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The role of curvature in entanglement

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HIGHLIGHTS

- The relationship between curvature and entanglement is subtle.
- There are regimes where increasing curvature increases entanglement.
- There are regimes where increasing curvature decreases entanglement.
- Supports the idea that supercoiling can inhibit DNA entanglement.

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ABSTRACT

Which tangles more readily: curly hair or straight hair? A perhaps natural thought, supported by some theoretical evidence, is to associate curvature and entanglement, and assume that they would grow together—that an increase in one fosters an increase in the other. However we have biological examples such as DNA in the chromosome, and mechanical examples such as coiled telephone cords, in which much more curvature is employed than is required for the packing, and in which tangling is presumably detrimental.

We offer a resolution to this conundrum. We show, that at least for simple but generally applicable models, the relationship between curvature and entanglement is subtle: if we keep filament density constant and increase curvature, the entanglement initially increases, passes through a maximum, then decreases, so there is a regime where increasing curvature increases entanglement, and there is also a regime where increasing curvature decreases entanglement. This has implications for filament packing in many circumstances, and in particular for the compaction structure of DNA in the cell—it provides a straightforward argument for the view that one purpose of DNA coiling and supercoiling is to inhibit entanglement. It also tells us to expect that wavy hair –neither the straightest nor the curliest – tangles most readily.

Q2

How would one best pack a long string into a small volume so as to minimize tangling? A little thought tells us that we could accomplish this by inhibiting the motion of the string entirely. However, in many circumstances this is not possible; often, as in the cases of the DNA and the suddenly obsolete telephone cords mentioned above, because motion is required for the purpose or function of the string.

In particular, DNA in the cell lives in a fairly volatile environment—there are free radical collisions which can cause breaks in the string, sections of the string must be manipulated and exposed for RNA copying, and of course the entire string must be unzipped and replicated for mitosis (cell division). To address these happenings and others, there is constant enzyme activity—cutting, joining, copying, repairing the string. All of these effects, and others, can lead to tangling and DNA

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tangling can cause, among other things, cell death [1]. There are several families of enzymes, most prominent of which are the topoisomerase, which address this tangling problem.

Many of our everyday filaments, such as hair and electronic cables, while they are not frequently cut and repaired, are also in dynamic environments.

In sum, this means that we can expect some noise or stochasticity to play a role in the filamentary behavior. So perhaps our question is better stated as: how would one best pack a long string into a small volume so as to minimize tangling, given that there will be some motion and stochasticity involved? The curvature is a local property of the filament, one of the fundamental descriptors of any filament, and so is natural as a first focus point in these sort of problems. For example, there has been considerable interest in the curvature of DNA [2–7].

Some basic connections between curvature and entanglement have been found. Milnor [8] showed that any knot in a closed loop would require at least 4Π of total curvature, where total curvature is defined as the integral or sum of the curvature over the length of the knot. One might think from this that entanglement patterns of increasing complexity require increasing curvature (here and henceforth by curvature we mean total curvature). However, as was shown in Buck–Simon [9], this is not the case, one can have knots of arbitrarily high complexity, as measured by crossing number, with curvature $4\Pi + \epsilon$, where ϵ is an arbitrarily small constant. But it was additionally shown there that this only happens in what are, at least for applications, somewhat special cases—the knot must have regions where it is long and thin, in the sense that one strand can wrap around another in such a way that their tangents are nearly parallel and they are arbitrarily close together over a long distance. Such conformations cannot be constructed if the filament has non-zero thickness (as is the case with most real-world filaments). In the same work it was shown that the entanglement is bounded by the product of the curvature and the ropelength, where the ropelength is the ratio of the length to the radius of the thickest rope (the thickest tube with no self-intersections) one can place about the conformation (use the knot curve as the centerline of the tube) [10,11].

If we pack a C^2 curve of length l into a ball of radius r, then the total curvature K is such that $K \geq (l/r) - 2$. This is a lower bound—it is how much the string is forced to curve to fit into the ball: certainly it could curve more [9]. We also note that this result requires a continuous string—one could cut the string into small bits and pack it into the ball with no curvature at all. If we assume unit thickness for the filament, and pack it as tightly as possible into the sphere, then we will have a sphere of radius $r \approx l^{1/3}$, so by the above K is at least $K \approx \frac{l}{l^{1/3}} = l^{2/3}$. But we have shown that in this case entanglement is bounded by $l^{4/3}$, so we have that entanglement is bounded by K^2 [11,12]. Note that one usually cannot find lower bounds for entanglement—because it is usually possible to make a conformation with no essential crossings (the unknot). We have developed, however, a theory of expected entanglement [12], and we have in general that for a long string the expected entanglement is bounded by K^2. This bound is not generally sharp: consider a string of trefoils tied in a rope. In this case both the curvature and the entanglement grow linearly with the number of knots in the rope. So it remains to generally characterize the relationship between curvature and entanglement. Numerical modelers have studied the total curvature of models of stochastic filaments, providing growth estimates for specific models of long strings [13].

We would like to focus on the effect of curvature on entanglement by considering the basic practical question above: given that we need to pack a certain amount of length in a certain volume, how should we manage the bending, the curvature, so as to minimize entanglement? So, we fix the density (the length per volume), and ask: how does entanglement tend to vary as we vary curvature?

We can do this analysis in the following model system. Let circles be centered at each lattice point in the cubic lattice (three dimensions) for some finite cube of fixed size, where the cube is large enough to contain many lattice points. Let the circles be randomly oriented with respect to one another. (A similar analysis could likely also be done for circles with randomly placed centers and random orientation). We will vary this system by changing the number of circles, that is, the distance between the lattice points, while keeping the total length constant—so we have to vary the radii of the circles as we vary the lattice spacing. The idea is that this way we are keeping the density constant—since it is just the length per unit volume, but varying the curvature, since the total curvature is simply $2\Pi N$, where N is the number of circles. Let us say that the total length is L. Then the length of each circle is $\frac{L}{N}$, so the radii are $\frac{L}{2\Pi N}$. There are N circles in the cube, so the distance between the centers of nearest neighbors is $N^{\frac{-1}{3}}$ (assuming a cube of width 1).

This system, for various N, is depicted in Fig. 1. A system of randomly placed circles with the possibility of linking has been used to model mitochondrial DNA from trypanosomes [14].

Now, how to measure the entanglement? In this system there is one straightforward method: simply count how many pairs of circles are linked. For an estimate, we will simply assume that some percentage of circles which could be linked are, that is, the pairs of circles whose centers are closer to one another than twice the radii. To be more precise, the probability of linking of two circles as a function of the distance between their centers has been studied [15,16], and we could use a better approximation, but we will continue on this track for the nonce. So the question becomes: for a given circle, how many other circles have their centers within two radii? The radii are $\frac{L}{2\Pi N}$, so the question becomes, how many lattice points, where the lattice unit is $N^{\frac{-1}{3}}$, are in a ball of radius $\frac{L}{\Pi N}$? But this is approximately:

$$\frac{4}{3}\Pi \left[\frac{\frac{L}{2\Pi N}}{N^{-1/3}} \right]^3 .$$