(RN^{-1/2}) - I_\nu(RN^{-1/2})K_\nu(\rho' N^{-1/2})}{K_\nu(RN^{-1/2})}\right) \tag{2.29}$$

at $\nu = 0$ to the function itself there. According to the development above, and especially (2.28), that ratio at large N yields

$$\langle\theta^2\rangle = \frac{(\ln(N))^2}{12}. \tag{2.30}$$

We can similarly obtain expressions for $\langle\theta^{2n}\rangle$ $(\propto(\ln(N))^{2n})$. The coefficient $\mathscr{A}_{2n}$ multiplying $(\ln(N))^{2n}$ in

$$\langle\theta^{2n}\rangle = \mathscr{A}_{2n}\,(\ln(N))^{2n} \tag{2.31}$$

is, as in (2.30), *independent* of R, the radius of the excluded region. Thus, even though it is necessary to keep the walker out of a finite region about the origin in order for second- and higher-order moments of the normalised winding angle distribution to be finite the moments themselves are independent of the size (and presumably other details) of the excluded region.

We now turn to a discussion of the behaviour of the distribution itself, with special emphasis on the large-θ tail. We recall that the behaviour at large argument of a function will be governed by the properties at small argument of its Fourier transform. In particular, the way in which a function falls off at large argument will be determined by those non-analyticities of its Fourier transform that lie closest to the origin, assuming that the Fourier transform possesses non-analyticities at finite argument. It is thus necessary to study the analytic properties of (2.29).

Once again the behaviour of interest is controlled by the modified Bessel function $K_\nu(RN^{-1/2})$ in the denominator. This function has zeros at imaginary values of ν that lie very close to the real axis when the product $RN^{-1/2}$ is very small, as it will be when the walk consists of a sufficient number of steps. Utilising (2.27) we see that when $\nu \to i\nu'$ (ν' small)

$$K_\nu(RN^{-1/2}) \to \frac{1}{\sinh(\nu'\pi)}\sin\{\nu'[\tfrac{1}{2}\ln(N) - \ln(\tfrac{1}{2}R)]\} \tag{2.32}$$

so that, when $\ln(R)$ is negligible compared to $\ln(N)$, the modified Bessel function goes to zero at $\nu' = 2\pi k/\ln(N)$, where k is an integer.

If we now carry out the integral over ν in (2.15) by contour integration it is immediately evident that the large-θ behaviour of $P_N(\theta)$ will be governed by the contribution to the integral of the residue at the pole in the integrand that is closest to the origin. According to the discussion immediately above that pole will be at $\nu=\pm 2\pi \mathrm{i}/\ln(N)$. Substituting this value of ν into $e^{i\nu\theta}$ we thus have

$$P_N(\theta) \propto \exp\left(-\frac{2\pi\theta}{\ln(N)}\right) \qquad \theta \gg 1. \tag{2.33}$$

The distribution decays *exponentially* with θ when θ is large. Note that the details of the exponential decay are independent of the size of the excluded region. The only thing that matters is its existence.

3. Simulations

As a supplement to and check of our theoretical analysis we have generated winding angle distributions numerically in two and three dimensions. The results of these calculations have been used to verify two of the central predictions of that analysis. Recall (2.30) and (2.33):

$$\langle\theta^2\rangle = \left(\frac{\ln(N)+C}{12}\right)^2 \tag{3.1}$$

and

$$P_N(\theta)_{\theta \gg \ln(N)} \sim \exp\left(-\frac{2\pi\theta}{\ln(N)+C'}\right) \to \exp\left(-\frac{2\pi\theta}{\ln(N)}\right). \tag{3.2}$$

If we write

$$[\langle\theta^2\rangle]^{1/2} \to b_1 \ln(N) + C_1 \tag{3.3}$$

$$-\theta[\ln(P_N(\theta))]^{-1} \equiv A \to b_2 \ln(N) + C_2 \qquad N \gg 1 \tag{3.4}$$

then, according to (3.1) and (3.2),

$$b_1 = (12)^{-1/2} = 0.289\ldots \tag{3.5}$$

and

$$b_2 = \frac{1}{2\pi} = 0.159\ldots. \tag{3.6}$$

We use our numerical calculations to check (3.3)-(3.6).

Winding angle distributions were generated using two different approaches. In the first we performed an exact enumeration of all unrestricted two-dimensional walks of up to 72 steps on a square lattice. The second was a Monte Carlo type simulation of much longer walks. The exact enumeration utilised the recursion relation

$$C_N(\boldsymbol{x}', \boldsymbol{x}) = \sum_{n=0}^{(z^*)-1} C_N(\boldsymbol{x}', \boldsymbol{x}+\boldsymbol{l}_n) \tag{3.7}$$

(see (2.2)) with the initial condition $C_1(\boldsymbol{x}', \boldsymbol{x}) = \delta_{\boldsymbol{x}',\boldsymbol{x}}$ and the constraint $C_N(\boldsymbol{x}', \boldsymbol{x}) = 0$, when x is at the origin. Our constraint thus creates an excluded region about the origin. All walks start on one of the lattice sites that is a nearest neighbour to the site at the origin. We then calculated the quantities $b_1(N)$ and $b_2(N)$, which are defined as follows:

$$b_1(N) = \frac{\langle\theta^2\rangle_{N+4}^{1/2} - \langle\theta^2\rangle_N^{1/2}}{\ln(N+4) - \ln(N)} \tag{3.8a}$$

$$b_2(N) = \frac{A_{N+4} - A_N}{\ln(N+4) - \ln(N)}. \tag{3.8b}$$

b_1 and b_2 as given by (3.5) and (3.6) ought to be the $N \to \infty$ limits of $b_1(N)$ and $b_2(N)$. Our results are summarised in table 1 and the linear extrapolation plotted against $1/N$ gives

$$D = 2 \qquad \begin{cases} b_1 = 0.301 \\ b_2 = 0.171. \end{cases}$$

The Monte Carlo type simulations utilised a standard random number generator. The walks were performed on a square and a simple cubic lattice. Once again, the starting point was one of the sites adjacent to the origin. The way in which we enforced an excluded-region constraint is worth mentioning. If a given walker happened to step on the origin (in two dimensions) or z axis (in three dimensions) we discarded the walk entirely and started over again. This replicates the effect of an absorbing wall and is the proper way to exclude the region (Feller 1968). Keeping the walkers off the origin by having them take a step in another direction whenever they happen to step on the origin, no matter how that other direction is determined, is equivalent to placing a reflecting wall around the excluded region and does *not* properly exclude the origin. We found that this latter procedure yields different winding angle statistics than does either the method we employed or our theoretical analysis.

We took 50 000 samples in our simulations for each of several values of N, where N ranged up to 724. The quantities b_1 and b_2 were obtained via least-squares fits to semilog plots. Figures 2 and 3 display the results of our simulations and the least-squares fits. Our results are also presented numerically in table 2. The quantities b_1 and b_2, as determined by least squares, are

Table 1. Values of $b_1(N)$ and $b_2(N)$ from exact enumeration on a square lattice. The linear extrapolation plotted against $1/N$ gives $b_1 = 0.3010$ and $b_2 = 0.1711$.

N	$b_1(N)$	$b_2(N)$
26	0.272 333 6044	0.211 252 3334
30	0.275 132 8123	0.205 836 6806
34	0.277 623 7972	0.201 692 6125
38	0.279 811 1752	0.198 424 6620
42	0.281 724 7061	0.195 788 6768
46	0.283 399 6102	0.193 622 6666
50	0.284 869 4462	0.191 813 9012
54	0.286 163 8237	0.190 281 3258
58	0.287 307 9999	0.188 965 2896
62	0.288 323 1889	0.187 821 1302
66	0.289 227 1002	0.186 814 9561
70	0.290 034 5091	0.185 920 7669

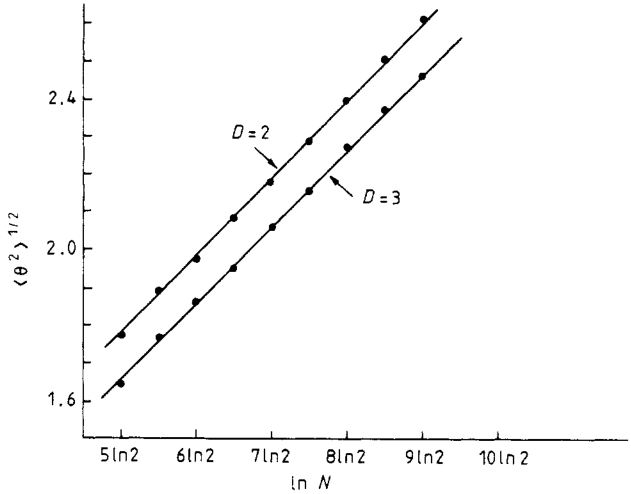

Figure 2. A plot suggesting $\langle\theta^2\rangle^{1/2}$ is asymptotically proportional to $\ln(N)$ for ordinary random walks on a square and cubic lattice. Our analytical results predict 0.289 for the slope. The simulation (by least-squares fitting) gives 0.301 for a square lattice and 0.293 for a cubic lattice.

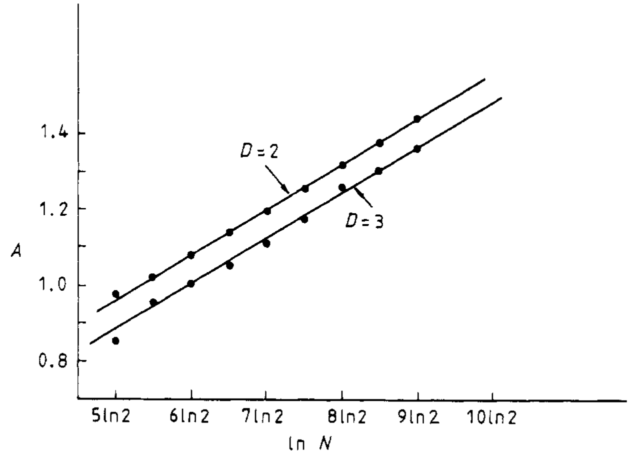

Figure 3. A plot suggesting the quantity A (see equation (3.4)) is linearly proportional to $\ln(N)$ with slope 0.175 for a square lattice and 0.174 for a cubic lattice. Comparing with the analytical result of 0.159 there are about 10% discrepancies. A few possible explanations are given in § 3.

$$D=2: \qquad \begin{cases} b_1 = 0.301 \pm 0.003 \\ b_2 = 0.175 \pm 0.001 \end{cases} \tag{3.9}$$

$$D=3: \qquad \begin{cases} b_1 = 0.293 \pm 0.003 \\ b_2 = 0.174 \pm 0.005. \end{cases} \tag{3.10}$$

Comparing the above with (3.5) and (3.6) we note small ($\leqslant 10\%$), but non-negligible, discrepancies between analytical predictions and numerical results. There are a few possible sources for these differences. First, our analytical results hold in the limit of very large N. This regime may not be fully entered in our simulations. Note, for

Table 2. Values of $\langle\theta^2\rangle^{1/2}$ and A (see equations (3.3) and (3.4)). These values are obtained by Monte Carlo simulation with 50 000 samples for each value of N.

	$d=2$		$d=3$	
$\ln(N)$	$\langle\theta^2\rangle^{1/2}$	A	$\langle\theta^2\rangle^{1/2}$	A
5.5 ln 2	1.7745	0.9571	1.6435	0.8512
6.0 ln 2	1.8847	1.0217	1.7666	0.9543
6.5 ln 2	1.9752	1.0784	1.8651	1.0084
7.0 ln 2	2.0782	1.1385	1.9515	1.0557
7.5 ln 2	2.1749	1.1982	2.0592	1.1120
8.0 ln 2	2.2827	1.2610	2.1592	1.1775
8.5 ln 2	2.3961	1.3217	2.2719	1.2580
9.0 ln 2	2.5047	1.3790	2.3685	1.3092
9.5 ln 2	2.6129	1.4472	2.4589	1.3679

example, that the values of $b_2(N)$ that are obtained in our exact enumeration are further away from the theoretical value of b_2 than is our least-squares result, obtained by fitting to much longer walks. This quantity, however, is not nearly as easy to obtain as b_1. First, we must fit a numerically generated winding angle distribution to a specific form for various N. Then it is necessary to perform a least-squares analysis of a plot of fitting parameters against N. The parameter of interest controls the distribution in the large θ wings and may, therefore, be sensitive to statistical fluctuations associated with the finite number of walks in our samples. We thus expect larger errors in our determination of this quantity. The way in which the large N limit is approached and, in particular, the size and qualitative behaviour of the next-to-leading-order contributions to the winding angle distribution is well worth studying.

A possibility that cannot be ruled out as yet is that the random number generator that we used may have been responsible for some anomalies in the random walk statistics.

Finally, there is the possibility of a fundamental shortcoming in our application of theory. The region excluded in our simulations is not circular and there may be some non-trivial effect on the winding angle distribution of the shape of the excluded region. Furthermore, the continuum approximation may not apply here. We do not expect either of these last two possibilities to pan out. Nevertheless we feel that there is a need for both more extensive simulations and a closer examination of our theoretical model.

4. Conclusion

The winding angle distribution for unrestricted walks has been calculated in the diffusion equation or continuum approximation. This represents a reappraisal of the problem as first addressed by Spitzer (1958). We find that the introduction of an excluded region about the origin changes the distribution in fundamental ways from the Cauchy form that Spitzer obtained. The new distribution, which decays exponentially for large winding angle rather than as the inverse square of the angle, possesses finite moments at all positive integer order. The fact that the second and higher moments of the Cauchy distribution are infinite renders it unacceptable as a complete description of the winding angle distribution of real random walks on a lattice. It most certainly rules it out as a description of the statistics of entanglement for a self-intersecting chain polymer grown in the vicinity of a long straight rod. The excluded region about the origin is well motivated physically in the latter case and is a natural consequence of the restrictions that limit configurations in the former.

We are able to formulate precise numerical predictions for the winding angle distribution, relating to both its behaviour at large winding angle and the relationship between its second moment and the number of steps in a long walk. In obtaining these predictions we relied on the existence of an excluded region, but the predictions, which are asymptotic in nature, are independent of details of that region, specifically its size. Our predictions were compared to both the results of exact enumeration of random walks with up to 72 steps and of simulations of walks consisting of up to 724 steps. In all cases discrepancies between numerical results and our analytical predictions are no larger than 10%. The discrepancies that do exist are thus small but not quite negligible. As yet we have no firm explanation for them.

At this point many questions remain to be answered. The most intriguing in our opinion have to do with the effects of excluded volume. Preliminary results from simulations of three-dimensional self-avoiding random walks indicate that their winding angle statistics are not strikingly different from those of unrestricted walks. The second moment of the distribution, $\langle\theta^2\rangle$, appears to scale with the same power—or with close to the same power—of $[\ln(N)]^2$ as it does for the unrestricted walk. This is in contrast to the case in two dimensions where, as noted in § 1, $\langle\theta^2\rangle \propto \ln(N)$ for the self-avoiding walk while $\langle\theta^2\rangle \propto (\ln(N))^2$ when the walk is unrestricted. A renormalisation group calculation seems an eminently worthwhile undertaking. This is especially so when we consider the physical implications of such a calculation. The self-avoiding walk models the statistics of a long-chain polymer. The desirability of precise quantitative results for the entanglement of a real chain polymer with a rod is evident.

There are questions concerning the analysis performed in this paper that ought to be answered as well. The diffusion equation limit applies when the distribution of interest varies slowly on the scale of a step length. This in turn implies that in order for this limit to be applicable when an excluded region is introduced the size of that region ought to be large compared to a step length. Nevertheless, we find that our predictions are independent of the size of that region in the limit of long walks and that we recover Spitzer's form for the distribution in the limit that its extent is vanishingly small. A more searching study of the way in which different limiting regimes arise seems an eminently worthwhile undertaking.

It is worth noting that the approach to the Cauchy distribution is *not uniform* as the size of the excluded region goes to zero. As long as the region has a finite extent, no matter how small, exponential decay is recovered in the extreme wings of the distribution, and for long enough walks positive moments depend uniquely and universally on their length. The issues that need to be addressed are those of crossover. Their full resolution will only follow from further and deeper analysis.

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Privman for enlightening discussions and for having brought the problem to our attention. After this article was submitted Dr Claude Belisle brought to our attention work of his own on the problem of winding angles. We are grateful to him for informing us of his work, which overlaps substantially the work reported above.

Appendix 1. The limit of large N

We are interested in extracting the coefficient of z^N in the power series expansion of $P(\theta, z)$, as given by (2.15) and (2.16). Combining the two we obtain

$$P(\theta, z) = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\nu\theta}\left(\frac{1}{\kappa^2}\int_0^{\infty} \frac{\cosh(\nu t)}{(\cosh(t))^2}\,\mathrm{d}t\right)\left(\frac{I_\nu(\kappa\rho_<)K_\nu(\kappa R) - I_\nu(\kappa R)K_\nu(\kappa\rho_<)}{K_\nu(\kappa R)}\right)\mathrm{d}\nu \tag{A1.1}$$

where, as noted in § 2, the quantity κ^2 is equal to $z^* - z$. We find the coefficient of z^N in (A1.1) by contour integration. In particular, we use the fact that if $P(\theta, z)$ is analytic in the vicinity of $z = 0$, then the coefficient of z^n in its power series expansion is

$$\frac{1}{2\pi\mathrm{i}}\oint \frac{P(\theta, z)}{z^{N+1}}\,\mathrm{d}z \tag{A1.2}$$

where the contour is counterclockwise, encloses the origin and has an infinitesimal radius.

We perform the integral by the method of steepest descents. This involves finding the extremum of the integrand. As it turns out, the z dependence in $P(\theta, z)$ that plays the controlling role in this part of the process is in the factor $1/\kappa^2$. We have to extremise

$$\frac{1}{z^N\kappa^2} = \exp[-\ln(z^* - z) - N\ln z] \tag{A1.3}$$

which is achieved when

$$z^* - z = z^*/N. \tag{A1.4}$$

This means that

$$\kappa = (z^*/N)^{1/2} \propto N^{-1/2}. \tag{A1.5}$$

In accord with the method of steepest descents, we replace the integral (A1.2) with the integrand, the quantities z and κ being eliminated with the use of (A1.4) and (A1.5). The expressions that follow (2.14) result from those substitutions—the constant z^* being, in addition, set equal to 1. This last substitution leads to great simplification of presentation and has absolutely no effect on our central results.

Appendix 2. The recovery of the limit of Spitzer

Recall equation (2.17), which is our result for the winding angle distribution in the limit of an excluded region of zero extent about the origin:

$$P_N(\theta) \propto \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\nu\theta} C(\nu) I_{|\nu|}(\rho' N^{-1/2})\,\mathrm{d}\nu. \tag{A2.1}$$

The argument of the modified Bessel function will be small for a long random walk. This allows us to use the limiting form (2.25). Thus we have for small ν (which determines the behaviour for large θ)

$$P_N(\theta) \propto \int_{-\infty}^{\infty} e^{i\nu\theta}[(\rho_</2)N^{-1/2}]^{|\nu|}\,d\nu = \int_{-\infty}^{\infty} e^{i\nu\theta} \exp(-|\nu| \ln[N^{1/2}2/\rho_<])\,d\nu$$
$$\propto \frac{\ln(N^{1/2}2/\rho)}{\theta^2+(\ln(N^{1/2}2/\rho))^2} \to \frac{C\ln(N)}{\theta^2+0.25(\ln(N))^2} \tag{A2.2}$$

where C is a constant. This is just the Lorentzian, or Cauchy, distribution predicted by Spitzer.

Appendix 3

In this appendix we demonstrate that the integration over real ν of (2.15) can be completed by closing in the upper half of the complex ν plane. We also derive a more general result for $P_N(\theta)$. From (2.15)

$$P_N(\theta) = \int_{-\infty}^{\infty} f(\nu)\,d\nu \tag{A3.1}$$

where

$$f(\nu) = \int_{\rho'}^{\infty} \rho K_\nu(\rho N^{-1/2}) \left(\frac{I_\nu(\rho' N^{-1/2})K_\nu(RN^{-1/2}) - I_\nu(RN^{-1/2})K_\nu(\rho' N^{-1/2})}{K_\nu(RN^{-1/2})} \right) d\rho. \tag{A3.2}$$

In the limit $x \to 0$ and small ν the modified Bessel functions approach the following limiting forms:

$$I_\nu(x) = [x/2]^\nu \tag{A3.3}$$

$$K_\nu(x) = \tfrac{1}{2}\pi \frac{I_{-\nu}(x) - I_\nu(x)}{\sin(\nu\pi)}$$
$$= \frac{\pi}{2\sin(\nu\pi)}([x/2]^{-\nu} - [x/2]^\nu). \tag{A3.4}$$

If we now take $N \gg 1$ and insert (A3.3) and (A3.4) into (A3.2) we obtain

$$f(\nu) = \int_{\rho'}^{\infty} \rho K_\nu(\kappa\rho) \frac{\sinh[\nu \ln(\rho'/R)]}{\sinh[\nu \ln(2/\kappa R)]}\,d\rho \tag{A3.5}$$

where $\kappa = N^{-1/2}$.

It can be readily verified from (A3.5) that $f(\nu)$ vanishes exponentially as the real part of ν goes to plus or minus infinity. This means that we can transform the integration of $f(\nu)$ over real ν into an integral around a closed contour by adding an infinite semicircle in the top half-plane. We then evaluate the integral by adding up the residues of the poles of the integrand that lie there. The relevant poles all lie on the positive imaginary axis, at

$$\nu_n = \frac{in\pi}{\ln(2/\kappa R)}\ . \tag{A3.6}$$

Now

$$\int_{\rho'}^{\infty} K_{\nu_n}(\kappa\rho)\rho\,\mathrm{d}\rho = \int_{\rho'\kappa}^{\infty} K_{\nu_n}(x)x\,\mathrm{d}x. \tag{A3.7}$$

As $\kappa \to 0$ (or as $N \to \infty$) this integral converges, so $\rho'\kappa$ can be replaced by its limit value of 0. Using an integral representation of the modified Bessel function $K_\nu(x)$ we have

$$\int_{\rho'\kappa}^{\infty} K_{\nu_n}(x)x\,\mathrm{d}x \simeq \int_{0}^{\infty} K_{\nu_n}(x)x\,\mathrm{d}x = \kappa^{-2}\int_0^\infty\int_0^\infty \exp(-x\cosh t)\cos\left(\frac{n\pi t}{\ln(2/\kappa R)}\right)x\,\mathrm{d}x\,\mathrm{d}t$$

$$= \kappa^{-2}\int_0^\infty (\cosh t)^{-2}\cos\left(\frac{n\pi t}{\ln(2/\kappa R)}\right)\mathrm{d}t. \tag{A3.8}$$

Because $\cos[n\pi t/\ln(2/\kappa R)] \to 1$ as $\kappa \to 0$ we are left in the limit of large N with the result

$$\int_0^\infty K_{\nu_n}(x)x\,\mathrm{d}x = \kappa^{-2}\int_0^\infty (\cosh t)^{-2}\,\mathrm{d}t = \kappa^{-2} = 1/N. \tag{A3.9}$$

We thus have the following result for $P_N(\theta)$:

$$P_N(\theta) = \kappa^{-2}\sum_{n=1}^{\infty} 2\pi\mathrm{i}[\cos(n\pi)]^{-1}\mathrm{i}\sin\left(n\frac{\pi\ln(\rho'/R)}{\ln(2/\kappa R)}\right)\exp\left(-\frac{n\pi\theta}{\ln(2/\kappa R)}\right)$$

$$= 2\pi\kappa^{-2}\sum_{n=1}^{\infty}(-1)^{n+1}\sin(nB)\exp(-n\theta/A)$$

$$= 2\pi\kappa^{-2}\frac{\sin(B)}{2[\cos(B)+\cosh(\theta/A)]} \tag{A3.10}$$

where

$$B = \frac{\pi\ln(\rho'/R)}{\ln(2/\kappa R)} \to 0 \qquad \text{as } N \to \infty \tag{A3.11}$$

and

$$A = \frac{1}{2\pi}\ln\left(\frac{2}{\kappa R}\right) = \frac{1}{2\pi}(\ln(N)+\ln(z^*)) + \text{constants}.$$

As $N \to \infty$

$$P_N(\theta) \to \frac{C_1}{2[1+\cosh(\theta/A)]} \tag{A3.12}$$

$$= \frac{C_1}{4[\cosh(\theta/2A)]^2} \tag{A3.13}$$

where C_1 is a constant.

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