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The shapes of high-dimensional random walks

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Abstract. The individual principal radii of gyration are computed for unrestricted random walks in a large number of spatial dimensions. A low order expansion in one over the dimensionality yields useful information regarding the distribution and average of these measures of the extent and spatial anisotropy of high-dimensional random walks. Such an expansion may well prove useful in the study of the shapes of other random fractal objects.

1. Introduction

It has been known for some time that the trail left by a random walker is elongated in overall shape rather than spherical (Kuhn 1934, Solc and Stockmeyer 1971, Solc 1971). This is true whether the walk is self-avoiding or not. The general realisation that other random fractal objects occurring in nature—such as the clusters resulting from kinetic aggregation or percolation processes—are also non-spherical has been more recent (Family *et al* 1985). In all cases, the anisotropy of the objects has important consequences on the nature and behaviour of these systems when in the condensed phase (see, for example, Petrie 1979). Indeed, for diffusion-limited aggregation, there are strong indications of an intimate connection between the overall shape of the cluster and its fractal dimension (Turkevich and Scher 1985, Ball *et al* 1985). Whilst, for random walks, it is well known that self-avoiding walks provide an asymptotically accurate model for the natural conformation of long chain polymers (de Gennes 1979 and references therein, also see Freed 1981). Thus, it is quite reasonable to expect interesting relationships between the asphericity of these macromolecules and various important physical properties, such as the effect of anisotropy on flow fields or mobilities of polymers in various porous media. Other examples can be cited, but it is clear that useful physics with interesting and important technological applications will emerge from a study of the extent to which random walk processes and other random generators of fractals give rise to aspherical objects.

This paper is a continuation of an earlier effort (Rudnick and Gaspari 1986) to quantify the shapes of random walks, focusing on analytical methods rather than numerical computations. There are a number of numerical studies in the literature in which the shape of either an unrestricted or a self-avoiding random walk is characterised in terms of the limiting ratios of the principal radii of gyration (see Bishop and Michels 1985 and references therein). These quantities are obtained numerically in a straightforward way but an analytical study of the individual radii poses considerable challenges. In our previous paper, we avoided the analytical difficulties arising in a calculation of the components of the radii of gyration by defining the following parameter, A_d, which measures the asphericity of the shape of the random walk:

$$A_d = \frac{\Sigma_{i>j}^{d} \langle (R_i^2 - R_j^2)^2 \rangle}{(d-1)\langle (\Sigma_{i=1}^{d} R_i^2)^2 \rangle} \tag{1.1}$$

where R_i^2 is the square of one of the principal radii of gyration of a random walk in d dimensions. The brackets in (1.1) represent an average over all walks. The analytical evaluation of A_d is tractable for both the unrestricted and the self-avoiding walk. In the case of the unrestricted walk, one has an exact result (Rudnick and Gaspari 1986)

$$A_d = \frac{2(d+2)}{(5d+4)} \tag{1.2}$$

while a renormalisation group calculation yields an ε expansion for A_d for the self-avoiding walk in $4-\varepsilon$ dimensions (Aronovitz and Nelson 1986).

We report here on a study of the individual principal radii of gyration of a d-dimensional walk in the regime $d \gg 1$. Our main result consists of the first two terms in a $1/d$ expansion for the individual radii. As expected, our expansion is in accord with exact results for unrestricted walks to the appropriate order in $1/d$. We find, furthermore, that the ratios of the squares of the largest principal radii of gyration lie close to the reported numerical values. Since self-avoiding walks have the same asymptotic statistics as unrestricted walks in more than four dimensions, our results apply to both kinds of walks when $d > 4$ but are not reliably applied to self-avoiding walks when $d < 4$. However, the results for unrestricted walks may have some relevance to real polymer systems at the theta point when the attractive and repulsive monomer forces cancel each other (Williams *et al* 1981).

The calculation outlined here is an example of a promising alternative approach to the problem of describing the shape of a random fractal object, and it may, in spite of its limitations, provide useful insights into both average shapes and the distribution of shapes of random walks and, possibly, other objects generated by important random processes.

The remainder of this paper is organised as follows. In the next section, the definition of key quantities used to describe the shape of the random walks are reviewed and some of their properties are developed. Chief among these quantities is the asphericity parameter, A_d, and exact analytical results for unrestricted walks in arbitrary dimensions are presented. Section 3 contains the discussion of high-dimensional walks, starting with the leading order walk in $d \to \infty$ limit. The moment of inertia tensor for this walk is derived and its eigenvalues are extracted. The next-to-leading order walks are then taking into account, yielding the next-to-leading order contributions to an expansion in $1/d$ of the average radii of gyration of the random walk. We find that the ratios of the three largest radii of gyration are as follows:

$$\langle R_1^2 \rangle : \langle R_2^2 \rangle : \langle R_3^2 \rangle = 9 : 2.25 : 1 \tag{1.3}$$

to within corrections of order $(1/d)^2$. These ratios compare favourably with numerical results. In appendix 1, a comparison between the exact results presented in § 2 and results that follow from our expansion are shown to match to the appropriate order. Appendix 2 contains the derivation of a conjectured form for the distribution of the principal radii of gyration.

2. Measures of the shape of a random walk

There are a number of ways to measure the anisotropy of a random walk (Kuhn 1934, Solc 1971, Ruben and Mazur 1975, 1977, Rubin *et al* 1976) all of which lead to a consistent picture of the walk. Here we are interested in developing analytical techniques to describe the shape of the walk itself and the usual way to quantify the overall shape of an N step random walk starts with the moment of inertia tensor, $\vec{T}$ (Solc 1971). The elements of $\vec{T}$ are given by

$$T_{ij} = \frac{1}{N+1} \sum_{k=1}^{N+1} (x_{ik} - \langle x_i \rangle)(x_{jk} - \langle x_j \rangle) \tag{2.1}$$

where x_{ij} is the ith component of the position vector of the kth 'node' in the walk. The quantity $\langle x_i \rangle$ is the average over the walk

$$\langle x_i \rangle = \frac{1}{N+1} \sum_{l=1}^{N+1} x_{il}. \tag{2.2}$$

Note that there are $N+1$ nodes in an N step walk, and the nodes can be thought of as the walker's 'footprints'. The d by d tensor $\vec{T}$ has as its eigenvalues the principal radii of gyration of the walk. Thus, when diagonalised,

$$\vec{T} = \begin{pmatrix} R_1^2 & & \\ & R_2^2 \ddots & 0 \\ 0 & & R_d^2 \end{pmatrix}. \tag{2.3}$$

The ratios of the individual eigenvalues describe the deviation from sphericity of the random walk when the components are averaged over all N step walks. Numerical calculations have been carried out by many investigators (for references see the paper by Bishop and Michels (1985)) and the results calculated by Solc (1973) for the ratios in the large-N limit for unrestricted walks and Mazur *et al* (1973) for self-avoiding walks in three dimensions are typical. These authors find that

$$\langle R_1^2 \rangle : \langle R_2^2 \rangle : \langle R_3^2 \rangle = 11.8 : 2.69 : 1.00 \tag{2.4}$$

for unrestricted walks and

$$\langle R_1^2 \rangle : \langle R_2^2 \rangle : \langle R_3^2 \rangle = 14.8 : 3.06 : 1.00 \tag{2.5}$$

when the walks are self-avoiding.

Unfortunately, the process of averaging the roots, R_i^2, of the characteristic equation of $\vec{T}$ is not readily susceptible to analytical methods. It has been shown (Rudnick and Gaspari 1986, Theodorou and Suter 1984, Aronowitz and Nelson 1986) how to avoid this difficulty by measuring the shape of the random walk in terms of appropriate low order invariants of the tensor $\vec{T}$ rather than the individual principal radii of gyration. We defined a parameter A_d which measures the asphericity of a random walk and thereby provides a useful description of deviations from spherical symmetry applicable to various fractal objects. Moreover, the asphericity parameter involves averages that can be readily obtained in the case of unrestricted walks and—with some effort—in the case of self-avoiding walks. To see this, we first express A_d in terms of the invariants of the moment of inertia tensor, $\overleftrightarrow{T}$,

$$
\begin{aligned}
A_d &= \frac{1}{d-1}\frac{\sum_{i>j}^{d}\langle (R_i^2-R_j^2)^2\rangle}{\langle(\sum_i R_i^2)^2\rangle} \\
&= \frac{1}{d-1}\frac{\sum_{i>j}\langle (R_i^4+R_j^4-2R_i^2R_j^2)\rangle}{\langle(\sum_j R_i^2)^2\rangle} \\
A_d &= \frac{d\,\sum_{i=1}^{d}\langle R_i^4\rangle-\langle(\sum_{i=1}^{d}R_i^2)^2\rangle}{(d-1)\langle(\sum_{i=1}^{d}R_i^2)^2\rangle}
\end{aligned}
\tag{2.6}
$$

which obviously is equal to

$$
A_d = \frac{d\langle T_r\overleftrightarrow{T}^2\rangle - \langle (T_r\overleftrightarrow{T})^2\rangle}{(d-1)\langle (T_r\overleftrightarrow{T})^2\rangle}. \tag{2.7}
$$

The quantity A_d is seen to be an invariant and varies between zero for a spherical walk and one for a walk with a single principal radii of gyration infinitely larger than the rest. The averages appearing in (2.7) can be exactly calculated for unrestricted walks. Using the generating function techniques described in our previous paper, it is straightforward to show that, for a hypercubic lattice in the large-N limit, the average becomes

$$
\begin{aligned}
\langle T_r\overleftrightarrow{T}^2\rangle &= d\langle T_{11}^2\rangle + d(d-1)\langle T_{12}^2\rangle \\
&= d\left(\frac{N^2}{20d^2}\right) + d(d-1)\left(\frac{N^2}{90d^2}\right) \\
\langle (T_r\overleftrightarrow{T})^2\rangle &= d\langle T_{11}^2\rangle + d(d-1)\langle T_{11}T_{22}\rangle \\
&= d\left(\frac{N^2}{20d^2}\right) + d(d-1)\left(\frac{N^2}{36d^2}\right)
\end{aligned}
\tag{2.8}
$$

which, when substituted into (2.7), reduces to our earlier result:

$$
A_d = \frac{2(d+2)}{(5d+4)}. \tag{2.9}
$$

As d becomes very large, we have

$$
A_d = \frac{2}{5} + \frac{12}{25}\frac{1}{d} + \mathrm{O}\left(\frac{1}{d^2}\right). \tag{2.10}
$$

We see from (2.10) that the infinite-dimensional unrestricted walk is neither spherical nor asymptotically linear. To get a deeper understanding of this result and insight regarding the shape of the high-dimensional walk we must go beyond the simple one-parameter description provided by A_d and study the eigenvalues of $\overleftrightarrow{T}$ directly. For walks in high dimensions, this becomes a tractable analytical problem which we now discuss.

3. High-dimensional walks

To simplify our discussion, we will place the random walker on a d-dimensional hypercubic lattice. The walker takes each step along one of the $2d$ links connecting a site to its nearest neighbour. If the walk is not too long, i.e. the number of steps, N, is much less than the spatial dimensionality, the most probable walk has the walker choosing a direction at each step that is orthogonal to all the previous steps that were taken. At the nth step there are $2(d-n+1)$ ways of doing this and $2(n-1)$ ways of walking in a direction that is not orthogonal to any previous steps (assuming that all previous steps were taken according to the above rule). There are $(2d)^N$ possible unrestricted N step walks from a given site.

$$\eta_0 = 2d(2d-2)\ldots(2d-2(N-1)) = \frac{2^N d!}{(d-N)!} \tag{3.1}$$

will be of the above kind. Using Stirling's formula, we have for η_0

$$\eta_0 = 2^N \exp\left[d \ln\left(\frac{d}{e}\right) - (d-N)\ln\left(\frac{d-N}{e}\right)\right] \approx (2d)^N \exp\left(-\frac{1}{2}\frac{N^2}{d}\right) \tag{3.2}$$

according to which we may expect our leading order walk to dominate all others when $N \ll \sqrt{d}$. The final result, however, holds more generally than implied by this inequality (Gaspari *et al* 1987).

To construct the matrix $\vec{T}$ for this leading order walk we renumber and, where necessary, reflect coordinate axes so that the walk is first along the positive '1' axis, then along the positive '2' axis, and so on. The coordinates of the $N+1$ nodes of the walk are

$$\begin{aligned} \boldsymbol{r}_1 &= (0,0,0,\ldots) \\ \boldsymbol{r}_2 &= (1,0,0,\ldots) \\ \boldsymbol{r}_3 &= (1,1,0,0,\ldots) \\ \boldsymbol{r}_4 &= (1,1,1,0,0,\ldots) \\ &\vdots \end{aligned} \tag{3.3}$$

Thus

$$\langle x_1 \rangle = \frac{N}{N+1} \qquad \langle x_2 \rangle = \frac{N-1}{N+1} \tag{3.4}$$

and, in general,

$$\langle x_j \rangle = \begin{cases} \dfrac{N-j+1}{N+1} & 1 \leqslant j < N+1 \\ 0 & N+1 \leqslant j. \end{cases} \tag{3.5}$$

The non-zero elements of $\vec{T}$ are contained in an $N+1$ by $N+1$ submatrix with elements given by

$$\begin{aligned} T_{ij} &= \frac{1}{N+1} \sum_{l=1}^{N+1} (x_{il} - \langle x_i \rangle)(x_{jl} - \langle x_j \rangle) \\ &= \frac{1}{N+1}\left[i\left(0 - \frac{N-i+1}{N+1}\right)\left(0 - \frac{N-j+1}{N+1}\right) \right. \\ &\quad + (j-1)\left(1 - \frac{N-i+1}{N+1}\right)\left(0 - \frac{N-j+1}{N+1}\right) \\ &\quad \left. + (N+1-j)\left(1 - \frac{N-i+1}{N+1}\right)\left(1 - \frac{N-j+1}{N+1}\right)\right] \\ &= \frac{1}{(N+1)^2}\, i(N-j+1) \end{aligned} \tag{3.6}$$

where we have assumed for simplicity that $j \geqslant i$. The result (3.6) holds *only* if $0 < i$, $j < N+1$. All other elements of $\tilde{T}$ are zero. It is a straightforward calculation to show that when $i > j$ the right-hand side of (3.6) is replaced by the same expression with i and j interchanged, so that in general

$$T_{i_1, i_2} = \frac{1}{(N+1)^2} i_<(N+1-i_>). \tag{3.7}$$

If we define

$$x_{1,2} = \frac{i_{1,2}}{(N+1)} \tag{3.8}$$

where $0 < x_{1,2} < 1$ we have

$$T_{i_1, i_2} = x_<(1-x_>). \tag{3.9}$$

This matrix occurs in a number of different contexts and its spectrum is known (Fixman 1962, Forsman and Hughes 1963). In the limit of large N, the x appearing in (3.9) can be treated as continuous variables. The operator on the right-hand side of (3.9) is then the inverse of the operator $-\mathrm{d}^2/\mathrm{d}x^2$ on the space of functions that go to zero at $x = 0$ and $x = 1$. Its eigenfunctions are

$$\psi_k(x) = A \sin kx \tag{3.10}$$

where $k = n\pi$. It can be verified by substitution that the eigenfunctions of (3.7), for the discrete walk, are

$$\psi_n(i) = \left(\frac{2}{N+1}\right)^{1/2} \sin\left(\frac{n\pi i}{N+1}\right) \tag{3.11}$$

and their associated eigenvalues are

$$\lambda n = \frac{1}{4(N+1)}\left[\sin^2\left(\frac{n\pi}{2(N+1)}\right)\right]^{-1}. \tag{3.12}$$

When $n \ll N+1$ the eigenvalues are approximately given by

$$\lambda n = \frac{N+1}{\pi^2 n^2} \approx \frac{N}{\pi^2 n^2}. \tag{3.13}$$

Now, since all walks of the type being considered are topologically equivalent, the average square of the principal radii of gyration become, for the largest $\langle R_n^2 \rangle$,

$$\langle R_n^2 \rangle = \frac{N}{\pi^2 n^2}. \tag{3.14}$$

Thus

$$\langle R_1^2 \rangle : \langle R_2^2 \rangle : \langle R_3^2 \rangle = 1 : \tfrac{1}{4} : \tfrac{1}{9} = 9 : 2.25 : 1. \tag{3.15}$$

It is encouraging that the largest $\langle R_n^2 \rangle$ scale linearly with the number of steps in the walk. This is the expected dependence of a characteristic linear dimension for an unrestricted random walk in arbitrary dimensions.

It is seen from the distribution of eigenvalues that the shape of the walk is neither spherical nor linear as previously observed. Indeed, it was found that $A_d \to \frac{2}{5}$ as $d \to \infty$ and therefore this limiting value for A_d is an independent check on the correctness of our result for the eigenvalues. This limit follows by noting that for large N

$$\begin{aligned} T_r\vec{\vec{T}} &= \sum_{n=1}^{\infty} \frac{N}{\pi^2 n^2} = \frac{N}{6} \\ T_r\vec{\vec{T}}^2 &= \sum_{n=1}^{\infty} \left(\frac{N}{\pi^2 n^2}\right)^2 = \frac{N^2}{90} \end{aligned} \tag{3.16}$$

and as $d \to \infty$

$$A_d \to \frac{Tr\vec{\vec{T}}^2}{(Tr\vec{\vec{T}})^2} = \frac{(N^2/90)}{(N^2/36)} = \frac{2}{5} \tag{3.17}$$

which confirms the correctness of not only the eigenvalues but also the class of walks described here as being the leading order contributions for high-dimensional random walks.

The next-to-leading-order walks offer an additional order in the $1/d$ expansion and an extra level of complication. Walks which lead to the next order are those where the random walker now takes one step in a direction that is *not* orthogonal to all the previous steps. We quantify this walk by identifying the step that is in the same—or opposite—direction as a previous step, along with the previous step. This walk will be an N step walk in which the ith step is in the positive 'i' direction with the *single exception* of the lth step which is either in the positive or negative 'j' direction ($j < l$). The derivation of the moment of inertia matrix $\vec{\vec{T}}$ for this walk involves a straightforward set of calculations like the one outlined in (3.6). When carried through we obtain the remarkably simple result that $\vec{\vec{T}}_{1\pm}$, the matrix for this walk, is given by

$$\vec{\vec{T}}_{1\pm} = (1 - l\rangle\langle l \pm j\rangle\langle l)\,\vec{\vec{T}}_0(1 - l\rangle\langle l \pm l\rangle\langle j) \tag{3.18}$$

where the '$\pm j$' in the subscript above identifies walks that have the lth step in the $+$ or $-j$ direction. The matrix $\vec{\vec{T}}_0$ on the right-hand side of (3.17) is the moment of inertia matrix for the leading order walk. The vectors $\langle l$ and $\langle j$ are unit vectors in the i and j direction and they are orthogonal, $\langle l|j\rangle = \langle j|l\rangle = 0$.

Expanding the right-hand side of (3.16)

$$\vec{\vec{T}}_{1\pm} = \vec{\vec{T}}_0 - (|l\rangle \mp |j\rangle)\langle l|\vec{\vec{T}}_0 - \vec{\vec{T}}_0|l\rangle(\langle l| \mp \langle j|) + (|l\rangle \mp |j\rangle)\langle l|\vec{\vec{T}}_0|l\rangle(\langle l| \mp \langle j|). \tag{3.19}$$

Transforming to a new basis, defined by

$$|A\rangle = |l\rangle \mp |j\rangle \tag{3.20}$$

and

$$|B\rangle = \vec{\vec{T}}_0|l\rangle \tag{3.21}$$

we have

$$\vec{\vec{T}}_{1\pm} = \vec{\vec{T}}_0 - |A\rangle\langle B| - |B\rangle\langle A| + |A\rangle\langle A|\langle l|\vec{\vec{T}}_0|l\rangle. \tag{3.22}$$

It can be verified that the perturbation represented by the last three terms on the right-hand side of (3.22) is small compared to the leading order contribution, $\vec{\vec{T}}_0$. Furthermore, it is of a particularly simple form. Defining an appropriate orthogonal basis those last three terms can be written as a two by two matrix, $\vec{M}_{\pm j,l}$. The eigenvalues of the matrix $\vec{T}_{1\pm j,l}$ are thus the eigenvalues of

$$\vec{T}_0 - \vec{M}_{\pm j,l}. \tag{3.23}$$

To find the eigenvalues of (3.22) we look for the poles of

$$(\vec{T}_0 - \vec{M}_{\pm j,l} - \lambda\vec{I})^{-1} \tag{3.24}$$

where $\vec{I}$ is the identity operator. Defining

$$\vec{T}_0 - \lambda\vec{I} \equiv \vec{L} \tag{3.25}$$

we have for (3.23)

$$(\vec{L} - \vec{M})^{-1} = \vec{L}^{-1} + \vec{L}^{-1}(\vec{M} + \vec{M}\vec{L}^{-1}\vec{M} + \vec{M}\vec{L}^{-1}\vec{M}\vec{L}^{-1}\vec{M} + \ldots)\vec{L}^{-1}. \tag{3.26}$$

The subscripts on $\vec{M}$ have been dropped for convenience. The poles of (3.24) will be the poles of the sum in square brackets in (3.26). We have for that sum

$$\begin{aligned}\vec{\Sigma} = \vec{M} + \vec{M}\vec{L}^{-1}\vec{M} + \ldots &= (\vec{M} + \vec{M}\vec{L}^{-1}(\vec{M} + \vec{M}\vec{L}^{-1}\vec{M} + \ldots) \\ &= \vec{M} + \vec{M}\vec{L}^{-1}\vec{\Sigma}\end{aligned} \tag{3.27}$$

or

$$(\vec{I} - \vec{M}\vec{L}^{-1})\vec{\Sigma} = \vec{M}. \tag{3.28}$$

Note that $\vec{\Sigma}$ is a two by two matrix in the basis set from which we construct the two by two matrix $\vec{M}$. To find $\vec{\Sigma}$ we must invert the two by two matrix that is $\vec{I} - \vec{M}\vec{L}^{-1}$ restricted to that basis. The poles of $\vec{\Sigma}$ and hence of (3.24) will be those of this inverted matrix. The poles of the inverse of a non-singular finite matrix are just the zeros of the determinant of that matrix, so our task is to find the zeros of $\det(\vec{I} - \vec{M}\vec{L}^{-1})$. A few steps lead to the following result for that determinant

$$\begin{aligned}\det(\vec{I} - \vec{M}\vec{L}^{-1}) \\ &= 1 - 2\langle A|\vec{L}^{-1}|C\rangle \pm \langle A|\vec{L}^{-1}|A\rangle\langle l|\vec{T}_0|j\rangle \\ &\quad + \langle C|\vec{L}^{-1}|A\rangle\langle A|\vec{L}^{-1}|C\rangle - \langle A|\vec{L}^{-1}|A\rangle\langle C|\vec{L}^{-1}|C\rangle\end{aligned} \tag{3.29}$$

where the vector $\langle C$ is given by

$$\begin{aligned}\langle C| &= \langle B| - \frac{\langle A|B\rangle}{\langle A|A\rangle}\langle A| \\ &= \langle B| - \tfrac{1}{2}(\langle l|\vec{T}_0|l\rangle \mp \langle j|\vec{T}_0|l\rangle)\langle A|.\end{aligned} \tag{3.30}$$

The condition that the right-hand side of (3.29) is zero yields an exact relation satisfied by the eigenvalues of $\vec{T}_{1\pm}$. To construct that relationship we note that

$$\vec{L}^{-1} = \sum_k \frac{|\phi_k\rangle\langle\phi_k|}{\lambda_k - \lambda} \tag{3.31}$$

where $|\phi_k\rangle$ is the kth eigenvecctor of $\vec{T}_0$, with associated eigenvalue λ_k. Each eigenvalue of $\vec{T}_{1\pm}$ will be close to one of the λ_k. We thus express an eigenvalue of $\vec{T}_{1\pm}$ as

$$\lambda_i + \Delta\lambda_i \tag{3.32}$$

where λ_i is the closest unperturbed eigenvalue. Using (3.31), (3.32) and keeping careful track of the relative magnitude of various contributions to the equation satisfied by $\Delta\lambda$ we obtain, after a series of algebraic manipulations,

$$1 \mp \frac{2\langle\phi_i|l\rangle\langle\phi_i|j\rangle\lambda_i}{\Delta\lambda_i} + \frac{1}{\Delta\lambda_i}\sum_{k\neq i}\frac{\lambda_i\lambda_k}{\lambda_k-\lambda_i}(\langle\phi_i|l\rangle\langle\phi_k|j\rangle - \langle\phi_i|j\rangle\langle\phi_k|l\rangle)^2$$

$$\pm 2\sum_{k\neq i}\frac{\lambda_k}{\lambda_k-\lambda_i}\langle\phi_k|l\rangle\langle\phi_k|j\rangle = 0. \tag{3.33}$$

Contributions to the relationship that are asymptotically less important than those retained in (3.33) in the limit of large N have been dropped. The solution of (3.33) to the desired order in N is

$$\Delta\lambda_i = \lambda_i(\pm 2\langle\phi_i|l\rangle\langle\phi_i|j\rangle) - \sum_{k\neq i}\frac{\lambda_k\lambda_i}{\lambda_k-\lambda_i}(\langle\phi_i|l\rangle\langle\phi_k|j\rangle + \langle\phi_i|j\rangle\langle\phi_k|l\rangle)^2. \tag{3.34}$$

This solution gives us information about the full distribution of principal radii of gyration to order $1/d$. In the body of this paper we restrict ourselves to a calculation of the average of $\Delta\lambda_i$ over all of the walks we have considered, and verifying that (3.34) is consistent with the exact results presented in § 2 to the required order in $1/d$. This latter comparison is carried out in appendix 1. In appendix 2, we develop a conjectured form for the distribution of the eigenvalues to order $1/d$.

To find the average $\Delta\lambda_i$ we note that the relative weight of each of the walks we have been considering is $1/2d$. Taking all topologically distinct walks into account involves a sum over all l, all $j<l$ and '+' and '−'. We thus have

$$\begin{aligned}
\langle\Delta\lambda_i\rangle &= \frac{\lambda_i}{2d}\left(\sum_{j<l}\sum_{\pm}(\pm 2\langle\phi_i|l\rangle\langle\phi_i|j\rangle) - \sum_{k\neq i}\frac{\lambda_k}{\lambda_k-\lambda_i}(\langle\phi_i|l\rangle\langle\phi_k|j\rangle + \langle\phi_i|j\rangle\langle\phi_k|l\rangle)^2\right)\\
&= \frac{1}{d}\sum_{\substack{j,l\\ j<l}}\sum_{k\neq i}\frac{\lambda_k\lambda_i}{\lambda_i-\lambda_k}(\langle\phi_i|l\rangle\langle\phi_k|j\rangle + \langle\phi_i|j\rangle\langle\phi_k|l\rangle)^2\\
&= \frac{1}{d}\sum_{k\neq i}\frac{\lambda_k\lambda_i}{\lambda_i-\lambda_k}\sum_{j<l}(\langle\phi_i|l\rangle^2\langle\phi_k|j\rangle^2 + \langle\phi_i|j\rangle^2\langle\phi_k|l\rangle^2\\
&\quad + 2\langle\phi_i|l\rangle\langle\phi_i|j\rangle\langle\phi_k|l\rangle\langle\phi_k|j\rangle)\\
&= \frac{1}{d}\sum_{k\neq i}\frac{\lambda_k\lambda_i}{\lambda_i-\lambda_k}\sum_{j\neq l}(\langle\phi_i|l\rangle^2\langle\phi_k|j\rangle^2 + \langle\phi_i|l\rangle\langle l|\phi_k\rangle\langle\phi_i|j\rangle\langle j|\phi_k\rangle)\\
&= \frac{1}{d}\sum_{k\neq i}\frac{\lambda_k\lambda_i}{\lambda_i-\lambda_k}[\langle\phi_i|\phi_i\rangle\langle\phi_k|\phi_k\rangle + (\langle\phi_i|\phi_k\rangle)^2 - 2\langle\phi_i|l\rangle^2\langle\phi_k|l\rangle^2].
\end{aligned} \tag{3.35}$$

The last term in the square brackets of (3.35) is negligible compared to the first two. Using $\langle\phi_i|\phi_i\rangle = 1$ for all i and $\langle\phi_i|\phi_k\rangle = 0$ if $i\neq k$, we are left with

$$\langle\Delta\lambda_i\rangle = \frac{\lambda_i}{d}\sum_{k\neq i}\frac{\lambda_k}{\lambda_i-\lambda_k}. \tag{3.36}$$

Thus, to order $1/d$ we have for the ith eigenvalue

$$\langle\lambda_i\rangle = \lambda_i\left(1 + \frac{1}{d}\sum_{k\neq i}\frac{\lambda_k}{\lambda_i-\lambda_k}\right). \tag{3.37}$$

Using (3.13) we have

$$\sum_{k\neq i}\frac{\lambda_k}{\lambda_i-\lambda_k}=\sum_{k\neq i}\frac{N/k^2}{N/i^2-N/k^2}=\sum_{k\neq i}\frac{i^2}{k^2-i^2}. \tag{3.38}$$

The sum on the left-hand side can be carried out exactly using contour integration methods. We find

$$\sum_{k\neq i}\frac{i^2}{k^2-i^2}=\frac{3}{4} \tag{3.39}$$

independent of i.

Thus

$$\langle\lambda_i\rangle=\lambda_i\left(1+\frac{3}{4d}\right)=\frac{N}{\pi^2 i^2}\left(1+\frac{3}{4d}\right). \tag{3.40}$$

An immediate consequence of this remarkable result is that the ratios of the three largest principal radii of gyration are independent of dimensionality to first order in $1/d$. High-dimensional walks have roughly the same shapes.

4. Summary

In this paper we have studied the shapes of random walks in high spatial dimensions. We were able to explicitly calculate the first two terms in a $1/d$ expansion for the square of the principal radii of gyration by considering appropriate subclasses of random walks. We show that the ratio of the squares of the principal radii of gyration lies close to numerical results in three dimensions and correspond to walks whose shape cannot be classified as either spherical or linear. Moreover, we found the remarkable result that the ratios of the average principal radii of gyration are independent of dimensionality to order $1/d$, indicating that the shapes of high-dimensional walks are insensitive to spatial dimensionality. These results hold for both self-avoiding and unrestricted random walks. Our findings are fully consistent with our earlier calculation of the asphericity of random walks and provides a deeper understanding of the high-dimensional limit for the asphericity parameter.

The analysis presented here provides an interesting and useful theoretical approach to characterising and quantifying the notion of a shape of a random walk. We expect our work to be fruitfully applied to measure the shapes of closed or polygon random walks, percolating clusters and other fractal clusters as well, which will lead to important and novel insights relating the anisotropy of random fractal objects to some of their interesting and technologically important physical behaviour.

Appendix 1

In this appendix we demonstrate that the principal radii of gyration calculated as described in the main text leads to the correct expansion of the asphericity parameter to order $1/d$. Recall that we had

$$A_d=\frac{d\,\Sigma_{i=1}^{d}\langle\lambda_i^2\rangle-\langle(\Sigma_{i=1}^{d}\lambda_i)^2\rangle}{(d-1)\langle(\Sigma_{i=1}^{d}\lambda_i)^2\rangle} \tag{A1.1}$$

which can be written as

$$A_d = \frac{\Sigma_{i=1}^d \langle \lambda_i^2 \rangle + (1/d)(\Sigma_{i=1}^d \langle \lambda_i^2 \rangle - \langle (\Sigma_{i=1}^d \lambda_i)^2 \rangle) + \ldots}{\langle (\Sigma_{i=1}^d \lambda_i)^2 \rangle}. \tag{A1.2}$$

Since terms of order $1/d$ are needed, the λ_i in the second term in the numerator can be replaced by their leading order expansion, $\lambda_i^0 = N/\pi^2 i^2$ and $\Sigma_i \langle \lambda_i^2 \rangle$ and $\langle (\Sigma \lambda_i)^2 \rangle$ need only be calculated to order $1/d$.

We take up the calculation of $\Sigma_i \langle \lambda_i^2 \rangle$ first. According to our previous result (see equation (3.34))

$$\begin{aligned} \langle \lambda_i^2 \rangle &= (\lambda_i^0)^2 + \frac{1}{2d} \sum_{j<l} \sum_{\pm} (2\lambda_i^0 \Delta\lambda_i + \Delta\lambda_i^2) \\ &= (\lambda_i^0)^2 + \frac{1}{d}\left(-\sum_{j<l} \sum_{k \neq i} \frac{2(\lambda_i^0)^2 \lambda_k^0}{(\lambda_k^0 - \lambda_i^0)} (\langle \phi_i | l \rangle \langle \phi_k | j \rangle + \langle \phi_i | j \rangle \langle \phi_k | l \rangle)^2 \right. \\ &\quad \left. + \frac{1}{d} \sum_{j<l} 4 \langle \phi_i | l \rangle^2 \langle \phi_i | j \rangle^2 (\lambda_i^0)^2 \right). \end{aligned} \tag{A1.3}$$

After some straightforward manipulations, the last two terms sum up to

$$\frac{1}{d} \sum_{j<l} \sum_{k=1}^{d} \lambda_i^0 \lambda_k^0 (\langle \phi_i | l \rangle \langle \phi_k | j \rangle + \langle \phi_i | j \rangle \langle \phi_k | l \rangle)^2 \tag{A1.4}$$

which allows us to write

$$\sum_{i=1}^{d} \langle \lambda_i^2 \rangle = \sum_{i=1}^{d} (\lambda_i^0)^2 + \frac{1}{d} \sum_{j<l} \sum_{k,i} \lambda_i^0 \lambda_k^0 (\langle \phi_i | l \rangle \langle \phi_k | j \rangle + \langle \phi_i | j \rangle \langle \phi_k | l \rangle)^2. \tag{A1.5}$$

The last term in (A1.5) can be further simplified by using the eigenvalue equation satisfied by the vector $|\phi_i\rangle$ and $|\phi_k\rangle$ leading to the following expression:

$$\sum_{i=1}^{d} \langle \lambda_i^2 \rangle = \sum_{i=1}^{d} (\lambda_i^0)^2 + \frac{1}{d} \sum_{j \neq l} (\langle l | T_0 | l \rangle \langle j | T_0 | j \rangle + \langle l | T_0 | j \rangle \langle j | T_0 | l \rangle). \tag{A1.6}$$

In the asymptotic limit of large N, the $j = l$ term contributes negligibly, so (A1.7) is equivalent to

$$\sum_{i=1}^{d} \langle \lambda_i^2 \rangle = \sum_{i=1}^{d} (\lambda_i^0)^2 + \frac{1}{d}\left[\left(\sum_{i=1}^{d} \lambda_i^0 \right)^2 + \sum_{i=1}^{d} (\lambda_i^0)^2 \right] \tag{A1.7}$$

which, when combined with (A1.3), yields

$$A_d = \frac{\Sigma_{i=1}^d (\lambda_i^0)^2 (1 + 2/d)}{\langle (\Sigma_i \lambda_i)^2 \rangle}. \tag{A1.8}$$

All that remains is to calculate the average of the trace squared to $1/d$. This is easily done by noting that the only terms which survive the averaging in the asymptotic limit are

$$\left\langle \left(\sum_i \lambda_i \right)^2 \right\rangle = \left(\sum \lambda_i^0 \right)^2 + \frac{1}{d} \sum_{j<l} \sum_i 4 \langle \phi_i | l \rangle^2 \langle \phi_i | j \rangle^2 (\lambda_i^0)^2. \tag{A1.9}$$

Again, neglecting the $j = l$ terms and using the fact that the vectors $|\phi_i\rangle$ are normalised,

$$\left\langle \left(\sum \lambda_i \right)^2 \right\rangle = \left(\sum_{i=1}^{d} \lambda_i^0 \right)^2 + \frac{2}{d} \sum_i (\lambda_i^0)^2. \tag{A1.10}$$

Thus our final result is

$$A_d = \frac{\Sigma_i (\lambda_i^0)^2}{(\Sigma_i \lambda_i^0)^2}\left(1+\frac{2}{d}-\frac{2}{d}\frac{\Sigma_i (\lambda_i^0)^2}{(\Sigma \lambda_i^0)^2}\right)+O\left(\frac{1}{d^2}\right) \tag{A1.11}$$

$$= \frac{2}{5}+\frac{12}{25}\frac{1}{d}+O\left(\frac{1}{d^2}\right) \tag{A1.12}$$

which are the correct leading and next-to-leading-order terms in the expansion for A_d in powers of $1/d$.

Appendix 2

In this appendix, we develop an expression for the distribution of the principal radii of gyration for high-dimensional random walks. The expression reflects contributions from the leading and next-to-leading-order walks and is thus accurate to the first two orders in $1/d$. The analysis leading to the final result is strongly motivated, and we believe correct, but no attempt has been made to present a mathematically rigorous derivation.

The n largest individual radii of gyration are the n largest eigenvalue of the tensor, $\vec{T}$, defined in (2.1). Let these eigenvalues be $\lambda_1, \lambda_2 \ldots, \lambda_n$ such that

$$\langle f(\lambda_1, \lambda_2 \ldots \lambda_n)\rangle = \int \ldots \int P(\lambda_1, \lambda_2 \ldots \lambda_n) f(\lambda_1, \lambda_2 \ldots \lambda_n) \mathrm{d}\lambda_1 \, \mathrm{d}\lambda_2 \ldots \mathrm{d}\lambda_n \tag{A2.1}$$

where $\langle f\rangle$ is the average of f over all N step walks. The Fourier transform of this distribution function, $p(K_1, K_2 \ldots K_n)$, is defined by

$$p(K_1, K_2, \ldots, K_n) = \int \ldots \int \exp[\mathrm{i}(K_1\lambda_1 + K_2\lambda_2 + \ldots + K_n\lambda_n)] P(\lambda_1, \lambda_2 \ldots \lambda_n) \, \mathrm{d}\lambda_1 \, \mathrm{d}\lambda_2 \ldots \mathrm{d}\lambda_n. \tag{A2.2}$$

By the normalisation of $P(\lambda_1 \ldots \lambda_n)$, it follows that

$$p(0, 0, \ldots, 0) = 1. \tag{A2.3}$$

To order $1/d$, the walks contributing to the average in (A2.1) are (i) the leading order walks described in § 3 and (ii) the next-to-leading-order walks, also described in that section. The number of walks of the first type is

$$\eta_0 \approx (2d)^N \exp(-N^2/2d) \approx (2d)^N (1 - \tfrac{1}{2}N^2/d). \tag{A2.4}$$

By direct counting, one verifies that the number of walks of the second type is

$$\eta_1 = (2d)^N \frac{1}{d} \sum_{l=2}^{N} \sum_{j<l} \approx (2d)^N \frac{N^2}{2d}. \tag{A2.5}$$

So, to order $1/d$

$$\eta_0 + \eta_1 = (2d)^N. \tag{A2.6}$$

The λ in the first kind of walk are equal to

$$\lambda_m = \frac{N}{\pi^2 m^2} \tag{A2.7}$$

and while for walks of the second kind,

$$\lambda_m^1 = \lambda_m\left(1 \pm \langle\phi_m|l\rangle\langle\phi_m|j\rangle - \sum_{k\neq m}\frac{\lambda_k}{\lambda_k-\lambda_m}(\langle\phi_m|l\rangle\langle\phi_k|j\rangle + \langle\phi_m|j\rangle\langle\phi_k|l\rangle)^2\right) \tag{A2.8}$$

where (A2.7) is equivalent to (3.13) and (A2.8) follows from (3.34). The quantities in the above two expressions are all defined in § 3.

For convenience of notation, we define

$$\alpha_{j,l}^m = \langle\phi_m|l\rangle\langle\phi_m|j\rangle\lambda_m \tag{A2.9}$$

and

$$\beta_{j,l}^m = \sum_{k\neq m}\frac{\lambda_k\lambda_m}{\lambda_k-\lambda_m}(\langle\phi_m|l\rangle\langle\phi_k|j\rangle + \langle\phi_m|j\rangle\langle\phi_k|l\rangle)^2. \tag{A2.10}$$

Then $p(K_1, K_2 \ldots K_n)$ becomes

$$\begin{aligned} p(K_1, K_2 \ldots K_n) &= \exp[\mathrm{i}(\lambda_1 K_1 + \lambda_2 K_2 \ldots + \lambda_n K_n)] \\ &\quad \times\left[1 - \frac{N^2}{2d} + \frac{1}{2d}\left(\sum_{j<l}\sum_{l}\prod_{m=1}^{n}\exp(\mathrm{i}K_m\alpha_{j,l}^m - \mathrm{i}K_m\beta_{j,l}^m)\right.\right. \\ &\quad \left.\left. + \sum_{j<l}\sum_{l}\prod_{m=1}^{n}\exp(-\mathrm{i}K_m\alpha_{j,l}^m - \mathrm{i}K_m\beta_{j,l}^m)\right)\right]. \end{aligned} \tag{A2.11}$$

On expanding the exponentials with respect to K_m and keeping only a few low order terms, a step that is justified *a posteriori*, the right-hand side of (A2.11) can be written

$$\begin{aligned} &\exp[\mathrm{i}(\lambda_1 K_1 + \ldots \lambda_n K_n)]\left[1 - \frac{N^2}{2d} + \frac{1}{2d}\sum_{l}\sum_{j<l}\left(2 - \sum_{m=1}^{n}(K_m\alpha_{j,l}^m)^2 - 2\mathrm{i}\sum_{m=1}^{n}K_m\beta_{j,l}^m\right.\right. \\ &\quad \left.\left. - 2\sum_{m_1\neq m_2}K_{m_1}K_{m_2}\alpha_{j,l}^{m_1}\alpha_{j,l}^{m_2} + \ldots\right)\right]. \end{aligned} \tag{A2.12}$$

The orthogonality of the eigenfunctions ϕ_k yields the following results:

$$\sum_{l=2}^{N}\sum_{j<l}(\alpha_{j,l}^m)^2 = 2\lambda_m^2 \tag{A2.13}$$

$$\sum_{l=2}^{N}\sum_{j<l}\alpha_{j,l}^{m_1}\alpha_{j,l}^{m_2} = 0 \qquad (m_1 \neq m_2) \tag{A2.14}$$

$$\sum_{l=2}^{N}\sum_{j<l}\beta_{j,l}^m = \sum_{k\neq m}\frac{\lambda_k\lambda_m}{\lambda_k-\lambda_m}. \tag{A2.15}$$

Thus

$$\begin{aligned} p(K_1, K_2, \ldots, K_n) &= \exp[\mathrm{i}(\lambda_i K_1 + \ldots \lambda_n K_n)] \\ &\quad \times\left(1 - \frac{1}{d}\sum_{m=0}^{n}\lambda_m^2 K_m^2 - \frac{\mathrm{i}}{d}\sum_{m=1}^{n}\sum_{k\neq m}\frac{\lambda_l\lambda_m}{\lambda_l-\lambda_m}K_m\right). \end{aligned} \tag{A2.16}$$

We now take the crucial step of exponentiating the term in curly brackets. Although we present no rigorous justification for this step other than noting that the exponential gives terms correct to $O(1/d^2)$ which is all that is required, we believe it leads to a correct result. Thus, (A2.16) is rewritten as

$$p(K_1, K_2, \ldots, K_n) = \exp\left(\mathrm{i}(\lambda_1+\langle\Delta\lambda_1\rangle)K_1+\mathrm{i}(\lambda_2+\langle\Delta\lambda_2\rangle)K_2+\ldots\mathrm{i}(\lambda_n+\langle\Delta\lambda_n\rangle)K_n-\frac{1}{d}\sum_m^n(\lambda_m K_m)^2\right) \tag{A2.17}$$

which leads to the following Gaussian form for $P(\lambda_1, \lambda_2 \ldots \lambda_n)$:

$$P(\lambda_1, \lambda_2 \ldots \lambda_n) = \prod_{i=1}^n P^i \tag{A2.18}$$

where

$$P^i = \left(\frac{d}{4\pi(\lambda_i^0)^2}\right)^{1/2} \exp\left(-\frac{(\lambda_i-\lambda_i^0-\langle\Delta\lambda_i\rangle)^2}{4(\lambda_i^0)^2/d}\right) \tag{A2.19}$$

and $\lambda_i^0 = N/\pi^2 i^2$.

Note that the width of the distribution for the individual radii of gyration is of order N and that the width goes to zero as $d \to \infty$. Thus, for high-dimensional walks, the probability distribution function for the individual principal radii of gyration is a strongly peaked function.

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