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LETTER TO THE EDITOR

The asphericity of random walks

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Abstract. The asphericity, $\langle A\rangle$, of a random walk is defined and calculated for non-self-avoiding walks. The definition of $\langle A\rangle$ generalises to self-avoiding walks, percolating clusters and other fractal objects and thus provides a generalised quantitative measure of the departure from spherical symmetry of the gross shape of these objects.

That the gross shape of linear polymers and random walks is not spherical has been known from some time (Kuhn 1934, Solc 1971). Numerical studies (Bishop and Michels 1985) have established that the radii of gyration of these objects are not equal, but possess ratios that approach limiting values significantly different from unity in the large system limit. What has been lacking up until now are analytical results for the anisotropy of these physically interesting fractal objects in various spatial dimensions. In this letter, we define and describe a quantity that measures the asphericity of a random walk and implement the calculation of this quantity for an unrestricted random walk, or equivalently, a self-intersecting chain polymer. This asphericity parameter can, in principle, be calculated for self-avoiding walks as well and provides a natural description of deviations from spherically symmetric shapes applicable to a wide variety of fractal objects.

We begin by defining the moment of inertia tensor for one configuration of a random walk (Bishop and Michels 1985). Imagining that a unit mass is located at every one of the N steps of the walk, we can construct a tensor $\overleftrightarrow{T}$, with components

$$\begin{aligned} T_{ij} &= \frac{1}{N}\sum_{l=1}^{N}(\bar{X}_{il}-\bar{X}_i)(X_{jl}-\bar{X}_j) \\ &= \frac{1}{N^2}\sum_{l>R}^{N}(X_{il}-X_{ik})(X_{jl}-X_{jk}) \end{aligned} \tag{1}$$

where X_{il} is the ith cartesian component of the position vector of the lth mass and $\bar{X}_i$ is the average over the walk of that component.

For three-dimensional walks, the matrix $\overleftrightarrow{T}$ has three eigenvalues, R_1^2 R_2^2 and R_3^2, the three principal radii of gyration squared of the walk. The matrix also has three invariants, Tr, M and D, where Tr and D are the trace and determinant, respectively, and M is the sum of its three minors. We have

$$\mathrm{M} = T_{11}T_{22}+T_{11}T_{33}+T_{22}T_{33}-T_{12}T_{21}-T_{13}T_{31}-T_{23}T_{32}. \tag{2}$$

A brief consideration of the characteristic equation of $\vec{T}$ reveals that

$$\begin{aligned}
\mathrm{Tr} &= R_1^2 + R_2^2 + R_3^2 \\
\mathrm{D} &= R_1^2 R_2^2 R_3^2 \\
\mathrm{M} &= R_1^2 R_2^2 + R_1^2 R_3^2 + R_2^2 R_3^2.
\end{aligned} \tag{3}$$

Thus, we can now define another invariant quantity which measures the walk's deviation from spherical symmetry

$$\mathrm{Tr}^2 - 3\mathrm{M} = \tfrac{1}{2}[(R_1^2 - R_2^2)^2 + (R_1^2 - R_3^2)^2 + (R_2^2 - R_3^2)^2]. \tag{4}$$

It is important to realise that the invariants of the inertia tensor are independent of the direction of a particular walk and consequently any characteristic anisotropy will persist in the averaging process.

We now define the 'asphericity' $\langle A\rangle$ by averaging (4) over all random walks:

$$\langle A\rangle = \frac{\langle(\mathrm{Tr}^2 - 3\mathrm{M})\rangle}{\langle \mathrm{Tr}^2\rangle}. \tag{5}$$

The normalisation has been chosen so that $\langle A\rangle$ ranges from zero for spherically symmetric objects to 1 for extremely elongated or 'cigar' shaped objects.

Thus, the parameter $\langle A\rangle$ is a useful measure of the instantaneous anisotropy or deviation from sphericity of the walk. Moreover, it can be calculated straightforwardly since it involves taking averages over products of the matrix elements of $\vec{T}$. This will not be the case if the radii of gyration are chosen to describe the anisotropy of the walk. These quantities are extremely cumbersome to average because of their complicated dependence on the invariants. Indeed, for spatial dimension greater than four, the roots themselves must be determined numerically. In contrast, however, $\langle A\rangle$ can be calculated quite easily, and for unrestricted walks, it has an exact expression which we now derive.

For unrestricted walks, the linear topology of the walk allows us to express the average over all configurations of an N step walk of any quantity $f(\boldsymbol{X}_{i_1}, \boldsymbol{X}_{i_2}, \ldots \boldsymbol{X}_{i_k})$ as follows:

$$N_{\mathrm{T}}\langle f\rangle = P \sum_{\substack{\boldsymbol{X}_{i_1}\ldots\boldsymbol{X}_{i_1} \\ \boldsymbol{X},\boldsymbol{X}'}} \sum_{\substack{n_1\ldots n_{k+1} \\ n_1+\ldots+n_{k+1}=N}} \Gamma_{n_1}(\boldsymbol{X}, \boldsymbol{X}_{i_1}) \ldots \Gamma_{n_{k+1}}(\boldsymbol{X}_{i_k}, \boldsymbol{X}') f(\boldsymbol{X}_{i_1} \ldots \boldsymbol{X}_{i_k}) \tag{6}$$

where P stands for all permutations of the $\boldsymbol{X}_i$, $\Gamma_{n_{i+1}}(\boldsymbol{X}_i, \boldsymbol{X}_{i+1})$ is the number of n_{i+1} step walks between $\boldsymbol{X}_i$ and $\boldsymbol{X}_{i+1}$ and N_{T} is the total number of N step walks. The average is much more easily computed using the generating function for a grand canonical ensemble of walks (Feller 1950, Fisher 1984, de Gennes 1979). It is easy to show that the right-hand side of (6) is simply the coefficient of Z^N of

$$P \sum_{\substack{\boldsymbol{X}_{i}\ldots\boldsymbol{X}_{i} \\ \boldsymbol{X},\boldsymbol{X}'}} C(\boldsymbol{X}, \boldsymbol{X}_{i_1}) \ldots C(\boldsymbol{X}_{i_k}, \boldsymbol{X}') f(\boldsymbol{X}_{i_1} \ldots \boldsymbol{X}_{i_k}) \tag{7}$$

where $C(\boldsymbol{X}_i, \boldsymbol{X}_j)$ is the generator of random walks

$$C(\boldsymbol{X}_i, \boldsymbol{X}_j) = \sum_{n=0}^{\infty} \Gamma_n(\boldsymbol{X}_i, \boldsymbol{X}_j) Z^n. \tag{8}$$

In the continuum limit (Feller 1950, Fisher 1984)

$$C(\boldsymbol{X}_i, \boldsymbol{X}_j) = \frac{1}{(2\pi)^3} \int \mathrm{d}\boldsymbol{k} \frac{\exp[i\boldsymbol{k}\cdot(\boldsymbol{X}_i - \boldsymbol{X}_j)]}{(1-qz)+(k^2/q)} \tag{9}$$

where the integral is over a Brillouin zone and q is the coordination number of the lattice on which the walk is taken. Using (7) and (9), we find the averages necessary to obtain $\langle A\rangle$ easy to evaluate and for a three-dimensional unrestricted walk, $\langle A\rangle = \frac{10}{19}$.

This quantity, as noted earlier, can be calculated for self-avoiding walks or other fractal objects. The calculation will be significantly more difficult and numerical procedures or techniques as the ε expansion will, no doubt, be required. Our exact result, however, will be a useful guide for such future numerical studies.

The application of interdimensional expansion will involve the generalisation of the quantity $\langle A\rangle$ to d dimensions. This generalisation is straightforward. The invariants of interest are the trace of $\tilde{T}$ and the generalisation of M. Denoting the d eigenvalues of T by $\lambda_1 \ldots \lambda_d$, if we define

$$\mathrm{M}_d = \frac{1}{2} \sum_{\substack{i,j=1 \\ i\neq j}}^{d} \lambda_i \lambda_j \tag{10}$$

and

$$\langle A_d\rangle = \frac{\langle[\frac{1}{2}(d-1)\,\mathrm{Tr}^2 - d\mathrm{M}_d]\rangle}{\frac{1}{2}(d-1)\langle\mathrm{Tr}^2\rangle} \tag{11}$$

then

$$\langle A_d\rangle = \frac{\Sigma_{i>j}\langle(\lambda_i-\lambda_j)^2\rangle}{(d-1)\langle(\Sigma_i \lambda_j)^2\rangle} \tag{12}$$

measures the asphericity of the d-dimensional fractal object. Again, as in the three-dimensional case, $0 \leqslant \langle A_d\rangle \leqslant 1$. For unrestricted walks, we find $\langle A_d\rangle = 2(d+2)/(5d+4)$ which has a limit of $\frac{2}{5}$ as $d \to \infty$. We note that these results for $\langle A_d\rangle$ have relevance to the self-avoiding walk problem for $d>4$ where the distinction between restricted and unrestricted walks becomes irrelevant. We also conjecture that the results for the unrestricted walk have application to the shapes of percolating clusters for $d>6$, the case when the cluster distribution can be approximated by Gaussian statistics.

Although there is some arbitrariness in defining the 'shapes' of these random objects, we propose that the asphericity parameter discussed here for random walks is an excellent measure of an object's departure from sphericity. It can be used to investigate the shapes of percolating clusters or other fractals as well.

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