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# SOME PROBLEMS IN APPLIED KNOT THEORY, AND SOME PROBLEMS IN GEOMETRIC TOPOLOGY


by

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# SOME PROBLEMS IN APPLIED KNOT THEORY, AND SOME PROBLEMS IN GEOMETRIC TOPOLOGY

**D. W. Sumners**

Modern knot theory was born out of physics in the 19th century. Gauss' considerations on inductance in circular wires gave rise to the "Gauss Integral," a formula for the linking number of two simple closed curves in 3-space [G]. William Thompson (Lord Kelvin), upon seeing experiments performed by P. G. Tait involving colliding smoke rings, conceived the "vortex theory of atoms," in which atoms were modelled as configurations of knotted and linked vortex rings in the aether [Th]. In this context, a table of the elements was--you guessed it--a knot table! Tait set about constructing this knot table, and the rest is history [Ta]!

Given the circumstances of its birth, it is not surprising that knot theory has, from time to time, been of use in science. One can think of 3-dimensional knot theory as the study of flexible graphs in $\mathbb{R}^3$, with emphasis on graph entanglement (knotting and linking). A molecule can be represented by its molecular graph--atoms as vertices, covalent bonds as edges. A large molecule can be very flexible. Such a flexible molecule does not usually maintain a fixed 3-dimensional configuration. It can assume a variety of configurations, driven from one to the other by thermal motion, solvent effects,

experimental manipulation, etc. From an initial configuration for a molecule (or set of molecules), knot theory can help identify all of the possible attainable configurations of that molecular system. It is clear that the notion of topological equivalence of embeddings of graphs in $\mathbb{R}^3$ is physically unrealistic--one cannot stretch or shrink molecules at will. Nevertheless, the topological definition of equivalence is, on the one hand, broad enough to generate a large body of mathematical knowledge, and, on the other hand, precise enough to place useful and computable limits on the physically possible motions and configuration changes of molecules. For molecules which possess complicated molecular graphs, knot theory can also aid in the prediction and detection of various spatial isomers [Si]. As evidence for the utility of knot theory (and other mathematics) in chemistry and molecular biology, see the excellent survey articles [Wa,WC], and the conference proceedings [ACG,KR,L].

Some of the problems posed below deal with configurations of random walks or self-avoiding (no self-intersections) random walks on the integer cubic lattice in $\mathbb{R}^3$. The statistics of random walks on the lattice are used to model configurations of linear and circular macromolecules. A macromolecule is a large molecule formed by concatenating large numbers of monomers--such as the synthetic polymer polyethylene and the biopolymer DNA. Conversion of circular polymers from one topological state (say unknotted and unlinked) to another (say knotted and

linked) can occur through the action of various agents, chemical or biological. Given constraints (energetic, spatial or temporal), linear polymers can exhibit entanglement (knotting and linking). Moreover, linear polymers can be converted to circular polymers in various cyclization reactions. If one wants a random sample of the configuration space of a macromolecule in $\mathbb{R}^3$, one can model the spatial configuration of a macromolecule as a self-avoiding random walk in $\mathbb{R}^3$, where the vertices represent the positions of carbon atoms, and adjacent vertices are connected by straight line segments (all the same length), representing covalent bonds. A discrete version of random walks in $\mathbb{R}^3$ is random walks on the integer cubic lattice. One studies the statistical mechanics of large ensembles of these random walks in hopes of detecting physically observable quantities (such as phase transition) of the physical system being modelled.

The problems below are stated in an informal style, and addresses of relevant people are included when known, in hopes that the interested reader will contact them.

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Consider random walks on a cubic lattice in $\mathbb{R}^3$ that start with $0 < y < n$, $n > 1$, and end when either $y = 0$ or $y = n$. An L-walk (R-walk) is a walk that starts with $y = 1$ ($y = n - 1$). (Think of an L-walk or R-walk as a walk that starts on one of the planes $y = 0$ or $y = n$ and takes its first step into the region between the planes.) An L-loop (R-loop) is an L-walk that ends with $y = 0$ ($y = n$). Assume step probabilities are all equal to 1/6 (pure isotropy). Given an L-walk L and an R-walk R, define the offset linking number olk(L,R) as follows: If each of L and R is a loop, complete it to a closed curve by joining its endpoints with an arbitrary path in its base plane, offset the lattice for R by the vector $(-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})$, and define olk(L,R) to be the homological linking number of the resulting (disjoint) closed curves. Otherwise, set olk(L,R) = 0. We say L links R if olk(L,R) $\neq$ 0.

Problem 1. Given an L-walk L and a family $\mathcal{R}$ of R-walks with density of starts d, what is the probability $P_{link}(n)$ that L will link a member of $\mathcal{R}$?

Problem 2. Compute $\lim_{n\to\infty} P_{link}(n)$.

Problem 3. Find the expected value $D_{link}(n)$ of the number of members of $\mathcal{R}$ that L links.

Problem 4. Compute $\lim_{n\to\infty} \dot{D}_{link}(n)$.

Problem 5. Find the expected sum $W_1(n)$ of the absolute values of the offset linking number of L with the members of $\mathcal{R}$.

Problem 6. Compute $\lim_{n\to\infty} W_1(n)$.

Problem 7. Find the expected sum $W_2(n)$ of the squares of the offset linking number of L with the members of $\mathcal{R}$. (Comment: $W_2(n)$ should be easier to deal with than $W_1(n)$.)

Problem 8. Compute $\lim_{n\to\infty} W_2(n)$.

Given an L-loop that starts at (0,1,0), define its reach to be its maximum y-value, its range to be its maximum x- or z-value, and its breadth b = range/reach. By analogy, define the breadth of any loop.

Problem 9. Compute the expected value of b as a function of n and its asymptotics. (Comment: Simulation statistics seem to indicate that b = 1.19. See [BL].)

Represent a loop by an isosceles triangle parallel to the y axis having its base on the base plane for

the loop. Its "breadth" b = altitude/2·base. Analogs of $D_{link}(n)$ and $P_{link}(n)$ for these simplified loops are

$$D(n) = 2b^2 d \sum_{i=1}^{n-1} d_i \sum_{j=n-i}^{n-1} [1-2b^2 d(i+j+1/2-n)^2 d_j], \text{ and}$$

$$P(n) = 1 - 1/n - \sum_{i-1}^{n-1} d_i \prod_{j=n-i}^{n-1} [1-2b^2 d(i+j+1/2-n)^2 d_j].$$

Asymptotics for D(n) are given in [BL].

Problem 10. Compute $\lim_{n\to\infty} P(n)$.

(Comment: We conjecture that $n\cdot(P(n) \sim 0(\log(n))$.)

Problem 11. Show that $\lim_{n\to\infty} P(n) = \lim_{n\to\infty} P_{link}(n)$, and that

$\lim_{n\to\infty} D(n) = \lim_{n\to\infty} D_{link}(n)$.

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There exist naturally occurring enzymes (topoisomerases and recombinases) which, in order to mediate the vital life processes of replication, transcription and recombination, manipulate cellular DNA in topologically interesting and nontrivial ways [WC, S1]. These enzyme actions include promoting writhing (coiling up) of DNA molecules, passing one strand of DNA through another via an enzyme-bridged break in one of the strands, and breaking a pair of strands and recombining to

different ends. If one regards DNA as very thin string, these enzyme activities are the stuff of which recent combinatorial knot theory is made! Moreover, relatively new experimental techniques (rec A enhanced electron microscopy) [KS] make possible the unambiguous resolution of the DNA knots and links produced by reacting circular DNA with high concentrations of a purified enzyme in vitro (in the laboratory). The experimental protocol is to manufacture (by cloning techniques) artificial circular DNA substrate on which a particular enzyme will act. As experimental control variables, one has the knot type(s) of the substrate, and the amount of writhing (supercoiling) of the substrate molecules. The product of an enzyme reaction is an enzyme-specific family of DNA knots and links. The reaction products are fractionated by gel electrophoresis, in which the molecules migrate through a resistive medium (the gel) under the forcing of an electric field (electrophoresis). Molecules which are "alike" group together and travel together in a band through the gel. Gel electrophoresis can be used to discriminate between molecules on the basis of molecular weight. Given (as is the case here) that all molecules are the same molecular weight, it then discriminates between molecules on the basis of average 3-dimensional "shape". Following electrophoresis, the molecules are fattened with a protein (rec A) coating, to enhance resolution of crossovers in an electron micrograph of the molecule. In this manner, the knot (link) type of the various reaction

products is an observable. This new observational power makes possible the building of knot-theoretic models [WC,WMC,ES] for enzyme action, in which one wishes to extract information about enzyme mechanism from the DNA knots and links produced by an enzyme reaction.

Problem 1: Build new models for enzyme action. The models now existing involve signed crossover number [WC], polynomial invariants [WMC], and 2-string tangles [ES]. The situation is basically this: as input to a black box (the enzyme), one has a family of DNA circles (of known knot type and degree of supercoiling). The output of the black box is another family of DNA knots and links. THE PROBLEM: What happened inside the box?

Problem 2: Explain gel electrophoresis experimental results. Gel electrophoresis is a race for molecules--they all start together, and the total distance travelled by a molecule when the electric field is turned off is determined by its gel mobility. At the finish of a gel run, the molecules are grouped in bands, the slowest band nearest the starting position, the fastest band farthest away. When relaxed (no supercoils) DNA circles (all the same molecular weight) run under certain gel conditions, the knotted DNA circles travel according to their crossover number [DS]! What is it about crossover number (an artifact of 2-dimensional knot projections) that determines how fast a flexible knot moves through a resistive

medium? The theory of gel mobility of molecules (linear or circular) is rather difficult to work out. See [LZ] for some results on the gel mobility of unknotted circular molecules under pulsed field electrophoresis.

Problem 3: What are the properties of a random knot (of fixed length)? Chemists have long been interested in the synthesis of molecules with exotic geometry; in particular, the synthesis of knotted and linked molecules [Wa]. One can imagine such a synthesis by means of a cyclization reaction (random closing) of linear chain molecules [FW]. Let N represent the number of repeating units in such a linear chain. A unit may represent a monomer of the substance, or the equivalent statistical length of the substance. For example, the equivalent statistical length for polyethylene is about 3.5 monomers, and for duplex DNA, about 500 base pairs. A randomly closed chain of length N is a random piecewise linear embedding of $S^1$, with all the 1-simplexes the same length. See [R1,R2] for a discussion of the topology of the configuration space of such PL embeddings. In order to make predictions about the yield of such a cyclization reaction, one needs answers to the following mathematical questions [S2]:

A. For random simple closed curves of length N (as above), what is the distribution of knot types, as a function of N?

B. What is the probability of knotting, as a function of N? One can show that, for simple closed curves of length N inscribed on the cubical lattice in $\mathbb{R}^3$, the knot probability goes to one exponentially rapidly with N [SW].

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I. EXPANSIVE VS. PSEUDO-ANOSOV

The references here are two preprints: [H] by K. Hiraide, Department of Mathematics, Tokyo Metropolitan University, Fukasawa 2-1-1, Setagaya, Tokyo 158, Japan, and [Le] by Jorge Lewowicz, Instituto de Mathematica, Casilla de Correo 30, Montevideo, Uruguay. In [H] and [Le], the authors independently prove that the concepts "expansive" and "pseudo-Anosov" coincide for surfaces.

A. What is the situation for 3-manifolds?

B. Find a good example of a 3-manifold (such as $S^3$) which does not support an Anosov diffeomorphism.

C. Prove some of the beginning lemmas of Lewowicz-Hiraide for 3-manifolds.

II. DYNAMICAL SYSTEMS

A. The two topics of zeta functions in dynamical systems and Alexander polynomials in knot theory are closely related: see [M]. For flows on $S^3$, periodic orbits are knots; thus there should be a combination

such as a 2 variable polynomial, combining knot theory (e.g., the degree of the Alexander polynomial) and dynamical systems (the length of the orbit). See [BW].

B. Branched surfaces can support Anosov endomorphisms. However, all that are known are shift equivalent to linear maps on the 2-torus, such as that induced by the 2x2 matrix $\begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix}$.

*Conjecture.* Given an Anosov endomorphism $g: K \to K$, there is a linear map $f: T \to T$, T the 2-torus, such that f is shift equivalent to g. See the Northwestern thesis of Lan Wen, Department of Mathematics, Beijing University, PRC.

*Definition.* $f: X \to X$ and $g: Y \to Y$ are shift equivalent provided that there exist maps $r: X \to Y$ and $s: Y \to X$ and an integer m such that $rf = gr$, $sg = fs$, $sr = f^m$, and $rs = g^m$.

*Definition.* $g: K \to K$ is Anosov, provided there is a sub-bundle E of the tangent bundle TK, such that dg leaves E invariant and contracts vectors, and such that the map induced on TK/E by dg expands vectors.

C. Hassler Whitney gives an example which is dear to the heart of all continuum theorists that know it--both of us! It is a carefully constructed arc A in the plane and a smooth function $f: A \to$ Reals with grad f = 0 (both partials are 0), yet f has different values at A's

endpoints. Contact Alec Norton, Boston University for his preprints and ideas on this subject. (Don't be afraid of smooth functions on manifolds. They have beautiful pathology and are crying out for continuum theorists to look at them. And they are really and truly easy to get the hang of.)

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