VIEW FROM THE PENNINES: IDEAL KNOTS

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The moorland rescue team takes itself seriously, and many walkers have reason to be grateful for their dedication. The team practice at weekends, and on Saturday evening it is not unusual to see them in the local pub. They are not hard to spot: their shirts and jackets are festooned with brightly coloured ropes and other equipment. The object pictured on the cover of *Mathematics Today* this month would not look out of place amongst the clips and climbing gear of the rescue team. It might have some obscure use during a difficult traverse. In fact, it is a mathematical object called an ideal link, computed by Ben Laurie [2], and has more to do with the complicated geometry of long molecules such as DNA than the life-preserving paraphernalia of the sociable climbers.

What makes Laurie's representation of this link special is that if the link is tied using rope with a given constant (inelastic) cross-section, then this form minimizes the length of rope used. If the same exercise is carried out with a knot rather than a link then the length-minimizing representation is called an ideal knot. The motivation for the study of ideal knots and links comes from the study of large molecules such as DNA [6, 7]. Length minimization is a simple model of energy minimization, so ideal knots represent minimum energy configurations. More realistic energy expressions have been investigated, and the results seem quite similar [15]. Ideas from knot theory have been used to explain supercoiling effects in DNA [16], and the ideal knot approach promises to give further insights.

Suppose that a piece of rope is tied loosely in a knot. Think of the rope as a tube with a fixed diameter and imagine trying to reduce the length of the rope. The knot needs to remain the same knot – a trefoil for example – as the length is reduced, and different strands of the rope must not intersect, giving two global constraints. Locally the curvature of the rope is limited by the cross-section: if the curvature is too great the skin of the tube will crease and self-intersect. Thus there is also a local constraint. Like many problems which involve both global and local constraints, one of the hardest parts of the solution is to determine the best way to phrase the problem. Most mathematical formulations of ideal knots concentrate on the core of the tube, which is a continuous curve in three dimensions, $\mathcal{C}$. Since it is a length minimizing problem it is natural to try an approach based on the calculus of variations. A first attempt to formalize the problem might go something like this. Denote the radius of curvature of a curve at $\mathbf{x}$ by $\rho(\mathbf{x})$ and the open ball of radius d about $\mathbf{x}$ by $B(\mathbf{x}, d)$. Now the problem is: given $\delta > 0$ (the radius of the tube) find a curve $\mathcal{C} = \{\mathbf{x}(t) \in \mathbb{R}^3 \mid 0 \leq t \leq 1, \mathbf{x}(0) = \mathbf{x}(1)\}$ which solves the problem

$$\text{minimize } L = \int_0^1 \left| \frac{d\mathbf{x}}{dt}(t) \right| dt$$

subject to the constraints

(i) $\mathcal{C}$ is a trefoil;
(ii) $B(\mathbf{x}, 2\delta) \cap \mathcal{C}$ is a curve segment for all $\mathbf{x} \in \mathcal{C}$; and
(iii) $\rho(\mathbf{x}) \geq \delta$ for all $\mathbf{x} \in \mathcal{C}$.

Constraint (i) determines the knot type, (ii) ensures that different strands of the

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tube do not intersect, and (iii) ensures that the tube does not self-intersect due to curvature. Of course, the fundamental scale invariant quantity of interest is not L but L/δ: the ratio of the minimal length to the rope thickness. Unfortunately, the constraints do not seem to lend themselves to expression in terms which allow the calculus of variations to be used, although this might be circumvented by working in a more complicated space of curves.

This sort of formulation is enough to make it possible to write computer programmes which calculate approximate ideal knot configurations. These were pioneered by Pieranski, and operate using a physical model of string tightening [11] or Monte Carlo style algorithms [2] on curves of the given knot type. These simulations generate some fabulous pictures (see for example Laurie's link on the cover of this issue and his ideal knot website [2] or Pieranski's home page [11]) and provide data which can be used to investigate properties of the ideal configuration. Some of these findings are described below, but first let us review other formulations of the problem.

A number of researchers have attempted to prove the existence of ideal knot configurations in restricted classes of curves by thinking of the knot as a finite set of nodes connected by particular types of curve (splines, polynomial knots, lattice knots...), or by considering open knots, and some progress has been made in these directions, e.g. [9, 13]. A more interesting general approach has been suggested by Gonzalez and Maddocks [5] in an attempt to unify the constraints (ii) and (iii) above. They have come up with a generalization of the radius of curvature which they call *global radius of curvature*. The radius of curvature of a curve at a point $\mathbf{x}$ is the radius of the circle which passes through $\mathbf{x}$, is tangential to the curve and has the same curvature (second derivative) as the curve at $\mathbf{x}$ – note that these three conditions specify a unique circle. There are other ways to specify a unique circle, and hence unique radius: one could use two distinct points, $\mathbf{x}$ and $\mathbf{y}$, on the curve and and look for the circle which passes through $\mathbf{x}$ and $\mathbf{y}$ and is tangential to the curve at $\mathbf{x}$ [15]. Or one could choose three distinct points, $\mathbf{x}$, $\mathbf{y}$ and $\mathbf{z}$, on the curve and look for the unique circle which passes through all three points. The radius of this circle, $r(\mathbf{x},\mathbf{y},\mathbf{z})$, is the starting point for Gonzalez and Maddocks; the radii of the other two circles can be obtained from it by taking appropriate limits. A bit of geometry gives

$$r(\mathbf{x},\mathbf{y},\mathbf{z}) = \frac{|\mathbf{x}-\mathbf{y}||\mathbf{y}-\mathbf{z}||\mathbf{z}-\mathbf{x}|}{4\mathcal{A}(\mathbf{x},\mathbf{y},\mathbf{z})}$$

where $\mathcal{A}$ is the area of the triangle defined by the three vectors. This can be rewritten in a number of ways, for example

$$r(\mathbf{x},\mathbf{y},\mathbf{z}) = \frac{|\mathbf{x}-\mathbf{y}||\mathbf{y}-\mathbf{z}||\mathbf{z}-\mathbf{x}|}{2|(\mathbf{x}-\mathbf{y})\times(\mathbf{x}-\mathbf{z})|}$$

which makes it easier to connect it to Gauss integrals [14] and is one reason why some people prefer to work with $1/r$ (cf. [8]). The global radius of curvature, $\rho_G(\mathbf{x})$, for $\mathbf{x}$ on a smooth curve $\mathcal{C}$ is the smallest possible value of r:

$$\rho_G(\mathbf{x}) = \min_{\mathbf{y},\mathbf{z}\in\mathcal{C}} r(\mathbf{x},\mathbf{y},\mathbf{z})$$

The ideal knot property now has a very simple description in terms of ρ_G. Fix the length of the rope $L>0$ and try to maximize the thickness of the rope; this is the dual problem of the original length-minimizing formulation of ideal knots. Let $\mathcal{K}$ denote the set of all simple smooth curves $\mathcal{C}$ of a given knot type and length L. For each such curve, the minimum global radius of curvature, $\Delta(\mathcal{C})$, determines the largest cross-section of a non-self-intersecting rope with core $\mathcal{C}$. The ideal knot representations are therefore those which maximize this thickness, i.e. if $\mathcal{C}^*$ is an ideal knot then

$$\Delta(\mathcal{C}^*) = \sup_{\mathcal{C}\in\mathcal{K}} \left(\inf_{\mathbf{x}\in\mathcal{C}} \rho_G(\mathbf{x}) \right)$$

This formulation of the problem feels much more elegant, although it is still not known whether the maximizing representations $\mathcal{C}^*$ are smooth.

Regardless of the precise details of the space of curves in which the ideal knot representations lie, numerical simulations produce approximate ideal knots whose properties can be studied, and it is here that some really surprising features emerge.

The first property suggested by the numerics is that the global radius of curvature of an ideal knot is piecewise constant. Laurie's figure makes this point clearly: the curvature looks uniform except for a few kinks where the different strands of the links change roles from axis to coil and back again. There is also some theoretical justification for this conjecture [5].

The most spectacular, though controversial, property of ideal knots is that the writhe appears to be quantized (see [1, 4], but also [12]). The writhe is an averaged measure of how a knot is seen in projection. Any two-dimensional projection of a knot will have a set of intersections where one strand passes 'over' or 'under' the other strand. An index can be assigned to each such crossing depending on whether the upper string crosses from right to left (index $+1$) or vice versa (index -1). The sum of these indices over the intersections of the projection averaged over all projections (i.e. integrated over a solid angle of 4π) is the writhe of the knot. It depends on the representation of the knot, and is connected to other properties (link and twist) by White's Theorem [16]. Pieranski [10] noticed that the numerically computed writhe of ideal knots appear to be quantized, i.e. the writhe difference between the writhes of ideal knots is a multiple of $\frac{4}{7}$ [12]. Theoretical support for this conjecture was provided by Cerf and Stasiak [4], see also [1], although further computations by Pieranski and Pryzbyl [12] suggest that the situation might be more complicated. If there is indeed some form of quantization then the theory of ideal knots may have profound implications for geometric physics.

The theory of ideal knots and links is still in its infancy. There is still no universally agreed best formulation of the problem, nor are there clean results about the existence of solutions or their properties. However, there is enough numerical evidence to suggest that the theoretical efforts of Gonzalez, Maddocks, Sullivan and others is worthwhile, and it is certainly creating new geometric avenues of investigation. It is not clear whether the more exciting expectations raised by the numerical simulations will be met, but this will not prevent it remaining one of the most fascinating problems I have read about in recent years.

And just in case you were wondering: the technical name for the two component link Laurie produced for the cover page is 2.10.1; this ideal link is interesting because although there are symmetric forms of the link, the ideal link has broken symmetry – the two loops on the right are parallel and the two on the left splay [3].

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