Knots in Hamilton Cycles

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Received June 7, 1994
Revised Manuscript Received July 18, 1994

Introduction

Following an abrupt quench from good to poor solvent conditions, an isolated polymer is expected to collapse from a swollen coil to a compact globule. An interesting conjecture[1–3] regarding this transition has been made. In good solvent, the swollen coils are expected to be relatively unknotted, while at equilibrium the globules are expected to be extensively knotted. Therefore, it is believed that the collapse transition occurs over two separate stages: a rapid folding or crumpling to a compact globule which occurs without changing the knottedness of the coil, followed by a slow knotting or entangling of the coiled globule via self-reptation.

This conjecture is supported by a number of exact and numerical results in statistical knot theory.[4–16] For example, we know that cyclic polymers with strong excluded volume are relatively unknotted. The probability that a cyclic polymer with well-developed excluded volume is not knotted is known to vary with chain length, N, as $\exp(-N/N_0)$.[7] Typical values of N_0 are on the order of 10^5 or 10^6.[8,9] In other words, sufficiently long chains ($N \gg N_0$) are knotted, indeed, extensively knotted with complicated knot states, but for N around a few thousand, almost no knots are seen. However, we also know that, as the strength of the excluded-volume interaction decreases, the knot probability increases significantly, with a tendency toward increasingly complex knots.[9] θ-State cycles also appear to follow the $\exp(-N/N_0)$ law, but with N_0 on the order of several hundred.[9,15] Therefore, since polymer collapse involves both a change in coil size and a change in knotting, the conjecture of a two-stage relaxation is logical.

Numerical studies in statistical knot theory[4–16] typically involve the generation of an ensemble of cyclic paths followed by the determination of the knot state of each path by the computation of a knot invariant, such as the Alexander polynomial. A number of ensembles with various statistical properties have been studied, but never an ensemble that would model the collapsed state of polymers. In this paper, I report numerical studies on the knot state of Hamilton cycles in boxes on the simple cubic lattice. Since these are space-filling, compact cycles, they are in many ways adequate models of polymers in the collapsed state.

Generation of Hamilton Cycles

Hamilton paths are walks on a finite lattice that visit each site of the lattice once and only once, while Hamilton cycles are Hamilton paths that also return to the site of origin. An efficient algorithm has already been described[17] that generates space-filling paths in simple cubic lattice boxes with periodic boundary conditions. Generation of Hamilton paths in the same boxes only requires suppression of the periodic boundaries. A Hamilton cycle is selected each time this algorithm produces a Hamilton path terminating at a site that neighbors the origin of the path.

Determination of Knot State

Once a cycle has been selected, its knot state is determined, usually by computation of the Alexander polynomial[4–16,18–20] of the cycle. Other polynomial knot invariants have been recently discovered[14,15,21,22] that are, in some ways, superior to the Alexander polynomials. However, the Alexanders, being older than the others, are more extensively tabulated[19,20] and furthermore are simpler to calculate.[9,15]

Evaluation of the Alexander polynomial of a complex cycle is time consuming, so most numerical studies include a step of cycle simplification, or "smoothing", in which the cycle in question is replaced by a simpler, shorter, "smoother" version that still has the same knot state as the original. In this study, no particularly heroic efforts were made at cycle simplification, except to remove every pair of steps j and $j + 2$ whenever these pointed in opposite directions. It is obvious that such a maneuver preserves the knot state of the original structure. In retrospect, it would have been advantageous to include other simplification schemes, especially with the longer cycles, but this approach still proves adequate.

The algorithm for computing the Alexander has been given elsewhere[4,9,18–20] and will not be reproduced here. The Alexanders, usually denoted $\Delta(t)$, are polynomials in a scalar t with integral coefficients. The following list summarizes those properties[18–20] of the polynomials that are relevant to our discussion.

(A) The polynomials $\Delta(t)$ are defined as any minor of the "Alexander matrix". Elements of this matrix are linear functions of t. Determination of $\Delta(t)$ therefore requires evaluation of a determinant.

(B) $\Delta(t)$ is a knot invariant, which is to say that two knots in the same knot state possess the same $\Delta(t)$, except as qualified by property F below.

(C) The converse of property B does not hold: Two knots with the same $\Delta(t)$ are not necessarily in the same knot state.

(D) Many knots are "composite", in the sense that they can be uniquely decomposed into two or more "prime" knots. The Alexander polynomial of a composite is the product of the Alexanders of its primes. On the other hand, factorizability of $\Delta(t)$ does not guarantee that the knot is prime; many primes possess Alexanders that factor into Alexanders of other prime knots.

(E) $\Delta(1) = \pm 1$ for all knots.

(F) The Alexander polynomials are indeterminate up to a factor $\pm t^m$, where m is an arbitrary integer. The Alexander polynomials of two knots of the same knot state (or even the same knot viewed in two different projections) may differ by this arbitrary factor. Standard knot tables[19,20] always give polynomials normalized according to some convention.

Property C obviously implies that the Alexander polynomials are not perfectly discriminating. This is not a terribly severe problem, however, especially with the simpler knots, since, among these, duplications are relatively rare. For example, excluding enantiomers, no duplications exist in knots of fewer than nine crossings. Nevertheless, employing only Alexander polynomials, we are never able to uniquely determine the knot state.

Property F would seem to disqualify the numerical computation of Alexander polynomials as an effective procedure, since this arbitrary factor is *a priori* unknown. Three different approaches have been employed to avoid this difficulty. The most common is the numerical determination of $|\Delta(-1)|$, from which the arbitrary factor obviously disappears. (It also disappears from $|\Delta(+1)|$, but this is useless since by property E it always equals 1.) $|\Delta(-1)|$ is, by itself, a valid knot invariant but is less discriminating than the full polynomial, since even more

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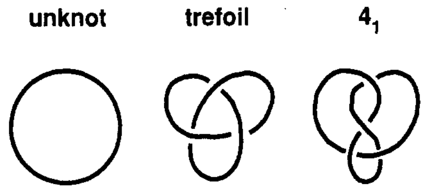

Figure 1. Three simplest knots.

knots generally map onto a unique element of the range. For example, the first duplication occurs with knots 4_1 and 5_1.[19] The second technique, employed so far only by Koniaris and Muthukumar,[9] is the exact computation of the polynomial by machine algebra, which obviously permits normalization of the final result and also avoids any possible danger of round-off error, overflow, or underflow during the calculation of large determinants. It is definitely the method of choice if one is willing to exert the necessary computational effort. The third approach, due to Deguchi and Tsurusaki,[14,15] is to augment the calculation of $|\Delta(-1)|$ with other knot invariants. They compute the Vassiliev numbers, which are defined as coefficients in the Taylor series of the Jones polynomial at $t = 1$ and which are considerably easier to calculate than the full Jones polynomial.[14,15,21,22] By computing two independent knot invariants, they avoid most of the duplications inherent in any single invariant.

In this work, I have introduced another approach. The function $F(t) = t^{-T}|\Delta(t)|$, where $T = \ln|\Delta(e)|$ and e is the base of the natural logarithms, is invariant under the transformation $\Delta(t) \rightarrow \pm t^m\Delta(t)$. $F(t)$ is also a knot invariant, and it inherits a number of properties from the Alexander polynomials: First, $F(1) = 1$ always. Second, F of a composite knot is the product of the F's of its prime factors. Obviously, $F(t)$ is uniquely determined by $\Delta(t)$ and therefore carries not more information than the latter.

Several authors tabulate Alexander polynomials for each of the 250 prime knots that can be drawn with 10 or fewer crossings.[19,20] From this list I construct a master table of Alexander polynomials that include the polynomials of these 250 primes, plus all possible second- and third-order composites of these primes. For each Hamilton cycle, $F(t)$ is computed at 10 different values of $t(^1/_4, ^2/_4, ^3/_4, ..., ^{10}/_4)$. This list of $F(t)$ values is compared with the corresponding list constructed from polynomials found on the master table. If no match can be found, then the knot is tabulated as having an unknown Alexander polynomial. In this way, the Alexander polynomial of a knot can be determined provided that it is equal to the polynomial of one of the prime knots 0_1 through 10_{165}, or else a second- or third-order composite of any of these primes.

Computation of the determinant $\Delta(t)$ through forward Gaussian elimination must include pivoting to avoid significant round-off errors. Following forward elimination, the determinant is obtained as the product of the matrix diagonal. Forming this product for large matrices can lead to underflows or overflows, since the exponent m in the factor t^m can be large. To avoid this, the logarithm of the product, not the product itself, must be accumulated. Then $F(t)$ can be determined from the logarithms of the relevant determinants. I performed the Gaussian elimination in double precision and found that $F(t)$ values agreed to at least five significant figures with the $F(t)$ values calculated directly from the normalized forms of the Alexander polynomials.

Results

Following the procedures outlined above, Hamilton cycles were generated on simple cubic lattices of size $i \times j \times k$, for all values of (i, j, k) satisfying $2 \leq i \leq j \leq k \leq 10$ and with $N = ijk$ even. Obviously, N is the total walk length, and no cycles exist when N is odd. For each set of (i, j, k) values, 10^5 cycles were generated for $N \leq 500$ and 10^4 for $N > 500$. The occurrence frequency of Alexander polynomials was tabulated for each set of (i, j, k) values. Results for the three Alexander polynomials $\Delta(t) = 1$, $\Delta(t) = t^2 - t + 1$, and $\Delta(t) = t^2 - 3t + 1$, corresponding respectively to the three simplest knots (Figure 1), are given in Figure 2. Also appearing in Figure 2 is the contribution from unknown knots, in the sense explained above. Figure 3 displays the contribution from unknots, plotted in a semilog fashion. The following observations may be made.

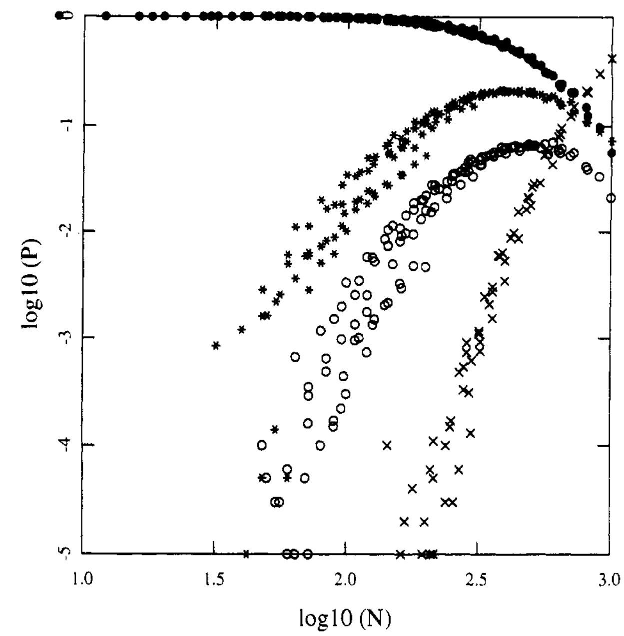

Figure 2. Occurrence frequency of the unknot (●), the trefoil (*), the knot 4_1 (O), and of knots of unknown Alexander polynomial (×) in ensembles of Hamiltonia cycles on compact simple cubic lattices of total volume N.

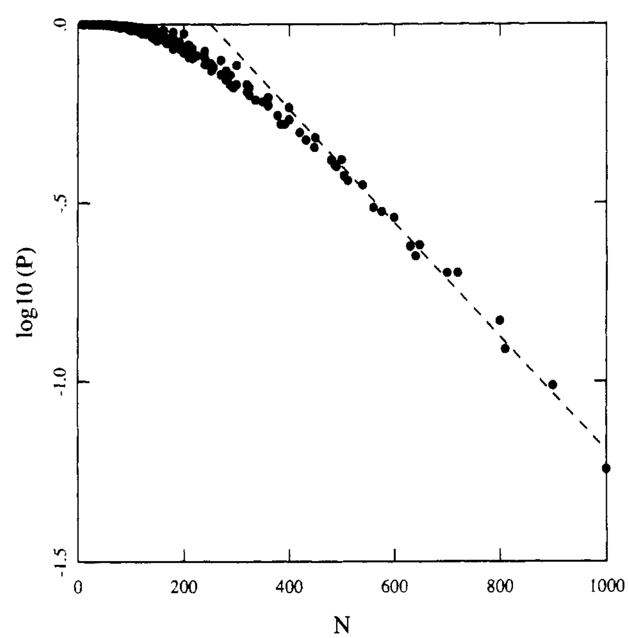

Figure 3. Semilog graph of the occurrence frequency of the unknot. The dashed line has a slope −1/270.

Unknots. When $N < 100$, the unknot is overwhelmingly dominant. Its dominance drops steadily with increasing N. By $N = 1000$, only about 6% of the cycles are not

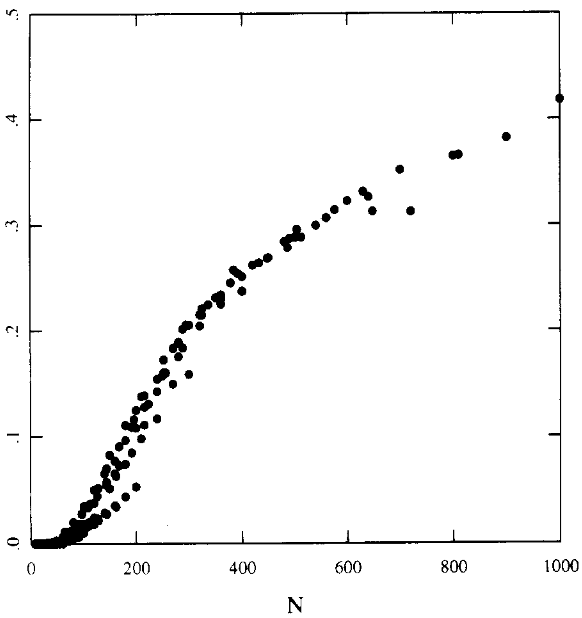

Figure 4. Fraction of Hamilton cycles, from among those whose Alexander polynomial could be determined, that possess an Alexander polynomial that contains the factor $(1 - t + t^2)$.

knotted. At larger N values, the unknot probability is approximately equal to $\exp(-N/270)$.

Simple Knots. The contributions due to the trefoil and to the knot 4_1 pass through a maximum near $N = 500$ and then decrease steadily for larger N. This behavior is typical of all knots except the unknot, although the maximum for any particular knot depends on its complexity.

Unknown Knots. The contributions from unknown Alexander polynomials increase dramatically beyond $N = 500$. Around $N = 500$, the contribution from unknowns is a few percent. At $N = 1000$, they contribute over 40% of the total.

Therefore, between $N = 100$ and $N = 1000$, Hamilton cycles on the simple cubic lattice go from being practically unknotted to being copiously and completely knotted. Other studies indicate that self-avoiding rings of length $N = 1000$ are almost completely unknotted. Therefore, the conjecture of a two-stage collapse transition is supported by this study.

Soteros et al.[12] have shown rigorously that very long self-avoiding rings are almost always composite and that trefoils are generally expected to dominate the primes composing these long rings. Their argument may be summarized by saying that any sequence of steps that can occur, will occur, indeed many times, if the ring is sufficiently long. Therefore, sufficiently long rings contain many prime knots, including trefoils. Although their argument applies specifically to self-avoiding rings, it at least suggests that the same should be true of Hamilton cycles. Figure 4 displays a test of this conjecture. It displays, as a function of N, the fraction of times that a knot whose Alexander could be determined contains the factor $(1 - t + t^2)$, i.e., $\Delta(t)$ for the trefoil. Unfortunately, not all knots having this factor are necessarily composites of the trefoil. However, only about 20% of the first 250 primes possess this factor;[19] therefore, the occurrence of over 40% in the longer Hamilton cycles and the steady increase of the curve in Figure 4 both seem to support the extension of the theorem of Soteros et al.[12] to Hamilton cycles.

Acknowledgment. Partial support for this research was provided by the National Science Foundation, Grant DMR-8822934.

References and Notes

(1) de Gennes, P.-G. *J. Phys. (Fr.)* **1985**, *46*, L-639.
(2) Grosberg, A. Yu.; Nechaev, S. K.; Shakhnovich, E. I. *J. Phys. (Fr.)* **1988**, *49*, 2095.
(3) Grosberg, A. Yu.; Kuznetsov, D. V. *Macromolecules* **1993**, *26*, 4249.
(4) Frank-Kamenetskii, M. D.; Lukashin, A. V.; Vologodskii, A. V. *Nature* **1975**, *258*, 398.
(5) Frank-Kamenetskii, M. D.; Vologodskii, A. V. *Sov. Phys-Usp.* **1981**, *24*, 679.
(6) Michels, J. P.; Wiegel, F. W. *Proc. R. Soc. London A* **1986**, *403*, 269.
(7) Sumners, D. W.; Whittington, S. G. *J. Phys. A: Math. Gen.* **1988**, *21*, 1689.
(8) Janse van Rensburg, E. J.; Whittington, S. G. *J. Phys. A: Math. Gen.* **1990**, *23*, 3573.
(9) Koniaris, K.; Muthukumar, M. *J. Chem. Phys.* **1991**, *95*, 2873.
(10) Janse van Rensburg, E. J.; Whittington, S. G. *J. Phys. A: Math. Gen.* **1991**, *24*, 3935.
(11) Janse van Rensburg, E. J.; Whittington, S. G. *J. Phys. A: Math. Gen.* **1991**, *24*, 5553.
(12) Soteros, C. E.; Sumners, D. W.; Whittington, S. G. *Math. Proc. Cambridge Philos. Soc.* **1992**, *111*, 75.
(13) Janse van Rensburg, E. J.; Sumners, D. A. W.; Wasserman, E.; Whittington, S. G. *J. Phys. A: Math. Gen.* **1992**, *25*, 6557.
(14) Deguchi, T.; Tsurusaki, K. *Phys. Lett. A* **1993**, *174*, 29.
(15) Deguchi, T.; Tsurusaki, T., preprint.
(16) Grosberg, A.; Nechaev, S. *Adv. Polym. Sci.* **1993**, *106*, 1.
(17) Mansfield, M. L. *J. Chem. Phys.* **1982**, *77*, 1554.
(18) Crowell, R. H.; Fox, R. H. *Introduction to Knot Theory*; Ginn: Boston, 1963.
(19) Burde, G.; Zieschang, H. *Knots*; de Gruyter: New York, 1985.
(20) Rolfsen, D. *Knots and Links*; Publish or Perish: Berkeley, CA, 1976.
(21) Jones, V. F. R. *Bull. Am. Math. Soc.* **1985**, *12*, 103.
(22) Wu, F. Y. *Rev. Mod. Phys.* **1992**, *64*, 1099.