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An Investigation of Polygonal 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 ideal polygonal knot configurations for small numbers of edges.

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

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. 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 correlate well with the averages of other physical characteristics over large random collections of the corresponding knot conformations[10,11,22,23]. They also correlate well with the observed gel speeds of the corresponding DNA knots.

The realizations of the knots employed here are 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 provides 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[14]. In order to make the calculations, one selects a starting vertex (we could require it to be (0,0,0)) and an adjacent vertex, establishing an order on the vertices. These choices allows one to realize the space of such equilateral polygonal knots as a subset of Euclidean space of dimension three times the number of vertices. 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 define 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, ref [1,2,15] and, in the second, one seeks quantities that can distinguish between distinct geometric knot types representing the same topological knot type, ref [3,15,16].

Physical or Spatial Characteristics of Knots

One physical characteristic of a knot conformation is its **breadth**. The breadth of a knot configuration K, $\beta(K)$, is defined to be the maximum of the distances between pairs of vertices of K. In a desire to use breadth in the study of knot spaces, as a function of n, we define the normalized breadth to be the breadth divided by the length of the knot. If **K** designates a geometrical knot type in Equ(n), let b(**K**) denote the greatest lower bound of $\beta(K)$ over all K representing the knot type **K**. Similarly, let B(**K**) denote the least upper bound of b(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. Both quantities are distinct measures of the spatial extent of the knot. While knots of small breadth and or small radius of gyration are quite compact, the conformations largest breadth and radius of gyration are quite distinct. The standard regular planar polygons have the largest radius of gyration while, for example, the least upper bound of the breadth is [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 a 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 the components of knots of the same topological type are examples of proposed ideal characteristics of knots and are intended to be related to characteristics of ideal knots.

Another approach to the determination of ideal characteristics of knots is to first determine an ideal knot conformation for a given equilateral polygonal knot type. One method is that of optimizing the **thickness** or, equivalently, the **ropelength** within the component defining the polygonal knot. There are several interesting definitions for this notion of ropelength, [9,14,23]. The conceptually simplest, 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 the definition employed by Stasiak and others. In work with Eric Rawdon [14], we used an approach that Rawdon, [18] developed as an analog of the smooth case: the injectivity radius is defined as the minimum of MinRad of an equilateral polygonal knot (defined as half the minimum of the doubly-critical self-distance) and the minimum of the radii of curvature at each of vertices (defined as the edge length divided by twice the tangent of half the exterior angle at the vertex). The thickness is the injectivity radius divided by the total length of the knot and the ropelength is the reciprocal of the thickness. The ropelength and the thickness are two among many physical characteristics of a polygonal knot.

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 randomly selected pair of vertices. The resulting conformations are "almost equilateral" and, as described in Millett and Rawdon[14], determine a geometrically equivalent equilateral knot. For each of the selected knot conformations, the breadth and radius of gyration is recorded. The knot presentation is determined and is used to compute the HOMFLY knot polynomial, [8,12] invariant using the Ewing-Millett program, [6,7]. This program accepts knot presentations of up to 240 crossings and, for the generic knot conformation, is 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 breadth 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 [21]. The 32 edge knots were gotten by subdivision of the 16 edge knots. All knots were check to insure that they satisfied the robustness requirement necessary to insure that an equilateral knot of this geometric type existed and was approximated by the data. Once an robust equilateral example of a topological knot type has been created, the simulated annealing process is applied to search for ropelength optimized conformations are discussed in Millett-Rawdon [14]. More data concerning the spatial characteristics of ropelength (and energy) optimized knots can be found there.

Analysis of Numerical Data

A portion of the data from the Monte Carlo exploration of the knot space average breadth and the breadths of the energy and ropelength optimized knots as a function of the knot type for equilateral knots with 8, 16 and 32 edges is given in Table 1. In Figure 2, we show, graphically, the optimized energy and ropelengths as a function of the average normalized breadth of the knot. This graph illustrates the expectation that the smaller the breadth of the knot, the larger the energy and ropelength but shows, in addition, that this dependence holds for the knot space average of breadths in the knot type.

Table 1. Knot Space Average, Energy and Ropelength Optimized Data.

	8 Ave	8EOp	8ROp	16Ave	16EOp	16ROp	32Ave	32EOp	32ROp
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	.10528	.1198	.1179	.13055	.1639	.1658
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	.1250	.1250	.10419	.1675	.1452	.12698	.1497	.1364
3.1#3.1	NA	.1257	.1257	.11017	.1874	.1714	.12952	.1944	.1758
3.1#-3.1	NA	.1250	.1250	.10962	.1674	.1470	.13139	.1958	.1752

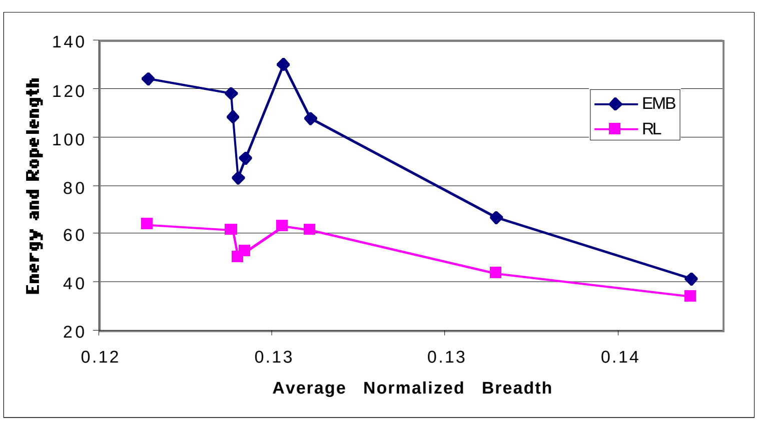

Figure 2. Optimized Energy and Ropelength versus Average Breadth

The proportion of knot space as a function of the normalized breadth as well as the number of distinct knot types, as measured by distinct HOMFLY polynomials, capture to fundamental facets 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 will employ a normalization of the breadth given by dividing the breadth by the length of the knot. Thus, the maximum normalized breadth is always 0.5. The minimum normalized breadth is 1/n, n equal to the number of edges.

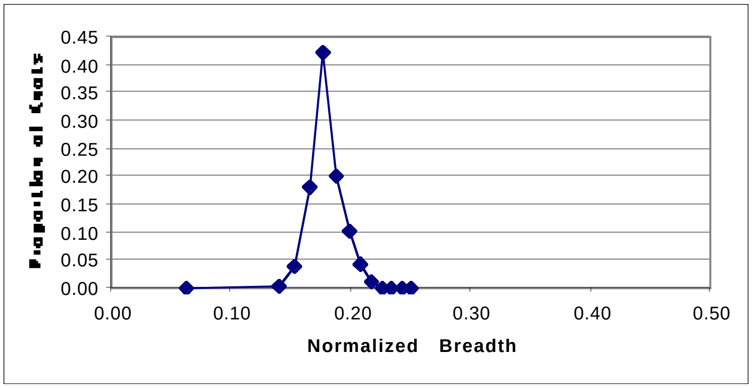

Figure 3. Equ(8) population distribution

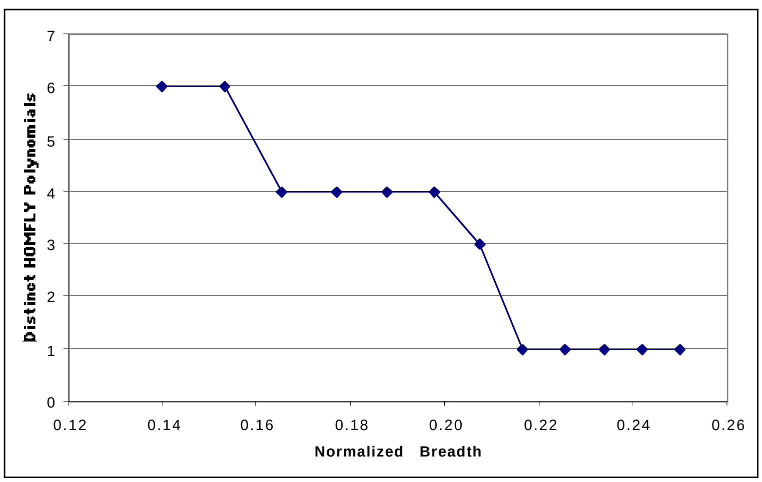

Figure 4. Distinct knot types in Equ(8) versus normalized breadth.

The relationship between the normalized breadth and the number of distinct knot types provides an important insight into the structure of knot space. In general, the larger the breadth of the knot, the simpler the structure. The precise nature of this property changes with the number of edges.

Proposition 1: The least upper bound on the breadth of a non-trivial knot in Equ(4n + 2) is equal to Sqrt$(4 + 1/n^2)/(4 + 2/n) = B(\mathbf{3_1})$.

Proof: This value is realized by a sequence of trefoil knots converging to the singular set represented by union of two isosceles triangles along their base, of unit length, and edge length equal to "n." Twice the altitude of the triangle gives the least upper bound. A configuration with a breadth greater than this value can have only two locally extreme "height" values along the direction parallel to the line connecting the vertices giving the breadth. As a consequence, any such configuration is a geometrically trivial knot.

As noted in the proof, this least upper bound is realized by the least upper bound of the normalized breadth 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 5. A close but non-singular configuration with normalized breadth .283338 is shown in Figure 6. Its vertex coordinates are:

{{0., 0., 0.}, {0.486131, 0.015706, 0.873745}, {-0.513209, -0.0166517, 0.857231},
{0.0277697, 0.000808531, 0.0163762}, {-0.972096, 0., 0.},
{-0.486048, -0.0167832, 0.873771}}.

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

The largest observed breadth 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.

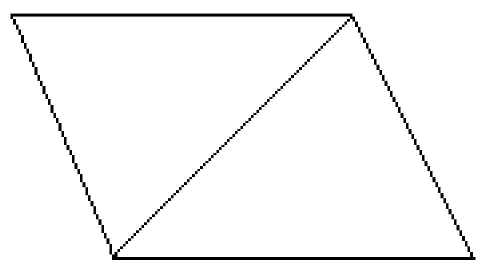

Figure 5. Singular Hexagonal Trefoil Position

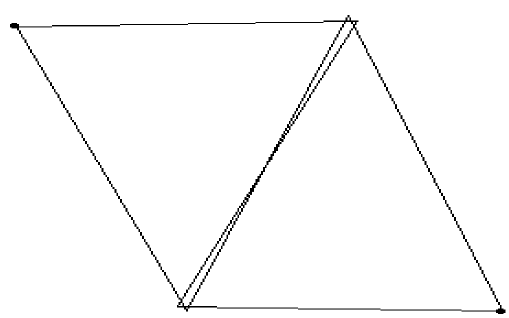

Figure 6. Hexagonal Trefoil with Large Breadth.

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.

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.

Proposition 2. In Equ(2n), $b(\mathbf{3_1}) = 1/2n$, for $n \geq 3$.

Proof: In Equ(6), using the model in which the individual edges lengths 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:

{{0, 0, 0}, {1.0, 0, 0}, {0.00299957, 0.07739435, -0.00049926},
{0.96018567, -0.21105152, -0.02486597},
{0.04083793, 0.1273103549, 0.17590997},
{0.99690190, -0.02499956, -0.07457634}}

shown in Figure 7. The breadth of this trefoil configuration is 1.00186874.

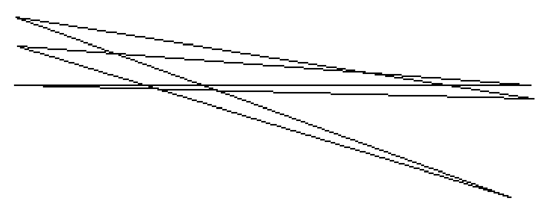

Figure 7. Trefoil of Breadth 1.00186874

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? Based on observations with mechanical models and some Monte Carlo evidence, the following conjecture seems appropriate:

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

The Monte Carlo evidence supporting the conjecture is that, taking into consideration the statistical implications of small sample size at this extreme breadth, the maximum number of distinct HOMFLY polynomials occurs for the smallest possible breadth.

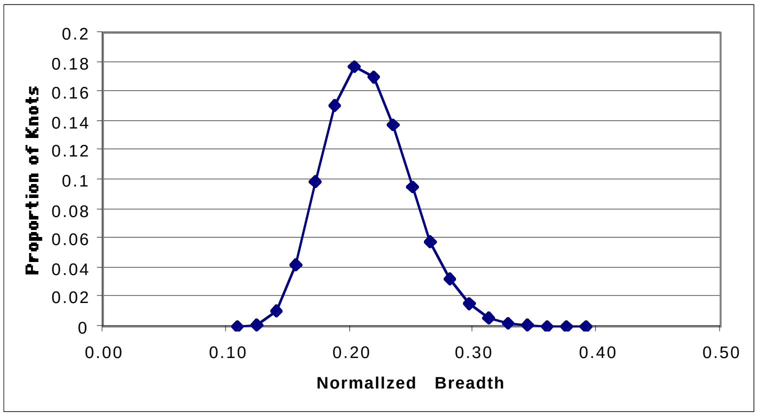

Figure 8. Equ(16) population distribution

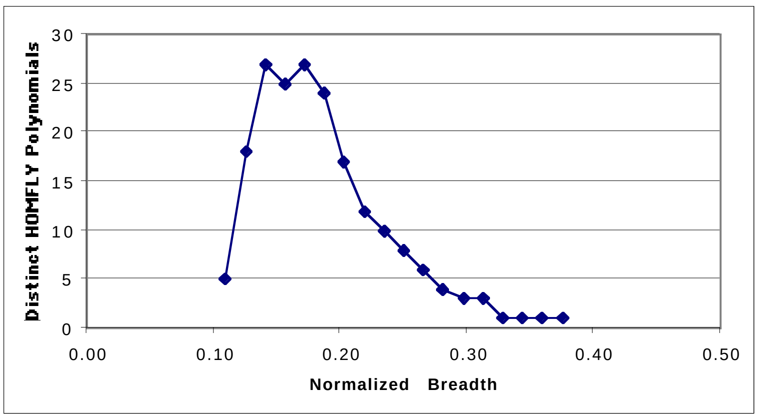

Figure 9. Distinct knot types in Equ(16) versus normalized breadth

In Figure 9, the global variation of the complexity of knotting is more clearly suggested by the data. The collection of knots of small breadth appear to have a greater diversity of knotting occurring in contrast with those of larger and very large breadth. For breadth near 0.5, the bridge number of the knot implies that only unknots can occur and provides a limiting factor on the complexity of the knotting that is possible. The variation of complexity for intermediate values of breadth is unknown but this data gives a hint of the nature of the function.

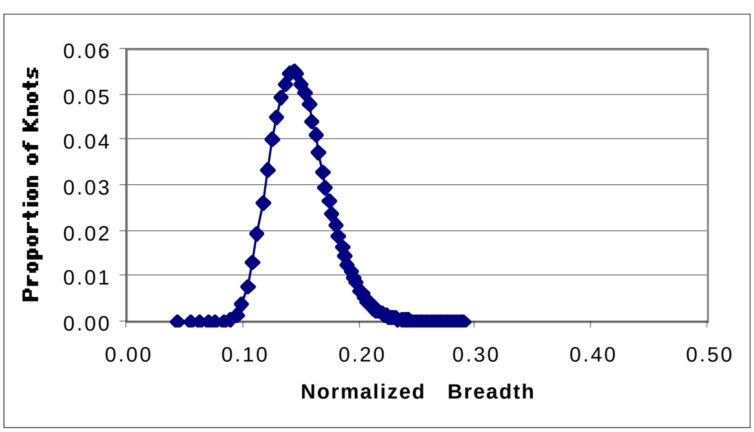

Figure 10. Equ(32) population distribution versus normalized breadth.

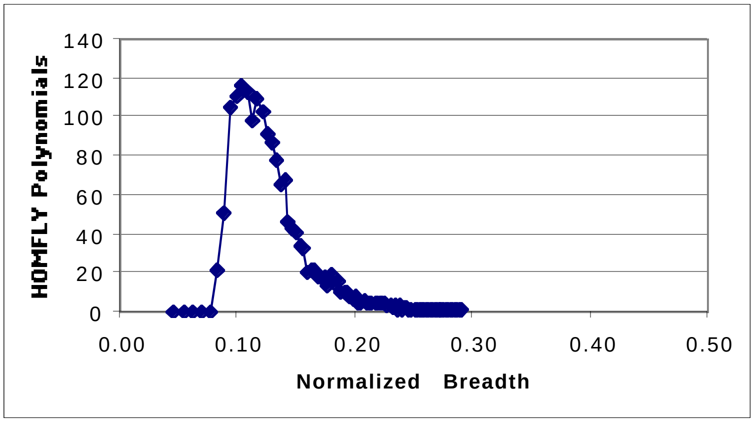

Figure 11. Distinct knot types in Equ(32) versus normalized breadth

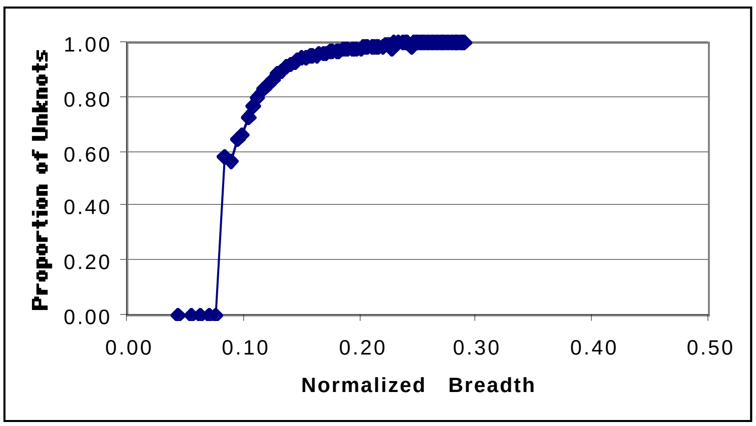

Figure 12. Equ(32) Proportion of unknots versus breadth.

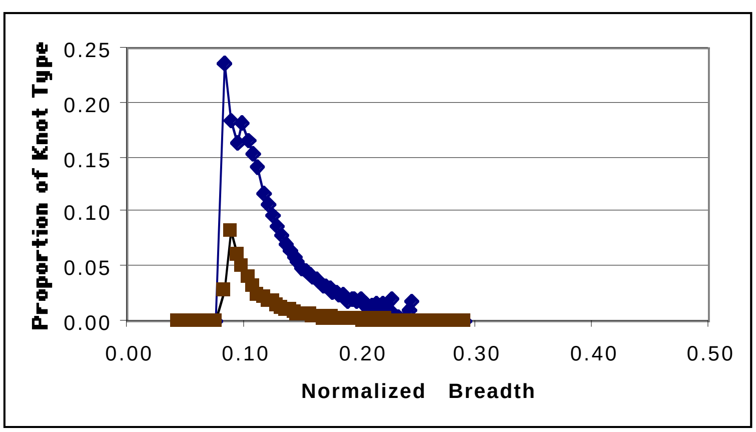

Figure 13. Equ(32) Proportion of Trefoil and Figure-Eight Knots

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 breadth are shown in Figures 10, 11, 12 and, 13 for 32 edge knots. The knot space average normalized breadth for all knots and for several knot types are show in Figure 14. This data gives further evidence of the domination of the unknot is knot space as well as the utility of the average normalized breadth as a measure of knot complexity.

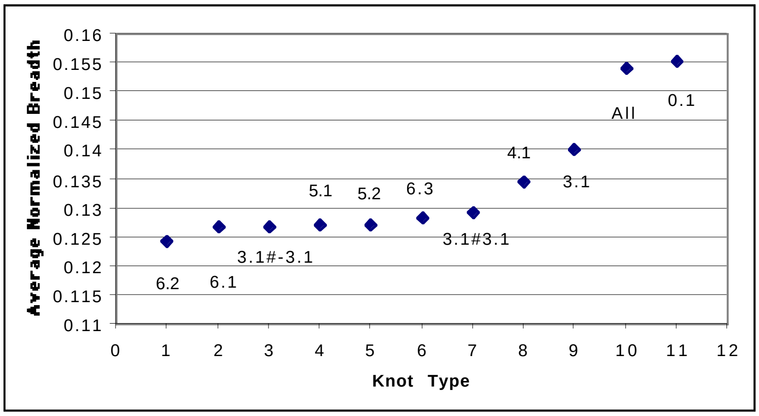

Figure 14. Knot Space Average Normalized Breadth

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 15 we show the relationship between the average breadth and the average radius of gyration of those knots appearing in the study of Equ(32). This data implies that the breadth and radius of gyration measure strongly correlated physical features of the average knot of each topological type.

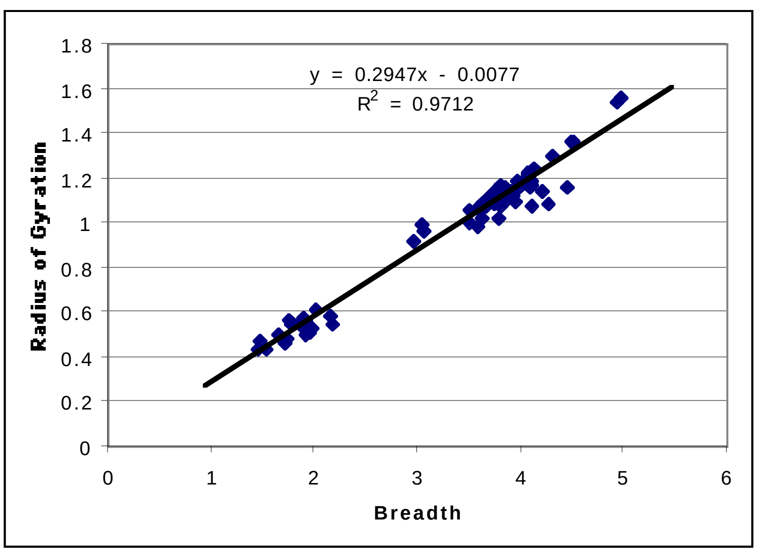

Figure 15. Average Radius of Gyration versus Average Breadth of a Knot Type

This correlation is also illustrated by view the radius of gyration as a function of the breadth of the knot. The data for Equ(32) are shown in Figure 16. The departure from a strictly monotonic relationship for configurations with larger breadth shown in the figure may be a consequence of the sparseness of the data in this range.

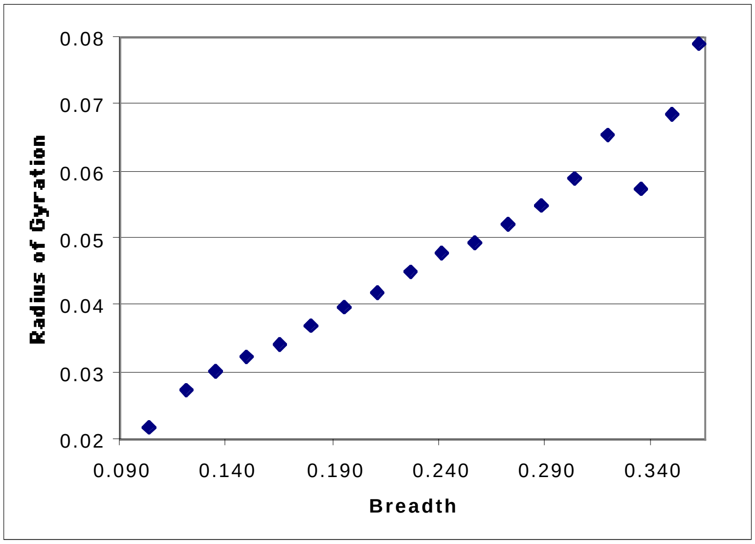

Figure 16. Radius of Gyration versus Breadth in Equ(32)

While there does appear to be a simple functional relationship between the knot space average breadth of the knot type and the breadth of the ropelength optimized knot, the statistical data is not yet sufficient to be conclusive. The case for Equ(32) knots is shown in Figure 17.

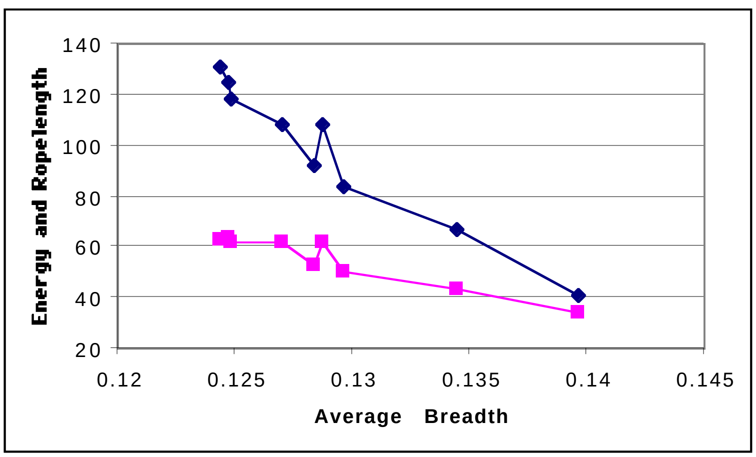

Figure 15. Knot space average versus optimized ropelength and energy breadths.

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 10. The maximum proportion is at breadth 0.148 compared to the knot space average of breadth 0.154.

The data also identifies the transition from **compact** knotted configurations, those with small breadth, to those that of greater extent, those which are **elongated** or with larger breadth. We have seen that the elongated knots are topologically simpler and but, we note, may contain connected sums. They are also are of very small probability. 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 shows 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 breadth, 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 breadth 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 14, we show how the knot space average normalized breadth 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 2 and 15, 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 breadth and radius of gyration as measured by the data from Equ(32). The data shows that they are, in the aggregate, measuring strongly related spatial characteristics of the configurations.

References

[1] J.A. Calvo, Geometric knot theory: the classification of spatial polygons with a small number of edges, Ph.D. thesis, University of California, Santa Barbara (1998).

[2] J.A. Calvo, Geometric knot spaces and polygonal isotopy, preprint (1999).

[3] J.A. Calvo, K.C. Millett, Minimal edge piecewise linear knots, Ideal Knots, V. Katritch, L. Kauffman, A. Stasiak (Eds.), World Scientific Publishing,1998, pp. 107-128.

[4] J.A. Calvo, personal communication (1998).

[5] Y. Diao, C. Ernst, & E. J. Janse van Rensburg, Thicknesses of knots. Math. Proc. Cambridge Philos., 126(2) 1999, 293-310

[6] B. Ewing, K.C. Millett, A load balanced algorithm for the calculation of the knot polynomials, The Mathematical heritage of C.F. Gauss, World Scientific Publishing, (1991), 225-266.

[7] B. Ewing, K.C. Millett, Computational algorithm and the complexity of link polynomials, Progress in knot theory and related topics, no. 56 in Travaux en Cours, Hermann, Paris, 1997, 51-68.

[8] P. Freyd, D. Yetter, J. Hoste, W.B.R. Lickorish, K. C. Millett, A. Ocneanu, A new polynomial invariant of knots and links, Bulletin of the American Mathematical Society 12 (2) (1985) 239-246.

[9] O. Gonzalez, J. H. Maddocks, Global curvature, thickness, and the ideal shape of knots, Proc. Nat. Acad. Sci. USA, 96 (1999), pp. 4769-77

[10] V. Katritch, J. Bednar, D. Michoud, R.G. Schrein, J. Dubochet, A. Stasiak, Geometry and physics of knots, Nature 384 (1996) 142-145.

[11] V. Katritch, W. K. Olson, P. Pieranski, J. Dubochet, A. Stasiak, Properties of ideal composite knots, Nature 388 (1997) 148-151.

[12] W.B.R. Lickorish, K. C. Millett, A polynomial invariant of oriented links, Topology 26 (1) (1987) 107-141.

[13] R. A. Litherland, J. Simon, O. Durumeric, and E. Rawdon, Thickness of knots, Topology Appl.91(3) 1999, 233-244

[14] K.C. Millett, E.J. Rawdon, Energy, thickness, and other physical aspects of equilateral knots, preprint (2000).

[15] K. C. Millett, Monte Carlo explorations of polygonal knot space, Knots in Hellas '98, C. McA. Gordon, V. F. R. Jones, L. H. Kauffman, S. Lambropoulou, J. H. Przytycki (Eds.), World Scientific Publishing, (2000), 306-334..

[16] K.C. Millett, Knotting of regular polygons in 3-space, Journal of Knot Theory and Its Ramifications 3 (3) (1994) 263-278.

[17] P. Pieranski, In search of ideal knots, Ideal Knots, V. Katritch, L. Kauffman, A. Stasiak (Eds.), World Scientific Publishing,1998, pp. 20-41.

[18] E. Rawdon, The thickness of polygonal knots, Ph.D. thesis, University of Iowa, 1997.

[19] E. Rawdon, Approximating the thickness of a knot, Ideal Knots, Knots, V. Katritch, L. Kauffman, A. Stasiak (Eds.),, World Scientific Publishing, 1998, 143-150.

[20] E. Rawdon, Approximating smooth thickness, J. Knot Theory Ramifications, 9(1), 2000, 113-145.

[21] R. Scharein, KnotPlot, http;//www.cs.ubc.ca/spider/scharein

[22] A. Stasiak, V. Katrich, J. Bednar, D. Michoud, J. Dubochet, Electrophoretic mobility of DNA knots, Nature 384 (1996) 122.

[23] A. Stasiak, J. Dubochet, V. Katritch, P. Pieranski, Ideal knots and their relation to the physics of real knots, Ideal Knots, V. Katritch, L. Kauffman, A. Stasiak (Eds.),, World Scientific Publishing,1998, pp. 1-19.