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AMS Special Session on
Physical Knotting and Unknotting
Las Vegas, Nevada
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Preface

The physical properties of knotted and linked configurations in space have been of interest to physicists and mathematicians for a long time. More recently and more widely, they have become interesting to biologists, computer scientists, and engineers. The depth of importance and breadth of application are now widely appreciated. Critical progress continues to be made each year. Nevertheless, many fundamental and basic questions in the general domain of physical knotting, unknotting, and linking remain completely unanswered or at least are not fully and satisfactorily answered.

At its core, physical knot theory lives on the fringes of topology. Here we search for the interconnection of the classical theory of knots – where arbitrary flexibility and zero thickness are the rules of thumb – and the physical world of solar coronal loops, molecules, geometric linkages, rope, and even cooked spaghetti. For obvious reasons, we sometimes refer to this field by oxymoronic or narcissistic terms such as "applied knot theory" or "real knot theory" as well as our preferred "physical knot theory."

For this volume we have invited papers which, together, provide a broad perspective on contemporary research questions in the areas of knotting and unknotting, linking and folding, and modeling and breaking geometric or physical objects in three (and occasionally two or four) dimensional space. Some of these papers are primarily theoretical; others are experimental. Some are purely mathematical in nature; others deal with the applications of mathematics to theoretical computer science, engineering, physics, biology, or chemistry. Together, they present a collection of topics covering the most critical questions as well as introducing several new ideas and approaches that will see application more widely as a result of the new conversations stimulated by this volume.

Most of these articles were presented at the *Special Session on Physical Knotting and Unknotting* at the Western Section Meeting of the American Mathematical Society in Las Vegas, Nevada, on April 21 and 22, 2001. This Special Session brought together twenty-three speakers from Mathematics, theoretical and experimental Physics, the Biological Sciences, and Computer Science. Participants came from Canada, Greece, Japan, Poland, Switzerland and the United States of America.

One of the principal organizing themes of the special session is the exploration of the theoretical and experimental properties of knots or links endowed with some important physical or spatial property. A fundamental question concerns the distribution of geometric or physical properties of individual or collections of equilateral knots or links. For example, what is the optimal thickness, or its reciprocal: the ropelength, of an equilateral polygonal knot of n edges of a fixed topological type?

What is the distribution of the thickness in the space of equilateral polygonal knots having n edges? What is the distribution if the knot type is specified? Other examples of the same spirit are the diameter, radius of gyration, average or minimum crossing numbers, the volume (as measured by its convex hull), and the various formulations of "knot energy." Another feature of research in this area are questions concerning the statistical distribution of knot types as a function of the number of edges. For example, what is the probability that an n edge equilateral polygon is knotted? Finally, how are these various characteristic spatial attributes related to other properties of the knots or links?

The first article, **"Physical knots"** by Jonathan Simon, provides an excellent introduction to these matters and explores the linkage between classical knot theory and the physical attributes of knots such as their "strength," ropelength, energy, minimal edge number of a knot type, and statistical knot theory. These themes will be taken up in subsequent articles. From one perspective, many of these properties and associated questions can be framed as concerning properties of spaces of knots. While much is still unknown concerning the topology and geometry of these knot spaces, several papers present current progress on basic questions or discuss some attractive open questions.

Richard Randell discusses the global structure in the second article, **"The space of piecewise-linear knots."** Randell explores the homology and cohomology groups of the space of piecewise-linear knots (or links). Here, a piecewise-linear knot or link of n edges is defined by n vertices in Euclidean space satisfying the condition that no edges may intersect each other. Thus, the set of all piecewise-linear knots (links) of n edges can be regarded as a subset of $\mathbb{R}^{3n}$. A path component in such a piecewise linear knot (link) space corresponds to a knot type. Thus, the number of path components bounds the number of different knots (links) a polygon of n edges can represent.

Jorge Alberto Calvo, **"Characterizing polygons in $\mathbb{R}^{3n}$,"** looks at the minimal edge number of a knot type as one facet of a "geometric" theory of polygonal knots. By comparing deformations which may change the length of edges against those that preserve these length, Calvo demonstrates that these are two distinct theories. He presents a series of open questions pertaining to these geometric knot theories and looks at some steps in a program towards understanding the geometric nature of these theories. He describes those topological knot types that can be constructed with eight or fewer edges giving the first proof that 8_{18} must have edge number nine.

Eric J. Rawdon and Robert G. Scharein,**"Upper bounds for equilateral stick numbers,"** establish a process for computing the minimal edge numbers of equilateral and non-equilateral knots. These results are obtained by using the software *KnotPlot* to make perturbations of configurations in knot space that allow fortuitous elimination of edges. They compute upper bounds for the equilateral edge number of knots through 10 crossings. Comparing the results to those for polygonal edge numbers, they identify seven knots, including 8_{19}, for which these may be different.

Kenneth C. Millett, **"An investigation of polygonal knot spaces and ideal physical knot configurations,"** presents the results of a Monte Carlo experiment that produces data on the distribution of diameters in the spaces of

equilateral knots with 8, 16, and 32 edges. These data provide a profile of the complexity of knot space as well as elementary information at the extremes.

Tetsuo Deguchi and Miyuki K. Shimamura, **"Topological effects on the average size of random knots,"** review observations of various nontrivial properties of the mean square radius of gyration of random polygons and self-avoiding polygons obtained by means of computer simulations. They discuss the case of small excluded volume and consider the effects of the imposition of topological constraints on the population.

The article by Akos Dobay, Pierre-Edouard Sottas, Jacques Dubochet, and Andrzej Stasiak, **"Bringing an order into random knots,"** describes the determination of the optimal edge length, i.e. the length at which a given knot type will reach its highest probability, of random walks leading to the formation of different knot types and shows that a power law accurately describes the relationship between this and the previously characterized lengths of ideal knots of the corresponding type.

If the continuous structure of polygonal knot space, in which the vertices of the knot are restricted only by the nature of the knot constraints, is replaced by the requirement that the vertices are at adjacent points of a lattice the resulting theory allows the application of many different methods. This has been an very fertile and productive direction of research. E. J. Janse van Rensburg, **"The probability of knotting in lattice polygons,"** considers the question: what is the probability of knotting, and what is the statistically averaged entanglement complexity of the random polygon? Knots are detected by computing the Alexander Polynomial and the entanglement complexity is measured by computing the torsion of the knots in the lattice polygons.

In a subsequent article, **"Knotting in adsorbing lattice polygons,"** Janse van Rensburg considers the case of knotting in adsorbing lattice polygons. There is an adsorption transition driven by the interaction between the polygon and an attractive wall. The article contains the results of simulations to estimate the knot probability and the entanglement complexity and a discussion of their implications.

Several papers consider these properties for knots with maximal thickness, so-called ideal knots. The article by Piotr Pieranski and Sylwester Przybyl **"In search of the ideal trefoil knot,"** describes a tightening process used to arrive at the shortest conformation of a trefoil using "perfect rope." They analyze the set of contact points of a thick tube about the knot and provide evidence that an ideal trefoil cannot lie on a standard torus.

Yuanan Diao and Claus Ernst, **"The crossing numbers of thick knots and links,"** derive a closed integral formula for a modification of the average crossing number of thick knots and links. By employing this formulation, they strengthen known inequalities between the crossing number of a thick knot or link and its arc length.

Rob Kusner, **"On thickness and packing density for knots and links,"** describes some problems, observations and conjectures concerning the thickness of a knot or link and their packing density in $\mathbb{R}^3$ and $\mathbb{S}^3$. Evidence and arguments supporting the conjecture that the density packing of thick links is generally less than the density of the hexagonal packing of unit disks in $\mathbb{R}^2$.

John M. Sullivan, **"Approximating ropelength by energy functions,"** considers a family of energy functions for knots, depending on a power p, which

approaches the ropelength as p increases. A numerically computed trefoil knot that seems to be a local minimum for ropelength is described along with supporting evidence provided by nearby critical points of the approximating energies, for large enough p.

R. Langevin and Jun O'Hara, **"Conformal geometric viewpoints for knots and links I,"** introduce energies of links in terms of the infinitesimal cross-ratio from a conformal geometric viewpoint. They consider the behavior of the Gauss integral formula of the linking number under Möbius transformations.

Oscar Gonzalez, John H. Maddocks, and Jana Smutny, **"Curves, circles, and spheres,"** explore variants of global radii of curvature that are defined in ways related to $q(s)$, defined as the smallest possible radius amongst all circles passing through this point and any two other points on the curve, coalescent or not. The minimum value of the global radius of curvature gave a convenient measure of thickness suggesting the potential value of its variants. In this article, the authors describe the interrelations between all possible global radius of curvature functions of this type, and show that there are two of particular interest. Their properties are illustrated with several examples that appear related to biological structure.

Giovanni Dietler, Piotr Pieranski, Sandor Kasas, and Andrzej Stasiak, **"The rupture of knotted strings under tension,"** give a very interesting description of a series of beautiful experiments on breaking strands of cooked spaghetti and explores the role that knotting plays in the breaking process. The experiments suggest that the breakage occurs at the first region of high curvature within the knot, a localization that results from joint contributions of loading, bending, and friction forces.

In the analysis of enzyme mechanisms describing the action of topoisomerase on DNA, the calculus of rational tangles has played an important role. Louis H. Kauffman and Sofia Lambropoulou, **"Classifying and applying rational knots and rational tangles,"** discuss a new combinatorial approach to the classification of rational tangles and of unoriented and oriented rational knots. They consider the classification of achiral and strongly invertible rational links as well as the relationships between tangles, rational knots and DNA recombination.

One of the historically motivating questions has been the search for an "energy" function which, when applied to knots in $\mathbb{R}^3$, would provide a systematic method of simplifying any unknotted configuration to that of the unknot by merely deforming in the direction that most rapidly decreases this energy. Dennis Roseman, **"Untangling some spheres in $\mathbb{R}^4$ by energy minimizing flow,"** provides a concise introduction to the subject of energy minimization techniques for studying knots and surfaces in four dimensional space.

One key feature of work is the existence of exemplars with specified properties and the development of algorithms that describe relationships between configurations. These algorithms provide sequences of spatial transformations that alter the geometric structure under consideration, but only in an allowable fashion. One of the more enduring questions has been the existence of planar polygonal knots, i.e. planar polygons that cannot be transformed to an "ideal" planar configuration. It is only recently that Connelly, Demaine and, Rote showed that every planar polygon was unknotted, i.e. equivalent to a standard convex model under a motion that preserves edge lengths and avoids self-intersections. The interest in a theorem for polygons or curves in three space that are topologically unknotted is the stimulus

for much of the study of knot energies and ropelength, i.e. the search for a method of systematically unknotting unknots. In this domain, spatial polygons are called linkages. In the spirit of such questions, Michael Soss and Godfried T. Toussaint, **"Convexifying polygons in 3D: a survey,"** provide a survey of the history of linkage folding in a unique combination of fields. To convexify a polygon is to reconfigure it with respect to a given set of operations until the polygon becomes convex. The problem of confexifying polygons has a long history in a variety of fields, including mathematics, kinematics, and physical chemistry.

In **"Infinitesimally locked self-touching linkages with applications to locked trees,"** Robert Connelly, Erik D. Demaine, and Günter Rote develop a generalization of rigidity theory in a constructive way so that one can easily determine if self-touching linkages are locked.

Finally, the closing contribution to this volume is a paper, **"Biologic,"** by Louis H. Kauffman presenting a wider vision of potential organizing principles that could amplify the applications of mathematical methods to the biological sciences.

Acknowledgments

We would like to thank Bernard Russo and the AMS for helping us organize the special session at the Las Vegas meeting out of which this volume grew. We would also like to thank Christine Thivierge for her efficient work in making this volume possible. Most especially, we thank our families for their support and patience in our mathematical endeavors.

Jorge Alberto Calvo
Kenneth C. Millett
Eric J. Rawdon

Based on a Special Session at the AMS Sectional Meeting in Las Vegas (NV) in April 2001, this volume discusses critical questions and new ideas in the areas of knotting and folding of curves in surfaces in three-dimensional space and applications of these ideas to biology, chemistry, computer science, and engineering.

Some of the papers are primarily theoretical; others are experimental. Some are purely mathematical; others deal with applications of mathematics to theoretical computer science, engineering, physics, biology, or chemistry. Connections are made between classical knot theory and the physical world of macromolecules, such as DNA, geometric linkages, rope, and even cooked spaghetti.

This book introduces the world of physical knot theory in all its manifestations and points the way for new research. It is suitable for a diverse audience of mathematicians, computer scientists, engineers, biologists, chemists, and physicists.

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