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## Geometric Knot Theory

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**ABSTRACT.** Geometric knot theory studies relations between geometric properties of a space curve and the knot type it represents. As examples, knotted curves have quadrisecant lines, and have more distortion and more total curvature than (some) unknotted curves. Geometric energies for space curves – like the Möbius energy, ropelength and various regularizations – can be minimized within a given knot type to give an optimal shape for the knot.

Increasing interest in this area over the past decade is partly due to various applications, for instance to random knots and polymers, to topological fluid dynamics and to the molecular biology of DNA. This workshop focused on the mathematics behind these applications, drawing on techniques from algebraic topology, differential geometry, integral geometry, geometric measure theory, calculus of variations, nonlinear optimization and harmonic analysis.

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### Introduction by the Organisers

The workshop *Geometric Knot Theory* had 23 participants from seven countries; half of the participants were from North America. Besides the fifteen main lectures, the program included an evening session on open problems. One morning session was held jointly with the parallel workshop “Progress in Surface Theory” and included talks by Joel Hass and Andre Neves.

Classically, knot theory uses topological methods to classify knot and link types, for instance by considering their complements in the three-sphere. But in recent decades there has been increasing interest in connecting these topological knot types with geometric properties of the various space curves representing them, and

in finding optimal geometric shapes for a given knot type by minimizing various energy functionals.

To find an optimal shape for a given knot, one usually minimizes some geometric energy. We emphasize that the concept of “energy” is very general here. For instance, we can build polygonal “stick knots” of fixed or varying edge length and let the energy be the number of sticks; we could also restrict these sticks to lie in a given grid or to form an arc presentation in an open book. Average crossing number and total curvature are classical examples of energy functions, for which the infimal value is not achieved but instead recovers diagrammatic information (minimum crossing number and bridge number, respectively).

It has long been hoped that following the gradient flow of a more suitable energy functional for curves would lead to an effective method for simplifying the shape of knots. For example, one might load a curve with electric charge and let its shape evolve by electrostatic repulsion. A scale-invariant version of the Coulomb potential, properly renormalized, was introduced by O’Hara and shown by Freedman, He and Wang to be Möbius-invariant. This gives a very useful energy for knots and links, where many open problems remain.

Another natural question asks how much rope is needed to tie a given knot or link. Mathematically the rope is idealized to have fixed circular cross-section: it is a normal tube around some core curve. We minimize the *ropelength*, the scale-invariant quotient of length over thickness. Here *thickness* (or reach in Federer’s terminology) is the maximal radius of a normal tube and has many equivalent formulations useful in different contexts. For instance it is bounded both by the local radius of curvature and by the closest approach of two different strands of the knot. On the other hand, it is also the maximal Menger curvature of all triples of points on the knot, that is, the infimal radius of circles intersecting the knot three times.

Replacing the maximum of Menger curvature (an  $L^\infty$  norm) by various  $L^p$  norms, one obtains a whole family of knot energies, interpolating between thickness on the one hand and repulsive Coulomb-type potentials on the other. When these energies are finite (or minimized) for a given curve, the smoothness of the curve and its geometric complexity are both controlled. Recently, the spaces of finite energy curves for these and related energies have been characterized in terms of fractional Sobolev spaces. A similar characterization for the Möbius energy made it possible to analyze its gradient flow, and there is hope that these techniques can be extended to study geometric flows for integral Menger curvature as well. In the limit, this could also lead to an analytic understanding of the gradient flow for ropelength. Moreover, intricate bootstrapping arguments for fractional orders of differentiability were recently developed to prove smoothness of critical points for several of these energies. In addition, integral Menger curvature and its interpolating relatives have successfully been generalized to submanifolds of arbitrary dimension and co-dimension in Euclidean space, which opens up the search for corresponding results in the context of higher dimensional (knotted)

submanifolds, such as finiteness of isotopy types with bounds on integral Menger curvature and regularity theorems for finite or minimal energy submanifolds.

Another set of interesting questions arises from considering the average values of geometric functionals over spaces of curves instead of the minimum values. For instance, we might ask for the average total curvature of a class of curves, or the average knot type. To get sensible answers here, we must restrict our attention to finite-dimensional spaces of curves such as the space of polygons with a given length and a given number of edges. We must also choose a natural probability measure to integrate our functionals against; this measure also provides the setting for a theory of random knots. Such random knotted polygons are thought to provide good models for knotted polymer molecules. The relationship between the averages over random polygons in a given knot type to the minimum values for this knot type (and to the topology) is an area of active research. Progress here could lead to important advances in the statistical physics of polymers and other entangled systems.

The fifteen talks and the open problem session are documented in the remainder of this report. The workshop schedule also left free time for informal mathematical interactions, and many fruitful discussions developed.

On the lighter side, Colin Adams directed an evening of mathematical theater based on some of his humorous columns for the *Mathematical Intelligencer*. More than half the workshop participants acted in one or more of the skits, and the appreciative audience included almost everyone from both workshops. In addition to the traditional Wednesday hike to St. Roman, many participants walked to the Museum for Minerals and Mathematics after the last talk on Friday afternoon.



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## Abstracts

### Turning knots into flowers

COLIN ADAMS

(joint work with Thomas Crawford, Benjamin DeMeo, Michael Landry, Alex Tong Lin, MurphyKate Montee, Seojung Park, Saraswathi Venkatesh, Farrah Yhee)

Traditionally, knots have been studied by considering their projections, where we allow exactly two strands to cross at a singular point. The minimal number of such crossings is denoted  $c(K)$ . In [6], the authors considered projections of graphs, where they allowed three strands to cross, each strand passing straight through the crossing. In that paper, they showed that most bipartite graphs do not possess a projection with only triple crossings of this type.

But this brings up the question, what is true with regard to triple crossings for knots? In [1], we first prove that every knot possesses a projection with only triple crossings. Therefore the minimal number of triple crossings for a knot  $K$ , denoted  $c_3(K)$  is well-defined. One can consider its relation to traditional crossing number, now denoted  $c_2(K)$ , and see that  $c_2K/3 \leq c_3(K)$ . Although we find links that realize this lower bound, it is still an open question as to whether any knots realize this lower bound.

Similar in spirit to the result of Kauffman [4], Murasugi [5] and Thistlethwaite [7] that  $\text{span}(\langle K \rangle) \leq 4c_2(K)$ , where  $\langle K \rangle$  is the bracket polynomial introduced by Kauffman, we prove that  $\text{span}(\langle K \rangle) \leq 8c_3(K)$ . We utilize this to determine triple crossing number for a variety of knots. Specifically, an alternating knot such that its reduced alternating projection decomposes into bigon sequences, each containing an even number of crossings will have  $c_3(K) = c_2(K)/2$ . An alternating knot such that its reduced alternating projection decomposes into a set of three crossings, all on a triangle and the rest in bigon sequences, each containing an even number of crossings, will have  $c_3(K) = (c_2(K) + 1)/2$ .

We also consider quadruple crossings in [3], where four strands of the knot pass straight through each crossing. We show that every knot has a quadruple crossing projection and hence a well-defined quadruple crossing number  $c_4(K)$ . We prove  $\text{span}(\langle K \rangle) \leq 16c_4(K)$ , and use this fact to determine the quadruple crossing number for a variety of knots and links.

A multi-crossing or  $n$ -crossing is a crossing in a projection with  $n$  strands of the knot passing straight through the crossing. We prove that every knot has an  $n$ -crossing projection and hence a minimal  $n$ -crossing number, denoted  $c_n(K)$ . We know that  $c_2(K) > c_3(K) \geq c_5(K) \geq c_7(K) \geq \dots$  and  $c_2(K) > c_4(K) \geq c_6(K) \geq c_8(K) \geq \dots$ . It remains an open question as to how the  $n$ -crossing numbers for  $n$  even and  $n$  odd are related.

A particularly intriguing question is whether every knot has a value  $n$  for which  $c_n(K) = 1$ . That is to say, does every knot possess a projection with just a single mult-crossing? In [2], we show that this is indeed the case. Moreover, there is

such a projection such that the loops hanging off the single multi-crossing are not nested. The projection resembles a flower. Such a projection is called a petal projection.

Hence we can define the übercrossing number (least  $n$  for the multi-crossing in a projection with a single multi-crossing) and the petal number (least  $n$  for the multi-crossing in a petal projection). Note that a petal projection is an arc projection, and hence  $\alpha(K) \leq p(K)$ .

We determine the petal number of all knots of nine or fewer crossings. We also use arc index to show that the petal number of the  $(r, r + 1)$ -torus knots is  $2r + 1$ .

A variety of open problems come out of this work. Instead of each knot having a single crossing number, now each knot has a spectrum of crossing number values. What is the behavior of this spectrum? Do certain families of knots come out of this viewpoint on knots? A petal projection is a braid representation of a very specific type. What can we say about the braids that result? And how do these new invariants relate to the traditional knot invariants?

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### Gradient flow for the Möbius energy

SIMON BLATT

In his 1991 paper [4], Jun O’Hara introduced the Möbius energy

$$E(\Gamma) := \int_{\Gamma} \int_{\Gamma} \left( \frac{1}{|y-x|^2} - \frac{1}{d_{\Gamma}(x,y)^2} \right) d\mathcal{H}^1(y) d\mathcal{H}^1(x)$$

for embedded curves  $\Gamma \subset \mathbb{R}^3$ , where  $d_{\Gamma}(x, y)$  denotes the length of the shorter arc connecting the two points  $x$  and  $y$  and  $\mathcal{H}^1$  is the one-dimensional Hausdorff measure. We want to discuss some recent results regarding the negative gradient flow of this energy. We are looking at a smooth family of embedded closed curves  $\Gamma_t$ ,  $t \in [0, \infty)$  which satisfies the evolution equation

$$(1) \quad \partial_t^{\perp} \Gamma_t = -\mathcal{H} \Gamma_t \quad \forall t \in [0, T)$$



where  $\mathcal{H}\Gamma_t$  is the  $L^2$ -gradient of the Möbius energy. Already Freedman, He, and Wang [2] showed that this gradient can be expressed by

$$\mathcal{H}\Gamma := 2 \lim_{\varepsilon \rightarrow 0} \int_{\Gamma - B_\varepsilon(x)} \left( 2 \frac{P_{\tau_\Gamma(x)}^\perp(y-x)}{|y-x|^2} - \kappa_\Gamma(x) \right) \frac{d\mathcal{H}^1(x)}{|y-x|^2}.$$

In the formula above  $\tau_\Gamma$  stands for the unit tangent along  $\Gamma$  and  $P_{\tau_\Gamma(x)}^\perp = id - \langle \cdot, \tau_\Gamma(x) \rangle \tau_\Gamma(x)$  denotes the orthogonal projection of  $\mathbb{R}^3$  onto the normal space of  $\Gamma$  in  $x$ .

Due to the Möbius invariance of this energy and based on numerical experiments, one expects that in general this flow develops singularities after finite or infinite time. In this talk we analyze these singularities by constructing a blowup profile.

The fundamental result is the following: There is an  $\varepsilon > 0$  such that either the solution of the gradient flow smoothly exists for all time or there exists a sequence of times  $t_j$ , radii  $r_j \rightarrow 0$  and points  $x_j \in \Gamma_{t_j}$  such that

$$\int_{\Gamma_{t_j} \cap B_{r_j}(x_j)} \int_{\Gamma_{t_j} \cap B_{r_j}(x_j)} \frac{|\tau_{\Gamma_{t_j}}(x) - \tau_{\Gamma_{t_j}}(y)|^2}{|x-y|^2} d\mathcal{H}^1(y) d\mathcal{H}^1(x) \geq \varepsilon,$$

i.e. a small quantum of energy concentrates as we approach the singularity. Furthermore, by picking the times  $t_j$  and points  $x_j$  a bit more carefully one can show that the rescaled curves

$$\tilde{\Gamma}_j := \frac{1}{r_j} (\Gamma_{t_j} - x_j)$$

satisfy

$$\|\partial_s^k \tilde{\Gamma}\|_{L^\infty} \leq C_k.$$

Hence, using Arzela-Ascoli's lemma we can choose a subsequence of  $\tilde{\Gamma}_j$  converging locally smoothly to a limit curve  $\tilde{\Gamma}_\infty$ , the *blowup profile*. Due to our construction, this profile will be properly embedded, has finite Möbius energy, cannot be a straight line, and satisfies the equation

$$(2) \quad \mathcal{H}\tilde{\Gamma}_\infty \equiv 0.$$

In the last part of the talk, we discussed compact and non-compact *planar* solutions of (2) using the following interpretation of this equation which is motivated by the work of He [3]. In contrast to He's approach, we do not explicitly use the Möbius invariance of the energy:

Given two points  $x, y \in \Gamma$  there is either a unique circle or a straight line – which we like to think of as a degenerate circle – going through  $x$  and  $y$  and tangent to  $\Gamma$  at  $x$ . Note that this is the same circle, used to define the integral tangent-point energies. We denote by  $\kappa_\Gamma(x, y)$  the curvature vector of this circle in  $x$  and set  $\kappa_\Gamma(x, y) = 0$  if the tangent on  $\Gamma$  in  $x$  is pointing in the direction of  $y$  – which is the curvature of the straight line. Since

$$\kappa_\Gamma(x, y) = 2 \frac{P_{\tau(x)}^\perp(y-x)}{|y-x|^2},$$

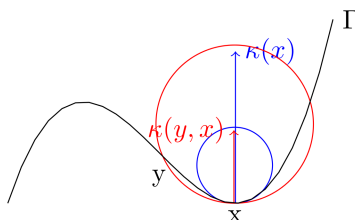


FIGURE 1. This picture shows the two circles playing a role in the geometric interpretation of the Euler-Lagrange equation of the Möbius energy: The blue circle is the osculating circle at  $x$  while the red circle is the circle going through  $x$  and  $y$  and tangent to  $\Gamma$  at  $x$ .

$H\Gamma \equiv 0$  is equivalent to

$$\lim_{\varepsilon \rightarrow 0} \int_{\Gamma - B_\varepsilon(x)} \frac{\kappa_\Gamma(x, y) - \kappa_\Gamma(x)}{|y - x|^2} \mathcal{H}^1(y) = 0$$

for all  $x \in \Gamma$ .

Using this geometric version of the equation, we can prove the following

**Theorem 1.** *Let  $\Gamma \subset \mathbb{R}^2$  be a properly embedded open or closed smooth curve of bounded curvature which satisfies*

$$\tilde{\mathcal{H}}\Gamma := 2 \lim_{\varepsilon \rightarrow 0} \int_{\Gamma \cap (B_{\frac{1}{\varepsilon}}(x) - (B_\varepsilon(x)))} \left( 2 \frac{P_{\tau_\Gamma(x)}^\perp(y - x)}{|y - x|^2} - \kappa_\Gamma(x) \right) \frac{d\mathcal{H}^1(x)}{|y - x|^2} = 0.$$

*Let furthermore  $x \in \Gamma$  be a point in which the curvature of  $\Gamma$  does not vanish, and such that the open ball  $B_x$  whose boundary is the osculating circle on  $\Gamma$  satisfies either  $B_x \cap \Gamma = \emptyset$  or  $\Gamma \subset \overline{B}_x$ . Then  $\Gamma = \partial B_x$ , i.e.  $\Gamma$  agrees with its osculating circle in  $x$ .*

Since all planar curves except the straight lines have such a point  $x$ , we get

**Theorem 2.** *The only properly embedded open or closed smooth curves  $\Gamma \subset \mathbb{R}^2$  which satisfy  $\tilde{\mathcal{H}}\Gamma$  are circles and straight lines.*

In [1] it was proven that near local minimizers the flow exists for all time and converges to a local minimizer on the same energy level as time goes to infinity. Combining this with the argument above, we get that the flow for closed planar curves exists for all time. A similar analysis of the asymptotic behavior for planar curves finally leads to

**Theorem 3.** *If  $\Gamma_0$  is a planar curve, the solution of (1) exists smoothly for all time and converges to a circle as  $t \rightarrow \infty$ .*

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### Universal constructions on spaces of knots with relations to finite-type invariants

RYAN BUDNEY

The topic of this presentation is spaces of knots, meaning spaces of embeddings such as  $Emb(S^j, S^n) = \{f : S^j \rightarrow S^n \text{ smooth embedding}\}$  with the ‘Whitney topology’. There is the corresponding space  $\mathcal{K}_{n,j}$ , which is the space of smooth embeddings  $\mathbb{R}^j \rightarrow \mathbb{R}^n$  which agree with the standard embedding  $x \mapsto (x, 0)$  outside of  $D^j \subset \mathbb{R}^j$ . We call  $\mathcal{K}_{n,j}$  the space of ‘long knots’. A basic theorem is that there is a homotopy-equivalence

$$Emb(S^j, S^n) \simeq SO_{n+1} \times_{SO_{n-j}} \mathcal{K}_{n,j}$$

provided  $n > j$ . The idea is to consider Euclidean space as a tangent space to  $S^n$ , so one-point-compactification gives a map  $\mathcal{K}_{n,j} \rightarrow Emb(S^j, S^n)$ , the action of  $SO_{n+1}$  on  $S^n$  and  $SO_{n-k}$  on  $\mathbb{R}^n$  fixing  $\mathbb{R}^j \times \{0\}$  gives the remaining map.

The Vassiliev approach to studying  $\mathcal{K}_{n,1}$  is to consider  $\mathcal{K}_{n,1} \subset E_{n,1}$  which is the space of smooth maps  $\mathbb{R} \rightarrow \mathbb{R}^n$  with  $x \mapsto (x, 0)$  for  $x \notin [-1, 1]$ .  $E_{n,1}$  is an affine vector space so it is contractible.  $E_{n,1} \setminus \mathcal{K}_{n,1}$  is a naturally stratified space, and essentially the Spanier-Whitehead dual of  $\mathcal{K}_{n,1}$ . In Vassiliev’s work he replaces  $E_{n,1}$  with a collection of contractible finite-dimensional subspaces of  $E_{n,1}$  that exhaust  $E_{n,1}$ , making the Spanier-Whitehead duality explicit. The stratification gives a spectral sequence for computing the homology and cohomology of  $E_{n,1} \setminus \mathcal{K}_{n,1}$ , known as the Vassiliev spectral sequence [5].

A parallel approach to studying embeddings is due to Goodwillie and Weiss [3]. This uses the formalism of Functor Calculus, which studies the Taylor approximations to the cofunctor  $\mathcal{O} \ni U \mapsto f|_U$  where  $\mathcal{O}$  is a category of open subsets of  $\mathbb{R}$  with morphisms given by inclusion. This functor is taking values in a category of embeddings of open subsets of  $\mathbb{R}$  into  $\mathbb{R}^n$ . Provided the open subset is not all of  $\mathbb{R}$ , these spaces have the homotopy-type of configuration spaces (labelled with tangent vectors). Such spaces (where the domain is not all  $\mathbb{R}$ ) form a diagram (maps given by restriction) whose homotopy-limit is called the Taylor approximation to the functor. If we restrict the intervals to have  $k$  or less connected components, again morphisms by restriction we get the  $k$ -th stage of the Taylor tower. The map is denoted  $\mathcal{K}_{n,1} \rightarrow T_k \mathcal{K}_{n,1}$ . Goodwillie, Weiss and Klein show that this map is  $(k-1)(n-3)$ -connected. There is a naturally-associated spectral sequence to such homotopy-limits, and this essentially agrees with the Vassiliev spectral sequence, up to a re-grading.

The Hatcher approach to spaces of knots uses the fibre bundles  $Diff(D^n) \rightarrow \mathcal{K}_{n,1}$  where  $Diff(D^n)$  is the group of diffeomorphisms of the  $n$ -disc  $D^n$  which restrict to the identity on the boundary  $\partial D^n = S^{n-1}$ . The point of this technique is it converts the study of spaces of knots to the study of the diffeomorphism groups of manifolds, which in dimension 3 there are many available tools from geometrization. At this point one has to restrict to  $n \leq 3$  as the homotopy-type of  $Diff(D^n)$  is not well-understood when  $n \geq 4$ . If we let  $\mathcal{K}_{3,1}(f)$  denote the path-component of  $f$  in  $\mathcal{K}_{3,1}$  we then have a sequence of fibre bundles  $Diff(D^3) \rightarrow \mathcal{K}_{3,1}(f)$  whose fibres have the homotopy-type of  $Diff(C_f)$ , where  $C_f$  is the complement of an open tubular neighbourhood of  $f$  in  $D^3$ , and the diffeomorphisms restrict to the identity on the boundary. Hatcher's theorem that  $Diff(D^3)$  is contractible has the consequence that  $\mathcal{K}_{3,1}(f) \simeq BDiff(C_f)$  or essentially equivalently,  $\Omega\mathcal{K}_{3,1}(f) \simeq Diff(C_f)$ , and theorems of Hatcher and Waldhausen imply that  $Diff(C_f)$  has the homotopy-type of the discrete group  $\pi_0 Diff(C_f)$ , so  $\mathcal{K}_{3,1}(f)$  is an Eilenberg-MacLane space of type  $K(\pi, 1)$ . This allowed Hatcher to show that

$$\mathcal{K}_{3,1}(f) \simeq \begin{cases} * & f \text{ is the unknot} \\ S^1 & f \text{ is a torus knot} \\ S^1 \times S^1 & f \text{ is a hyperbolic knot} \end{cases}$$

Moreover, if  $C_f$  has a non-trivial JSJ-decomposition,  $Diff(C_f)$  fits in an extension of groups, leading to an fiber-bundle description of  $\mathcal{K}_{3,1}(f)$  in terms of simpler knots and links, from the point of view of the JSJ-decomposition.

My work in this area started by completing the fiber-bundle description begun by Hatcher. The first result is that there is an action of the operad of 2-cubes on  $\mathcal{K}_{3,1}$  extending the connect-sum operation  $\mathcal{K}_{3,1} \times \mathcal{K}_{3,1} \rightarrow \mathcal{K}_{3,1}$ . The main theorem of [1] states that  $\mathcal{K}_{3,1}$  is *freely generated* by the 2-cubes operad  $\mathcal{C}_2$  by the subspace  $\mathcal{P} \subset \mathcal{K}_{3,1}$  of knots which are prime. This has the consequence that

$$\mathcal{K}_{3,1} \simeq \bigsqcup_{n \geq 0} \mathcal{C}_2(n) \times_{\Sigma_n} \mathcal{P}^n.$$

To put this into context:  $\mathcal{C}_2(n)$  has the homotopy-type of the configuration space of  $n$  distinct, labelled points in the plane. So if we take the component of the connect-sum of  $n$  trefoils in  $\mathcal{K}_{3,1}$  the above theorem states that it has the homotopy-type of  $\mathcal{C}_2(n) \times_{\Sigma_n} (S^1)^n$ , this is the configuration space of  $n$  distinct points in the plane, each of which has an associated unit tangent vector. If on the other hand the summands were all distinct torus knots, this theorem states the component has the homotopy-type of  $\mathcal{C}_2(n) \times (S^1)^n$ .

There is a construction called the *bar construction* whose role is to turn the multiplicative structure of a wide array of objects (such as groups, monoids and categories) into that of a loop space. In the above, the concatenation operation turns  $\mathcal{K}_{3,1}$  into a monoid, also describable in terms of the 2-cubes action. So there is a 'group completion' construction, which is a map  $\mathcal{K}_{3,1} \rightarrow \Omega B\mathcal{K}_{3,1}$  which has the property that any monoid map out of  $\mathcal{K}_{3,1}$  to a loop space must factor through this map. A theorem of Peter May's tells us what the homotopy-type of

the group-completion of a free  $\mathcal{C}_2$ -object is, which combined with the above tells us that

$$\Omega BK_{3,1} \simeq \Omega^2 \Sigma^2(\mathcal{P} \sqcup \{*\}).$$

Thus  $\Omega BK_{3,1}$  contains as a retract the double loop space on a countable wedge of spheres (countably-infinite many in each dimension  $\geq 2$ ). This is very interesting since the homotopy-limits in the Goodwillie Calculus naturally fiber over the homotopy-fiber of the Faddell-Neuwirth diagram of fibrations, so it is very similar to iterated loop spaces on wedges of spheres. So one might ask, is there a reason for this? I think there is. Precisely,

**Theorem:** There is an action of the little intervals operad  $\mathcal{C}_1$  on the Taylor tower  $T_k \mathcal{K}_{3,1}$  such that the Taylor approximation map  $\mathcal{K}_{3,1} \rightarrow T_k \mathcal{K}_{3,1}$  is  $\mathcal{C}_1$ -equivariant. Thus the Goodwillie-Weiss Taylor approximation map factors to a map  $\Omega BK_{3,1} \rightarrow T_k \mathcal{K}_{3,1}$ .

The satisfying aspect of this theorem is it starts to give a hint as to what objects like the Taylor tower and the Vassiliev spectral sequence may be converging to, in the 3-dimensional case. There are further operads that act on the space of knots  $\mathcal{K}_{3,1}$  such as the *splicing operad* [2], and so one might ask, does the Taylor approximation factor through these further bar constructions?

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### On the ropelength problem of knots

YUANAN DIAO

#### 1. Definition of the ropelength of a knot and a knot type.

Let  $K$  be a smooth knot. For any point  $x$  on the knot, the (geometric) disk of radius  $d$  centered at  $x$  on the tangent plane of  $K$  at  $x$  is denoted by  $D(x, d)$ . The *thickness* of  $K$  is defined as  $T_D(K) = \sup\{d : D(x, d) \cup D(y, d) = \emptyset, \forall x, y \in K\}$ . The ropelength of a knot  $K$  as a fixed space curve (denoted  $R(K)$ ) is the ratio between its arc length  $L(K)$  and its thickness:  $R(K) = L(K)/T_D(K)$ . The ropelength of a knot type  $\mathcal{K}$  is defined as  $R(\mathcal{K}) = \inf R(K)$  where the infimum is taken over all  $K$  with knot type  $\mathcal{K}$ .

Intuitively, this means that the ropelength of a particular knot is the minimum amount of a unit thickness rope needed to tie that knot.

A main problem concerning the ropelength of a knot type is: For a given knot type  $\mathcal{K}$ , what is its ropelength (or a good estimate of it)? When the ropelength problem was first studied, the following problem served as a good motivational

“open question”: Can one tie a non-trivial knot with a one foot long rope of diameter one inch? In other word, is the smallest ropelength of all non-trivial knots less than or equal to 24 (keep in mind that the thickness defined here is the radius)?

## 2. Knots on the simple cubic lattice

A counterpart of the ropelength problem in a discrete setting is the problem concerning the minimum length of knots realized on the simple cubic lattice. Advantages of studying knots on the cubic lattice include:

- The minimum length of any given knot exists;
- A lattice knot can be made into a smooth thick knot. In general, if  $K$  is a lattice knot with knot type  $\mathcal{K}$  and the length of  $K$  is  $L(K)$ , then the ropelength of  $\mathcal{K}$   $R(\mathcal{K}) < 2L(K)$ . In other word, if you can realize a particular knot on the cubic lattice, then one also obtains an upper bound for the ropelength of the corresponding knot type;
- The converse of the above statement is also true: If  $L(\mathcal{K}) = m$ , then  $\mathcal{K}$  can be realized on the cubic lattice with a length at most  $12m$  (Diao, Ernst and Rensburg 1999 [12]).

Thus the ropelength of a knot type and its minimum length on the cubic lattice are equivalent up to a scalar multiplication. Various bounds on the ropelength of knots can be obtained by studying the length required to realize these knots on the cubic lattice.

## 3. Global minimum ropelength of non-trivial knots

Let  $R_g$  be the global minimum ropelength for all non-trivial knots. The first “big open question” regarding ropelength asks whether  $R_g \leq 24$ ? The following is a brief history showing the progress on this problem.

- Litherland et al (1999):  $R_g \geq 5\pi \approx 15.708$  [16];
- Cantarella, Kusner and Sullivan (2002):  $R_g \geq 2(2 + \sqrt{2})\pi \approx 21.452$  [4];
- Diao (2003):  $R_g > 24$  [6];
- Denne, Diao and Sullivan (2006):  $R_g > 31.32$  [7].

The main ideas in the proof of  $R_g > 31.32$ : Using the fact that every  $C^{1,1}$  non-trivial knot has an alternating essential quadrisecant (Denne 2004), combined with a careful analysis of the minimum length of each arc of the knot separated by the intersection points on the alternating quadrisecant.

In the case of lattice knots, it is known that the minimum length of any non-trivial knots realized on the cubic lattice is 24 [5]. The proof is based on a combinatorial approach. This has recently been extended to establish the minimum length for the knots  $4_1$  and  $5_1$ : the minimum length for  $4_1$  is 30 (Ishihara 2009) and the minimum length for  $5_1$  is 34 (Ishihara, Shimokawa and Yamaguchi 2009).

## 4. General lower bounds on ropelength in terms of crossing number

Given a knot (type)  $\mathcal{K}$ , the question here asks for a lower bound of its ropelength in terms of its minimum crossing number  $Cr(\mathcal{K})$ . The following is a brief summary of some progress concerning this problem:

- $R(\mathcal{K}) \geq 4\sqrt{\pi Cr(\mathcal{K})} = \frac{1}{2}\sqrt{64\pi Cr(\mathcal{K})}$  (Buck and Simon 1999 [1]);
- $R(\mathcal{K}) \geq \frac{1}{2} \left( 17.334 + \sqrt{17.334^2 + 64\pi Cr(\mathcal{K})} \right)$  (Diao 2003 [6]);
- $R(\mathcal{K}) \geq 1.105(Cr(\mathcal{K}))^{\frac{3}{4}}$  (Buck and Simon 1999 [1]);
- The  $3/4$  power in the ropelength lower bound formula  $R(\mathcal{K}) \geq 1.105(Cr(\mathcal{K}))^{\frac{3}{4}}$  is sharp. That is, there exists a family of infinitely many knots such that  $R(\mathcal{K}) \leq a(Cr(\mathcal{K}))^{\frac{3}{4}}$  for some constant  $a > 0$ . (Diao and Ernst 1998, Cantarella, Kusner and Sullivan 1998 [8, 3]);
- There exists a family of infinitely many prime knots such that  $R(\mathcal{K}) \geq b \cdot Cr(\mathcal{K})$  for any  $\mathcal{K}$  in this knot family, where  $b > 0$  is some constant (Diao, Ernst and Thistlethwaite 2003 [13]).

The proves of the first three results above were all based on the analysis of the average crossing number of the knot  $K$  expressed as the following double integral

$$\frac{1}{4\pi} \int_K \int_K \frac{|\dot{\gamma}(t), \dot{\gamma}(s), \gamma(t) - \gamma(s)|}{|\gamma(t) - \gamma(s)|^3} dt ds,$$

where  $\gamma(t)$  is an arc length parameterized equation for  $K$  (Freedman and He 1991 [15]). The other two results are obtained by direct construction and the last result means that the  $3/4$ -power lower bound is not a general upper bound for all knots.

## 5. Upper bounds on ropelength in terms of crossing number

Given a knot (type)  $\mathcal{K}$ , the question here asks for an upper bound of its ropelength in terms of its minimum crossing number  $Cr(\mathcal{K})$ . The following is a brief summary of some progresses concerning this problem:

- $R(\mathcal{K}) \leq d \cdot (Cr(\mathcal{K}))^2$  for some constant  $d > 0$ . In fact,  $R(\mathcal{K}) \leq 1.64(Cr(\mathcal{K}))^2 + 7.69Cr(\mathcal{K}) + 6.74$  (Cantarella et al [2]);
- $R(\mathcal{K}) \leq O((Cr(\mathcal{K}))^{\frac{3}{2}})$  (Diao, Ernst and Yu [14]);
- If  $\mathcal{K}$  can be realized by a closed braid with  $n$  crossings, then  $R(\mathcal{K}) \leq O(n^{6/5})$  (Diao and Ernst [10]);
- For many knots,  $R(\mathcal{K}) \leq O(Cr(\mathcal{K}))$ . For example, the family of all Conway algebraic knots, which includes all 2-bridge knots and Montesinos knots as well as many other knots (Diao and Ernst [9]);
- $R(\mathcal{K}) \leq O(Cr(\mathcal{K}) \ln^5(Cr(\mathcal{K})))$  for any knot  $\mathcal{K}$ . That is, the general upper bound of  $R(\mathcal{K})$  is almost linear in terms of  $Cr(\mathcal{K})$ . However, It remains open whether  $O(Cr(\mathcal{K}))$  is the general ropelength upper bound for any knot  $\mathcal{K}$  (Diao, Ernst, Por and Ziegler [11]).

The approaches/methods used in the proofs of the above results include the page presentation of a knot, divide and conquer technique used in graph theory and VLSI layout used in computer science, as well as direct constructions and some other results from graph theory.

## 6. Some open questions

- Prove or disprove the existence of infinitely many knots  $\{\mathcal{K}_n\}$  whose ropelength grows faster than  $O(Cr(\mathcal{K}_n))$ .
- Prove or disprove that any alternating knot  $\mathcal{K}$  has a ropelength at least of the

order  $O(Cr(\mathcal{K}))$ .

- A less ambitious version of the last question: find any alternative knot family  $\{\mathcal{K}_n\}$  with a small bridge number but with a ropelength at the order of  $O(Cr(\mathcal{K}_n))$ .

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**The effect of confinement on knotting and geometry of random polygons**

CLAUS ERNST

(joint work with Y. Diao, E. Rawdon, U. Ziegler)

In this talk we discuss equilateral random polygons in spherical confinement. The motivation to study such an equilateral random polygon model is the well known fact that generic material (long DNA chains) is often packed with a very high density in most organisms. For example, in the prototypic case of the P4 bacteriophage virus, the  $3\mu m$ -long double-stranded DNA is packed within a viral capsid with a caliper size of about  $50nm$ , corresponding to a 70-fold linear compaction [10]. Analysis of DNA extracted from bacteriophage P4 shows topologically interesting aspects: packed DNA is chirally organized and extraced DNA molecules are circles that are non-trivially knotted with very high probability [2]. Our works models the condensed DNA by equilateral polygons in confinement and investigates the influence of the restrictiveness of the confinement on topological and geometric aspects of the polygons. In this study no special packing mechanisms is used, but polygons are generated based on their probabilities.

Many theoretical aspects of equilateral random polygons without confinement are well understood. For example, the mean squared distance between two vertices on an equilateral random polygon of length  $n$  that is  $k$  vertices apart is  $k(n-k)/(n-1)$  and the mean squared radius of gyration of such a random polygon is  $(n+1)/12$  [11]. Additionally, certain measurements with a topological flavor such as the mean ACN (average crossing number) of an equilateral random polygon are also well researched [8, 1]. Unlike equilateral random polygons without confinement, the confined equilateral random polygons have not been thoroughly studied and there are many unanswered questions. The first issue is how to define the models to reflect the various packing properties the DNA or polymer chains may have. Once a confined random polygon model is defined, the next issue is determining the probability distributions of the random polygons based on the model, and the third issue is the actual generation of the random polygons in accordance with these (theoretical) probability distributions. In a series of papers, the presenter and his collaborators have developed algorithms for several models to generate equilateral random polygons that are confined inside a sphere of fixed radius [4, 5, 6].

This talk concentrates on sample data generated with the model presented in [5]. The model can be described as follows: Consider equilateral random polygons that are “rooted” at the origin and assume that there is an algorithm that samples such objects with uniform probability. Now consider a confinement sphere  $S_R$  of radius  $R \geq 1$  and with center at the origin. Only those sampled equilateral random polygons are kept which are contained in the confinement sphere  $S_R$ . Using this algorithm a large sample of random polygons was generated of lengths ranging from 10 steps to 90 steps in increments of steps of 10. The confinement radii range from  $R = 1$  to  $R = 4.5$ . The total sample space consists of 162 sets each containing 10,000 polygons for a total of 1,620,000 random polygons.

For each polygon various geometric quantities such as curvature, torsion, the average crossing number (ACN), and the writhe are computed as well as the HOMFLYPT polynomial. (For information on knot polynomials see any standard book in knot theory [3].) The latter was used to determine the knot type of each polygon. This generates some (hopefully few) knot identification errors due to the fact that there exist different knot types with identical HOMFLYPT polynomials. If there are two knots  $K_1$  and  $K_2$  with identical HOMFLYPT polynomial and  $Cr(K_1) < Cr(K_2)$  then we identify the knot as  $K_1$ .

These computations generates a wealth of data whose evaluation is still in progress. Figures 1 and 2 give examples of the effects of the confinement radii  $R$  on some topological and geometric properties of the random polygons. In Figures 1 and 2 the  $x$ -axis is the radius of confinement and there are 9 curves, one for each length of the polygons from length 10 (bottom) to length 90 (top).

For an unconfined polygon the mean total curvature is approximately  $n\pi/2 + 3\pi/8$  [9]. To isolate the excess curvature per edge due to knotting and confinement we compute an adjusted curvature  $c_{adj}$  from the total curvature  $c_{tot}$  of a polygon by using the following formula:  $c_{adj} = (c_{tot} - 3\pi/8)/n - \pi/2$ . The two curvatures  $c_{tot}$  and  $c_{adj}$  are shown in Figure 1. By looking at the curvature of unknotted polygons we concluded that most of the excess curvature  $c_{adj}$  is due to confinement and not due to knotting.

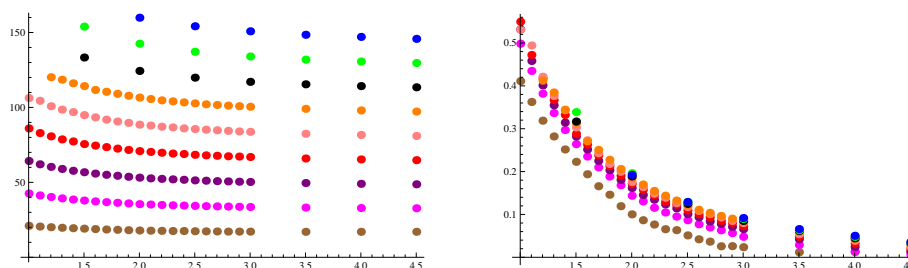


FIGURE 1. On the left, the total curvature  $c_{tot}$  of the polygons, on the right the excess curvature per edge  $c_{adj}$ .

Figure 2 shows the probability of knotting on the left and the ACN of knotted polygons on the right. This demonstrates clearly that confinement increases the knotting probability and the ACN even for relatively short random polygons. For example it is known [1] that the ACN of unconfined random polygons of length  $n$  is asymptotically  $3/16n \log(n)$ . However this formula gives only an ACN of about 76 for a random polygon of length 90. Figure 2 shows that already for polygons of length 30 the ACN exceeds 76 as the confinement radius approaches one.

Of special interest is the effect of confinement on the knot spectrum. At what confinement radius  $R$  and at what length  $n$  of the polygons are certain knots more likely? This analysis is ongoing and should be completed in the months to come. As far as future work is concerned, we already know that confinement alone cannot

reproduce the knot spectrum observed in the bacteriophage P4 capsid. In order to achieve this we need to add additional considerations to our model of confined random polygons. Obvious candidates are a stiffness parameter that makes large curvature angles less likely or giving a volume to the segments of our random polygons.

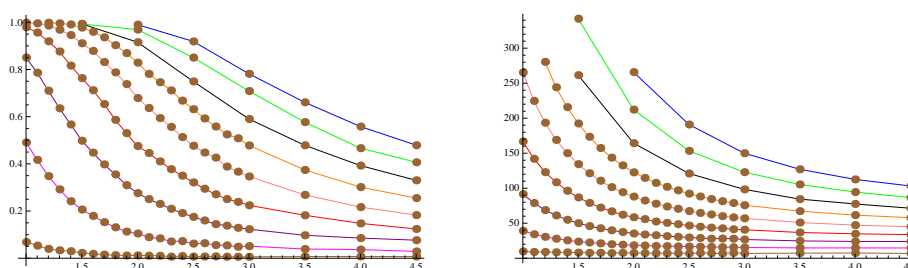


FIGURE 2. On the left, the probability of knotting. On the right the ACN of knotted polygons. The  $y$ -axis shows the probability of knotting and the ACN, respectively.

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## Distinguishing physical and mathematical knots and links

JOEL HASS

(joint work with Alexander Coward )

The theory of knots and links studies one-dimensional submanifolds of  $\mathbb{R}^3$ . These are often described as loops of string, or rope, with their ends glued together. Real ropes however are not one-dimensional, but have a positive thickness and a finite length. Indeed, most physical applications of knot theory are related more closely to the theory of knots of fixed thickness and length than to classical knot theory. For example, biologists are interested in curves of fixed thickness and length as a model for DNA and protein molecules. In these applications the thickness of the curve modeling the molecule plays an essential role in determining the possible configurations.

Two fundamental problems concerning physical knots and links are to show the existence of a *Gordian Unknot* and a *Gordian Split Link*. A Gordian Unknot is a loop of fixed thickness and length whose core is unknotted, but which cannot be deformed to a round circle by an isotopy fixing its length and thickness. A Gordian Split Link is a pair of loops of fixed thickness whose core curves can be split, or isotoped so that its two components are separated by a plane, but cannot be split by an isotopy fixing each component's length and thickness.

In recent joint work with Alexander Coward, we established the existence of a Gordian Split Link. We thus showed for the first time that the theory of physically realistic curves of fixed thickness and length is distinct from the classical theory of knots and links.

**Theorem 1.** *A Gordian Split Link exists.*

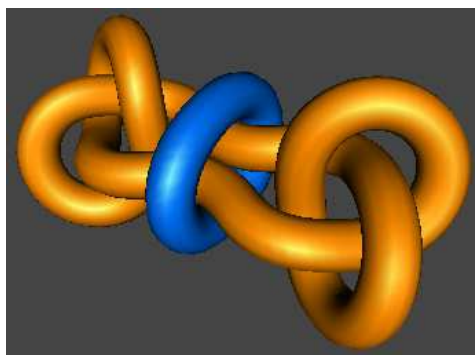


FIGURE 1. A Gordian Split Link.

The proof of Theorem 1 is by a construction of a link, illustrated in Figure 1, that can be split topologically but not physically. While this property is intuitively quite clear, its proof is not so simple, and involves new arguments involving isoperimetric inequalities for families of curves.

The existence of a Gordian Unknot remains open.

Theorem 1 is a consequence of the following result, which gives an explicit lower bound on the length required for  $L_1$ , the unknotted component of  $L$ , under the assumption that  $L$  can be split by a physical isotopy.

**Theorem 2.** *If there is a physical isotopy of  $L = L_1 \sqcup L_2$  that splits its two components, then the length of  $L_1$  must be at least  $4\pi + 6 \approx 18.566$ .*

Since the link  $L$  can be constructed with the length of the unknotted component  $L_1$  equal to  $4\pi + 4$ , this result implies Theorem 1. Details are available in [3].

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### Tabulation of prime knots by arc index

GYO TAEK JIN

(joint work with Hyuntae Kim)

Every knot can be presented on the union of finitely many half planes which have a common boundary line, so that each half plane contains a single arc of the knot. Such a presentation is called an arc presentation of the knot. The arc index of a knot is the minimal number of half planes needed in its arc presentations [2].

A grid diagram of a knot is a knot diagram constructed by finitely many vertical line segments and the same number of horizontal line segments such that at each crossing a vertical segment crosses over a horizontal segment. A grid diagram with  $n$  vertical segments is easily converted to an arc presentation on  $n$  half planes, and vice versa. Grid diagrams are useful in several ways. A slight modification of a grid diagram gives a front projection of its Legendrian imbedding. Grid diagrams are used to compute Heegaard Floer homology and Khovanov homology.

Various authors have determined the arc index of prime knots up to 11 arcs [1, 3, 4, 5, 6, 7]. In this work, we've tabulated prime knots of arc index twelve up to 16 crossings. This is achieved by generating grid diagrams of twelve arcs which contain all prime knots of arc index twelve. Among the prime knots with arc index

twelve, the torus knot of type (5,7) has the largest crossing number 28 and it is the only one with this crossing number.

Crossings	3-9	10	11	12	13	14	15	16
Prime knots with arc index 12	0	123	0	627	1412	3180	6216	7955

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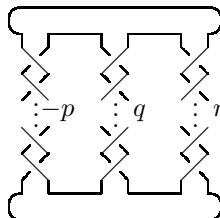
### Arc index of pretzel knots of type $(-p, q, r)$

GYO TAEK JIN

(joint work with Hwa Jeong Lee)

The arc index is equal to the crossing number plus two for alternating knots and alternating nonsplit links [1, 5]. For nonalternating prime knots and links, it is not bigger than the crossing number [3, 4].

We've determined the arc index of some nonalternating pretzel knots. A pretzel link of type  $(-p, q, r)$  is a knot if and only if at most one of  $p, q, r$  is an even number. We consider the cases that  $p, q, r \geq 2$ ,  $r \geq q$  and at most one of  $p, q, r$  is even.



**Theorem 1.** *Let  $\alpha(K)$  and  $c(K)$  denote the arc index and the crossing number of  $K$ , respectively.*

(1) If  $K = P(-2, q, r)$  is a knot with  $3 \leq q \leq r$ , then

$$\alpha(K) \leq c(K) - 1.$$

(2) If  $K = P(-p, 2, r)$  is a knot with  $p \geq 3$ ,  $r \geq 3$ , then

$$\alpha(K) = c(K).$$

(3) If  $K = P(-p, 3, r)$  is a knot with  $p \geq 3$ ,  $r \geq 3$ , then

$$\alpha(K) = c(K) - 1.$$

(4) If  $K = P(-p, 4, r)$  is a knot with  $p \geq 5$ ,  $r \geq 5$ , then

$$\alpha(K) = c(K) - 2.$$

(5) If  $K = P(-3, 4, r)$  is a knot with  $r \geq 7$ , then

$$c(K) - 4 \leq \alpha(K) \leq c(K) - 2.$$

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### Menger-type curvature in higher dimensions

SŁAWOMIR KOLASIŃSKI

For three points  $x$ ,  $y$  and  $z$  lying on a rectifiable curve  $\gamma$  in  $\mathbb{R}^n$  one defines the Menger curvature by the formula

$$c(z, y, z) = \frac{1}{R(x, y, z)} = \frac{4\mathcal{H}^2(\text{conv}(x, y, z))}{|x - y||y - z||z - x|},$$

where  $R(x, y, z)$  denotes the radius of the circumcircle of  $x$ ,  $y$  and  $z$ ,  $\mathcal{H}^2$  is the 2-dimensional Hausdorff measure and  $\text{conv}(x, y, z)$  denotes the convex hull of the set  $\{x, y, z\}$ . In 1999, Gonzalez and Maddocks [4] suggested the use of *curvature energies* given as integrals of  $c(x, y, z)$  in some power  $p$  to solve topologically constrained variational problem of finding the ideal shape (i.e. with the smallest “curvature”) of a given knot realized as a curve embedded in  $\mathbb{R}^3$ . This program has been adopted by many mathematicians - see e.g. [2, 3, 7, 8, 9].

Generalizing Menger curvature to higher dimensional objects is not as straightforward as it seems. If one defined the curvature to be the inverse of the radius of the smallest sphere passing through 4 points lying on a surface, then there exist  $C^\infty$ -smooth surfaces on which this curvature would be unbounded. In fact,

the graph of the function  $(x, y) \mapsto xy$  is an example of such surface (cf. [10, Appendix B]). Better definitions, which give rise to curvatures which are bounded whenever the points lie on a  $C^2$ -smooth surface, were given by Strzelecki and von der Mosel in [10] and [11].

In my talk I shall focus on the following *discrete curvatures*

$$\mathcal{K}(x_0, \dots, x_{m+1}) = \frac{\mathcal{H}^{m+1}(\text{conv}(x_0, \dots, x_{m+1}))}{\max\{|x_i - x_j| : i, j \in \{0, 1, \dots, m+1\}\}^{m+2}}$$

$$\text{and } \mathcal{K}_{tp}(x, y) = \frac{1}{R_{tp}(x, y)} = \frac{2 \text{dist}(x - y, T_x \Sigma)}{|x - y|^2}$$

defined for  $x, y, x_0, \dots, x_{m+1} \in \Sigma$ , where  $\Sigma$  is an  $m$ -dimensional, countably rectifiable subset of  $\mathbb{R}^n$ . It is worth noting that whenever  $\Sigma$  is  $C^2$ -smooth submanifold of  $\mathbb{R}^n$ , the curvatures  $\mathcal{K}$  and  $\mathcal{K}_{tp}$  are bounded. The *curvature energies* I consider are

$$\mathcal{E}_p^l(\Sigma) = \int_{\Sigma} \dots \int_{\Sigma} \sup_{x_l, \dots, x_{m+1} \in \Sigma} \mathcal{K}(x_0, \dots, x_{m+1})^p d\mathcal{H}_{x_0}^m \dots d\mathcal{H}_{x_{l-1}}^m$$

and  $\mathcal{E}_{tp,p}^l$  given by the same formula but with  $\mathcal{K}$  replaced by  $\mathcal{K}_{tp}$ . Note that, these energies are invariant under scaling if  $p = ml$ . Next, we define the class of “good” subsets of  $\mathbb{R}^n$  which contains e.g. all  $C^1$ -immersed manifolds and all finite sums of such immersions as well as their bilipschitz images. If  $p > ml$ ,  $\Sigma$  is a “good” set and  $\mathcal{E}_p^l(\Sigma) \leq E$  or  $\mathcal{E}_{tp,p}^l(\Sigma) \leq E$ , then  $\Sigma$  is in fact an embedded,  $C^{1,\alpha}$ -smooth submanifold of  $\mathbb{R}^n$ , where  $\alpha = 1 - \frac{ml}{p}$  (cf. [5, 11]). Moreover, there exist a scale  $R = R(E, m, l, p)$  and a constant  $C_H = C_H(E, m, l, p)$  such that for each  $x \in \Sigma$ ,  $\Sigma \cap \mathbb{B}(x, R)$  is a graph of some function  $f$ , such that  $\|Df(y) - Df(z)\| \leq C_H|y - z|$ . The exponent  $\alpha$  is optimal as a result of [1, 6].

Rigid control over the graph representation of  $\Sigma$ , resulting from finiteness of the curvature energy, allows, in consequence, to prove a compactness theorem for the class of normalized “good” sets with uniformly bounded energy. Then the existence of minimizers of the energy follows due to lower semi-continuity of both  $\mathcal{E}_p^l$  and  $\mathcal{E}_{tp,p}^l$  with respect to  $C^1$ -convergence.

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### Average geometric and topological properties of open and closed equilateral polygonal chains

KENNETH C. MILLETT

(joint work with Jorge A. Calvo, Akos Dobay, Laura Plunkett, Eric Rawdon, Andrzej Stasiak)

Equilateral polygonal chains, both open and closed, in 3-space provide fundamental models for the spatial structure of biological and physical macromolecules in addition to being of interest in their own right. The proof of the Frisch-Wasserman-Delbrück conjecture that the probability that a open or closed chain in 3-space goes to one as the length goes to infinity coupled with the advent of an appreciation of the role of knotting in DNA and proteins and, more generally, in polymeric materials has intensified the desire to understand their geometrical and topological structure and consequences.

The desire to determine the probability of knotting of closed polygonal  $n$ -gons lead to the development of methods to randomly sample them and the need to prove that the proposed algorithms did so. For example, in 1994 [2], we proved that the **polygonal fold method** provides one way to create a Markov Chain Monte Carlo,  $MC^2$  sampling algorithm. Underlying this theorem is the description of closed equilateral  $n$ -gon as an ordered list of  $n$  unit “edge” vectors, i.e. points in the unit 2-sphere, subject to the requirement that they sum to the zero vector and that they determine an embedded polygon. The elementary step of the polygonal fold method is to randomly select two of its vertices and to randomly rotate one to they segments they determine through a random angle to create a new polygonal conformation, checking that it is embedded. Another widely used method is the **crankshaft method** in which one randomly selects two edge vectors, employs them to determine an isosceles triangle with is randomly rotated about its base to define two new vectors which then replace the original pair. The result is a new polygonal configuration which we proved, [5] also creates a  $MC^2$  sampling method. The *HOMFLY* [3] polynomial knot invariant is then computed for each of the generated conformations and employed as a surrogate for the knot type

identity to estimate the proportion of configurations of each type as a function of the number  $n$  of edges for closed chains.

For open chains, the challenge is quite different as it is very easy to generation random samples, just take a sequence of random unit vectors and confirm that the resulting chain is embedded there being no closure constraint. The identification of the knot type, however, is a matter that lead to a variety of approaches and associated problems. In an effort to address these issues, we proposed a new method in 2005 [1, 4]. One determines the center of mass of the chain, placing unit mass at each vertex, and closes the initial and terminal vertices to a single point on a sphere of extremely large radius (compared to the diameter of the conformation). The resulting closed chain is, with probability one, embedded and thereby determines a knot type associated to the closure point. This process is locally constant and defined almost everywhere thereby allowing to determine its knotting spectrum, that is the distribution of proportions of the sphere associated to each of the finitely many knot types. If one type occurs more than half the time, one designates that as being the knot type of the open chain. In practice one estimates the spectrum by considering the closures to an appropriately large number of uniformly distributed points on the sphere.

The ability to determine the knotting of an open chain enables one to identify the locus, scaled and shape of knotting in knotted open and closed polygonal chains [6] including proteins [7]. In addition, one is now able to locate slipknots, i.e. knotted subchains contained in unknotted subchains, which are now known to exist in protein structures and occur with probability going to one as the number of edges in a walk or equilateral polygon goes to infinity [9]. We have applied these methods to study the existence, scale, and dynamic persistence of knots in open chains in the simple cubic lattice under “**inchworm**” moves which we have proved provide an ergodic sampling of embedded configurations. Intrinsic to embedded chains in the lattice is an excluded volume that has important consequences for the character of these structures. Interested in evaluating the consequences of excluded volume in 3-space chains, Laura Plunkett [8] has developed the ergodic **double reflection sampling method** that conserves the desired excluded volume of configurations during the sampling.

By employing these methods we are able to determine the dependence the presence of knots and slipknots in open and closed polygonal chains on the number of edges and, with Plunkett’s  $MC^2$  sampling method, on the excluded volume. Among other properties one is able to study are the squared radius of gyration, diameter, end-to-end distance or, for example, the persistence of knots in lattice walks under inchworm dynamics.

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### Min-max theory and the energy of links

ANDRE NEVES

(joint work with Ian Agol and Fernando Marques)

Let  $\gamma_i : S^1 \rightarrow \mathbb{R}^3$ ,  $i = 1, 2$ , be a 2-component link. The *Möbius cross energy* of the link  $(\gamma_1, \gamma_2)$  is defined to be

$$E(\gamma_1, \gamma_2) = \int_{S^1 \times S^1} \frac{|\gamma_1'(s)| |\gamma_2'(t)|}{|\gamma_1(s) - \gamma_2(t)|^2} ds dt.$$

The Möbius energy has the remarkable property of being invariant under conformal transformations of  $\mathbb{R}^3$  [1]. In the case of knots other energies were considered by O'Hara [5].

It is not difficult to check that  $E(\gamma_1, \gamma_2) \geq 4\pi |\text{lk}(\gamma_1, \gamma_2)|$ , where  $\text{lk}(\gamma_1, \gamma_2)$  denotes the linking number of  $(\gamma_1, \gamma_2)$ . This is an immediate consequence of the Gauss formula:

$$\text{lk}(\gamma_1, \gamma_2) = \frac{1}{4\pi} \int_{S^1 \times S^1} \frac{\det(\gamma_1'(s), \gamma_2'(t), \gamma_1(s) - \gamma_2(t))}{|\gamma_1(s) - \gamma_2(t)|^3} ds dt.$$

By considering pairs of circles which are very far from each other, we see that the cross energy can be made arbitrarily small. If the linking number of  $(\gamma_1, \gamma_2)$  is nonzero, the estimate says that  $E(\gamma_1, \gamma_2) \geq 4\pi$ . It is natural to search for the optimal configuration in that case.

It was conjectured by Freedman, He and Wang [1], in 1994, that the Möbius energy should be minimized, among the class of all nontrivial links in  $\mathbb{R}^3$ , by the stereographic projection of the standard Hopf link. The standard Hopf link  $(\hat{\gamma}_1, \hat{\gamma}_2)$  is described by

$$\hat{\gamma}_1(s) = (\cos s, \sin s, 0, 0) \in S^3 \quad \text{and} \quad \hat{\gamma}_2(t) = (0, 0, \cos t, \sin t) \in S^3,$$

and it is simple to check that  $E(\hat{\gamma}_1, \hat{\gamma}_2) = 2\pi^2$ . Here we note that the definition of the energy and the conformal invariance property extend to any 2-component

link in  $\mathbb{R}^n$  [3]. A previous result of He proved that the minimizer must be isotopic to a Hopf link [2].

In the talk I explained how to prove this conjecture using the min-max theory of minimal surfaces.

We now briefly sketch the proof. For any link  $(\gamma_1, \gamma_2)$  in  $\mathbb{R}^3$ , we associate a continuous 5-parameter family of surfaces (integral 2-currents with boundary zero, to be more precise) in  $S^3$  such that the area of each surface in the family is bounded above by  $E(\gamma_1, \gamma_2)$ . This family is parametrized by a map  $\Phi$  defined on  $I^5$ , and is constructed so that

- $\Phi(x, 0) = \Phi(x, 1) = 0$  (trivial surface) for any  $x \in I^4$ ,
- $\Phi(x, t)$  is an oriented round sphere in  $S^3$  for any  $x \in \partial I^4$ ,  $t \in [0, 1]$ ,
- $\{\Phi(x, t)\}_{t \in [0, 1]}$  is a homotopically nontrivial sweepout of  $S^3$  for any  $x \in I^4$ ,
- $\sup\{\text{area}(\Phi(x, t)) : (x, t) \in I^5\} \leq E(\gamma_1, \gamma_2)$ .

This map  $\Phi$  has the crucial property that its restriction to  $\partial I^4 \times \{1/2\}$  is a homotopically nontrivial map into the space of oriented great spheres, which is homeomorphic to  $S^3$ . Therefore the min-max theory developed in [4] shows that

$$2\pi^2 \leq \sup\{\text{area}(\Phi(x, t)) : (x, t) \in I^5\} \leq E(\gamma_1, \gamma_2)$$

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### Three topics in knot energies

JUN O’HARA

#### 1. HÖLDER–LIPSCHITZ MIXED CONTROL

Recently, Marta Szumańska, Paweł Strzelecki, and Heiko von der Mosel [7] showed that the boundedness of the *integral Menger curvature* imposes geometric constraints called *diamond property* on knots, where the integral Menger curvature of a knot  $K$  is given by  $\mathcal{M}_{p'}(K) = \iiint_{K^3} dx dy dz / R(x, y, z)^{p'}$ , where  $R(x, y, z)$  is the radius of the circle through  $x, y$ , and  $z$ . We have quite similar situation when some type of the  $(j, p)$  *energy* is bounded, where the  $(j, p)$  energy [9] is given by  $E^{j,p}(f) = \iint_{S^1 \times S^1} \left( |f(s) - f(t)|^{-j} - |s - t|_{S^1}^{-j} \right)^p ds dt$ , where  $j$  and  $p$  must satisfy

$jp \geq 2$  and some other conditions so that the functional is well-defined, and  $f$  is an embedding from  $S^1 = \mathbb{R}/\mathbb{Z}$  into  $\mathbb{R}^3$  which is parameterized by the arc-length. In both cases, we use “*sub-critical*” parameters for the functionals,  $p' > 3$  or  $jp > 2$ , so that the functionals have more restrictive effects on knots than scale-invariant ones. What is essential is the boundedness of both Hölder and Lipschitz norms. To be precise, if the integral Menger curvature or  $(j, p)$  energy is bounded above, then we have

$$(1) \quad |f(s) - f(t)| > C_L |s - t|_{S^1}, \quad |f'(s) - f'(t)| < C_H |s - t|_{S^1}^\alpha$$

for some  $0 < \alpha < 1$ ,  $C_H > 0$ , and  $1 \geq C_L > 0$ , where  $|s - t|_{S^1}$  denotes the (shorter) arc-length between  $s$  and  $t$  in  $S^1$ . This bound gives the control of the variation of the tangent vector on short subarcs and of the closest approach between pairs of distant subarcs, in other words, a knot cannot make a sudden turn in a short subarc, whereas a pair of distant strands cannot be very close to each other.

Let  $\mathcal{S}^{HL}(\alpha, C_H, C_L)$  be the set of knots that satisfy the condition (1). If the Hausdorff distance between two knots in  $\mathcal{S}^{HL}(\alpha, C_H, C_L)$  is small then they are close with respect to  $C^1$ -topology and belong to the same knot type. We can also prove that there are finitely many solid tori  $\{N_i\}$  so that if  $f \in \mathcal{S}^{HL}(\alpha, C_H, C_L)$ , then, after a motion of  $\mathbb{R}^3$ ,  $f(S^1)$  can be contained in some  $N_i$  in a good manner [10]. If there is a sequence of knots in  $\mathcal{S}^{HL}(\alpha, C_H, C_L)$  which belong to a single knot type  $[K]$  then the limit of any convergent subsequence also belong to the same knot type<sup>1</sup>. These facts imply the existence of the energy minimizers in each knot type since there is no fear of having pull-tight phenomena, and the finiteness of knot types under any threshold of the energy.

## 2. ENERGY MINIMIZING TORUS

This topic is concerned with the characterization of the Clifford torus, just like the one by the Willmore functional recently proved by Fernando C. Marques and André Neves [6].

Let  $S$  be an embedded surface in  $\mathbb{R}^3$  without boundary. Let  $k_1(x)$  and  $k_2(x)$  be principal curvatures at a point  $x$  on  $S$ ,  $\Delta(x)$  given by  $\Delta(x) = (k_1(x) - k_2(x))^2$ , and  $K$  the Gauss curvature;  $K = k_1 k_2$ . Then the *surface energy in the sense of David Auckly and Lorenzo Sadun* [2] is given as follows:

$$(2) \quad \begin{aligned} V(x; S) &= \lim_{\varepsilon \rightarrow 0} \left( \int_{S \setminus B_\varepsilon(x)} \frac{d^2 y}{|x - y|^4} - \frac{\pi}{\varepsilon^2} + \frac{\pi \Delta(x)}{16} \log(\Delta(x) \varepsilon^2) + \frac{\pi K(x)}{4} \right), \\ E(S) &= \int_S V(x; S) d^2 x, \end{aligned}$$

where  $d^2 x$  and  $d^2 y$  mean the volume elements of  $S$ . The factor  $\Delta(x)$  in the log term of  $V(x; S)$  is put to make the resulting energy scale invariant. Auckly and Sadun proved that this energy  $E(S)$  is invariant under Möbius transformations [2]. We remark that if  $S$  is not embedded then  $E(S) = +\infty$ .

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<sup>1</sup>This statement has been improved by John Sullivan’s comment at the talk

**Theorem** [5]. *Let  $T_R$  be a torus of revolution whose generating circle has radius 1 and center at distance  $R$  ( $R > 1$ ) from the axis of revolution. Then  $E(T_R)$  attains the minimum only at  $R = \sqrt{2}$ . Namely, among Dupin cyclides, only the images of a stereographic projection of the Clifford torus give the minimum energy.*

**Problem.** (Energy version of the Willmore conjecture) Is it true that if  $S$  is an immersed torus in  $\mathbb{R}^3$  then  $E(S) \geq E(T_{\sqrt{2}})$  and the equality holds if and only if  $S$  is the Clifford torus up to Möbius transformations?

### 3. SYMPLECTIC MEASURE OF A 2-COMPONENT LINK

This topic is concerned with the characterization of the “best Hopf link”, just like the one by the Möbius cross energy given by Ian Agol, Marques, and Neves ([1]).

Let  $L = K_1 \cup K_2$  be a link in  $S^3$ . Then the product torus  $K_1 \times K_2$  is contained in  $S^3 \times S^3 \setminus \Delta$ , where  $\Delta$  is the diagonal. We can use two structures of  $S^3 \times S^3 \setminus \Delta$  to assign geometric quantities to  $K_1 \times K_2$ .

First is the symplectic structure under the identification  $S^3 \times S^3 \setminus \Delta \cong T^*S^3$ . Let  $\omega$  be the pull-back of the canonical symplectic form of  $T^*S^3$ . Since it is exact,  $\int_{K_1 \times K_2} \omega$  vanishes, but  $\int_{K_1 \times K_2} |\omega|$  doesn't in general. Let it be denoted by  $A(K_1, K_2)$ , and call it the *symplectic measure* of the link  $L$ . Since  $\omega$  is invariant under diagonal action of Möbius transformations on  $S^3 \times S^3 \setminus \Delta$ , so is the symplectic measure.

The second is the semi-Riemannian structure (i.e. the indefinite metric with sign  $- - + + +$ ) of the Grassmannian under the identification  $S^3 \times S^3 \setminus \Delta \cong SO(4, 1)/SO(1, 1) \times SO(3)$ .

**Theorem** [11]. (1) *The symplectic measure  $A(K_1, K_2)$  is equal to the measure of the product torus  $K_1 \times K_2$  with respect to the natural indefinite metric of  $SO(4, 1)/SO(1, 1) \times SO(3)$  mentioned above.*

(2) *Let  $\theta_L(x, y)$  be the angle at  $y$  between  $L$  and the circle which is tangent to  $L$  at  $x$  that passes through  $y$ . Then the symplectic measure can be expressed as*

$$A(K_1, K_2) = 2 \int_{K_1} \int_{K_2} \frac{|\cos \theta_L(x, y)|}{|x - y|^2} dx dy.$$

(3) *The symplectic measure of a 2-component link takes its minimum value 0 if and only if  $L$  is the “best” Hopf link up to Möbius transformations, i.e.  $L$  is the image of a stereographic projection of*

$$\{(z, w) \in \mathbb{C}^2; |z| = 1, w = 0\} \cup \{(z, w) \in \mathbb{C}^2; z = 0, |w| = 1\} \subset S^3.$$

We remark that the finiteness of  $A(K_1, K_2)$  does not prevent each knot  $K_i$  from having self-intersections.

For a 2-component link type  $[L]$ , define  $A([L]) = \inf_{L' = K_1 \cup K_2 \in [L]} A(K_1, K_2)$ . Then, if  $L$  is a separable link or a satellite link of a Hopf link, then  $A([L]) = 0$ . On the other hand, if  $L = K_1 \cup K_2$  is a hyperbolic link each component of which

is a non-trivial knot, then there is no solid torus  $H$  so that  $K_1$  is contained in  $H$  and  $K_2$  in  $\mathbb{R}^3 \setminus H$ .

**Problem.** What is  $A([L])$ ? Is it positive when  $L$  is a hyperbolic link?

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### Knotted arcs in open chains, closed chains, and proteins

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(joint work with Kenneth C. Millett, Joanna I. Sułkowska, Andrzej Stasiak)

In traditional knot theory, knots are closed non self-intersecting loops. The closure condition traps the knotting in the curve so that the curve cannot change its “type of knotting” without passing a portion of the curve through itself. In contrast, what the general public calls knots, like knotted shoelaces and garden hoses, are not mathematically knotted since they have two free ends. Clearly, shoelaces and garden hoses contain entanglement; the question is how to classify that entanglement.

Beyond the simple curiosity of understanding knotting in open curves, there are potential applications in the sciences. There are many entangled chain-like open objects in nature (e.g. DNA, proteins, and polymers) and the knotting can determine physical properties of the objects. These considerations have motivated researchers to study knotting in open curves. While a variety of techniques have been proposed to classify the knotting in a frozen open configuration, we concentrate on a version inspired by writhe and the average crossing number. Namely, for each direction in the unit sphere  $S^2$ , we add edges from the endpoints of the configuration in the given direction and connect them at infinity [1, 2] to define a closed curve. This procedure then determines a probability distribution of knot types, the spectrum of which we consider the “knot type” of the open configuration.

We are motivated currently by two questions. First, given a closed knot configuration, what is the minimal length arc that creates the knotting in the closed curve? In analyzing random closed knot configurations, the presence of slipknots forces one to consider whether the knotting in a proposed minimal length knotted subarc persists as length is added to one or both ends. But slipknots can be added after the minimal knotted arc is created as well, so a rigorous definition becomes delicate. Second, we are interested in knotted proteins. Proteins need to fold quickly and reproducibly to be functional, so folding into a knot would seem to be a big disadvantage. The earliest papers found only shallowly embedded knots, and suggested that the knotting may not be present in the non-crystallized form of the protein [3, 4]. Later, deeply embedded knots were found, revealing that knotting can be a feature in protein structures (see, for example, [5, 6]). Recently, we showed that the entanglement profile in knotted proteins that have the same function in different organisms were remarkably similar despite large differences in amino acid sequence and evolutionary separation spanning hundreds of millions of years [7]. This suggests that knotting has a real function in proteins.

The analysis of knotting in open polygons is still early in its development. However, the application of the techniques have great potential in understanding how entanglement affects physical properties of chain-like macromolecules.

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### Regularity theory for knot energies

PHILIPP REITER

(joint work with Simon Blatt)

We focus on analytical properties of *knot energies*, i.e. self-avoiding functionals being bounded below, see O’Hara [14, Def. 1.1]. They are the central object of *geometric knot theory* which aims at investigating geometric properties of a given knotted curve in order to gain information on its knot type.

As one is first of all interested in distinguishing between different knot types, the fundamental idea is to model some repulsive “force” which prevents the curve from leaving the ambient knot class by forming a self-intersection. Moreover, one



hopes to retrieve a notion of “optimal shape”, having strands particularly wide apart, by minimizing the respective energy. Such a functional can in fact be seen as a measure of “entangledness”. Following the negative gradient flow of this functional should simultaneously “untangle” the curve and preserve its knot type.

Knot energies can help model repulsive forces of fibres, whenever self-interaction of strands should be avoided. Vice versa, attraction phenomena may also be characterized by *maximizing* a suitable energy, see [1] for a model in theoretic biology for the interaction between pairs of stiff filaments via cross-linkers.

The first example of a knot energy was defined by O’Hara [13]. It is the element  $E^{2,1}$  of the family

$$(1) \quad E^{\alpha,p}(\gamma) := \iint_{\mathbb{R}/\mathbb{Z} \times [-\frac{1}{2}, \frac{1}{2}]} \left( \frac{1}{|\gamma(u+w) - \gamma(u)|^\alpha} - \frac{1}{D_\gamma(u+w, u)^\alpha} \right)^p |\gamma'(u+w)| |\gamma'(u)| \, dw \, du.$$

Here  $\alpha, p > 0$ ,  $\alpha p \geq 2$ ,  $(\alpha - 2)p < 1$ , and  $\gamma \in C^{0,1}(\mathbb{R}/\mathbb{Z}, \mathbb{R}^n)$ . The quantity  $D_\gamma(u+w, u)$  measures the intrinsic distance between  $\gamma(u+w)$  and  $\gamma(u)$  on the curve  $\gamma$ .

While this energy family, and in particular the so-called “Möbius energy”  $E^{2,1}$ , received much attention, there was a lack of a characterization of finite-energy curves. A preliminary result on O’Hara’s energies addressed necessary conditions for finite energy. We could prove [5] that finite energy implies differentiability in the sub-critical case  $\alpha p > 2$  which fails in the critical (scale-invariant) case  $\alpha p = 2$ . Later on, Blatt was able to fully settle this problem by characterizing finite-energy curves in terms of Sobolev-Slobodeckii spaces [4].

With the aid of sophisticated geometric arguments highly relying on Möbius invariance, Freedman, He, and Wang [10] proved a regularity result for  $E^{2,1}$  stating that any local minimizer is  $C^{1,1}$ , i.e. it possesses a Lipschitz continuous tangent. Later on, using completely different techniques involving pseudo-differential operators, He [11] showed how to improve this result to  $C^\infty$  by setting up a bootstrapping process.

The latter result was the origin for studying the regularity of stationary points in the case of the one-parameter sub-family  $E^{\alpha,1}$ ,  $\alpha \in [2, 3)$ . Any stationary point of  $E^{\alpha,1}$  in the class of injective, arc-length parametrized curves, belonging to the fractional Sobolev space  $W^{\alpha,2}(\mathbb{R}/\mathbb{Z}, \mathbb{R}^n)$  with cube integrable curvature, is  $C^\infty$ -smooth [15, 16]. Furthermore, a rigorous proof of Fréchet differentiability is added.

However, it was not clear whether  $W^{\alpha,2} \cap W^{2,3}$  was the optimal space for starting the bootstrapping. In fact, this is not the case: the identification of the energy spaces by Blatt [4] led to a significant improvement of the regularity result, providing more elegant proofs and omitting any claim of initial regularity [7].

We do not expect this situation to carry over to the parameter range  $p > 1$  as these energies seem to be “degenerate”.

In a next step, we have been able to establish similar results for other knot energy families such as the *generalized tangent-point energies*

(2)

$$\text{TP}^{(p,q)}(\gamma) = \int_{\mathbb{R}/\mathbb{Z}} \int_{-1/2}^{1/2} \frac{|P_{\gamma'(u)}^{\top}(\gamma(u+w) - \gamma(u))|^q}{|\gamma(u+w) - \gamma(u)|^p} |\gamma'(u+w)| |\gamma'(u)| \, dw \, du.$$

Here  $P_{\gamma'(u)}^{\top} a := \left\langle a, \frac{\gamma'(u)}{|\gamma'(u)|} \right\rangle \frac{\gamma'(u)}{|\gamma'(u)|}$  and  $P_{\gamma'(u)}^{\perp} a := a - P_{\gamma'(u)}^{\top} a$  for  $a \in \mathbb{R}^n$  denote the projection onto the tangential and normal part along  $\gamma$  respectively. Originally, the tangent-point energies have been considered in the case  $p = 2q$  only where the integrand amounts to the  $(-q)$ -th power of the radius of the circle passing through  $\gamma(u+w)$  and being tangent to  $\gamma(u)$ . Unfortunately, similarly to O'Hara's energies for  $p > 1$ , these energies are degenerate.

However, in the non-degenerate sub-critical range  $p \in (4, 5)$ ,  $q = 2$  one can state the following regularity result: any stationary point of  $\text{TP}^{(p,2)}$  with respect to fixed length, injective and parametrized by arc-length is  $C^\infty$ -smooth [6]. Restricting to  $C^1$ -curves, our method of proof, which bases on Blatt's characterization of energy spaces [2], works completely without using the techniques developed by Strzelecki and von der Mosel [18].

Interestingly, many arguments employed for O'Hara's energies can also be applied to the generalized tangent-point energies. Therefore, albeit modeling different geometrical concepts, these two energy families are not too different from an analytical viewpoint.

Similar results can be proven for a generalized version of *integral Menger curvature* [8]

(3)

$$\text{intM}^{(p,q)} := \iiint_{\mathbb{R}/\mathbb{Z} \times [-\frac{1}{2}, \frac{1}{2}]^2} \frac{|\gamma'(u)| |\gamma'(u+v)| |\gamma'(u+w)|}{R^{(p,q)}(\gamma(u), \gamma(u+v), \gamma(u+w))} \, dw \, dv \, du, \quad p, q > 0,$$

where  $R^{(p,q)}$  denotes some variant of the circumcircle function. In the classical case  $p = q$ , Strzelecki, Szumańska and von der Mosel [17] already derived necessary conditions for finite energy which have been improved by Blatt [3], and Hermes [12] computed the first variation.

Although our method fundamentally relies on the sub-critical range on which we can make use of the continuity of  $\gamma'$ , the statement should also hold for the non-degenerate *critical case*. Together with Schikorra [9], we could establish a corresponding result for the Möbius-energy  $E^{2,1}$  that—using sophisticated methods from harmonic analysis—improves the above-mentioned results by Freedman, He, Wang [10] and He [11]. In light of the technical difficulties arising here we expect these situation for the respective elements  $\text{TP}^{(4,2)}$  and  $\text{intM}^{(7/3,2)}$  to be quite involved.

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### The symplectic geometry of polygon space

CLAYTON SHONKWILER

(joint work with Jason Cantarella)

The statistical physics of long-chain polymers such as DNA is based on modelling a polymer by a space polygon. Physicists then study the statistics of geometric and topological properties of the polygons with respect to various probability measures on the space of polygons. This is reasonably straightforward for linear polymers, but when the ends of the polymer join together to form a ring polymer, the closure condition imposes subtle global correlations between the individual edges and the analysis becomes considerably more difficult.

Numerical experiments have been the mainstay of this field for several decades (e.g. [9, 7, 12]), but even these experiments are hampered by the state of development of sampling algorithms for equilateral polygons. There exist a number

of Markov chain methods (see [1] for a survey) which appear to work fairly well in practice and which have mostly been proved to be ergodic, but their rates of convergence are unknown.

Our basic belief is that geometric structures on the moduli space of polygons can facilitate the search for good sampling algorithms. In earlier work [4] we used methods originally developed by the algebraic geometers Hausmann and Knutson [11] to give a fast new direct sampling algorithm for closed polygons with total length 2 (but varying edgelengths). In addition, this theoretical framework gave us the tools to prove several new exact results on the expectation of physically relevant geometric invariants of these polygons, such as their radius of gyration and total curvature [5].

The present work [6] is focused on fixed edgelength polygons (including equilateral polygons). To set notation, let  $\text{Pol}(n; \vec{r})$  be the moduli space of  $n$ -gons in  $\mathbb{R}^3$  with edgelengths given by the vector  $\vec{r} = (r_1, \dots, r_n)$ . The key point is that this space has a natural *symplectic* structure:

**Theorem 1** (Kapovich–Millson [13]). *Pol( $n; \vec{r}$ ) is the symplectic reduction of  $\prod_{i=1}^n S^2(r_i)$  by the Hamiltonian diagonal  $SO(3)$  action. In particular,  $\text{Pol}(n; \vec{r})$  is a  $(2n - 6)$ -dimensional symplectic manifold, and the measure induced by the symplectic volume form agrees with the standard measure.*

In fact, Kapovich and Millson proved that any triangulation of the standard  $n$ -gon yields a Hamiltonian action of  $T^{n-3}$  on  $\text{Pol}(n; \vec{r})$  where the angle  $\theta_i$  acts by folding the polygon around the  $i$ th diagonal of the triangulation (called a *bending flow* in symplectic geometry and a *polygonal fold* or *crankshaft move* [1] in random polygons). The induced moment map  $\mu : \text{Pol}(n; \vec{r}) \rightarrow \mathbb{R}^{n-3}$  records the lengths  $d_i$  of the diagonals in the triangulation. If the “fan triangulation” shown in Figure 1 is used, then the inequalities determining the moment polytope are

$$(1) \quad 0 \leq d_1 \leq r_1 + r_2 \quad \begin{array}{l} r_{i+2} \leq d_i + d_{i+1} \\ |d_i - d_{i+1}| \leq r_{i+2} \end{array} \quad 0 \leq d_{n-3} \leq r_n + r_{n-1}$$

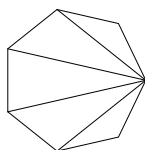


FIGURE 1. The fan triangulation of a polygon

The image of the moment map is a convex polytope called the *moment polytope* [3, 10]. Since the torus is half-dimensional (and hence the manifold is *toric*), the Duistermaat–Heckman theorem [8] implies that the pushforward of the symplectic measure on  $\text{Pol}(n; \vec{r})$  to the moment polytope is a constant multiple of Lebesgue measure.

We can now give a strategy for sampling fixed edgelength polygons. In general, when  $M^{2n}$  is a toric manifold with moment polytope  $P$  such that the moment map

can be inverted, we can construct a map  $\alpha : P \times T^n \rightarrow M$  which parametrizes a full-measure subset of  $M$  by “action-angle” coordinates. Moreover, this map is measure-preserving. Therefore, a general procedure for sampling a toric symplectic manifold uniformly with respect to its symplectic measure is to sample  $P$  and  $T^n$  independently and uniformly. In particular, since the symplectic measure and the standard measure agree on  $\text{Pol}(n; \vec{r})$ , we have

**Theorem 2** (with Cantarella [6]). *Polygons in  $\text{Pol}(n; \vec{r})$  are sampled according to the standard measure if and only if the diagonal lengths  $d_1, \dots, d_{n-3}$  are uniformly sampled from the moment polytope defined by the inequalities (1) and the dihedral angles  $\theta_1, \dots, \theta_{n-3}$  are sampled independently and uniformly in  $[0, 2\pi)$ .*

Note that these uniformity conditions give concrete criteria for evaluating the quality of *any* polygon sampling algorithm.

Since a polygon  $P \in \text{Pol}(n; \vec{1})$  is in *rooted spherical confinement* of radius  $r$  if each diagonal length  $d_i \leq r$ , the moment polytope for rooted sphere-confined polygons is determined by the inequalities (1) plus the additional inequalities  $d_i \leq r$  for all  $i$ . Thus, Theorem 2 easily extends to the case of confined polygons.

For small  $n$  the moment polytope can be sampled directly by decomposing it into standard simplices. For large  $n$  direct sampling seems challenging, but the moment polytope can certainly be sampled using the hit-and-run algorithm [2], which is a Markov chain algorithm known to produce approximately uniformly distributed sample points on arbitrary convex polytopes in  $\mathbb{R}^m$  in time  $O^*(m^3)$  [14]. In particular, we can sample fixed edgelenh  $n$ -gons in any chosen confinement by generating points in the  $(n - 3)$ -dimensional moment polytope using hit-and-run and then pairing each point with  $n - 3$  independent uniform dihedral angles. Figure 2 shows two equilateral 100-gons (not to scale) sampled using this algorithm.

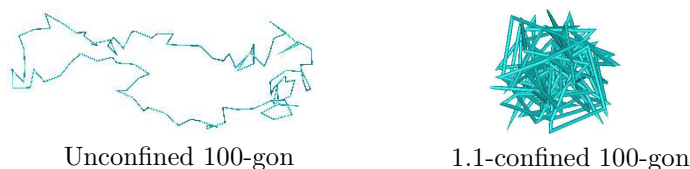


FIGURE 2. Two equilateral 100-gons with all edgelenhs equal to 1. The 100-gon on the left is completely unconfined, while the 100-gon on the right is confined by a sphere of radius 1.1.

To close, here are two open questions whose answers would give significant insight into the space of fixed edgelenh polygons:

- (1) Can the volume of the space of confined polygons be bounded below? If so, this should give lower bounds on the probability of complicated knots, since such knots will almost certainly be highly confined.
- (2) Is there a combinatorial description of the fan triangulation polytope (e.g. a simplicial decomposition)? Such a description would give a *direct* sampling algorithm for fixed edgelenh polygons.

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**Menger curvature as a knot energy**

PAWEŁ STRZELECKI

(joint work with Heiko von der Mosel and Marta Szumańska)

We consider closed rectifiable curves parametrized by arc length,  $\gamma: [0, L] \rightarrow \mathbb{R}^3$  with  $\gamma(0) = \gamma(L)$  and  $|\gamma'| = 1$  a.e. A priori, we allow  $\gamma$  to have self-intersections, multiply covered arcs etc. The *integral Menger curvature* of  $\gamma$  is defined as

$$\mathcal{M}_p(\gamma) = \iiint_{\gamma \times \gamma \times \gamma} \frac{dx \, dy \, dz}{R^p(x, y, z)},$$

where  $R(x, y, z)$  is the circumradius of three points  $x, y, z \in \mathbb{R}^3$ ; all integrations are w.r.t. the arc length on  $\gamma$ . This is one of the energies proposed by Gonzalez and Maddocks in the last section of [3]. (It is worth noting that  $\mathcal{M}_2(\cdot)$  has found remarkable applications in harmonic and complex analysis, see e.g. David [2].)

$\mathcal{M}_p$  is scale invariant for  $p = 3$ ; therefore, by an easy scaling argument, all polygons have infinite  $\mathcal{M}_p$  energy for  $p \geq 3$ . This is a first hint that the finiteness of

the integral Menger curvature  $\mathcal{M}_p(\gamma)$  for  $p \geq 3$  might enforce smoothing and self-avoidance effects. This is indeed the case, as the following two theorems confirm.

**Theorem 1.** *Assume that  $\mathcal{M}_p(\gamma) < \infty$  for some  $p \geq 3$ . Then  $\gamma(\mathbb{S}^1)$  is homeomorphic either to  $\mathbb{S}^1$  or to  $[0, 1]$ .*

(The condition  $\mathcal{M}_p(\gamma) < \infty$  does not imply the injectivity of  $\gamma$ . To see this, it is enough consider e.g. a doubly covered circle.)

**Theorem 2.** *If  $\mathcal{M}_p(\gamma) \leq E < \infty$  for some  $p > 3$  and  $\gamma$  is injective, then  $\gamma \in C^{1,\alpha}$  for  $\alpha = 1 - (3/p)$ , and*

$$|\gamma'(t) - \gamma'(s)| \leq C(p) \left( \iiint_{[s,t]^3} \frac{dx dy dz}{R^p(x, y, z)} \right)^{1/p} |s - t|^{1-(3/p)}$$

for all  $s, t \in [0, L]$  with  $|s - t| \leq \delta(p)\mathcal{M}_p(\gamma)^{-1/(p-3)}$ . Both constants  $C(p)$  and  $\delta(p)$  depend only on  $p$ , and not on  $\gamma$  itself.

Informally, if the integral Menger curvature  $\mathcal{M}_p(\gamma) \leq E$  for some  $p > 3$ , then there is a length scale  $d_0 = d_0(p, E)$  determined only by  $p$  and the energy bound  $E$  (and not by  $\gamma$  itself!) such that all the arcs of  $\gamma$  shorter than  $d_0$  are nearly straight. Besides, their bending, i.e. the rotation of the unit tangent to  $\gamma$ , is controlled by the local integral averages of  $1/R^p$ . Please note that Theorem 2 resembles closely the classic Sobolev–Morrey imbedding: we integrate over a three-dimensional ‘domain’,  $1/R$  replaces the curvature, i.e., plays the role of the second derivative, and we require the exponent  $p$  to exceed the ‘dimension’. The Hölder exponent  $\alpha$  is computed precisely according to the Sobolev–Morrey recipe.

There are three different parts the proof of Theorem 2. The first one is to obtain a control of the P. Jones’ *beta numbers* of the curve. For  $x \in \gamma$  and  $d > 0$ , set

$$\beta_\gamma(x, d) := \frac{1}{d} \inf \left\{ \sup_{y \in \gamma \cap B(x, d)} \text{dist}(y, G) : G \text{ is a straight line through } x \right\}.$$

In plain words,  $\beta_\gamma(x, d)$  measures how thin the *thinnest* cylinder is that contains the portion of  $\gamma$  in a given ball  $B(x, d)$  centered at  $x \in \gamma$ . An elementary argument based on energy estimates and continuity of  $1/R$  shows that  $\beta_\gamma(x, d) \leq C(p, E)d^\kappa$  where  $\kappa = (p - 3)/(p + 6)$ . The second part is to iterate this estimate as  $d$  goes to zero geometrically fast; this allows to conclude that  $\gamma \in C^{1,\kappa}$ . Finally, the third part of the proof is to improve the Hölder exponent from  $\kappa$  to  $\alpha = 1 - (3/p)$  by means of an iterative argument which is modelled on PDE techniques.

In the second step of the above proof we achieve in fact more than just showing  $\gamma \in C^{1,\kappa}$ . Let us explain that in more detail. For  $x \neq y \in \mathbb{R}^3$  and  $\varphi \in (0, \frac{\pi}{2})$  we denote by  $C_\varphi(x; y)$  the double with vertex at  $x$ , the cone axis passing through  $y$ , and opening angle  $\varphi$ ,

$$C_\varphi(x; y) := \{z \in \mathbb{R}^3 \setminus \{x\} : \exists t \neq 0 \text{ such that } \angle(t(z - x), y - x) < \frac{\varphi}{2}\} \cup \{x\}.$$

**Definition (the diamond property).** A curve  $\gamma$  has the *diamond property* at scale  $d_0$  and with angle  $\varphi \in (0, \pi/2)$ , in short the  $(d_0, \varphi)$ -*diamond property*, if and

only if for each couple of points  $x, y \in \gamma$  with  $|x - y| = d \leq d_0$  two conditions are satisfied: we have

$$(1) \quad \gamma \cap B(x, 2d) \cap B(y, 2d) \subset C_\varphi(x; y) \cap C_\varphi(y; x)$$

and moreover each plane  $a + (x - y)^\perp$ , where  $a \in B(x, 2d) \cap B(y, 2d)$ , contains exactly one point of  $\gamma \cap B(x, 2d) \cap B(y, 2d)$ .

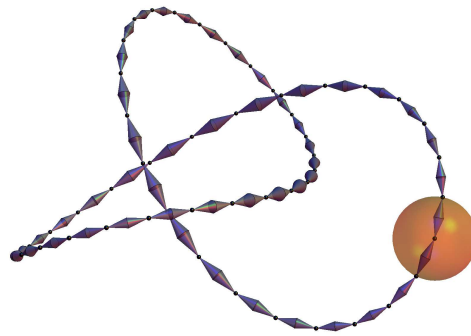


FIGURE 1. Small double cones with vertices on  $\gamma$  have pairwise disjoint interiors.

To obtain  $\gamma \in C^{1,\kappa}$ , we prove in fact that if  $\gamma$  satisfies  $\mathcal{M}_p(\gamma) \leq E$  for  $p > 3$ , then it has the  $(d, \varphi)$ -diamond property for all distances  $d \leq \delta(p)E^{-1/(p-3)}$  and all angles  $\varphi \geq C(p)E^{1/(p+6)}d^\kappa$ . Moreover, if the points  $x_1, x_2, \dots, x_N, x_{N+1} = x_1$  are evenly spaced along  $\gamma$ , at distances  $|x_i - x_{i+1}| \equiv d$  proportional to  $E^{-1/(p-3)}$ , then each ball  $B(x_i, d)$  contains *only* the arcs of  $\gamma$  coming from the two double cones with common vertex at  $x_i$  and the opening angle (say)  $1/4$ , see Figure 1. The arcs contained in all the other double cones but these two must not enter  $B(x_i, d)$ . All such double cones along the curve must have disjoint interiors. This observation can be used to prove the following result.

**Theorem 3.** *Assume that a curve  $\gamma$  of unit length satisfies  $\mathcal{M}_p(\gamma) \leq E < \infty$  for some  $p > 12$ . Then, the average crossing number of  $\gamma$  satisfies*

$$\text{acn}(\gamma) \leq C_1(p) + C_2(p) \left( \mathcal{M}_p(\gamma)^{1/p} \right)^{\frac{4}{3} \cdot \frac{p}{p-3}}.$$

The two constants  $C_i$  blow up as  $p \rightarrow 3$  but remain stable for  $p \rightarrow \infty$ . As  $p \rightarrow \infty$ ,  $\mathcal{M}_p(\gamma)^{1/p}$  tends to  $1/\Delta[\gamma]$ , the inverse of thickness of  $\gamma$ , which for curves of length one equals the ropelength. Thus, passing to the limit, we recover a weaker form of the estimate of  $\text{acn}(\gamma)$  in terms of ropelength, due to Buck and Simon [1],

$$\text{acn}(\gamma) \leq \frac{11}{4\pi} \cdot \left( \frac{1}{\Delta[\gamma]} \right)^{4/3}.$$



(Our constants are worse than  $11/4\pi$ . Examples due to Cantarella, Kusner and Sullivan – using thick  $(n, n - 1)$  torus knots – show that the above estimate is qualitatively sharp.)

Other applications of Theorem 2 and the shape control given by the diamond property include the following.

**Theorem 4.** *For each  $p > 3$  the integral Menger curvature  $\mathcal{M}_p$ , considered as a knot energy on the class of all rectifiable simple loops of fixed length, is strong (there are only finitely many different knot types under each energy level), minimizable (the energy minimum in each knot class is achieved) and tight (the pull-tight phenomenon cannot happen unless the energy blows up to infinity).*

Numerous questions concerning the integral Menger curvature are open, e.g.:

- (1) Is the round circle a unique minimizer of  $\mathcal{M}_p$  under fixed length constraints? (The numerical evidence suggests a positive answer).
- (2) Does the condition  $\mathcal{M}_3(\gamma) < \infty$  imply that  $\gamma'$  exists everywhere?
- (3) How regular are the local minimizers and stationary points of  $\mathcal{M}_p$ ?

One of the difficulties is that a local change of the curve leads to global changes of the integrand  $1/R$ .

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#### Minutes of the Open Problem Session

We briefly document the questions posed at the problem session on the evening of April 29.

- (1) **Pulling a hair tight.** Tight open knots are usually modelled mathematically with the two ends pulled straight in opposite directions. But physically, when a knot is tied tight in a hair or thread or cable, the ends seem to form a characteristic angle once they are released. Presumably the knot is held tight by friction, but each end straightens out to minimize elastic bending energy. What is an appropriate mathematical model for this variant of the ropelength problem? How does the angle between the ends depend on the knot type? [R. KUSNER]

- (2) **Ropelength-minimal knots.** Can we explicitly describe any ropelength-minimal (or even ropelength-critical) knot? (The explicit examples known so far are links in which each component is planar.) Is the minimizing trefoil piecewise  $C^2$  or even piecewise  $C^\infty$ ? [J. SULLIVAN]
- (3) **Ropelength vs. crossing number.** In terms of the crossing number  $n$  of a knot or link type, it is known that the minimum ropelength grows at least like  $n^{3/4}$  and at most like  $n(\log n)^5$ . The lower bound is sharp but the upper bound is probably not. Are there families for which the ropelength grows more than linearly in  $n$ ? Is there a better lower bound (perhaps linear in  $n$ ) if we restrict to alternating knots? [Y. DIAO]
- (4) **Menger vs. acn, higher-dimensional.** The Menger integral curvature  $\mathcal{M}_p(\gamma)$  of a space curve  $\gamma$  can be used to give upper bounds on geometric quantities like the average crossing number of  $\gamma$  and on invariants like stick number of its knot type. One can define similar energies  $\mathcal{M}_p(\Sigma)$  for  $k$ -submanifolds in  $\mathbb{R}^n$ . What are the analogous geometric quantities and topological invariants that might be bounded in terms of  $\mathcal{M}_p(\Sigma)$ ? [H. VON DER MOSEL]
- (5) **Loop number.** Given a knot diagram  $D$ , recall that an orientation-preserving smoothing of a crossing divides it into two loops. Define the *loop number* of  $D$  to be the minimum number of crossings that can be smoothed such that each of the resulting loops is a Jordan curve. That is, the remaining crossings are between distinct loops. Suppose  $D$  is a diagram of the unknot with writhe  $w$ . Is its loop number at least  $|w|$ ?  
 Now define the *loop number*  $\text{loop}(K)$  of a knot type  $K$  to be the minimum loop number over all diagrams for  $K$ . Clearly  $\text{loop}(K)$  is bounded above by crossing number. One can show that it is also bounded above by stick number minus 2 and thus also by a linear function of ropelength. Are there other relations between loop number and known knot invariants? [Y. DIAO]
- (6) **Average strangeness.** The writhing number of a space curve can be computed by averaging the signed crossing number of its projections over the sphere of possible projection directions. Can we get other interesting measurements of the geometry of space curves by averaging other diagram invariants over projection directions? For instance, Arnol'd gave three invariants of plane curves: strangeness,  $J^+$  and  $J^-$  which characterize an immersed plane curve up to ambient isotopy in the plane. So what does the "average strangeness" of a space curve tell you about the curve? [J. CANTARELLA]
- (7) **Critical unknots via complexity theory.** If we consider energy functionals on the space of loops in  $S^3$ , it seems to be the case that the space of unknots always contains numerous critical points. We can't prove this (yet), in part because techniques for establishing the existence of such minima seem to be hard to come by. We know by Hatcher's theorem that

the space of unknots in  $S^3$  is contractible, so unknotted critical points for knot energies are not dictated by the topology.

On the other hand, there are several suggestive results which lead one to believe that there may be a useful connection with complexity theory. Nabutovsky (1995) proved the existence of infinitely many critical “thick”  $S^5$ 's in  $\mathbb{R}^6$  using the algorithmic unrecognizability of the  $n$ -sphere in  $\mathbb{R}^{n+1}$  for  $n \geq 5$ . Freedman recently (2009) used the complexity theory assumption that  $P^{\#P} \neq NP$  (a much weaker assumption than  $P \neq NP$ ; the details don't matter much here) to derive a statement about the geometric complexity of links in “thin position” in  $S^3$ .

Can similar ideas be applied to show the existence of nontrivial local minima for interesting knot energies? Suppose one could prove a good lower bound on the computational complexity of unknot recognition. If there is only one energy-critical unknot for a given energy function  $F$ , then gradient descent with respect to  $F$  provides an algorithm for recognizing the unknot whose computational complexity is determined by the complexity of computing  $F$  and its gradient and the initial energy of an input configuration. If such an algorithm would recognize the unknot “too quickly”, this would show that  $F$  must have more than one unknotted critical point. [J. CANTARELLA]

- (8) **Polygons.** Is the space of embedded equilateral  $n$ -segment arms connected? Is the space of unknotted embedded equilateral closed  $n$ -gons connected? (This is known to be the case for  $n \leq 6$ .) How many knot types have stick number  $n$ ? (We know the answer only for  $n \leq 8$ .) [K. MILLETT]
- (9) **Random walks.** Consider an equilateral random walk (an open curve) with  $n$  edges of unit length inside the sphere of radius  $r \geq 1/2$ . Clearly the (total) curvature tends to  $\pi(n-1)$  as  $r \rightarrow 1/2$ . What happens to the torsion is not so clear. The conjecture is: The (unsigned total) torsion tends to  $(n-2)\frac{\pi}{3}$  as  $r \rightarrow 1/2$ ? Does the same apply for a (closed) *equilateral random polygon*, that is the average torsion angle tends to  $\frac{\pi}{3}$  as  $r \rightarrow 1/2$ ? [C. ERNST]
- (10) **Arc index for mutants.** Knot mutation preserves crossing number. Does it also preserve arc index? (This is true for alternating knots, since their arc index equals crossing number plus two.) [G. T. JIN]
- (11) **Frisch–Wasserman–Delbrück exponent.** The conjecture of Frisch, Wasserman and Delbrück (proved by Sumners–Whittington and Pippenger for lattice polygons and by Diao for equilateral polygons) states that the probability that an  $n$ -gon is unknotted goes to 0 as  $n \rightarrow \infty$ . In fact, Diao proved that the probability that an equilateral  $n$ -gon is unknotted is  $\leq e^{-n^\varepsilon}$  for some  $\varepsilon > 0$ . What is the constant  $\varepsilon$  in this statement? [C. SHONKWILER]
- (12) **Slipunknot.** It is known that the probability for an equilateral  $n$ -gon (or walk) to contain a *slip knot* goes to 1 as  $n \rightarrow \infty$ . (The same is true for polygons and walks in the lattice.) Since unknots are exponentially rare,

these results also hold when restricted to *knotted* polygons and walks. Do they also hold for *unknots*? [K. MILLETT]

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