The tangled web of self-tying knots

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Mathematician Leopold Kronecker stated "God created the integers, all else is the work of man," alluding to the fact that the natural numbers most likely arose from physical counting, as in one's fingers or goats in the pasture. Topology, however, is arguably a different creature altogether and may have had its own independent origins from the physical world in the ubiquitous knot—something that cannot be undone without using the free ends because the individual strands cannot move through each other (1). One imagines a primordial knot getting tied accidentally in Cro-Magnon times and then tugged at to no avail . . . perhaps eventually cut. Of course, knots went on to have their uses in early societies, still far from any theoretical considerations but very much related to their ability to bind or secure things such as animals, sails, hair, etc. Knotted strings were also used by the Inca civilization for record-keeping and possibly even communication (2), still a few centuries before Euler began counting bridge-crossings in Königsberg.

The discovery and synthesis of polymers, long-chain molecules such as DNA, has brought a renewed physical relevance and context to knots (3, 4), and with it a new direction of study. For instance, it has been shown by the electrophoresis of loop DNA that knot types from the simplest trefoil to a knot with 10 crossings can occur at the molecular level (5). Although knots were actually tied recently in surfactant nanotubes by micromanipulation (6), molecular knots mostly occur in a spontaneous way, driven by competition between a fluctuating exploration of space due to Brownian motion and the excluded-volume effect (the string cannot pass through itself). Knots are a natural and sometimes irreversible result of this process, and despite scientific study, it is still true that ". . . a complete statistical mechanical description of knots remains unattained" (7).

So, how exactly does DNA or anything like it become knotted? And are all of the knots equally easy to tie? In a recent issue of PNAS, Raymer and Smith (8) provide specific answers to some of these questions, including a macroscopic experimental study and a statistical model reproducing the main observations. Interestingly, their model connects back to the already well developed mathematical idea of a braid, one of several ways of deconstructing a knot (1, 9). This latest effort joins the long history of interactions between the physical and the mathematical in the study of knots, including famously the theory proposed by Lord Kelvin that atoms are vortex knots; this led to, among other things, the compilation of the first knot tables, with the hopes of explaining the periodic table of the elements (for an excellent discussion, see ref. 9).

Knot Theory vs. Knotted Things

Mathematically speaking, a knot is a closed loop that is tied up in some way in 3D space. One way of labeling a knot is by the minimum number of crossings it has; an index is then added to denote the distinct types of knot with those many crossings. For instance, ignoring issues of chirality, there is only one knot with three crossings (the trefoil 3_1) and one with four crossings (the figure eight 4_1), but there are three with six crossings (the 6_1, 6_2, and 6_3) (1).

Topologically, any rearrangements of a given knot that do not involve cutting and untying (by making free ends) are equivalent versions or representations of that knot; there is no issue of tight or loose in knot topology. Conversely, two knots are only considered different if they cannot be rearranged into each other in this way. However, one can always introduce additional things mathematically that distinguish between different representations of the same knot, such as being symmetric, as tight as possible, or minimal with respect to some global function such as total curvature or generalized "knot energy" (10). This has been done and has indeed helped to make knot theory more physically relevant to knotted filaments, molecules, strings, and other physical things (11). In dealing with an unwanted everyday knot, say in an extension cord, pulling on it often makes it worse by making it tighter. The question of a knot's smallest size or tightest configuration, known as its ideal configuration (10), is akin to the close packing problem for spheres, but with a topological twist.

In the physical world, however, it is usually strings with free ends, and not loops, that get knotted, either accidentally or with a purpose. Knots derive their importance by the way that they bind tightly, either by snagging on themselves or by attaching and holding something strongly. In terms of the one-dimensional coordinate along the string, a tight knot is nonlocal; points distant in arc length actually come into physical contact within the knot. It is at these points that the tension decreases because of the friction between the two parts of the string (12, 13), allowing for the main technological importance of certain knots: they hold. Exactly which knots do or do not slip off not only determines their utility but also plays a role in the probability of finding a particular knot tied spontaneously (8, 14, 15).

An extension of the definition of a topological knot was made by defining an "open" or "long" knot—meaning that a standard "closed" or "compact" knot is cut somewhere and the two free ends mapped out straight to infinity (16, 17). There can be several nonidentical "openings" for a given knot, depending on its symmetries; for the most symmetric class of knots, the torus knots, there is only one kind of open knot. For instance, there is only one open knot realization of the 6_1 but several for the 6_3. These open knots are closer to what can tie and untie (in a string or chain) (14, 18) and what was studied by Raymer and Smith (8).

Spontaneous Knotting—Not So Random

The fact is that open knots are everywhere. Although the classic example of a knotted phone cord may soon become a dimly remembered problem of an old technology, the fundamental ubiquity of knots comes from the fact that they tie themselves: knots are generated by the combination of a long string with some sort of random motion. This is a sort of derivative law of nature stemming from the Second Law of Thermodynamics (maximize entropy) as applied to long floppy things: Long Things Get Tangled. Some of you may have experienced this as part of the 1% of the population with a knotted umbilical cord at birth (19). Perhaps more readily, put a piece of twine in your pocket for a day or two and see for yourself what a tangle you may weave.

Thus, the random motions in everyday life mimic the effects of Brownian

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motion on long molecules—spontaneous knots writ large. There have been a number of recent studies on the dynamics of spontaneous knotting in the macroscopic world, in either a shaken hanging chain (14) or a chain bouncing on a vibrating plate (18, 20). However, the study by Raymer and Smith (8) is remarkable for the sheer scope of its statistics: $>$3,000 knots were tied. Among the issues now coming to light is that spontaneous knotting is apparently not a random process. Whereas an initial, naive hypothesis would be that the distribution of observed knots will be the same as if drawn by a random walk (this is a common modeling assumption), further reflection indicates why this might not be true. As Raymer and Smith show, the probability of spontaneous knotting and the distribution of knot types are determined by the tying process itself: the mechanics by which the free end threads itself through the other parts, and the physics of the string that puts it in that position before the knot is tied.

Their experiments involve shaking a string of various lengths in a closed box, then removing it and looking at the knots. Of course, it seems reasonable that the longer the string, the more likely it will tie itself up, but surprisingly, they find that the probability of knotting stops increasing at some length; this was also observed independently for a bouncing chain (20). The reasons for this resistance to knotting are dynamic: the string was too stiff or otherwise did not have enough room to move about in the box (8). This may have implications for the knottedness of confined DNA. And if you don't want the drawcords on your venetian blinds to knot themselves up, get some stiffer cord—or a smaller room.

Another experimental surprise came in the types of self-tied knots that were seen: "prime" knots were almost always observed, meaning only one big tangled knot, as opposed to several linked "composite" knots (1). Again, a random hypothesis would have predicted both kinds, something that is also often assumed in modeling. These experimental observations are reproduced in the model proposed by Raymer and Smith (8): a statistical treatment of the dynamics of the free end as it passes around loops in the string, which are represented mathematically by the braid structure of the knot (1, 9). In this model, the knot forms in two stages: First, a loop or series of loops come together, and then the free end finds its way through the tangle. This is treated as an "equilibrium" process, in that a rate of untying is also included by the opposite process: unbraiding by the free end. In other physical systems, different untying mechanisms have been observed, such as slipping (14, 15) or a diffusion-like process (18). All of these processes should be included in developing a Physical Theory of Knots, meaning essentially the proper mechanics and dynamics of knotted things. Fundamentally, these are all answers to the following question: Besides its topology, what other characteristics does a physical knot have?

The fundamental ubiquity of knots comes from the fact that they tie themselves.

Like caging a tiger or trapping a single atom for study, Raymer and Smith (8) have isolated a string in a small box and studied the statistics of its spontaneous knotting in detail. Future implications extend in both directions: mathematically, one wonders whether new results will spring from the knot statistics implicit in this braid-move model, while physically any number of complicating factors could be included next. Would a prime knot pre-tied at the center of the string (either tightly or loosely) induce or inhibit further knotting? Would two strings more readily tie together or individually self-tie? More importantly, will these observations turn out to be universal for physical knots, or will there be several different types of self-tying knots? Are there universal laws for the dynamics of knots? There is much to be done. It seems increasingly clear that the study of physical knots has come into its own as an experimental science.

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