

An Investigation of Equilateral Knot Spaces and Ideal Physical Knot Configurations

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ABSTRACT. Spaces of polygonal knots, subject to specified constraints such as the number of nondegenerate edges or the requirement of having fixed edge lengths, provide the context within which it is appropriate to study configurations which are ideal with respect to a variety of natural physically motivated constraints. Even for polygonal knots with relatively few vertices, the high dimensionality and complexity of the knot space structure makes analytical investigations impractical. In this note, we will discuss the methods and the results of a Monte Carlo investigation of several fundamental approaches to defining an ideal polygonal knot configuration. The analysis takes place in the context of polygons with a small number of edges.

1. Introduction

One goal of this note is the exploration of the global structure of equilateral knot space from the perspective of a fundamental spatial quantity, the diameter of the knot. It is used to separate knot space into bands bordered by the strata of configurations with equal diameter. Each of these bands consists of some fraction of knot space. The variation of this proportion as a function of the diameter captures a critical facet of the geometric structure of knot space. Each band also supports a specific collection of polygonal knot types at proportions whose variation is also of interest. Each of these varying quantities provides a measure of the complexity profile of knot space as a function of diameter. The data also give estimates of the knot space averages of the diameter of the knot for each topological knot type. These will be estimated for small numbers of edges (the tight knotting regime, that is, near the number of edges for which one is first able to construct the knot type). They are compared to other quantities that reflect the spatial characteristics of polygonal knot configurations achieving optimal values of ropelength or other spatial measures.

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2. Equilateral Polygonal Knots and Knot Spaces

A knot is a placement of a closed curve in three dimensional space that is regular, e.g. smooth or piecewise linear, and which does not intersect itself. The collection of all such knots which can be deformed into each other, avoiding any singular configuration or pathological behavior, determines a knot type whose members are representatives of this type. Among all such representatives there are some which may be considered as better representatives, according to an established criterion, than others in that their properties best reflect those of the aggregate. In this note, the term **"ideal knot"** will mean a configuration that is optimal with respect to a spatial property among all equivalent configurations. There are, therefore, different ideal knots according to which spatial property is optimized. The search for such "canonical" or "ideal" conformations and the determination of the extent to which they do characterize the collective properties continues to be an important research goal of physical knot theory and in its applications to the natural sciences. For example, the average crossing number and average writhe of thickness optimized configurations correlate well with the averages of other physical characteristics over large random collections of the corresponding knot conformations [16, 17, 18, 38]. They also correlate well with the observed gel speeds of the corresponding DNA knots.

The knots employed here are realized as equilateral (we require that all edges have unit length) polygons in 3-space. Because the simulations are all approximate, one is actually operating in the space of polygonal knots near the subspace of equilateral knots. If the data provide a knot that is sufficiently close to being equilateral and the minimum of the distances between non adjacent edges is sufficiently large, then there is an equilateral knot of the same polygonal knot type [23]. In order to make the calculations easier to accomplish, one selects a starting vertex (we could require it to be $(0, 0, 0)$) and an adjacent vertex, thereby establishing an order on the vertices. These choices allow one to realize the space of such equilateral polygonal knots with n edges, denoted by $Equ(n)$, as a subset of Euclidean space of dimension three times the number of edges. The closure is a compact subspace whose added points define singular "knot" conformations. The topology and geometry of the relatively open subset of non singular conformations defines the structure of knot space. For example, if there is a path in knot space connecting one conformation to another, we say that the two conformations are equivalent and represent the same equilateral knot type. The problems of whether or not a given topological knot type can be realized by an equilateral polygon or whether or not two equilateral polygons are equivalent are examples of questions in domain of geometric knot theory. In the first question, one seeks the equilateral edge number of the knot, [1, 4, 3, 22, 30], and in the second, one seeks quantities that can distinguish between distinct geometric knot types representing the same topological knot type, [2, 22, 27].

3. Physical or Spatial Characteristics of Equilateral Polygonal Knots

One physical characteristic of a knot conformation is its (normalized) **diameter**. The diameter of a knot configuration K , $\delta(K)$, is defined to be the maximum of the distances between pairs of vertices of K divided by the arc length of the knot. If K designates a geometrical knot type in $Equ(n)$, let $d(K)$ denote the greatest lower bound of $\delta(K)$ over all K representing the knot type K . Similarly, let $D(K)$

denote the least upper bound of $d(K)$ over all K representing the knot type K . Another interesting physical characteristic of the conformation is the **radius of gyration**, $\rho(K)$, the average distance of the vertices from the average position of the vertices divided by the length of the equilateral knot. Both quantities provide different measures of the spatial extent of the knot. The radius of gyration has been the subject of research concerning the conjecture that the topological knot type of the configuration influences the scaling, [6, 7, 8, 14, 16]. While knots of small diameter and or small radius of gyration are quite compact, the conformation's largest diameter and radius of gyration appear to be quite different. The standard regular planar n edge polygons have the largest radius of gyration while, for example, the least upper bound of the diameter is approximately $n/2$ and occurs for polygons of even numbers of edges at the singular conformation with the edges maximally stretched out along a line. Another physical characteristic is the minimal distance between non adjacent edges of the knot, $\mu(K)$. This is a measure of the **robustness** of the conformation, especially when the number of edges is close to the edge number of the knot type. It is one measure of the extent to which one may move vertices in knot space and still preserve the polygonal knot type. Their averages over all of knot space or over a specific region of knot space such as a component consisting of knots of the same topological type are examples of proposed ideal characteristics of knots. They will be compared to similar characteristics of ideal knot configurations.

One approach to the determination of the spatial characteristics of a knot type is to first identify an ideal knot conformation for a given equilateral polygonal knot type. For example, one may choose to optimize the polygonal thickness or, equivalently, the polygonal ropelength within the component defining the polygonal knot, [29, 31, 32]. There are several interesting definitions for this notion of ropelength of smooth knots, [5, 13, 9, 21, 40]. I believe that the conceptually simplest analog, for a given equilateral knot, is to keep the length of the knot fixed (indeed, fix the lengths of each of the edges) and expand a tube surrounding the knot (defined as the union of balls centered at each vertex and cylinders centered on each edge, all of the same radius) until it is no longer possible to do so without creating a singular tube, even by changing to an equivalent knot conformation of the same polygonal knot type. The optimized quantity is L/D , the ratio of the length of the knot and the diameter of the maximal tube, is called the ropelength. Its reciprocal is called the thickness of the knot. This is comparable to the definition employed by Stasiak and others. In work with Eric Rawdon [23], we used an approach that Rawdon, [29] developed as an analog of the smooth case. Let $DCSD$ denote the doubly-critical self-distance of the knot and let MinRad denote minimum of the radii of curvature (defined as the edge length divided by twice the tangent of half the exterior angle at a vertex) at the vertices of the knot. The injectivity radius of an equilateral polygonal knot is defined as the minimum of $1/2 * DCSD$ of the knot and MinRad . In this paper, the **thickness** is defined to be the injectivity radius divided by the total length of the knot and the **ropelength** is defined to be the reciprocal of the thickness. The ropelength and the thickness are two among many physical characteristics of a polygonal knot.

4. Monte Carlo Investigations

The population studied in this research was generated by a Monte Carlo sampling of equilateral polygonal knot spaces of knot conformations with 8, 16, and 32 edges. The sampling is accomplished by a random rotation about an axis determined by a pair of randomly selected pair of vertices. The resulting conformations are "almost equilateral," and as described in Millett and Rawdon [23], determine a geometrically equivalent equilateral knot. For each of the selected knot conformations, the diameter and radius of gyration is recorded. The knot presentation is determined and is used to compute the HOMFLY knot polynomial, [12, 19, 20] invariant using the Ewing-Millett program, [10, 11]. This program accepts knot presentations of up to 240 crossings, and for a generic knot conformation, has proved to be an effective tool to estimate the number and frequency of topological knot types. These data provide estimates of the variation of the number of distinct knot types as a function of diameter as well as the relative proportion of those knot types that do occur.

In the work with Rawdon, we determined estimates for the ropelength optimized knot conformations for many equilateral polygons with 8, 16, and 32 edges. These values are reached by the use of a random walk with a simulated annealing effect. The values are local minima, and we show, are quite close to actual global minima. The initial conformations for the 8 and 16 edge knots used in Millett-Rawdon were created by Rob Scharein using KnotPlot [35]. The 32 edge knots were gotten by subdivision of the 16 edge knots. All knots were checked to insure that they satisfied the robustness requirement necessary to insure that an equilateral knot of this geometric type existed and was closely approximated by the data. Once a robust equilateral example of a topological knot type was created, the simulated annealing process was applied to search for ropelength optimized conformations as discussed in Millett-Rawdon [23]. More data concerning the spatial characteristics of ropelength (and energy) optimized knots can be found there.

5. Analysis of Numerical Data

A portion of the data from the Monte Carlo explorations of equilateral knot spaces with 8, 16 and 32 edges is given in Table 1. The knots are denoted using the

TABLE 1. A Comparison of Average Diameter and Diameters of Energy and Ropelength Optimized 8, 16, and 32 Edge Equilateral Knots

Knot	8 Ave	8 En	8 RL	16 Ave	16 En	16 RL	32 Ave	32 En	32 RL
All	.17981			.11436			.15307		
0 ₁	.17993			.11453			.15433		
3 ₁	.17021	.2212	.2037	.10926	.1926	.1855	.13920	.1883	.1841
4 ₁	.16129	.1945	.1985	.10717	.1630	.1512	.13314	.1611	.1451
5 ₁	.13975	.1607	.1507	.10258	.1743	.1620	.13055	.1639	.1659
5 ₂	.14865	.1518	.1507	.10522	.1692	.1740	.12834	.1684	.1609
6 ₁	NA	.1562	.1510	.10785	.1522	.1434	.13008	.1587	.1488
6 ₂	NA	.1485	.1470	.10629	.1888	.1800	.12549	.1563	.1390
6 ₃	NA	.1392	.1391	.10419	.1675	.1452	.12698	.1487	.1364
3 ₁ #3 ₁	NA	.1276	.1275	.11017	.1874	.1714	.12952	.1944	.1758
3 ₁ # - 3 ₁	NA	.1250	.1250	.10962	.1674	.1470	.13139	.1958	.1752

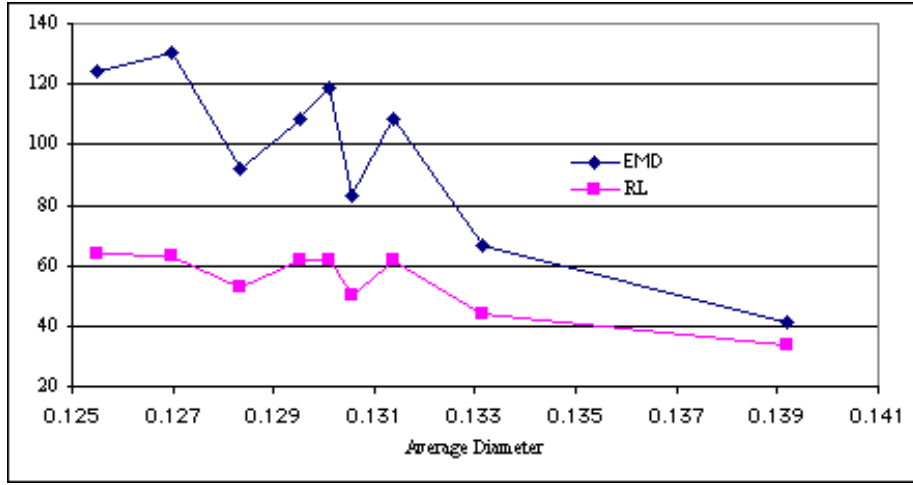


FIGURE 1. Optimized Energy and Ropelength versus Average Diameter

Alander-Briggs notation $0_1, 3_1, 4_1$, etc. standard representations of which are found in the tables of knot [33]. Note that $3_1 \# 3_1$ and $3_1 \# -3_1$ denote the connected sums of the trefoil, 3_1 , or its mirror reflecton, -3_1 . The average diameter over the entire space, Ave , and the diameters of the energy and ropelength optimized knots, En and RL respectively, are given as a function of the topological knot type. In Figure 1, we show, graphically, the optimized energy and ropelengths as a function of the average diameter of the knot. This graph illustrates the expectation that the smaller the diameter of the knot, the larger the energy and ropelength but shows, in addition, that this dependence holds for the knot space average of diameters in the knot type.

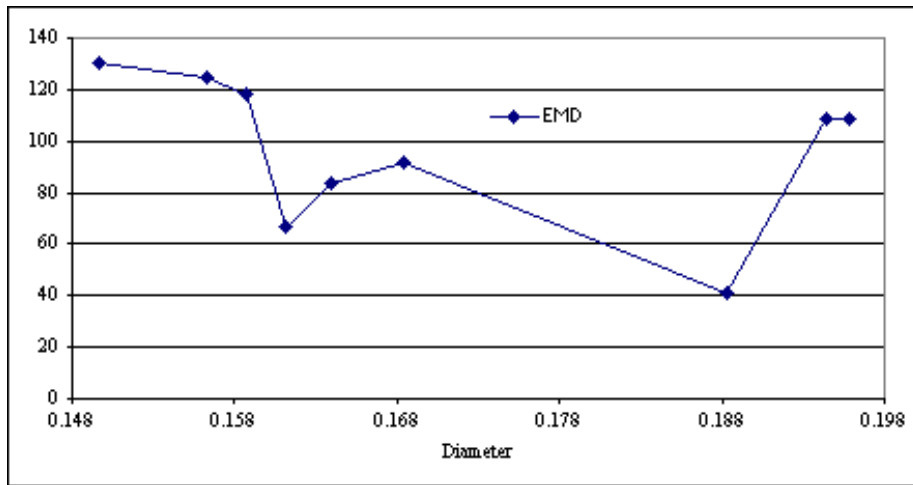


FIGURE 2. Optimized Energy versus Diameter

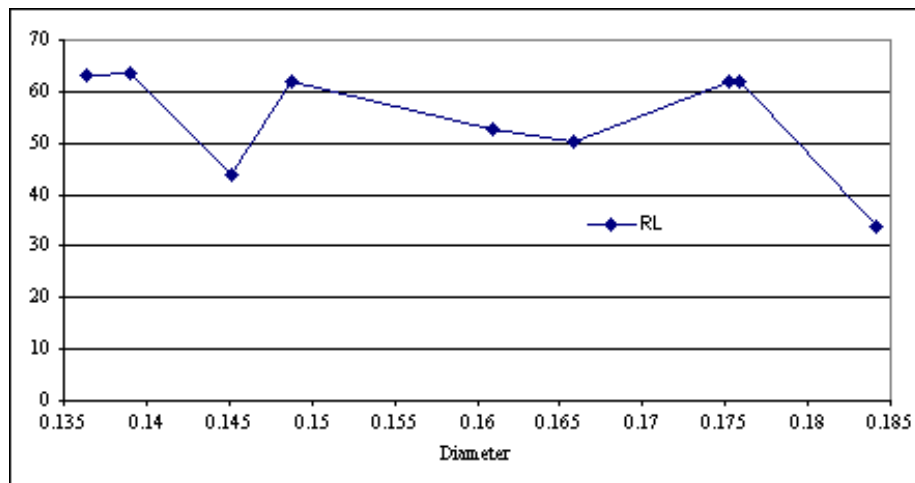
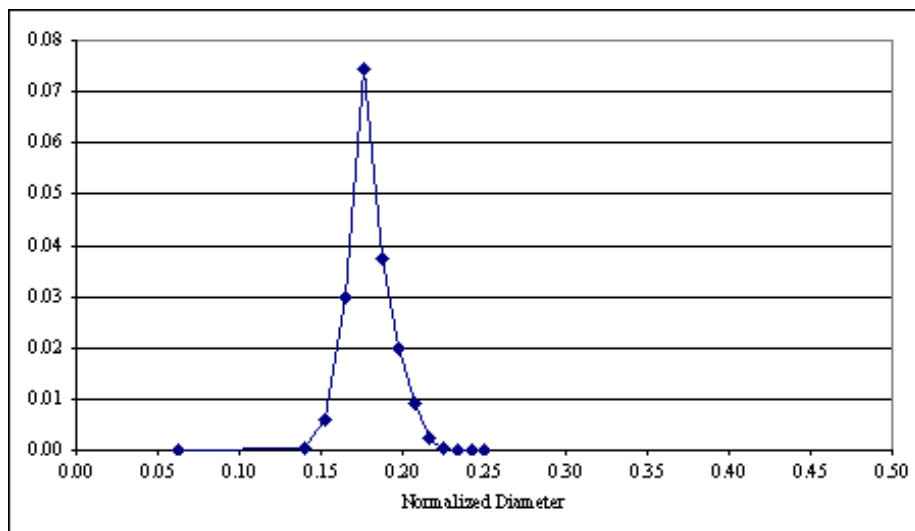
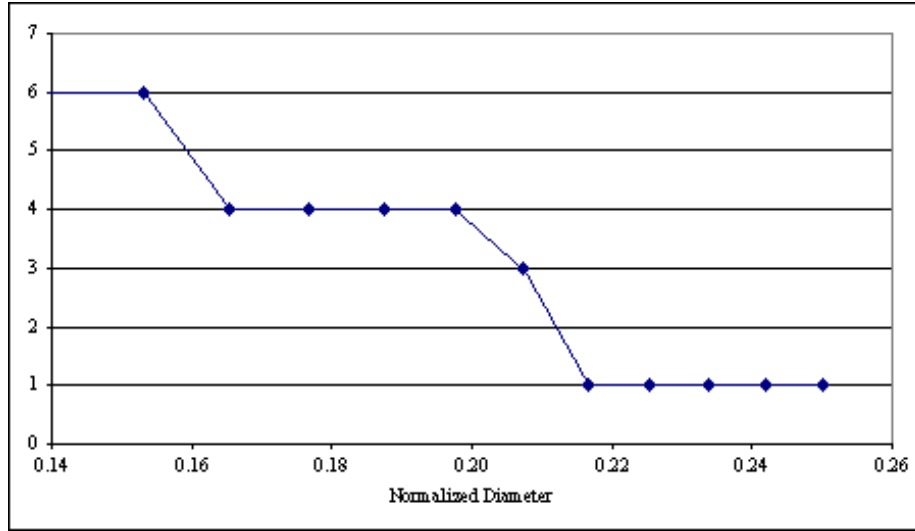


FIGURE 3. Optimized Ropelength versus Diameter

While this relationship appears to be quite weak, it is much stronger than the relationship between the energy or ropelength and the diameter of the optimized configuration. The graph of these data are shown in Figures 2 and 3.

The proportion of knot space as a function of the diameter and the number of distinct knot types, as measured by distinct HOMFLY polynomials, capture two fundamental features of the structure of knot space. These data are presented for the spaces of equilateral knots with 8, 16, and 32 edges. In order to better indicate the evolution of the shape of knot space as a function of the number of edges, we continue to employ a normalization of the diameter given by dividing the diameter

FIGURE 4. $Equ(8)$ Population Distribution

FIGURE 5. Distinct knot types in $Equ(8)$ versus normalized diameter

by the length of the knot. Thus, the maximum normalized diameter is always 0.5. The minimum normalized diameter is $1/n$, where n is the number of edges.

The data represented in Figures 4 and 5, and those in analogous graphs later in this paper, was generated by taking an equal subinterval partition of the range of diameters, and thereby, partitioning knot space into the corresponding family of regions. The Monte Carlo knot space data, collected over the entire space, was then partitioned according to the region of knot space, thereby giving the knot space proportion and knot diversity data determining the corresponding graphs. This method allows one to more easily generate and evaluate data that accurately reflect the nature and structure of these slices of knot space as parameterized by the knot diameter.

The relationship between the diameter and the number of distinct knot types illustrated by these graphs suggests an important feature of the structure of knot space. The preponderance of knot space is found in the "middle range of diameters" with the regions of extreme diameters being much more sparsely populated. Figure 4 gives a quantitative expression of this functional relationship. In general, the larger the diameter of the knot, the simpler the structure, as illustrated in Figure 5. The precise nature of this property changes, however, with the number of edges.

For each geometrical knot type K in $Equ(n)$, there will be a least upper bound of the knot type, denoted by $B(K)$. Except in the simple case of the Proposition 1, there are no exact calculations of $B(K)$ known at this time.

THEOREM 5.1. *The least upper bound on the diameter of a non-trivial knot in $Equ(4n + 2)$ is equal to $\sqrt{\frac{4-1/n^2}{4+2/n}} = B(3_1)$.*

PROOF. In this proof, we use knot models which are equilateral $(4n + 2)$ -gons having unit length edges and rescale the calculated value to account for the $(4n + 2)$ length of the knot. The limiting value is realized by a sequence of trefoil knots converging to the singular set represented by union of two isosceles triangles

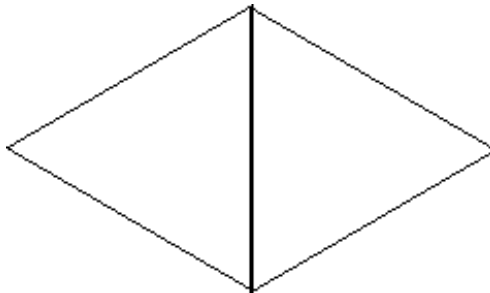


FIGURE 6. Singular Hexagonal Trefoil Position

along their base, of unit length, and whose other edges have length equal to " n ," as illustrated in Figure 6. Twice the altitude of the triangle gives the least upper bound. A configuration with a diameter greater than this value can have only two locally extreme "height" values along the direction parallel to the line connecting the vertices giving the diameter. As a consequence, any such configuration is a geometrically trivial knot. \square

As noted in the proof of the proposition, the least upper bound is realized by the least upper bound of the normalized diameter of the trefoil knot. For $n = 6$, this value is .28867 and the best Monte Carlo generated values observed do approach this value. The limit corresponds to the singular position shown in Figure 6. A close but non-singular configuration with normalized diameter .283338 is shown in Figure 7. Its vertex coordinates are:

$$\begin{aligned} &\{ \{0., 0., 0.\}, \{0.486131, 0.015706, 0.873745\}, \\ &\quad \{-0.513209, -0.0166517, 0.857231\}, \{0.0277697, 0.000808531, 0.0163762\}, \\ &\quad \{-0.972096, 0., 0.\}, \{-0.486048, -0.0167832, 0.873771\} \}. \end{aligned}$$

It has curvature of 12.6945, quite close to $4\pi \approx 12.566$, the minimal value.

The largest observed diameter in the Monte Carlo study of $Equ(6)$ is .251377, about 87.1% of the least upper bound. For $Equ(8)$, the largest observed value is .332723. For $Equ(10)$, this is .329364159, 79.88% of the theoretical value of .41231056. This reflects the extremely small probability of a randomly selected equilateral octagonal knot to have this character.

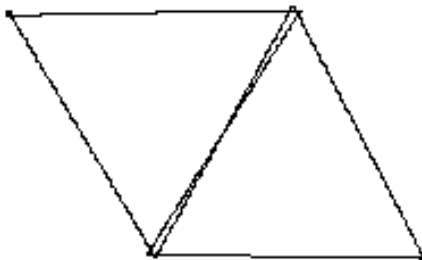


FIGURE 7. Hexagonal Trefoil with Large Diameter

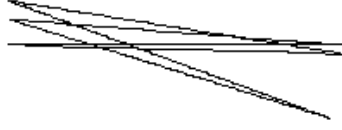


FIGURE 8. Trefoil of Diameter .16697812333

For the case of even numbers of vertices, for example " $2n$," the greatest lower bound over all configurations in $Equ(2n)$ is $1/2n$, corresponding to the singular locus of a single edge to which all edges converge. Let $b(K)$ denote the greatest lower bound of the diameter of all configurations in $Eq(n)$ equivalent to " K ".

THEOREM 5.2. *In $Equ(2n)$, $b(3_1) = 1/2n$, for $n > 3$.*

PROOF. In $Equ(6)$, using the model in which the individual edge length is 1, there is a sequence of trefoil knots converging to the single edge singular locus. Vertices 1, 3, and 5 converge to $\{0, 0, 0\}$ and vertices 2, 4, and 6 converge to $\{1, 0, 0\}$. One approximation is the hexagonal trefoil example with vertices:

$$\begin{aligned} &\{\{0, 0, 0\}, \{1.0, 0, 0\}, \\ &\quad \{0.00299957, 0.07739435, -0.00049926\}, \\ &\quad \{0.96018567, -0.21105152, -0.02486597\}, \\ &\quad \{0.04083793, 0.1273103549, 0.17590997\}, \\ &\quad \{0.99690190, -0.02499956, -0.07457634\}\} \end{aligned}$$

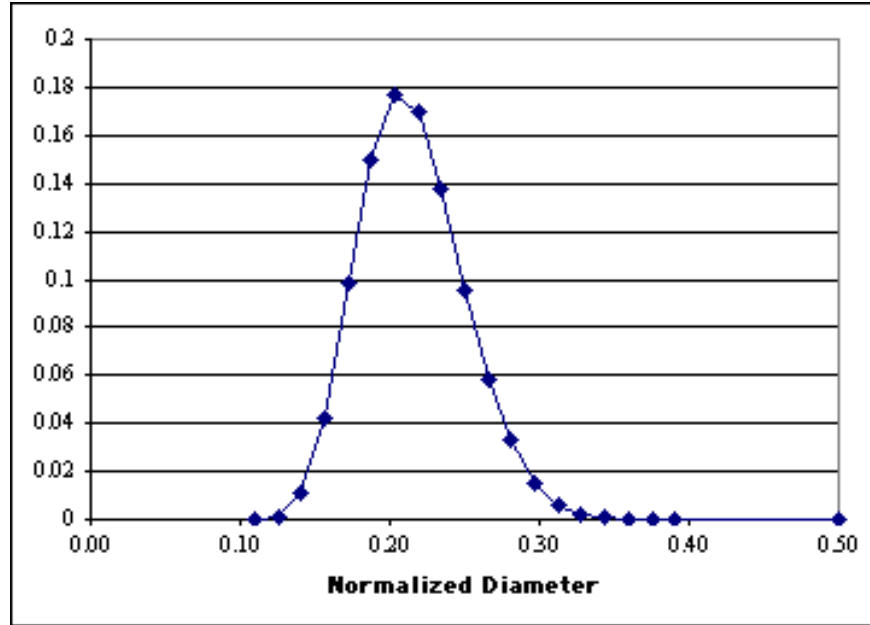
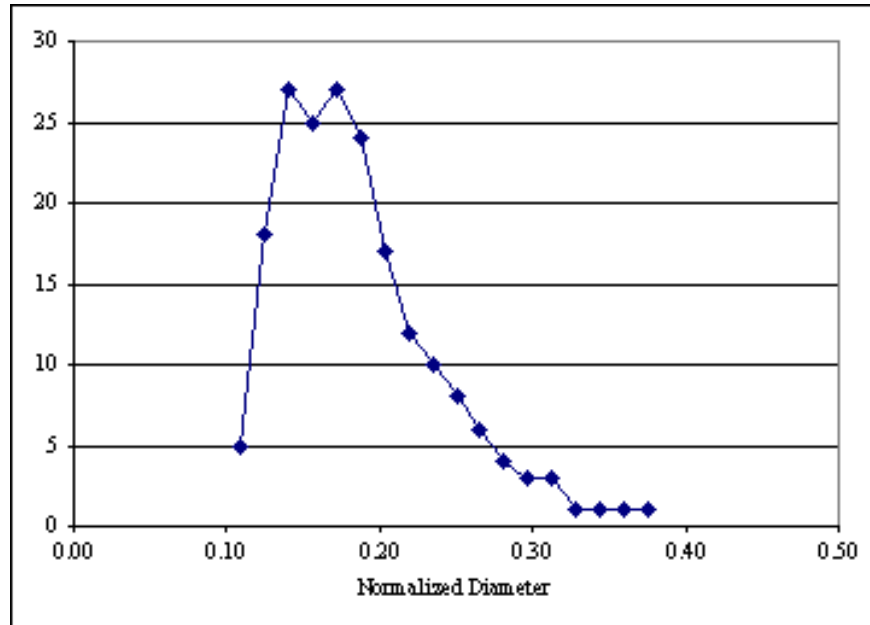
shown in Figure 8. The diameter of this trefoil configuration is .16697812333. \square

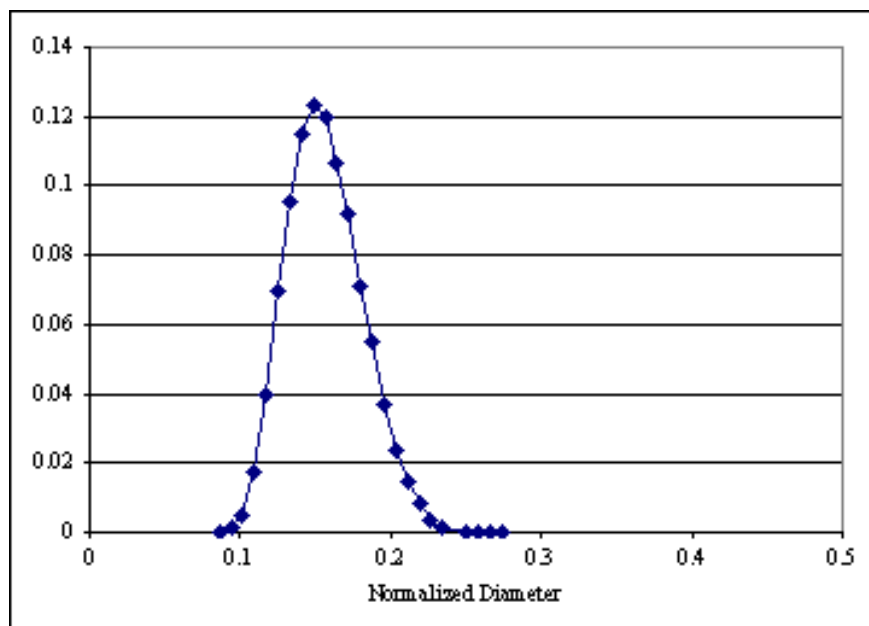
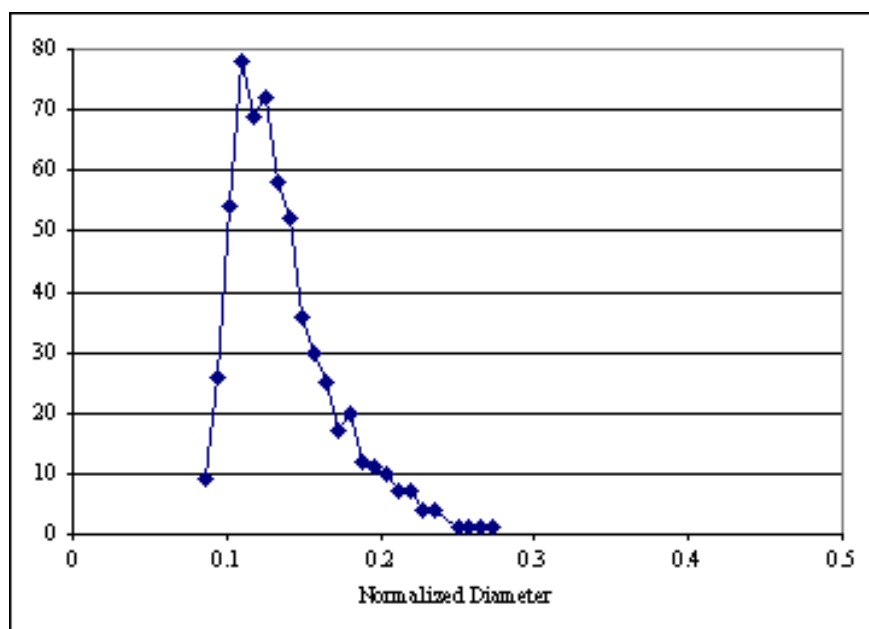
In the case of octagons, the edge connecting $\{0, 0, 0\}$ to $\{1, 0, 0\}$ is replaced by a small perturbation of three edges making sure that this connection that does not change the knot type. What occurs for other knot types? Monte Carlo evidence supports the conjecture that, taking into consideration the statistical implications of small sample size at extremely small diameters, the maximum number of distinct HOMFLY polynomials occurs for the smallest possible diameter. Based on observations with mechanical models and this Monte Carlo evidence, the following conjecture seems appropriate:

Conjecture 3: For each knot type in $Equ(2n)$, K , $b(K) = 1/2n$.

In Figure 10, the global variation of the complexity of knotting is more clearly suggested by the data. The collection of knots of small diameter has a greater diversity of knotting than those of larger diameter. Note that, for diameter near 0.5, the bridge number of the knot implies that only unknots can occur. This provides a limiting factor on the complexity of the knotting that is possible. The variation of complexity for intermediate values of diameter is unknown but these data give a hint of the nature of the function.

The distribution of the knot population and the dependence of the proportion of knot space for the unknot, trefoil and figure 8 knot as functions of normalized diameter are shown in Figures 11, 12, 13, and 14 for 32 edge knots. The average

FIGURE 9. $Equ(16)$ population distributionFIGURE 10. Distinct knot types in $Equ(16)$ versus normalized diameter

FIGURE 11. $Equ(32)$ population distribution versus normalized diameterFIGURE 12. Distinct knot types in $Equ(32)$ versus normalized diameter

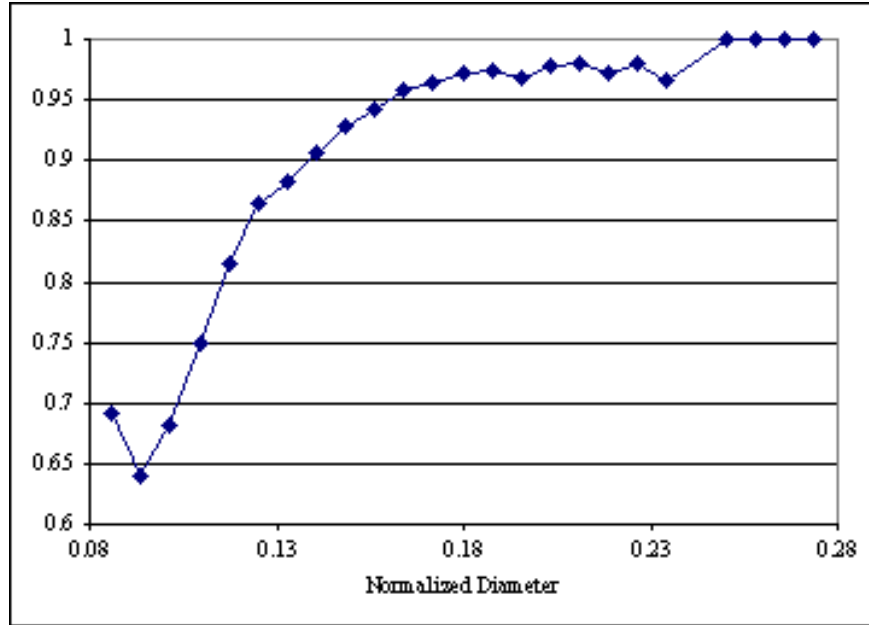


FIGURE 13. *Equ*(32) Proportion of unknots versus normalized diameter

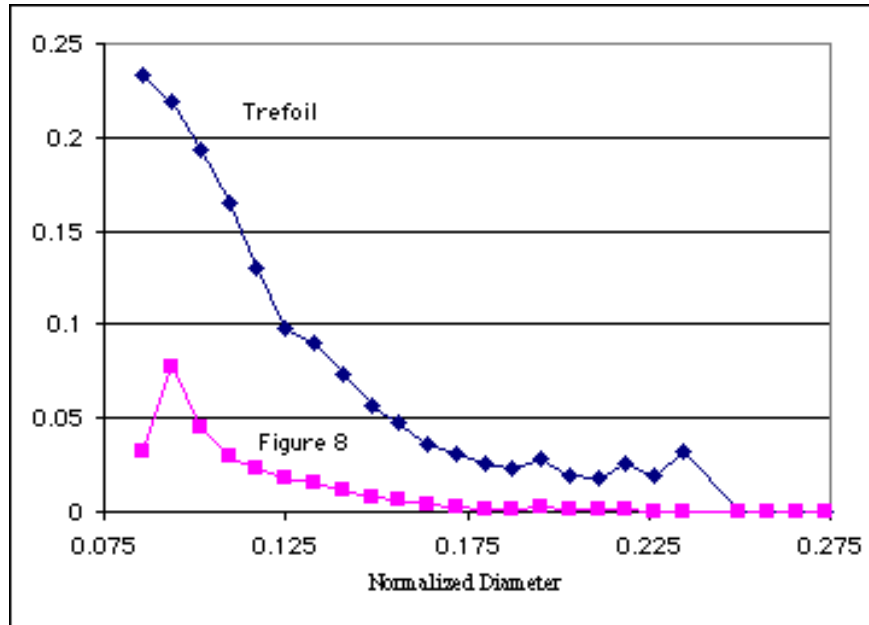


FIGURE 14. *Equ*(32) Proportion of Trefoil and Figure 8 knots versus normalized diameter

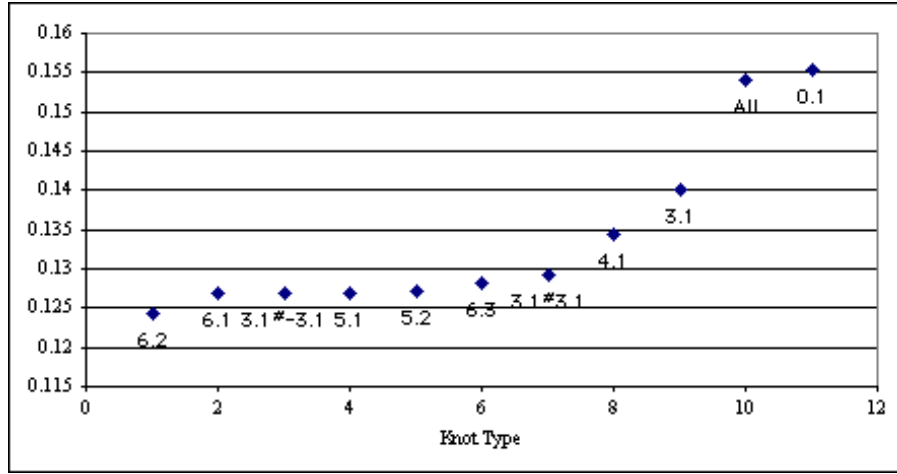


FIGURE 15. Average normalized diameter versus knot type

normalized diameter for all knots and for several knot types are shown in Figure 15. These data give further evidence of the domination of the unknot in knot space as well as the utility of the average normalized diameter as a measure of knot complexity.

The radius of gyration is an important measure of the spatial character of an equilateral polygonal knot that has been widely employed in applications of physical knot theory. In Figure 16 we show the relationship between the average

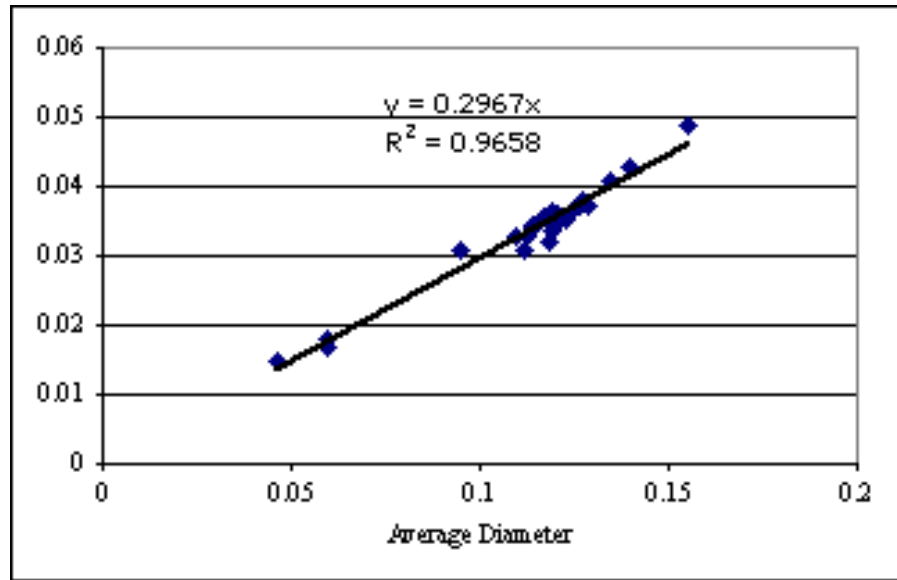


FIGURE 16. Average radius of gyration versus average diameter of a knot type

diameter and the average radius of gyration of those knots appearing in the study of $Equ(32)$. These data imply that the diameter and radius of gyration measure strongly correlated physical features of the average knot of each topological type.

6. Conclusions

The data developed in this project give a quantitative estimate of the degree to which the random knot in $Equ(n)$ is concentrated in a central portion of the knot space. About 80% of $Equ(32)$ lies between the two inflection points in the distribution shown in Figure 11. The maximum is at diameter 0.148 compared to the knot space average of diameter 0.154. The data also identify the transition from **tight** knotted configurations, those with small diameter, to those that of greater extent, that is, those which are **elongated** or having larger diameter. We have seen that the elongated knots are topologically simpler and, we note, may contain connected sums. They also have a very small probability of occurrence. While the compact knots are far more complex, on the average, and can be conjectured to contain exemplars for every topological knot type occurring in the knot space, they too have a very small probability of occurrence. The data show the existence of a phase transition between the compact and extended knot regimes, occurring at the point at which the concavity changes in the graph of the number of HOMFLY polynomials as a function of the diameter, about 0.148 for $Equ(32)$.

We have proved that the "longest knot" occurring in $Equ(2k)$ is a trefoil and have identified the singular limiting configuration. Similarly, we have shown the existence of a sequence of trefoil knots whose diameter is the minimum possible and have identified the singular limiting configuration. The region of compact knotting is still quite mysterious. Further investigation is necessary to put its structure in evidence.

In Figure 15, we show how the knot space average normalized diameter of a knot type provides a measure of knot complexity. This measure appears to be very similar to those provided by orderings imposed by means of other knot properties such as optimal energy, optimal ropelength, etc.

In Figures 1 and 16, we have taken a look at the relationship between ideal configurations, as determined by energy and ropelength, and compared their properties to those of knot space average configurations of the same topological type. While there is a general correspondence between the characteristics, it appears likely that they are independent.

Finally, we have explored the relationship between diameter and radius of gyration as measured by the data from $Equ(32)$. The data show that they are, in the aggregate, measuring strongly related spatial characteristics of the configurations.

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