MONTE CARLO EXPLORATIONS OF POLYGONAL KNOT SPACES

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ABSTRACT

Polygonal knots are embeddings of polygons in three space. For each n, the collection of embedded n-gons determines a subset of Euclidean space whose structure is the subject of this paper. Which knots can be constructed with a specified number of edges? What is the likelihood that a randomly chosen polygon of n-edges will be a knot of a specific topological type? At what point is a given topological type most likely as a function of the number of edges? Are the various orderings of knot types by means of "physical properties" comparable? These and related questions are discussed and supporting evidence, in many cases derived from Monte Carlo explorations, is provided.

Keywords: Monte Carlo, polygonal knots, energy, thickness, HOMFLY, geometric knots, physical knot theory

1. Introduction

The topological and geometric knotting of circles occurs in many contexts in the natural sciences: in the biology of DNA, in the chemistry of relatively small molecules, in the physics of macromolecules, in the spatial structure of trajectories of dynamical systems and line field conformations, and in complex movements of robots. Whereas topological knots have been studied from the time of Gauss, the study of geometric knots is a relatively recent event stimulated by these applications to the natural sciences. Geometric knotting, in contrast to topological knotting, concerns the imposition of geometric constraints on spatial polygons. Thus, constraints of length and of angle on allowed configurations of spatial polygons and their transformations define new notions of knotting and equivalence of knots. These constraints represent an effort to capture the local "stiffness" of molecular structures, as found in some mathematical models of DNA and other macromolecules, or other limitations on the physical system under consideration.

To systematize the study of polygonal knots it is convenient to consider functions taking the standard polygon of n sides into three-dimensional Euclidean space such that the edges go to line segments connecting the images of the corresponding vertices. Such maps are determined by a list of n distinct points, each corresponding to the image of the respective vertex of the polygon. The maps need not necessarily respect the lengths of edges nor the angles between successive edges. Each successive pair of points is therefore connected by a straight line segment, with the first and last points being connected to close the loop. For polygonal knots, care is necessary to insure that edges do not intersect except as necessary to connect adjacent edges. When a first and a second vertex are specified (giving an initial vertex and orientation of the polygon), the collection of all such maps corresponds to the product of n three-dimensional Euclidean or, equivalently, a 3n-dimensional Euclidean space. The entire collection such knots determines an open subset of this space, Geo(n). Requiring that each of the segments has length one determines a subspace of Geo(n), another knot space denoted by Equ(n), whose dimension is twice the number of vertices. This formulation of polygonal knot space and its topology is studied in the foundational papers of Dick Randell and, later, in those of Jorge Alberto Calvo.

Global properties of these knot spaces and the specific instances of knots within them provide information employed in their application to questions arising in the natural sciences mentioned earlier. The structure of these polygonal knot spaces is, however, extremely complex and resistant to direct study. In the case of lattice knot models, one method of gaining information and making quantitative estimations of underlying structure is the statistical sampling of the population of the space. The asymptotic occurrence of knotting has been a long time objective of research and is the subject of papers of Diao, Sumners, Pippenger, Whittington, Van Rensburg, and others. Prior to and concurrent with these theoretical advances, numerical studies have been undertaken.

Among the more successful methods used to investigate the asymptotic properties of knot spaces is the Metropolis Monte Carlo sampling of the space. The objective of this paper is the application of this and other similarly random methods in a new investigation of the nature of polygonal knotting. The estimations of knot types are accomplished by use of the HOMFLY polynomial. While this knot invariant does not, in general, provide a faithful representation of knot types, it is a much finer filter than those more commonly used, such as the Alexander polynomial or certain Vassiliev invariants arising as evaluations of knot polynomials. The second section of the paper reviews some of the fundamental definitions, concepts and results, and identifies some of the more central questions. It also describes some of the key relevant results of current research. The third section contains a short discussion of the key elements of the computer exploration of knot spaces. The fourth section presents the results of the Metropolis Monte Carlo studies. The fifth, and final section, focuses on conclusions derived from this study and discusses suggestions for directions of further research.

In addition to my own work some of the results reported here are due to Jorge Alberto Calvo, while others are the result of joint work with him. Still others reflect results of research underway in collaboration with Eric J. Rawdon.

2. Definitions, Fundamental Concepts, Questions and Results

The general context for studying spaces of polygonal knots is described in Randell [1, 2]. In this paper, I will employ the specific description used in Calvo [3] and in Calvo and Millett [4]. Let P_n be the standard regular polygon with n unit length edges in , equipped with a distinguished first vertex, called the base point, at $(r_n, 0)$, where $r_n = 1/\sin(\pi/n)$. Ordering the vertices in the counter clockwise direction places the m^{th} vertex at $r_n e^{2i\pi(m-1)/n} = (r_n \cos(2\pi(m-1)/n), r_n \sin(2\pi(m-1)/n))$, thereby determining an orientation on P_n. Let Map(n) denote the space of maps from P_n into $\mathbf{R}^3$ that are linear on the edges of P_n. Such maps uniquely correspond to points in $\mathbf{R}^{3n}$ by associating to each map the list of the images of the successive vertices, beginning at the base point and proceeding in the direction of the orientation. This association provides an identification of Map(n) with the structure of a topological space, $\mathbf{R}^{3n}$, that we will use in this study. Polygonal knots are the images of those maps that are embeddings, i.e. homeomorphisms of the regular n-gon to its image. The requirement that it be an embedding adds constraints giving rise to a 3n-dimensional dense open subspace of $\mathbf{R}^{3n}$, denoted by Geo(n). The constraints determine the discriminant, the set of maps which are not embeddings, as the closure of a finite set of semi-algebraic varieties. This set separates Map(n) into a finite number of connected components. Each component defines a distinct geometric knot type. Imposing the extra condition that these embeddings be length-preserving, we obtain a 2n dimensional submanifold Equ(n) of Geo(n), whose components define equilateral knot types.

Knot spaces are typically non-compact manifolds. For example, the space of based oriented equilateral triangles is homeomorphic to $\mathbf{R}^3$x SO(3); here, the first factor corresponds to the position of the first vertex in space. In order to simplify the analysis we consider the subspaces in which the first vertex goes to the origin. These are denoted by $Map_0(n)$, $Geo_0(n)$, and $Equ_0(n)$ respectively. In this paper we will also study the subset of Geo(n) whose vertices lie within the cube $[0,1]^3$. It is denoted by Cube(n).

The path components of Geo(n), Cube(n), and Equ(n) define potentially distinct theories of geometric knotting as well as models of interest in different natural contexts. For each n, we know that there are only finitely many geometric knot types [1, 5]. Note also that Cube(n) and Equ_0 (n) have compact closures in Map(n) and $Map_0(n)$, respectively. In order to provide a compact model in which to study the structure of Geo(n) we observe that Geo(n) has a radial structure that respects geometric knot types. Any expanding or contracting homothety preserves the geometric knot type and is isotopic to the identity. Thus, any representative of a geometric knot type is equivalent to one whose vertices determine points lying on the unit sphere in $\mathbf{R}^{3n}$. Furthermore, the proportion of geometric knots in Geo(n), the proportion in a ball in Geo(n) centered at the origin, or the proportion lying on a sphere in Geo(n) centered at the origin, are equal.

The function which assigns to each point in Map(n) the sum of the lengths of the edges of the image polygon defines a family of "level hypersurfaces" consisting of polygons of constant total length. For any non-zero total length, the corresponding hypersurface meets each ray from the origin exactly once thereby defining a diffeomorphism of the level surface to the standard sphere. As a consequence, each geometric knot is equivalent to one lying on the smooth sphere of images of total edge length equal to one. With an appropriate normalization of edge lengths, Equ(n) can be realized as a 2n-dimensional subset of this (3n - 1)-dimensional smooth sphere of geometric knots.

An important consequence of the discussion in the previous two paragraphs is that, in Metropolis Monte Carlo explorations of Geo(n), one may require that knots correspond to a collection of vertices lying within a specified ball. The proportion of their occurrence is equally an estimation of the proportion of the ball or in its boundary sphere consisting of knots of this type.

As soon as one begins to look closely at geometric and equilateral knots, three initial questions are posed.

QUESTION 1. For each topological knot type, K, what is the smallest n for which there is a realization with n edges?

This has been variously called the "stick number," "edge number," "broken line number," or "minimal polygon index" of the topological knot type. In this paper we will employ the term "polygon number" for this concept.

QUESTION 2. Is the polygon number the same for geometric knots and equilateral knots?

QUESTION 3. How many distinct geometric or equilateral knot types are there as a function of n, the number of edges?

Cube(n), Geo(n) and, Equ(n) are connected for $n \leq 5$. This is a "folk" result. One nice proof is attributed to Nicholas Kuiper [1, 2]. Stimulated by discussions with biologists, chemists, and, most directly, by participation in a 1991 NATO conference on "Topological Fluid Dynamics" organized by Moffat, Zaslavsky, Comte, and Tabor [6], I first constructed equilateral models of the hexagonal trefoil knot, the heptagonal figure eight knot, and several eight crossing knots as well as a variety of more complex knots. I also began to study "random knotting" with the assistance of undergraduate summer interns. One of these was Jorge Alberto Calvo whose doctoral research results are discussed later in this paper. Colin Adams has also directed summer undergraduate research projects which have provided important contributions to the determination of the polygon number [7, 8, 9], especially for composite knots. The polygon number has also been explored by Jin in connection with Kuiper's super bridge number [10, 11].

In his 1998 UCSB Ph.D. dissertation research [3,12,13], Calvo showed that, for n = 6, each of these spaces have exactly five components. That the set of topological unknots in Equ(6) and Geo(6) is connected is an earlier result of unpublished joint work with Rosa Orellana during summer 1993. This was discussed in [14]. Calvo has provided a new proof of this basic result in his thesis as part of his complete analysis of these spaces. He shows that there is one component of topologically trivial knots and two each of right handed and left handed trefoils. He also shows that Geo(7) has exactly five components. There is one component each of trivial knots and right and left hand trefoils and two components of figure eight knots. For n = 8, by direct construction there are known to be at least twenty components since only the unknot, the figure eight, 6_3, and the sum of the left and right trefoil knots (the square knot) are achiral among the twelve constructed topological knot types. In his thesis, Calvo showed that these, and possibly, the knot 8_{18} are the only topological knot types that can be realized in Geo(8). Subsequently, he proved that 8_{18} cannot occur. Monte Carlo searches have provided realizations of all these knot types in Equ(8) with the exceptions of 3.1#3.1 and 8_{19}.

In her 1997 Ph.D. dissertation, Monica Meissen, [15, 16], constructed nine-gon realizations of all seven crossing prime knots as well as 8_{21}. In addition, nine-gon realizations have been achieved for 8_{16}, 8_{17}, 8_{18}, 8_{21}, 9_{40}, 9_{41}, 9_{42}, and 9_{46}. As a consequence of Calvo's results, all of these knots must have geometric polygon number equal to nine.

I have employed several random knot generation and sampling strategies in order to provide some data relevant to these questions and to estimations of the complexity of knot spaces for larger numbers of vertices, including estimates of asymptotic properties. These data also give one rough sketch of the gross structure of these spaces for smaller numbers of vertices [14]. In the case of Cube(n), randomly generated coordinates of the vertices were selected with respect to the uniform distribution on the cube. In the case of Geo(n), n points in the unit three ball are selected with respect to the uniform distribution and collectively rescaled to define a point on the unit sphere in R^{3n}. In the case of Equ(n), the pivot transformation with randomly selected pairs of vertices and randomly selected angles was used. The pivot transforms the map by fixing one of the pieces determined by the pair of vertices and rotating the image of the other piece about the axis determined by the images of the designated vertices by the given angle. Up to Euclidean rotation, about the same axis, the map is equivalent to one given by reversing the roles of the two pieces. If the map is an embedding and the angle is sufficiently small, the result of the pivot is an equivalent embedding. In order to insure that one could sample the entire equilateral knot space, a couple of theorems are required.

THEOREM 1. [14] For any two maps in Map(n) there is a finite sequence of translations, rotations, and pivots taking one map to the other.

The proof of this result can be modified to prove the following theorem.

THEOREM 2. Any path connecting two maps in Map(n) can be approximated as closely as desired by a sequence of pivots.

The first theorem insures that any equilateral knot can be connected to the standard regular polygon by a sequence of these operations. The second is used to seek optimal representations of a geometric knot type by random perturbations of an instance of the knot. It implies that any knot equivalent representative can be reached by some sequence of pivots.

QUESTION 4. What proportion of knot space consists of knots of a given topological or geometric type?

In effect, we are asking, "If a polygonal knot is chosen at random, what is the likelihood that a knot of this type will be selected?" In the context of ring polymers, the asymptotic behavior of the probability of knotting has had a long history. Frisch and Wasserman [17] and Delbruck [18] conjectured that the asymptotic probability of knotting is one. This conjecture has been the subject of both numerical and well as theoretical study in a variety of contexts. In 1988 Sumners and Whittington [19] and, independently, Pippenger [20], established the conjecture in the context of the simple cubic lattice. Diao, Pippenger, and Sumners established the conjecture in the case of Gaussian random polygons [21]. Diao later studied the structure of equilateral spatial knots as well as minimal knots in the cubic lattice [22, 23]. Data from the current study concerning the proportion of distinct HOMFLY [24, 25, 26] polynomials, corresponding to specific knot types or small families of knot types, is reported later in the paper. Beyond the cases studied by Calvo, the question of geometric knot types is currently intractable due to the absence of effective invariants distinguishing geometric knot types. In Calvo's study of hexagonal knots and heptagonal knots, volume preserving involutions of the knot space demonstrate that all components of the a given topological knot type occupy the same proportion of the knot space.

QUESTION 5. How does the likelihood of a knot type depend on the number of edges? For example, how do the probabilities of the unknot, of prime and of composite knots depend on the number of edges?

In the cubic lattice, the likelihood of having a trefoil summand, or perhaps any other prime knot, goes to one as the number of edges goes to infinity. Van Rensburg and Whittington [27, 28] have estimated the probability, P(n), that an n-gon is knotted is given by $P(n) = 1 - \exp(-\alpha n + o(n))$ where $\alpha = (7.6 \pm 0.9)\mathrm{x}10^{-6}$. Another approach is to consider "Gaussian" random polygons in which the edge lengths satisfy a Gaussian distribution. Diao, Pippenger and Sumners [21] have shown that the probability of knotting tends to one exponentially with n. Specifically, they prove "There exists a constant $\varepsilon > 0$ such that P(n) is at least $1 - \exp(-n^{\varepsilon})$ provided that n is large enough."

In this study I have used the HOMFLY polynomial as a filter to attempt to identify (families of) topological knot types. In estimations of knot types I will not identify chiral presentations, as least to the extent that they are distinguished by their HOMFLY polynomials. Data will be presented concerning likelihood of a knot type for knots through the eight crossing knots as well as a selection of composite knots. The number of edges for which a given knot type occurs with its maximal relative probability as well as the numerical likelihood of the knot type occurring as a 16 edge knot will be also reported. An interesting analysis occurs when regarding these as providing parameters by which knot types can be given a linear order much in the same way that knots have been ordered by their minimal number of crossing representations. The optimal relative occurrence provides a measure suggesting "ideal" polygonal representations analogous to minimal crossing number or minimal polygon number representations. This line of study is the setting of the next question.

QUESTION 6. For each fixed n, what are their "ideal" configurations associated to each geometric knot type?

The question of what one means by an "ideal" configuration is one of great complexity and importance [29]. It is, in fact, the subject of an entire book [4]. One reason for the importance of this question is the possibility that the properties of ideal configurations correspond to physically observed behaviors of macromolecules under a wide range of conditions. An example of this is the electrophoretic mobility of DNA knots. Another is the desire to exhibit some intrinsic symmetries that have been observed physically. Thus, a central question is to provide an appropriate definition of the "ideal configuration".

One approach has been to define a function of the configuration such as an energy, a thickness, or another property of the specific spatial conformation to be optimized through deformations that respect the relevant structure determining the knot space. A key property of an energy function, for example, is being a positive function on the space of knots that it tends to infinity as singular maps are approached. Minimal energy configurations are discrete and finite in number. These can, in theory, be determined and compared in an effort to select one that is "ideal." An interesting historic objective was the creation of an energy such that a topological unknot would "flow" to a standard configuration by moving in a reverse gradient direction toward a minimal energy conformation, the standard unknot. While this approach has yet to bear definitive theoretical fruit, there have been many proposals for "energies" for smooth and polygonal knots. A particularly interesting family of functions have been proposed by O'Hara [30, 31, 32, 33] and Freedman, He, and Wang [34]. Kusner and Sullivan have proposed a mobius energy [35]. Another has been proposed for polygonal knots by Jonathon Simon, [36, 37]: the sum, over non-adjacent edges of the polygon, of the product of the lengths of the edges divided by the square of the minimum distance in three-space between the edges. By subtracting an intrinsic term from the Simon's energy, for example given by summing the product of the lengths of the edges divided by the square of the minimal arc distance along the portion of the knot connecting the two non-adjacent edges. This defines a discrete version of the Freedman, He, and Wang energy. The resulting energy function, denoted by $\varepsilon(K)$, has the attractive property that it is finite for polygonal knots.

However, it is not a "good" polygonal knot energy in the sense proposed by Diao, Ernst, and van Rensburg [38, 99] as it fails to be "asymptotically finite." This means that sequence of values $\varepsilon(K)$ fails to converge under subdivision of the polygonal knot K.

Another example of an "ideal property" is the thickness of the polygonal knot. The "thickness" of a smooth knot is the radius of the thickest tube, or tubular neighborhood consisting of normal non intersecting discs, whose axial curve is a representative of the knot type of unit length [40, 41, 42]. In this paper we will use Eric Rawdon's [43, 44, 45] definition of thickness for polygonal knots. It has the property that the thickness of inscribed polygonal approximations of a smooth curve approach the thickness of the curve. For a polygon of unit length, Rawdon's thickness, $\tau(K)$, is the minimum of a polygonal version of the doubly-critical self-distance function (distances between two points on the curve) and a minimal radial distance arising from adjacent edges due to curvature. For non unit length polygons, the value is divided by the length of the polygon. For many purposes the "length" of a knot, defined to be the reciprocal of the thickness, appears to possess a more natural structure and is preferred.

Our investigations of these quantities make an allowed random perturbation of the configuration, calculate the quantity to be optimized, compare it to the current value, and keep the new value and configuration if it represents an improvement over the currently held value. In order to improve the effectiveness of this simple method, we keep track of the nature of the perturbation and increase or decrease its magnitude and apply it again if an improvement has occurred. One might think of this as a choice of step size along a randomly selected path in knot space. We have not used some of the more complex methods associated with annealing approaches to optimization as this approach has proved to be adequately effective. Rather than seeking "ideal" knot conformations,
I search for "optimal" knot conformations with respect to a specific criterion. This search for optimal knots was be taken over conformations within a specific equilateral knot type or over families of related knot types, i.e. all representing a given topological knot type for varying numbers of edges. The question of optimization across all equilateral knot types representing the same topological knot type is being explored in ongoing research.

Thus, as the number of edges vary, another notion of optimization arises by seeking the maximum of the relative probability, for each fixed n, of the topological knot type. For a given optimal energy or thickness knot configuration we will also look at such physical knot theoretical properties as the average crossing number and the average writhe. These are averages over all projections of the given configuration of the number of crossings and, respectively, the signed sum of the crossing types. A crossing is given the value of 1 or -1 as shown in the Figure 1. Note that, for a knot, this value does not depend on the orientation of the knot.

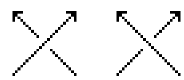

FIGURE 1. Crossing Convention

3. FOUNDATIONAL ASPECTS OF COMPUTER EXPLORATIONS OF KNOT SPACE

One important tool in the study of knot spaces has been the calculation of knot invariants. Historically, the Alexander polynomial has been the principal invariant used. It continues to be the most popular invariant, due to the relative ease of its calculation. Since 1984, however, other alternatives have become possible with the creation of the Jones polynomial and its successors, the HOMFLY polynomial, the Kauffman polynomial and, more recently, the "quantum" and Vassiliev finite type invariants [46, 47]. While, in theory, these are impractical due to the complexity of their computation, they have proven remarkably effective in our studies. The program used in this project was developed in collaboration with Bruce Ewing [48, 49]. It is able to calculate the HOMFLY polynomial for knots with up to 120 crossings. The HOMFLY polynomial is a finite Laurent polynomial in two variables, l and m, with integer coefficients, which is associated to each topological knot type. For the 2977 knot represented with fewer than 13 crossings there are only 76 cases that have the same first term as the trivial knot. By considering the entire invariant, these are easily eliminated. There are small families of knots having the same invariant and most, but not all, chiral knots are distinguished by the HOMFLY polynomial.

Many of the quantitative questions such as the probability of knotting or polygon number for a topological knot type are extremely difficult if not intractable through traditional geometric or algebraic topological methods. The Monte Carlo method [50], therefore, remains the most accessible. There are several obstacles to its application, however. First is the question of taking a uniformly distributed random sample of the space of knots.

In the case of Geo(n) or Cube(n), the Monte Carlo approach is quite straight forward. With respect to the uniform distribution on [0,1], one selects a list of 3n numbers to represent the coordinates of the n vertices of the polygon in Cube(n). For Geo(n), one randomly selects points n points on the unit sphere with respect to the uniform distribution and randomly selects n-1 radii randomly with respect to the uniform distribution on [0,1]. By allowing the first vertex to have magnitude one and the remaining vertices to lie within the unit ball with radii determined above, one has identified the vertex of a polygon in Geo(n) of largest magnitude, applied a homothety to place the polygon within the unit ball in 3-space, and used this largest vertex as the starting vertex. Direct calculation of the desired quantity, for example the curvature or the HOMFLY polynomial, provides the necessary data.

In the case of Equ(n) a Monte Carlo strategy is also possible. Using the pivot transformation with randomly selected axis vertices and rotation angle as described above, one can act upon the polygonal maps preserving the length and the linearity of the edges. Theorem 1 states that every polygonal knot can be reached (the transformation is irreducible) and every walk has the same probability of occurring (the transformation is reversible). Unfortunately, in order to insure that sampling by means of a pivot transformation is uniform with respect to the intrinsic measure, one needs to know that the pivot transformation is measure preserving. This, however, has not been demonstrated. So, although, I will later present results gained from the pivot sampling they will be representative of a limit measure that may differ from some more natural or intrinsic measure on the knot space.

QUESTION 7. What is the limit measure associated to the pivot transformation on Equ(n)?

Another context in which one can employ the pivot transformation is the study of ideal configurations. In this setting one uses a variation of the pivot transformation in which one dynamically selects, as a function of the current polygon, the range of the random rotation so as to insure that the geometric knot type is preserved throughout the rotation. In effect, one selects a short path determining a motion of the knot that does not change its knot type. Such transformations can be used to minimize energy, thickness, etc. This research is the subject of a study undertaken in collaboration with Eric Rawdon, [51]. Some preliminary elements of this research will be reported in the next section.

In all of the computer simulations and Metropolis Monte Carlo explorations extreme care must be exercised in the interpretation of the results. One example is the calculation of the HOMFLY polynomial in which integer algebra must be employed. A more delicate dimension is the determination of the topological knot type via the calculation of the HOMFLY polynomial or in the modification of an equilateral knot via the pivot transformation. All of these have implicit approximations as part of the method. Thus one must verify that the program is sufficiently accurate for the purpose of the study. A concrete example is provided by the creation of equilateral knots or their optimization with respect to some criterion. The computer approximation must be sufficiently accurate so as to insure that, although the precise data may not represent an equilateral knot, there is a nearby geometrically equivalent knot which is equilateral. Furthermore, transformations of "nearly equilateral" geometric knots imply that there exists a nearby transformation of the associated nearby equilateral knots. All this is necessary, of course, in order to be able to demonstrate that computer created nearly equilateral knots imply the existence of equivalent equilateral knots. These results will be found in the report the collaboration with Rawdon, [51].

4. The Results of the Metropolis Monte Carlo Studies

In this section, I will describe results of several recent simulations and numerical calculations as they concern the questions discussed above.

Question 1: What is the smallest number of edges required for an equilateral or geometric knot to realize a given topological knot type? A recent report is provided in Calvo and Millett [4]. Since then further progress has occurred, both Monte Carlo and theoretical. The consequences of this work is reflected in Tables 1 and 2.

Question 2: Is the polygon number the same for geometric and equilateral knots?
Question 3: How many distinct geometric or equilateral knot types are there as a function of n, the number of edges? The data represented in Figures 2 and 3 provide evidence in support of the conjecture that there are differences between the polygon numbers for geometric and equilateral knots. These data are also consistent with the exponential growth in distinct knots expected for the two knot theories. With respect to question 1, however, there is a remote possibility that the differences in numbers of knot types observed is an artifact of very small relative probabilities for equilateral representatives of the topological knot type rather than the non existence of representatives. An explicit example of this difference is required in order to settle this question.

These data are derived from a specific sample and are not a prediction of the actual number of distinct HOMFLY polynomials occurring for equilateral or geometric knots with a specific number of edges. The larger number of distinct polynomials observed for 24-gons is the result of a significantly larger sample size. The prediction of the total number of distinct polynomials is a more delicate question. An example of this later question is the effort to predict the number of distinct HOMFLY polynomials that arise for equilateral 50 edge knots. The growth in the number of distinct types can analyzed as a function on the number of observations and this sequence of data used to estimate the total number of types. The graph of the data is shown in Figure 4 from Calvo and Millett [4].

In that paper, we used this data to give an estimate of about 3,472 distinct knot polynomials occurring for knots in Equ(50). Of this, 2935 gave been observed. This is significantly smaller than the more than 124,359 HOMFLY polynomials of geometric knots that have been observed in Cube(32) but is comparable to the number observed for geometric knots with 18 to 19 edges. In order to give a credible prediction for either the equilateral or geometric knots a similar analysis would have to be undertaken for each of the sample points.

Question 4: What proportion of the knot space consists of knots of each type?" The estimation of an answer to this question, for any given knot type and knot space, requires a substantial collection of Monte Carlo studies and an analysis of the data for each knot type or HOMFLY polynomial, as is the case here. For Cube(n), the current status of calculation is shown in Figures 5, 6, 7, and 8 for selected knot types.

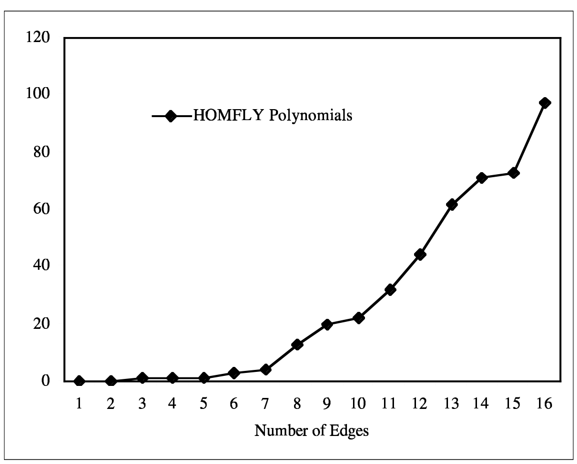

FIGURE 2. Knot Growth in Equ(n)

TABLE 1: Observed geometric polygon numbers p(.) for knots with nine or fewer crossings. Stars (*) indicate cases for which the minimal polygon number is shown.

K	p(K)	K	p(K)	K	p(K)
0	3*	8_{13}	10	9_{22}	12
		8_{14}	10	9_{23}	13
3_1	6*	8_{15}	12	9_{24}	12
		8_{16}	9*	9_{25}	13
4_1	7*	8_{17}	9*	9_{26}	12
		8_{18}	9*	9_{27}	12
5_1	8*	8_{19}	8*	9_{28}	12
5_2	8*	8_{20}	8*	9_{29}	12
		8_{21}	9*	9_{30}	13
6_1	8*	$3_1 + 5_1$	11	9_{31}	13
6_2	8*	$3_1 - 5_1$	11	9_{32}	12
6_3	8*	$3_1 + 5_2$	12	9_{33}	12
$3_1 + 3_1$	8*	$3_1 - 5_2$	11	9_{34}	12
$3_1 - 3_1$	8*	$4_1 + 4_1$	11	9_{35}	13
				9_{36}	14
7_1	9*	9_1	13	9_{37}	14
7_2	9*	9_2	14	9_{38}	14
7_3	9*	9_3	12	9_{39}	13
7_4	9*	9_4	14	9_{40}	9*
7_5	9*	9_5	13	9_{41}	9*
7_6	9*	9_6	12	9_{42}	9*
7_7	9*	9_7	12	9_{43}	10
$3_1 + 4_1$	9*	9_8	13	9_{44}	10
		9_9	13	9_{45}	10
8_1	11	9_{10}	13	9_{46}	9*
8_2	10	9_{11}	12	9_{47}	12
8_3	11	9_{12}	12	9_{48}	10
8_4	11	9_{13}	13	9_{49}	10
8_5	12	9_{14}	10	$3_1 + 6_1$	12
8_6	11	9_{15}	14	$3_1 - 6_1$	11
8_7	11	9_{16}	14	$3_1 + 6_2$	13
8_8	10	9_{17}	13	$3_1 - 6_2$	12
8_9	10	9_{18}	13	$3_1 + 6_3$	13
8_{10}	10	9_{19}	13	$4_1 + 5_1$	14
8_{11}	10	9_{20}	13	$4_1 + 5_2$	14
8_{12}	10	9_{21}	13	$3_1 + 3_1 \pm 3_1$	10*

TABLE 2: Observed equilateral polygon numbers ep(.) for knots with nine or fewer crossings. Stars (*) indicate cases for which the minimal polygon number is shown.

K	ep(K)	K	ep(K)	K	ep(K)
0	3*	8_{13}	12	9_{22}	??
		8_{14}	12	9_{23}	??
3_1	6*	8_{15}	16	9_{24}	??
		8_{16}	13	9_{25}	??
4_1	7*	8_{17}	13	9_{26}	19
		8_{18}	??	9_{27}	18
5_1	8*	8_{19}	9	9_{28}	??
5_2	8*	8_{20}	9	9_{29}	??
		8_{21}	10	9_{30}	15
6_1	8*	$3_1 + 5_1$	14	9_{31}	??
6_2	8*	$3_1 - 5_1$	15	9_{32}	16
6_3	8*	$3_1 + 5_2$	14	9_{33}	??
$3_1 + 3_1$	9	$3_1 - 5_2$	16	9_{34}	??
$3_1 - 3_1$	9	$4_1 + 4_1$	15	9_{35}	??
				9_{36}	18
7_1	9*	9_1	??	9_{37}	??
7_2	11	9_2	??	9_{38}	??
7_3	11	9_3	??	9_{39}	16
7_4	12	9_4	??	9_{40}	??
7_5	11	9_5	??	9_{41}	??
7_6	11	9_6	??	9_{42}	9*
7_7	11	9_7	??	9_{43}	13
$3_1 + 4_1$	11	9_8	??	9_{44}	13
		9_9	??	9_{45}	11
8_1	14	9_{10}	??	9_{46}	12
8_2	12	9_{11}	??	9_{47}	14
8_3	14	9_{12}	15	9_{48}	14
8_4	13	9_{13}	16	9_{49}	16
8_5	13	9_{14}	??	$3_1 + 6_1$	15
8_6	13	9_{15}	??	$3_1 - 6_1$	??
8_7	13	9_{16}	??	$3_1 + 6_2$	??
8_8	14	9_{17}	16	$3_1 - 6_2$	??
8_9	16	9_{18}	??	$3_1 + 6_3$	??
8_{10}	13	9_{19}	18	$4_1 + 5_1$	??
8_{11}	12	9_{20}	18	$4_1 + 5_2$	??
8_{12}	12	9_{21}	??	$3_1 + 3_1 \pm 3_1$	??

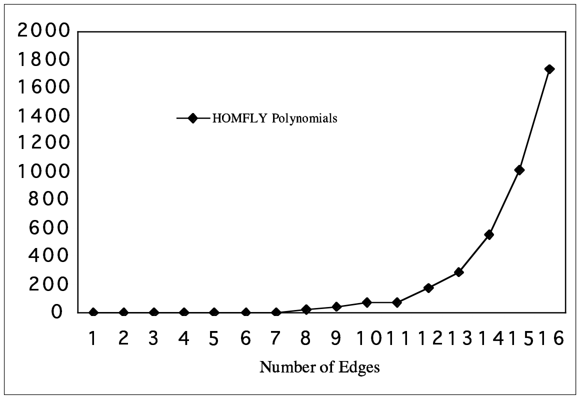

FIGURE 3. Knot Growth in Cube(n)

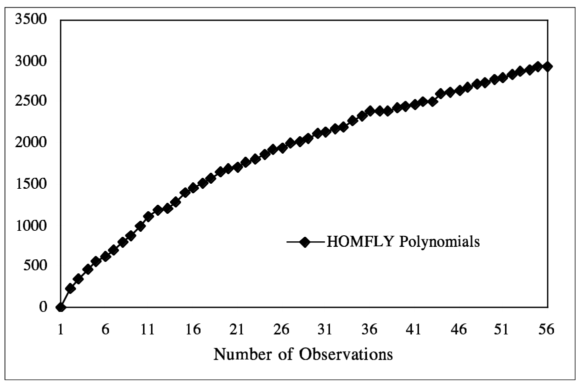

FIGURE 4. Distinct HOMFLY Polynomials of 50 Edge Knots

Question 5: How does the likelihood of a knot type depend on the number of edges? For example, how do the probabilities of randomly choosing an unknot, a prime or a composite knots occurring depend on the number of edges?

For Cube(n), the data shown in the previous figures are qualitatively consistent with the behavior exhibited in lattices and the case of Gaussian random polygons explored by Deguchi and Tsurusaki [52, 53]. Taking the perspective of scaling in statistical mechanics and considering the context of critical phenomena of second order phase transitions, they propose asymptotic formulae for random knotting, for a knot type K, of the form

$$P_K[n - 4] = C_K(n - 4)^{\upsilon_K}\mathrm{Exp}[-\kappa_K(n - 4)].$$

An analysis of the data collected in this study shows that is model is not sufficient to faithfully represent the data. Instead, it appears that a quadratic term in the exponential is required. At this time, the reason for this term is unexplained. Thus, the model proposed in this paper is

$$P_K[n - 4] = C_K(n - 4)^{\upsilon_K} \mathrm{Exp}[\kappa_K(n - 4) + \delta_K(n - 4)^2].$$

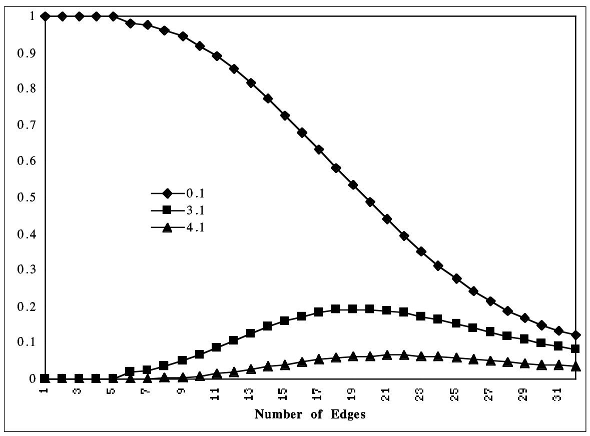

FIGURE 5. Proportion of Knot Types in Cube(n)

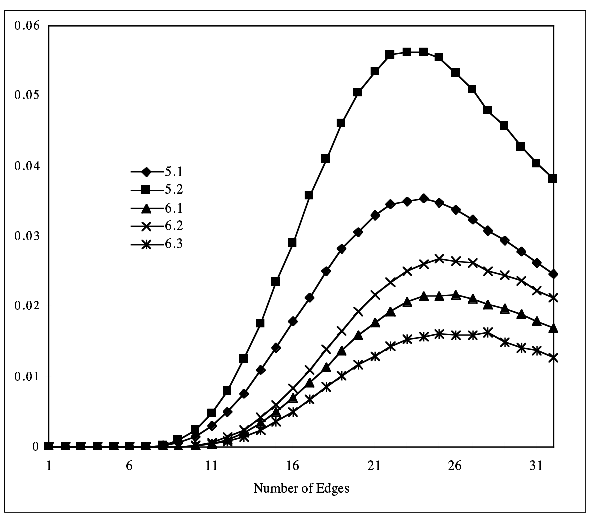

FIGURE 6. Proportion of Knot Types in Cube(n)

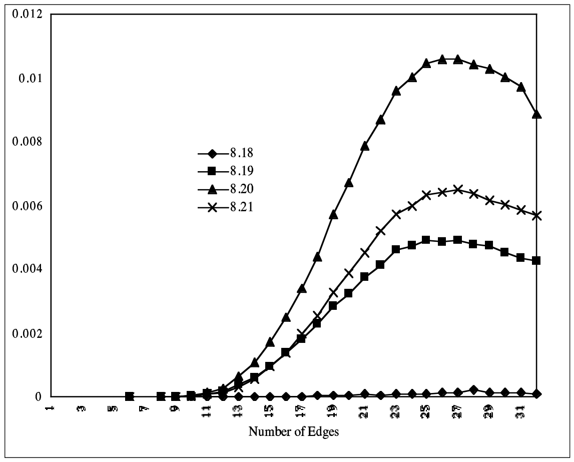

FIGURE 7. Proportion of Knot Types in Cube(n)

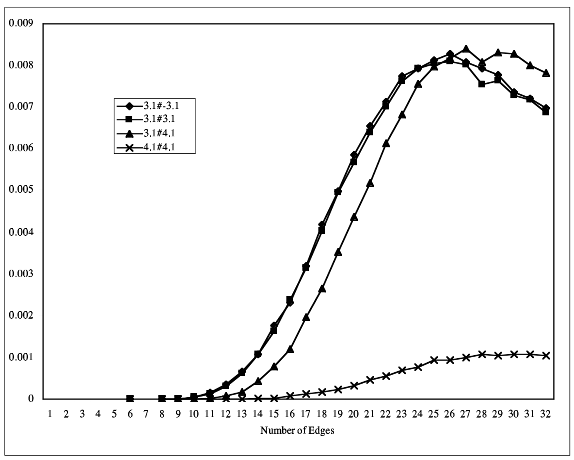

FIGURE 8. Proportion of Knot Types in Cube(n)

For the unknot, the predicted lattice dependence is of the form

$$P_0[n - 4] = \mathrm{Exp}[-\kappa(n - 4) + o(n)]$$

but the data for the case of geometric unknots, see Figure 9, gives the form

$$P_0[n - 4] = 0.988966(n - 4)^{-0.0270147}\mathrm{Exp}[0.0154788(n - 4) - 0.0034218\,(n - 4)^2].$$

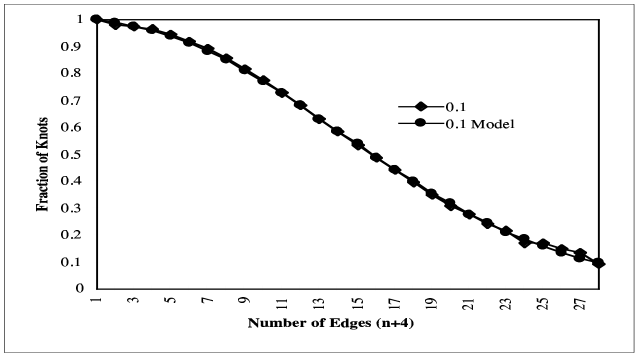

FIGURE 9. Cube(n) Unknot Occurrence Model

For the trefoil knot the data gives, see Figure 10,

$$P_{3.1}[n - 4] = 0.0135348(n - 4)^{0.523199}\mathrm{Exp}[0.192969\ (n - 4) - 0.0034218\ (n - 4)^2].$$

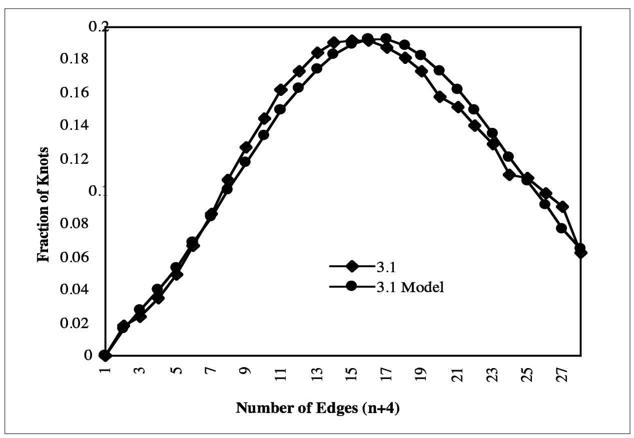

FIGURE 10. Cube(n) Trefoil Occurrence Model

For the 4.1, the figure 8 knot, see Figure 11, one has

$$P_{4.1}[n - 5] = 0.000712362(n - 5)^{1.69835}\mathrm{Exp}[0.0828738(n - 5) - 0.005909\ (n - 5)^2].$$

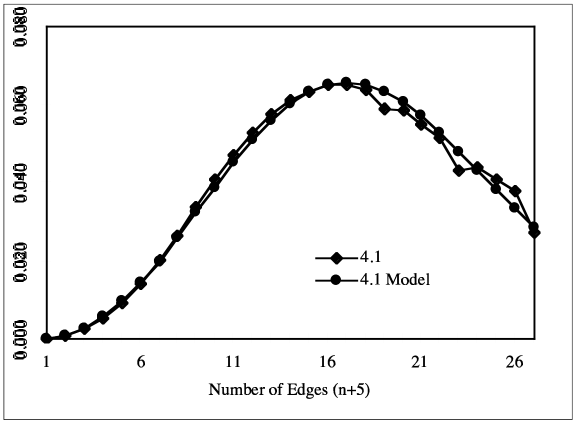

FIGURE 11. Cube(n) Figure Eight Occurrence Model

TABLE 3. Knotting as a function of the number of edges:

$$P_K[n] = C_K(n - n_0)^{\upsilon K}\mathrm{Exp}[\upsilon_K(n - n_0) + \delta_K(n - n_0)^2]$$

where $n_0 + 1$ is the number of edges required to construct the geometric knot.

Knot	$\ln(C_K)$	κ_K	υ_K	δ_K
0.1	-0.01110	-0.027015	0.015479	-0.0034218
3.1	-4.30249	0.523199	0.192969	-0.0073583
4.1	-7.24692	1.69835	0.082874	-0.0059091
5.1	-8.85832	1.93224	0.121593	-0.00690878
5.2	-8.43491	1.9929	0.115512	-0.00698158
6.1	-12.502	3.62345	-0.00817	0.00500914
6.2	-11.705	2.94066	0.102771	-0.00680935
6.3	-12.2566	2.95392	0.105574	-0.00691127
8.19	-14.1467	3.63823	-0.016296	-0.00424356
8.20	-15.0832	4.96809	-0.191126	-0.00124664
8.21	-13.317	3.19543	0.0541537	-0.00582986
3.1#-3.1	-14.6166	4.64039	-0.163117	-0.00197747
3.1#3.1	-12.1329	2.96944	0.0226628	-0.00498713
3.1#4.1	-12.7173	3.10306	0.0379747	-0.00516541

Table 3 contains the various knot parameters that have been calculated for the cube knot data. They represent one manner in which the various knot types can be ordered in terms of their statistical occurrence in this knot space. In the exploration of the physical properties of the various knot types arising in the natural sciences, another important parameter appears to be the number of edges at which a knot type attains its maximal relative probability of occurrence. This has been the subject of applications in molecular biology, for example in the papers of Stasiak and collaborators [54, 55, 56, 57, 58, 59]. Another example of this sort is probability of occurrence for a specified number of edges. The number of edges giving the maximal likelihood of a topological knot type, together with its probability of occurrence in Cube(16) are reported in Table 4.

TABLE 4. Maximal Geometric Knotting Probabilities

Knot Type	maximal likelihood	16 edge probability
3.1	20	0.173646
4.1	21	0.0472002
5.1	26	0.0179719
5.2	24	0.0289013
6.1	26	0.0069933
6.2	28	0.00832214
6.3	28	0.00505106
8.19	30	0.00134359
8.20	27	0.00243887
8.21	27	0.00137309
3.1#-3.1	23	0.00226923
3.1#3.1	26	0.00238724

Question 6: For each fixed n, how do the various "ideal" configurations associated to each geometric knot type order the knots types? How do these ideal configuration orders vary with n?

Tables 5 and 6 report some initial results of joint work with Eric Rawdon on energy, rope length, and the average crossing number of the energy minimized configuration of geometric knots. Note that these tables report similar but distinct orderings of the various topological knot types depending on the number of edges and the characteristic.

5. CONCLUSIONS AND AREAS FOR FURTHER RESEARCH

The determination of the polygon number for a given topological knot type is a very challenging problem for any specific example. As demonstrated by the results of Calvo, even for small numbers of edges, the systematic determination of all knots types occurring for a specific number of edges is even harder. Calvo has determined the geometric octagonal topological knot types and all have been observed in the Metropolis Monte Carlo sampling of Geo(8). In the study of a much larger number of samples taken

TABLE 5: 16 Edge Equilateral Knot Orders

Position	Probability	Energy	Rope Length	Average Crossing Number
1	0.1	0.1	0.1	0.1
2	3.1	3.1	3.1	3.1
3	4.1	4.1	4.1	4.1
4	5.2	5.1	5.1	5.1
5	5.1	5.2	5.2	5.2
6	6.2	3.1#3.1	8.19	3.1#3.1
7	6.1	6.1	3.1#3.1	6.1
8	6.3	8.19	6.1	6.2
9	3.1#-3.1	6.2	6.3	6.3
10	3.1#3.1	6.3	3.1#-3.1	8.19
11	8.2	8.20	6.2	7.1
12	8.19	3.1#-3.1	7.1	8.20
13	8.21	7.1	9.46	3.1#-3.1
14	7.3	7.2	8.20	3.1#4.1
15	7.2	3.1#4.1	7.2	7.2
16	7.5	7.3	7.4	7.3
17	7.7	9.46	3.1#4.1	9.46
18	7.6	7.4	7.5	7.6
19	7.1	7.5	7.3	8.21
20	3.1#4.1	8.21	7.6	7.5
21	7.4	9.42	10.144	7.4
22	9.42	10.144	8.21	3.1#5.1
23	8.2	7.6	3.1#5.1	9.42
24	9.46	9.43	9.42	3.1#5.2
25	9.44	3.1#5.1	3.1#5.2	8.1
26	8.11	8.1	9.45	10.144
27	8.6	3.1#5.2	9.49	9.43
28	8.1	8.7	8.7	8.7
29	8.14	9.45	8.15	4.1#4.1
30	8.9	10.151	10.145	8.9
31	8.10	9.49	8.9	7.7

TABLE 6: 32 Edge Equilateral Knot Orders

Position	Probability	Energy	Rope Length	Average Crossing Number
1	0.1	0.1	0.1	0.1
2	3.1	3.1	3.1	3.1
3	4.1	4.1	4.1	4.1
4	5.2	5.1	5.1	5.1
5	5.1	5.2	5.2	5.2
6	6.2	3.1#-3.1	3.1#-3.1	3.1#-3.1
7	3.1#3.1	3.1#3.1	6.1	3.1#3.1
8	6.1	6.1	3.1#3.1	6.1
9	3.1#-3.1	6.2	6.3	6.2
10	6.3	6.3	6.2	6.3
11	3.1#4.1	7.1	8.19	7.1
12	7.5	8.19	8.2	3.1#4.1
13	3.1#-5.2	3.1#4.1	7.1	8.19
14	8.2	7.2	7.2	7.2
15	7.6	7.3	7.3	8.2
16	8.19	8.2	3.1#4.1	7.7
17	7.7	7.4	8.21	7.3
18	8.21	7.5	7.6	7.4
19	7.4	7.7	9.46	7.5
20	7.3	8.21	7.7	7.7
21	7.2	7.6	9.42	8.21
22	9.44	3.1#5.1	7.4	7.6
23	8.11	8.1	9.43	3.1#5.1
24	9.42	3.1#5.2	7.5	3.1#5.2
25	7.1	9.42	10.144	4.1#4.1
26	8.15	9.46	3.1#5.1	8.1
27	8.9	8.2 .	8.1	8.2
28	8.4	4.1#4.1	3.1#5.2	9.42
29	9.46	9.43	9.49	9.46
30	8.6	8.6	8.1	9.43
31	8.7	8.9	4.1#4.1	8.8

from Equ(8), the knots 8.19, 8.20 and 3.1 $\pm$ 3.1 have not yet been observed. Despite having constructed equilateral models for these knots and being quite convinced that equilateral instances of them exist, this can not be confirmed by the current Monte Carlo data. Stronger evidence suggesting that geometric and equilateral polygon numbers must differ for most knot types is provided by comparison of the substantial differences in the growths of observed HOMFLY polynomials shown in Figures 2 and 3. The determination of a specific case in which the equilateral and geometric polygon numbers differ, however, remains unachieved. As a consequence, the determination of growth rate for equilateral and geometric knots is also still open. The data suggest that, asymptotically, the number of distinct HOMFLY polynomials of geometric knots with n edges is about ten times the number of distinct HOMFLY polynomials of equilateral knots with n^2 edges.

The proportion of the space of geometric knots appears to be given by a function of the form

$$P_K[n - 4] = C_K(n -4)^{\upsilon_K} \mathrm{Exp}[\kappa_K(n - 4) + \delta_K(n - 4)^2]$$

where the specific coefficients vary with the associated knot type. This model differs from those proposed for lattice knots or appearing in Deguchi and Tsurusaki by the presence of a quadratic term. The presence of this term does not yet have a theoretical explanation.

The various quantities such as the relative probability of occurrence, the number of edges at which this is probability is maximal, any of the knot energies, or the thickness of the polygonal knot can be used to impose an order on the topological knot types. The data has shown that these orders, while similar in many respects, are not entirely equivalent. Of particular interest, in terms of the present research, is the relationship between the order arising from relative probability and that arising from the energy or thickness. Unfortunately, the data in this study suggest that the relative probability order may change with increasing numbers of edges. Further research is necessary to confirm this assertion is necessary. A deeper investigation into the properties of pairs or families of knots that exhibit this behavior could also be important. Another fundamental question to be explored would be whether the probability of the unknot is ever smaller than that of any other knot, e.g. the trefoil knot.

In this paper we have considered Monte Carlo data generated for Equ(n), Geo(n), and Cube(n) and have noted the occurrence of quantitative differences in the data despite qualitative similarities. A. Stasiak has suggested that an important factor in accounting for the quantitative differences may be the influence of spatial constraints on the distributions. Effectively, in the case of the cube knots, the observed distribution may be the superposition of two or more distributions reflecting distinctive contributions arising from spatial constraints or barriers as well as one reflecting the intrinsic knotting. Further work, whose consequences will be reported in a sequel to this paper, is underway to explore these possibilities.

A somewhat different perspective on these questions arises by exploring the geometric structure of the various polygonal knot spaces and the components that determine the associated polygonal knot types. While the Monte Carlo simulations provide average data on the extent of these components, their precise geometric nature is a mystery. Are these components "uniformly long, skinny, thread-like" entities or do they have "fat" or "thick" regions that account from the preponderance of the relative probability? This question and the relationship of the answers to the relative probability and to a wide range of physical knot invariants provides the stimulus for a new collection of questions. These are the subject of a research collaboration with Eric Rawdon and the subject of another paper.

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