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LETTER TO THE EDITOR

Worm-like polymer loops and Fourier knots

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Abstract
Every smooth closed curve can be represented by a suitable Fourier sum as a function of an arbitrary parameter τ. We show that the ensemble of curves generated by randomly chosen Fourier coefficients with amplitudes inversely proportional to spatial frequency (with a smooth exponential cutoff) can be accurately mapped on the physical ensemble of inextensible worm-like polymer loops. The $\tau \to s$ mapping of the curve parameter τ on the arc length s of the inextensible polymer is achieved at the expense of coupling all Fourier harmonics in a non-trivial fashion. We characterize the obtained ensemble of conformations by looking at tangent–tangent and position–position correlations. Measures of correlation on the scale of the entire loop yield a larger persistence length than that calculated from the tangent–tangent correlation function at small length scales. The topological properties of the ensemble, randomly generated worm-like loops, are shown to be similar to those of other polymer models.

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(Some figures in this article are in colour only in the electronic version)

Classical polymer theories, from Debye to Flory to De Gennes [1] , use the analogy between conformation of a chain molecule and a Brownian random walk (BRW). In mathematically idealized form, such a random walk is thought of as a Wiener trajectory $\mathbf{r}(\tau)$ generated by the measure $P\{\mathbf{r}(\tau)\} \propto \exp\left[-\text{const}\int(\partial\mathbf{r}/\partial\tau)^2\,\mathrm{d}\tau\right]$, where τ is a parameter running along the trajectory. Despite its successes, the BRW model cannot reproduce the finite extensibility of polymer chains stretched by a strong force [2] and fails miserably in the study of polymers with knots. Indeed, simulations of discrete polymer models, or random polygons with N steps, show [3–5] that the probability of trivial knot configuration decays exponentially with N as $P_0(N) \sim \exp(-N/N^*)$, where N^* defines the crossover from an unknotted to a knotted regime. It was argued that Wiener trajectory polymer models cannot be used to calculate this probability [6], since they correspond to the limit $N \to \infty, l \to 0$ (l is a step length); $Nl^2 = \text{const}$, in which the probability of a trivial knot vanishes. Note that the contour length of Wiener trajectory diverges, $Nl \to \infty$, so it is not surprising that these models do not exhibit finite extensibility. A better continuum model of polymers which can handle the constraints imposed both by finite extensibility and by the presence of knots, and can describe the elastic response of such objects, is that of a worm-like chain. However, while the statistical physics of linear worm-like polymers is well understood, little is known about the conformations and the topology of worm-like loops (WLL). Our goal in this letter is to work out a method allowing computational generation of an ensemble of smoothly curved conformations of such polymers and to carry out the statistical analysis of their geometric and topological properties.

The conformations of worm-like polymers are generated by the measure $P\{\mathbf{r}(s)\} \propto \exp\left[-\text{const} \int (\partial^2\mathbf{r}/\partial s^2)^2 \, \mathrm{d}s\right]$ (i.e., are Boltzmann weighted by the bending energy proportional to the squared curvature), subject to the constraint of non-extensibility, $|\partial\mathbf{r}/\partial s| = 1$. In more general models [7], the three generalized curvatures describing the object could be treated as independent Gaussian variables. However, this is true only for open filaments and attempts to generalize these methods to the case of closed loops failed because the loop closure conditions introduce a non-local coupling between the curvatures that makes the problem practically intractable (except for the case of small fluctuations of a ring [8]). One way to generate the conformations of a closed loop is to expand each component $r^i(\tau)$ in a Fourier series,

$$r^i(\tau) = \sum_{n=1} \left[A_n^i \cos\left(\frac{2\pi n \tau}{T}\right) + B_n^i \sin\left(\frac{2\pi n \tau}{T}\right)\right]. \tag{1}$$

Here, τ is a parameter along the curve $\mathbf{r}(\tau)$ ($0 \leqslant \tau \leqslant T$) and the summation goes up to some cutoff frequency $n_{\max}$ (if the series converges sufficiently rapidly, the cutoff can be replaced by infinity). Any conformation of a sufficiently smooth closed loop can be fully described by the set of Fourier coefficients $\left\{A_n^i, B_n^i\right\}$, giving rise to the concept of Fourier knots introduced in [9, 10].

Using the above prescription one can generate an ensemble of loops of different shapes by taking the Fourier coefficients from some random distribution. However, even though all the loops have the same period T, their contour lengths $L_T = \int_0^T \mathrm{d}\tau' |\mathrm{d}\mathbf{r}/\mathrm{d}\tau'|$ are different for each realization of the Fourier coefficients. Even more importantly, since, in general, $|\partial\mathbf{r}/\partial\tau| \neq 1$, loops generated by (1) do not obey the inextensibility condition and cannot be used to model worm-like polymers. In order to generate an ensemble of different conformations of an inextensible loop, one has to transform to a representation in which trajectories are parametrized by the inextensible arclength s,

$$s(\tau) = \int_0^\tau \mathrm{d}\tau' |\mathrm{d}\mathbf{r}/\mathrm{d}\tau'|, \qquad |\partial\mathbf{r}/\partial s| = 1. \tag{2}$$

The non-trivial character of this transformation follows from the fact that in this representation, the contour parameter becomes a stochastic functional of the random process $\mathbf{r}(\tau)$ it parametrizes! Since one is interested in the ensemble of polymers a of well-defined contour length, one then brings all the generated conformations to the same contour length by a suitable affine transformation of all lengths and coordinates (this transformation does not affect the topology since the latter is independent of the parametrization). Thus, we can replace $L_T = s(T)$ by any standard length L, provided that we rescale all lengths using the affine transformation, $\mathbf{r} \to \mathbf{r}L/L_T$. Therefore, in three steps (generation of random coefficients and Fourier summation (1), reparametrization (2), and affine transformation $s \to sL/L_T$), of which the latter two couple all Fourier harmonics together in a complex way, we obtain a statistical ensemble of smoothly bent conformations of an inextensible loop of length L.

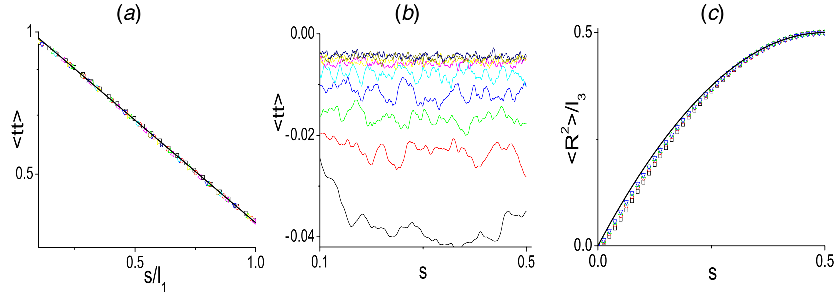

Figure 1. (*a*) Universal semi-log plot of the short length scale behaviour of the tangent–tangent correlation function versus the scaled distance, s/l_1; the best fit $\exp(-(s/l_1 - 0.07))$ is given by the solid line. (*b*) Large-scale behaviour of the correlation function, for different values of n_0 (the height of the curves increases with n_0). (*c*) Scaled (by l_3) mean-squared distance between points on the loop. The BRW expression is plotted by the solid line. Different values of n_0 are represented by black ($n_0 = 30$), red ($n_0 = 50$), green ($n_0 = 70$), blue ($n_0 = 100$), cyan ($n_0 = 150$), magenta ($n_0 = 200$), yellow ($n_0 = 220$), dark yellow ($n_0 = 250$) and navy ($n_0 = 270$).

Let us now check if this ensemble is representative of physical conformations of a worm-like loop which possesses some characteristic bending and (possibly) twist rigidities.

On length scales much larger than some microscopic cutoff, the conformations of a worm-like polymer are well represented by those of a BRW. For the latter, the amplitudes of the Fourier components can be readily shown to be of the form $\{A_n^i, B_n^i\}_{\mathrm{BRW}} = \lambda/n$ for $n \leqslant n_{\max}$ and zero otherwise, where λ is a random number (say, uniformly distributed between -1 and 1; the choice of another symmetric interval is equivalent to rescaling the contour length, see below). As will be demonstrated in the following, short scale behaviour characteristic of WLL can be obtained by replacing the abrupt cutoff $n_{\max}$ by Fourier coefficients that decrease smoothly with a characteristic decay frequency n_0,

$$\{A_n^i, B_n^i\}_{WLL} = \lambda\, \mathrm{e}^{-n/n_0}/n, \tag{3}$$

(note that the WLL and the BRW expressions for the coefficients coincide for $n \ll n_0$).

We expect that on small scales, the conformations of linear worm-like polymers and WLL are quite similar and that for the latter the persistence length is represented in Fourier space in terms of n_0 (the analogy is meaningful only for $n_0 \gg 1$, when there is a sufficiently broad range of length scales between the persistence length and the contour length of the knot). The characteristic property of the worm-like chain model is exponential decay, as $\exp(-s/l_1)$, of the tangent–tangent correlation function, which defines the persistence length l_1; similarly, for WLL, on length scales sufficiently small compared to the entire loop, one expects that $\langle\langle t(s) \cdot t(0)\rangle\rangle \simeq \exp(-s/l_1)$, where $\langle\langle\,\rangle\rangle$ denotes averaging both over the contour of a given loop and over the ensemble of loops. This expectation is confirmed in figure 1(*a*), where the logarithm of the correlation function is plotted against the dimensionless arclength s/l_1. The choice $l_1 = 0.43/n_0$ allows us to superimpose data for different values of n_0 in the range $30 \leqslant n_0 \leqslant 270$ (the small shift of the exponent is the result of the finite discretization of the contour length s).

At first sight, analogy with worm-like chain models of linear polymers suggests that on length scales much larger than l_1 the conformations of the loops are those of BRW with step size (Kuhn length) given by twice the persistence length, $2l_1$. However, because the large scale behaviour of a loop is strongly affected by the loop closure constraint, it is not clear, *a priori*, whether the same length controls both the small and the large scale behaviours. We

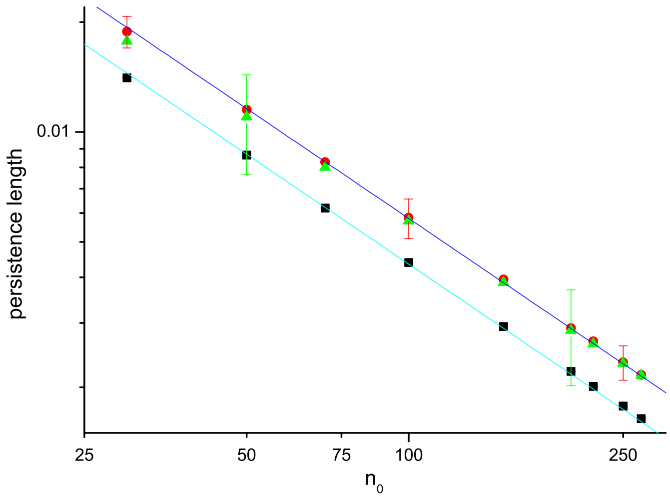

Figure 2. Log–log plot of persistence lengths l_1, l_2, l_3 (black squares, green triangles and red circles respectively) versus n_0. The expressions $0.435/n_0$ and $0.57/n_0$ are shown as solid lines. The standard deviations are represented by error bars.

therefore decided to generate a representative ensemble of configurations of WLL and use it to compute the tangent–tangent correlation function and the mean-squared distance between two well-separated points s and s' ($|s - s'| \gg l_1$) along the contour.

A simple estimate shows that on length scales much larger than the persistence length, the tangent–tangent correlation function of a WLL approaches a constant negative value $\langle\langle t(s) \cdot t(0)\rangle\rangle \simeq -2l_2/L$, where l_2 is, in general, different from l_1 (the negative value of the correlation follows from the fact that the tangent has to turn back on itself in order to come back to its initial direction upon traversing the contour of the loop). In figure 1(*b*) this correlation function is plotted in the interval $0.1 < s < 0.5$ (here and in the following we take $L = 1$) for different values of n_0. Upon averaging the correlation functions over the oscillations, all the results for different values of n_0 can be collapsed to a single horizontal line by dividing them by $l_2 = 0.575/n_0$. We therefore establish that WLL have at least two distinct 'persistence lengths', with $l_1/l_2 \simeq 3/4$.

We now proceed to compute the mean-squared distance between two points on the loop separated by a contour distance s, $\langle\langle R^2(s)\rangle\rangle = (1/L)\left\langle \int_0^L \left|\mathbf{r}(s'+s) - \mathbf{r}(s')\right|^2 \mathrm{d}s'\right\rangle$. Since we expect WLL to behave like BRW on scales much larger than some persistence length l_3, the probability distribution of $R^2(s)$ can be easily written assuming that both $s \gg l_3$ and $L - s \gg l_3$. Apart from a normalization factor, this probability is equal to the product of two Gaussian functions: $\exp[-R^2/(2s\ell_3)]\exp[-R^2/(2(L-s)\ell_3)]$. Averaging with this distribution yields the well-known relation (see, e.g., [11]), $\langle R^2(s)\rangle_{\mathrm{BRW}} = 2l_3 s(1 - s/L)$. This result indicates that the plot of $\langle\langle R^2(s)\rangle\rangle/l_3 L$ against $\sigma = s/L$ is universal, i.e., it is the unit height parabola $4\sigma(1-\sigma)$, independent of either persistence length l_3 or total contour length L. Figure 1(*c*) shows that the data averaged over 1000 different configurations collapse quite accurately on the expected parabolic master curve. Furthermore, by looking at our data for $\langle\langle R^2(s = L/2)\rangle\rangle$, we were able to relate l_3 to the cutoff n_0. Within the accuracy of our simulation, l_3 coincides with l_2 (see figure 2).

The conclusion that local and global statistical properties of worm-like loops are characterized by two different persistence lengths, l_1 and $l_2(=l_3)$, respectively, is a new result of this work. Although analytical theory of worm-like loops does not exist at present, we can offer some tentative considerations about the origin of the two persistence lengths, based on the study of small fluctuations of elastic rings [8]. For rings of zero linking number that possess both bending and twist persistence lengths, it was shown that while on small scales writhe fluctuations depend only on the bending persistence length (on such scales the ring is essentially straight and bending and twist decouple [13][3]), both bending and twist persistence lengths contribute to the writhe on larger scales, for which the global geometry of the closed ring becomes important. Extrapolating this result to the case of a strongly fluctuating loop considered in this work suggests that while l_1 represents the pure bending contribution to the persistence length, l_2 contains both the bending and the twist contributions and is therefore larger than l_1.

We now turn to the topological properties of WLL and examine the probability, P_0, that the randomly generated loop is an unknot, or, in other words, a trivial knot. Clearly, the topology of the loop does not depend on its parametrization and, in particular, it can be established based on the loop specified by the τ-representation. However, in order to formulate the question of a trivial knot probability in a physically meaningful way, we should collect statistics for the loops of different flexibilities. Indeed, it is clear that a very flexible loop is more likely to self-entangle and form a non-trivial knot than, e.g., a very rigid loop, which hardly deviates from a planar circle and thus forms a trivial knot with probability approaching certainty. In our approach, this means that we have to consider the dependence of P_0 on the cutoff frequency n_0. Since n_0 determines the Kuhn length defined as either $2l_1$ or $2l_2$, we can then bring our knotting probability data to a form comparable to that for discrete polymer models, where trivial knot probability depends on the number of segments N. In our case, we generate Fourier knots as completely smooth curves, but we can define the number of effective segments as the ratio of the contour length to the Kuhn length. For long random-walk-like polymers, this definition coincides with the standard one accepted in polymer physics for the Kuhn segments [11] but there remains an ambiguity associated with the choice of $N_1 = L/2l_1$ or $N_2 = L/2l_2$. In order to avoid this ambiguity we will measure the probability to obtain a trivial knot as a function of the cutoff frequency n_0.

To address the topology of the loops computationally, we employ the knot analysis routine due to Lua [12] which identifies knots by computing the Alexander polynomial invariant $\Delta(t)$ at one value of argument, $t = -1$, and Vassiliev invariants of degrees 2, v_2, and 3, v_3. This set of invariants is widely considered powerful enough for reliable identification of the trivial knot for all lengths achievable in practical computations. The data on the trivial knot probability are shown in figure 3. As this figure indicates, the trivial knot probability fits well to the exponential

$$P_0(n_0) \sim \exp[-n_0/242]. \tag{4}$$

Note that since this relation involves only the cutoff on the Fourier series, formula (4) can be re-interpreted in a purely mathematical form, not involving any references to polymers, or, for that matter, to any physics. While there is no fundamental understanding of the origin of this large cutoff ($n_0^* = 242$) at present, our formulation hints at the existence of a hitherto unexplored connection between Fourier analysis and topology of space curves.

In summary, we have shown that the choice of random Fourier coefficients with amplitudes that decay with frequency as $n^{-1}\exp(-n/n_0)$ generates a statistical ensemble of Fourier knots whose local properties coincide with those of worm-like polymers with persistence length that scales as $1/n_0$. Importantly, while random Fourier sum represents well the overall shape of

[3] This effect is expected only for worm-like loops; for linear worm-like chains it can be shown that twist degrees of freedom can be integrated over and that the spatial conformations of the polymer depend on the bending rigidity only.

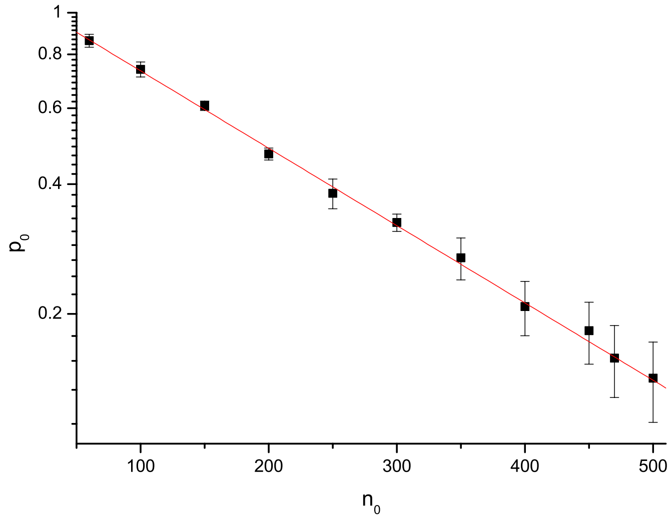

Figure 3. Semi-log plot of the trivial knot probability as a function of n_0.

a worm-like polymer loop, the polymer inextensibility condition leads to highly non-trivial coupling between Fourier harmonics, which is explicitly taken into account in our work. We found that even though WLL behave on large scales as BRW, as expected, the effective step size of this BRW is larger than that calculated from the local persistence length of the loop. This new prediction can in principle be directly tested by experiments on double stranded DNA loops that can monitor both local (persistence length) and global (e.g., radius of gyration) properties of the polymers (see, e.g., [14–16]). It would be interesting to test these results and predictions against Monte Carlo simulations along the lines of [17] (where worm-like chain is modelled as the set of short straight segments with torsional and bending angles properly chosen to approach the smooth limit). We also demonstrated that Fourier knots exhibit exponential decay of the unknotting probability with the characteristic cutoff frequency of the Fourier expansion. The characteristic cross-over determined by this exponential decay represents a large number, which, although in the same ballpark as for other known models, remains an unexplained puzzle.

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