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Exact shapes of random walks in two dimensions

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Abstract

Since the random walk problem was first presented by Pearson in 1905, the shape of a walk which is either completely random or self-avoiding has attracted the attention of generations of researchers working in such diverse fields as chemistry, physics, biology and statistics. Among many advances in the field made in the past decade is the formulation of the three-dimensional shape distribution function of a random walk as a triple Fourier integral plus its numerical evaluation and graphical illustration. However, exact calculations of the averaged individual principal components of the shape tensor for a walk of a certain architectural type including an open walk have remained a challenge. Here we provide an exact analytical approach to the shapes of arbitrary random walks in two dimensions. Especially, we find that an end-looped random walk surprisingly has an even larger shape asymmetry than an open walk.

The shape of a random walk taking place in a d-dimensional space is often described by d principal components arranged in descending order, i.e., $S_1 \geqslant S_2, \geqslant \cdots \geqslant S_d$, of the shape tensor **S** [7, 11, 15, 17]. This tensor **S** is related to the inertia tensor **I** of an n-vertex walk by the equality $\mathbf{I} = n(s^2\mathbf{1} - \mathbf{S})$ where unit mass is assumed for each vertex, **1** is the identify matrix, and s^2 is the trace of S, i.e., $s^2 = \mathrm{tr}(\mathbf{S})$ with s historically termed the radius of gyration [3, 5], i.e., the square root of the arithmetic mean of n squared distances of the vertices from their center of mass. For convenience, unit step length is further assumed for the walk.

A walk may be either completely random or self-intersecting [1–3, 5] (the large-n limit of the gaussian model) or self-avoiding (Edwards model) [2, 4, 10, 12, 15, 16] and may have different architectural types [21] usually specified by the architecture or Kirchhoff matrix **K**. Let $\mathbf{\Lambda}$ denote the diagonal matrix of all $n-1$ nonzero eigenvalues of **K** times n^2. The eigenpolynomials of $\mathbf{\Lambda}$, i.e., $P_{n-1}(x) = |\mathbf{1} + x\mathbf{\Lambda}^{-1}|$ for an end-looped or dumbbell-like walk, i.e., two identical large rings connected by a doubly-sized chain, may be written down with the use of graph theory, with the result that $D(x) \equiv P_\infty(x^2) = U(x)U^2(x/2)\ B(x, -1/3)\ B(x, 2/3)$, where $U(x) = 4\,\mathrm{sh}(x/4)/x$ and $B(x, a) = [\mathrm{ch}(x/4) - a]/(1 - a)$. From the

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above eigenpolynomial, one can obtain an analytic expression for the function $S_m(x)$ defined as the large-n limit of $\mathrm{tr}(\mathbf{\Lambda} + x^2\mathbf{1})^{-m}$.

For arbitrary random walks in two dimensions, we find by using the method of Solc and Gobush [9] that shape factors, i.e., the δ_α defined as $\langle S_\alpha\rangle/\langle s^2\rangle$ which is the ratio of the averaged principal component of **S** to the mean square radius of gyration, and shape variance factors, the σ_α defined as $(\langle S_\alpha^2\rangle - \langle S_\alpha\rangle^2)/\langle s^2\rangle^2$, are given by $\delta_\alpha = 1/2 + (-1)^\alpha \chi_1$ and $\sigma_\alpha = (1 + 3\mu_2)/4 + (-1)^\alpha \chi_2 - \delta_\alpha^2$, respectively. Here, $\mu_m = S_m(0)/S_1^m(0)$ and χ_m is defined as

$$\chi_m = S_1^{-m}(0) \int_0^\infty |xD(x + \mathrm{i}\,x)|^{-1}\, \mathrm{Im}[F_m(x + \mathrm{i}x)]\, \mathrm{d}x,$$

with $F_1(x) = S_1(x), F_2(x) = S_2(x) + 2^{-1} S_1^2(x)$ and $\mathrm{Im}(x + \mathrm{i}y)$ denoting the imaginary part of $x + \mathrm{i}\,y$. Similarly, we can write down expressions for δ_α and σ_α for the $d = 3$ case. However, a complication occurs in this case as it involves triple integrals over the restricted domains of the rotation group SO(3), which are difficult to evaluate accurately even by numerical means. Therefore, for random walks in a space with $3 \leqslant d < \infty$ and for self-avoiding walks, the exact evaluation of δ_α or σ_α remains a challenge. Numerical evaluations of δ_α and σ_α for two common types and one new type of random walks in two dimensions, i.e., open, closed and end-looped walks, based on the above general formulas have been made and the results are tabulated in Table 1. We note that our general formulas reproduce the earlier results for a closed random walk [9].

From Table 1, we find that the simulation results of Bishop and Michels [22] for shape factors of 2D chains and rings of finite length ($n = 64$), i.e., 0.839 and 0.161 for chains and 0.755 and 0.245 for rings, are very close to our exact values for open and closed random walks; and that shape variance factors are in descending order, i.e., $\sigma_1 > \sigma_2$, for all three types of random walks, implying a broader distribution of the largest principal component. For an end-looped random walk, it is seen from Table 1 that it is more elongated than other types of random walks and even more asymmetrical than an open random walk though its average size is smaller than that of the latter (with a shrinking factor, i.e., the ratio of its mean square radius of gyration to that of the open walk, of $51/64 \cong 0.796875$). This large shape asymmetry of the

Table 1
Shape and shape variance factors for open (1), closed (2) and end-looped (3) random walks in two dimensions

Type	δ_1	δ_2	σ_1	σ_2
1	0.832938	0.167062	0.369214	0.009090
2	0.754323	0.245677	0.155901	0.014739
3	0.852352	0.147648	0.439593	0.006567

end-looped random walk may have important implications for the improvement of the rheological properties of end-looped linear polymers yet to be made or discovered.

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