Knots and Links

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Knots appear in a variety of contexts in physics, chemistry and biology. This article is an introduction to the science of knots and links for the uninitiated and it outlines why scientists find them fascinating.

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1. Knotted Fish

Think of an organism that has four hearts, one nostril, no stomach but with teeth on its tongue! This may seem like creature out of a science fiction story, but a fish with all these attributes exists. It is the *hagfish*, which is one of the lowest forms of fish and is an archaic (very old) form of life. It can secrete a thick slime on its skin, which makes the fish very slippery to hold. Because of this, it is also known as the *slime eel*. The hagfish usually burrows into either dead or live fish and eats the flesh and internal organs. It takes hold of the flesh using its teeth and pulls it out. The most surprising thing about the hagfish is that, if it needs extra leverage to pull the flesh out, it loops itself into a *knot* and presses the knot against the body of the prey, as shown in *Figure* 1. The knot that it makes is known as the half hitch. If you take hold of the hagfish, it would then secrete the slime and use the knot mechanism to pull itself out. Once free, the fish has to get rid of the slime, as otherwise, its gills and nostril would be blocked with the slime and it would suffocate. This too, it does, by moving the knot from one end of it to the other. It can form not only the half hitch, but also the figure eight knot. An old article by Jensen, gives more details on the hagfish [1].

Figure 1. The hagfish bites into the prey, knots itself up, and uses the knot for leverage for pulling the flesh out. (taken from reference [5]).

2. Mathematics of Knots

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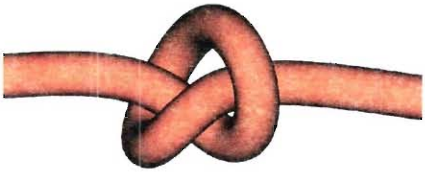
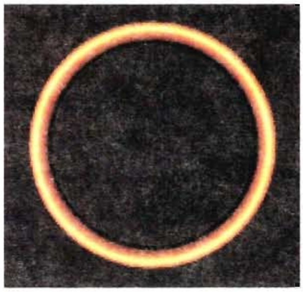
Knot, link, molecular knot, knot polynomial, catenanes.

Every one of us has made the half hitch knot (see *Figure* 2) on a string. Mathematicians, however, prefer their





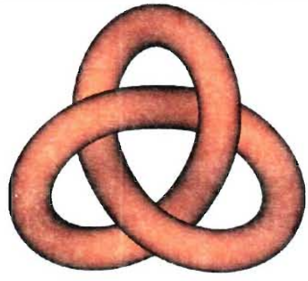
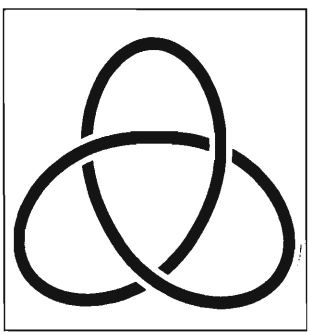


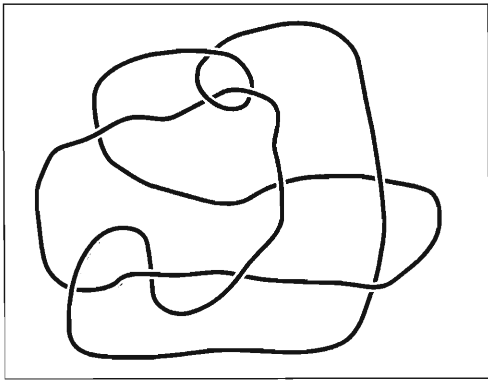
Figure 2(left). The half hitch, which is converted into a trefoil knot by joining the two ends to form a loop.
Figure 3 (center). The unknot.
Figure 4 (right). The trefoil, which is denoted as 3_1, as it has the crossing number three.

knots to be loops. The reason is simple. Moving one of the loose ends of the string in *Figure* 2 through the knot can untie it easily. This can be avoided if the two ends are joined together to form a loop. Then the knot is embedded in the string for ever. The simplest such "mathematician's knot" is obtained if one takes the two ends of a straight string and joins them together to form a simple loop, and this is called the unknot (see *Figure* 3). The knot obtained by joining together two ends of the knotted hagfish shown in *Figure* 4 is known as the trefoil. It is the simplest nontrivial knot and has the interesting property that it is not superimposable on its mirror image. This means that if one had a substance, whose molecules are made of a long chain, looped and knotted to form the trefoil, then the substance would be optically active. The trefoil is a three dimensional object, but it can be easily represented on two-dimensional paper. Such a representation would have crossings, which are represented by interrupting the line that represents the lower strand (see *Figure* 5).

Figure 5. Two dimensional representation of the trefoil. Note that at each intersection, the lower strand is represented by a line that is broken.



Two knots are considered equivalent (same) if one can be deformed into the other. Obviously, one is not allowed to cut the loop and rejoin. Thus the knot in *Figure* 6 is equivalent to the unknot. A characteristic of a knot is the crossing number. The unknot has no crossing, but its equivalent representation shown in the *Figure* 6 has ten crossings. The minimum number of crossing with which a knot can be represented in two dimensions is known as the crossing number. The trefoil thus has the



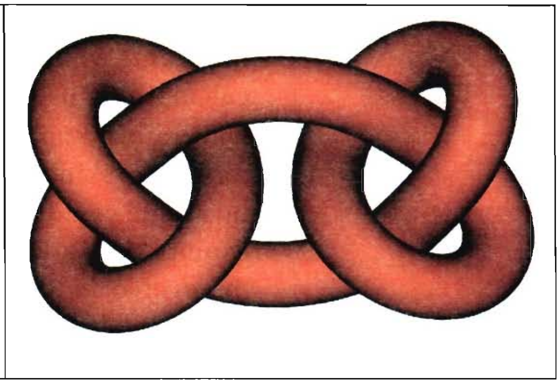


Figure 6 (left). A knot equivalent to the unknot.
Figure 7 (right). Composing two trefoil knots to get a square knot. Obviously, the square knot is not prime. If one composed a trefoil knot with its mirror image, the result is a different knot, known as the granny knot.

crossing number three and is denoted as 3_1. The figure-eight knot (*Figure* 8) has four crossings and is denoted by 4_1.

Two knots can be cut and joined to get a more complex knot. The mathematician would say that the two knots have been composed (multiplied!) to get a new complex knot. An example is shown in *Figure* 7. Obviously composing the unknot with any knot leaves the knot unchanged. Thus, the unknot, among all the possible knots, is like unity (multiplicative identity) among the set of integers N (remember $1 \times n = n$ for any $n \in N$). Further, it may be possible to deform a knot such that it is seen to be composed of simpler knots. A knot that cannot be simplified in this fashion, is known as a prime knot. Obviously, this is analogous to the prime numbers which cannot be decomposed and written as a product of two smaller primes. An interesting question is: given a knot, does it have an inverse? That is, for a given knot K_1, do we have another knot K_2, such that the composition of K_1 and K_2 is the unknot? If such a K_2 exists, then it would be referred to as the inverse of K_1. Interestingly, non trivial knots do not have inverses.

A knot that is not composed of two simpler knots is known as a prime knot.

Knots are difficult to work with, and often, it can be very hard to say whether two planar diagrams represent the same knot or not. Therefore, mathematicians have thought up clever ways for this purpose. They use the knot invariants. The idea in introducing an invariant

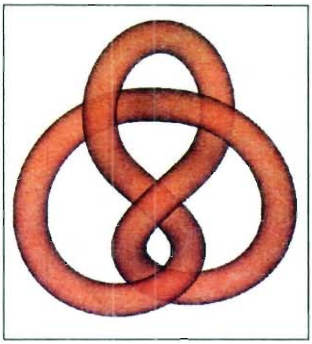
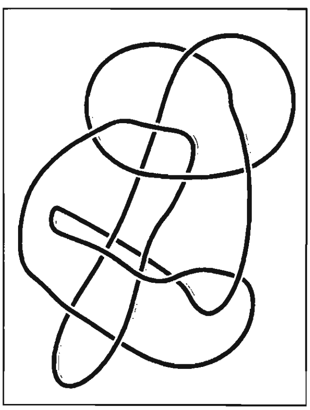


Figure 8. The figure eight knot, which can be represented only with a minimum of four crossings and is labeled as 4_1.

is the following: Given any knot, one can calculate the invariant, which is unique and is unchanged even if one calculates it using a deformed version of the same knot. Naturally a knot invariant remains unchanged if one performs any kind of deformation on the knot. The knot invariant could be a number or a polynomial. The first example of a knot invariant is the Alexander polynomial, discovered in 1927. The Alexander polynomial for the trefoil knot is $t^2 - t + 1$ and the polynomial for 4_1 (the figure-eight knot of *Figure* 8) is $t^2 - 3t + 1$. As these two polynomials are different one concludes that the knots are different. The Alexander polynomial for the unknot is equal to 1 (unity). A table of all the knots having up to 9 crossings is given in the Appendix 1 of the book by Livingston [14]. The Appendix 2 of the same book lists the Alexander polynomial of each one of these knots.

The next to be introduced was the Jones polynomial. This polynomial involves not only positive powers of $\sqrt{t}$, but negative powers too. Almost immediately after the introduction of Jones polynomials, the HOMFLY polynomial, was found independently by Hoste, Ocneanu, Millet, Freyd, Lickorish and Yetter and it is named after them (there were others too, who invented the same, but they published their results slightly later). However, given a knot polynomial, it may not be possible to identify the knot uniquely. Thus the knot shown in *Figure* 9 and the unknot have the same Alexander polynomial associated with them. The Jones polynomial is better in this respect, but this too has the same problem. For more information on polynomial invariants, see the article by Sunder [2] in *Resonance*, or the books by Adams [3] or Sossinsky [4].

Figure 9. A knot having the same Alexander Polynomial as the unknot. Both have Alexander polynomial equal to unity.



In addition to knots, mathematicians also like to think of links, the simplest example of which is the Hopf link, shown in *Figure* 10. A more complicated link called the Borromean link, which has three rings connected together, is shown in *Figure* 11. The interesting thing about this link is that any two of the rings are not interlocked, while the three are. Thus cutting any one of the rings causes the other two to fall apart. The link was known from prehistoric times, but got its name from the 15th century Italian family Borromeo which used this symbol extensively on crests and statues commissioned by them. Interestingly, molecules with this kind of interconnectedness have been synthesized [5]. See *Figure* 12 for three dimensional representation of the geometry of such a molecule.

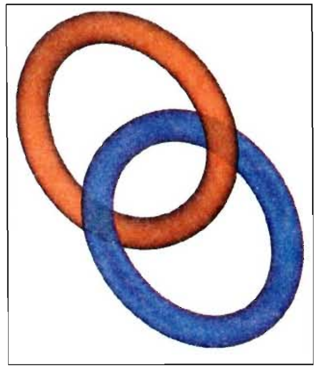


Figure 10. A Hopf link.

3. Knot Physics

Knots were taken up for serious scientific study first in the field of physics. In the 19th century, physicists believed in all-pervading ether. Electromagnetic waves, of which radio and microwaves and visible light are examples, were believed to be waves in the medium of ether, in a fashion similar to sound waves, whose medium is air. Ether was believed to be an ideal fluid. Helmholtz had investigated flows in such fluids. In particular, he analyzed vortices in such fluids and showed that vortex tubes (collection of vortex lines) had to close up and such closed loops of vortex tubes are quite stable. At that time one knew nothing about atoms and there was no evidence for their existence. Still, some scientists believed them to exist, though one had no idea of their nature. In 1867, Thomson (who later became Lord Kelvin) proposed that atoms were knots of vortex tubes in ether. The existence of different elements would then be due to the possibility of having different kinds of knots in three dimensional space. Further, spectral lines observed in the radiation from atoms could be due to vibrations of these loops. These ideas were supported by Maxwell, the founder of electromagnetic theory of light. The physicochemical properties of each element would then be due to their different knotted-ness. This started off an attempt at the problem of classifying knots by Tait. This is a rather difficult problem, as it is usually very difficult to

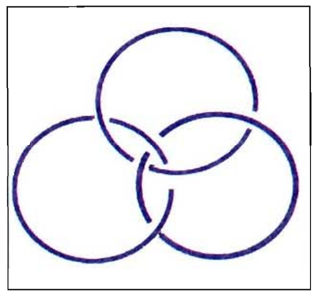
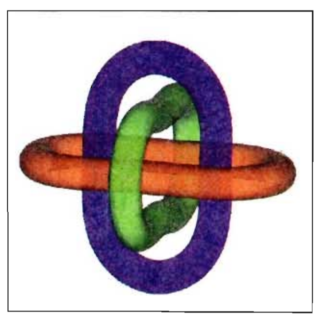


Figure 11.Two dimensioal representation of Borromean rings.

Figure 12. Three dimensional representation of the Borromean link.



There are 1,701,935 knots with 16 or fewer crossings.

say whether two knots are identical or not. Further, the number of primary knots increase rapidly with the number of crossings. Thus there is only one knot with three crossings (excluding mirror images), one with four, two knots with five crossings, three with six and seven with a crossing number of seven. Beyond this, the number increases rapidly. Thus there are 12,965 knots with 13 or fewer crossings and 1,701,935 with 16 or fewer crossings. However, soon due to the discovery of the electron and the nucleus, one had a better understanding of the structure of the atom and therefore physicists lost their interest in knots. Surprisingly, this interest has been revived in the recent past. This is because the theory that is presently believed to be the most fundamental one is the string theory, in which particles are considered to be stringlike objects that are closed. A very interesting idea is that such loops may be knotted [6]. This is very much like the original idea of Thomson. Physicists seem to have come around a full unknot (circle)!

At a more macroscopic level, knots have become important in the area of polymer physics. Suppose one has a large number of long chain molecules, which are present in solution. Imagine now that the two ends of any given molecule can react together to form a loop when they come together. The result will usually be an unknot. However, it is also possible that the result could be a non-trival knot, like the trefoil. So, one can ask: what is the probability that the loop will be an unknot? This question has been answered by a recent simulation of Windwer [7], who finds that it decreases exponentially with the number of units in the polymer N He finds that it behaves like $Ce^{-\mu N}$ where $\mu = 0.0051130$.

The probability that a polymer molecule composed of N units, joined together at the two ends to form knot, is an unknot decreases exponentially with N.

Suppose one has the half-hitch of *Figure* 2. One takes hold of the two free ends and pulls apart so that the string breaks. Where would it break? The observation is that the breaking occurs at the knot. Interestingly,

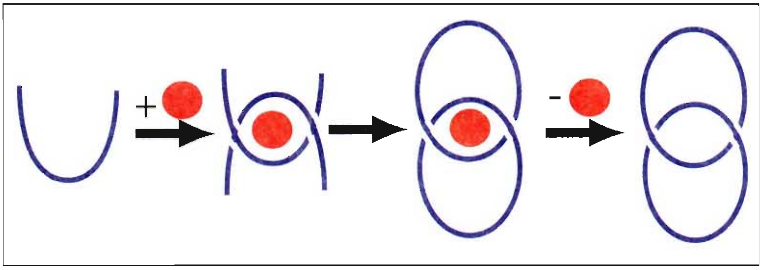


Figure 13. Templated synthesis of [2]catenane.

experimental observation of the dynamics of such breaking is easy with knotted spaghetti and therefore, physicists have experimented with spaghetti [8]. At a more fundamental level, there have been very interesting connections discovered between statistical physics, quantum field theory and knots. These are rather advanced topics and we shall leave it to the interested reader to pursue the literature [6].

4. Molecular Links and Knots

Chemists have long been interested in making linked molecules. The first type to be made are called catenanes. *Catena* is a Latin word, meaning chain. The simplest of these is the [2]catenane which has the topology of the Hopf link. Chemists use the [2] to indicate that two rings have been linked together. The first catenane was synthesized by Wasserman. The way in which they were prepared is the following: One first makes a ring molecule which is big enough that a second linear chain molecule can thread through it. Then the two ends of the linear molecule are joined together. The molecules that are threaded through the ring at the time of closing will lead to the [2]catenane. Such synthesis has been facilitated by templating – that is, one uses a species (invariably a metal ion) around which two long chain molecules will wrap around as in *Figure* 13 [9]. Then the ends of the two chains are closed to obtain a [2]catenane. This elegant synthesis was performed by the group of Sauvage [9]. Several catenanes have been synthesized and are of considerable interest, because many of them

'Templating' can be used efficiently to synthesize molecules that are knotted/linked.

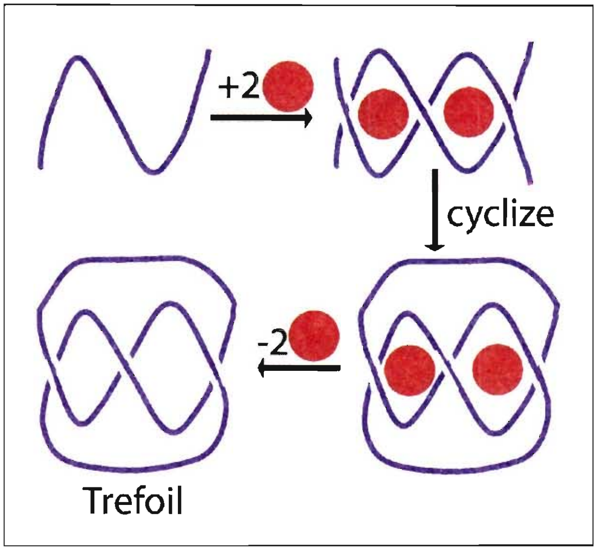


Figure 14. Templated synthesis of trefoil.

have been designed to perform as molecular devices. For a description of such interesting applications, see chapter 5 of the recent book on nanotechnology [10].

The synthesis of molecular Borromean ring [5] is a beautiful demonstration of the use of molecular modeling in synthetic organic chemistry.

The same kind of strategy has been used to obtain a trefoil knot (see *Figure* 14) [9]. One of the most interesting molecules that has recently been made is a molecule analogous to the Borromean link, shown in *Figure* 12. The synthesis of this molecule is a beautiful demonstration of the power of theoretical modeling as an aid to the chemist. Usually, synthesizing an organic molecule would involve a large number of steps. The more steps one has, the lower would be yield of the final desired product. The system was first designed on the computer so that it would tend to self assemble in the desired form. The use of metal ions was crucial for this. The molecule could be made in one step (chemists call this as one pot synthesis) with high yield. *Figure* 15 gives an idea of the strategy adopted. The reader may refer to the original article for more details [5]. Obviously more synthetic challenges remain. For example, how would one synthesize a molecule with topology of figure eight knot shown in *Figure* 8?

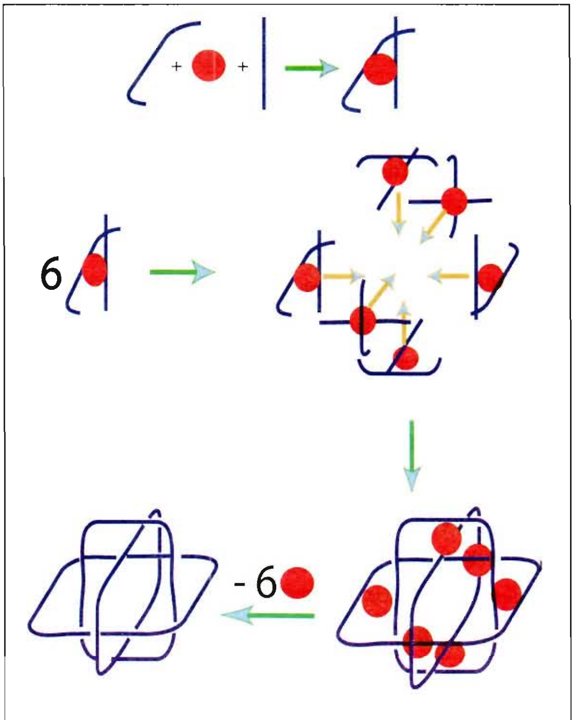


Figure 15. Templated synthesis of the Borromean rings. The red circle is a metal ion (in actual synthesis, Zn^{2+} ions) which acts as a template causing the rod like and bow like parts (molecules) to assemble in the correct orientation, thus facilitating the synthesis. For details see the reference [5].

Interestingly, naturally occurring DNA can be knotted. Knotting would reduce the size of the molecule in solution, as a result of which the molecule, in general, can diffuse faster. A lot of interesting work has been done with DNA and the first Borromean type link has been made with DNA [11]. Living cells have enzymes known as topoisomerases that can knot and unknot DNA.

5. Drawing and Experimenting with Knots and Links

A computer programme called *KnotPlot*, for drawing knots is available for free. Using it, one can draw and experiment with knots and links. It can be downloaded from *http://knotplot.com*. It is developed and maintained by Robert G Scharein. Using it one can draw two dimensional representations of knots/links. In addition, it has a catalogue of knots and other interesting objects.

KnotPlot is an interesting software which can be used to play with knots. All the knots in this article were drawn using *KnotPlot*.

An elementary introduction to knots may be found in the book by Sossinsky [4] for which an Indian edition is available.

Once drawn, the knot's shape in three dimensions can be changed, so that it has the optimum shape (based upon an energy criteria that one can choose). The program can also calculate the HOMFLY polynomial. All the knots/links shown in this article have been drawn using this software. To determine whether a given two-dimensional representation of a knot is equivalent to the unknot is a rather tedious thing to find out manually. For not too complex knots, this can be easily done using the *KnotPlot.* All that is needed is to draw it using the software, and then allow the knot's shape to change dynamically. One can imagine that the knot is immersed in a liquid and its shape is allowed to change so that it has the least energy. The resultant shape, usually is simpler. The reader is urged to try the following exercise using the software: Draw the knot in *Figure* 6 using *KnotPlot* and evolve it to show that it reduces to the unknot.

Further Reading

Plenty of information on knots and links is available on the web. Interesting and more recent information as well as movies of the hagfish too can be found. A few elementary books on knots are available, of which the most interesting is the book by Adams [3]. It contains a lot of material and is written for the uninitiated. It even has knot jokes and pastimes. An even more elementary level book is the one by Sossinsky, for which an Indian edition has come out [4] recently. But it contains far fewer topics than the book by Adams. In *Resonance* itself, there has been an article on the mathematics of knots by Sunder [2]. An intermediate level book is by Livingston [14]. At a more advanced level is the book by Kauffman [12], who has made significant contributions to knot theory. A brief and concise introduction to knots is given in the book by Kleinert [13], but it is by no means elementary.

Suggested Reading

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The Turk's-Head is a tubular knot that is usually made around a cylindrical object, such as a rope, a stanchion, or a rail. It is one of the varieties of the Binding Knot, and serves a great diversity of practical purposes but it is perhaps even more often used for decoration only; for which reason, it is usually classed with "fancy knots." Representations of the Turk's-Head are often carved in wood, ivory, bone, and stone.

Clifford W Ashley in The Ashley Book Of Knots