

# Spontaneous knotting of an agitated string

Dorian M. Raymer\* and Douglas E. Smith\*

Department of Physics, University of California at San Diego, 9500 Gilman Drive, Mail Code 0379, La Jolla, CA 92093

Edited by Leo P. Kadanoff, University of Chicago, Chicago, IL, and approved July 30, 2007 (received for review December 21, 2006)

It is well known that a jostled string tends to become knotted; yet the factors governing the “spontaneous” formation of various knots are unclear. We performed experiments in which a string was tumbled inside a box and found that complex knots often form within seconds. We used mathematical knot theory to analyze the knots. Above a critical string length, the probability  $P$  of knotting at first increased sharply with length but then saturated below 100%. This behavior differs from that of mathematical self-avoiding random walks, where  $P$  has been proven to approach 100%. Finite agitation time and jamming of the string due to its stiffness result in lower probability, but  $P$  approaches 100% with long, flexible strings. We analyzed the knots by calculating their Jones polynomials via computer analysis of digital photos of the string. Remarkably, almost all were identified as prime knots: 120 different types, having minimum crossing numbers up to 11, were observed in 3,415 trials. All prime knots with up to seven crossings were observed. The relative probability of forming a knot decreased exponentially with minimum crossing number and Möbius energy, mathematical measures of knot complexity. Based on the observation that long, stiff strings tend to form a coiled structure when confined, we propose a simple model to describe the knot formation based on random “braid moves” of the string end. Our model can qualitatively account for the observed distribution of knots and dependence on agitation time and string length.

Jones polynomial | knot energy | knot theory | random walk | statistical physics

Knots have been a subject of scientific study since as early as 1867, when Lord Kelvin proposed that atoms might be described as knots of swirling vortices (1). Although this theory fell into disfavor, it stimulated interest in the subject, and knots currently play a role in many scientific fields, including polymer physics, statistical mechanics, quantum field theory, and DNA biochemistry (2, 3). Knotting and unknotting of DNA molecules occurs in living cells and viruses and has been extensively studied by molecular biologists (4–6). In physics, spontaneous knotting and unknotting of vibrated ball-chains have recently been studied (7–9). In mathematics, knot theory has been an active field of research for more than a century (3).

Formation of knots in mathematical self-avoiding random walks has been extensively studied (10–16). In the 1960s, Frisch and Wasserman (10) and Delbruck (11) conjectured that the probability of finding a knot would approach 100% with an increasing walk length. In 1988, Sumners and Whittington (15) proved this conjecture rigorously by showing that exponentially few arcs would remain unknotted as the length tends to infinity. Numerical studies of finite-length random walks find that the probability of knotting and the average complexity of knots increase sharply with the number of steps (16).

Here, we describe a simple physical experiment on knot formation. A string was placed in a cubic box and the box was rotated at constant angular velocity about a principle axis perpendicular to gravity, causing the string to tumble. We investigated the probability of knotting, the type of knots formed, and the dependence on string length. Before tumbling, the string was held vertically above the center of the box and dropped in, creating a quasirandom initial conformation. After tumbling, the box was opened and the ends of the string were

lifted directly upward and joined to form a closed loop. A digital photo was taken whenever a complex knot was formed. The experiment was repeated hundreds of times with each string length to collect statistics.

## Results

Most of the measurements were carried out with a string having a diameter of 3.2 mm, a density of 0.04 g/cm, and a flexural rigidity of  $3.1 \times 10^4$  dynes·cm<sup>2</sup>, tumbling in a  $0.30 \times 0.30 \times 0.30$ -m box rotated at one revolution per second for 10 sec (see *Materials and Methods*). Photos of the string taken before and after tumbling are shown in Fig. 1, and movies of the tumbling are provided as [supporting information \(SI\) Movies 1–5](#). The measured dependence of knotting probability  $P$  on string length  $L$  is shown in Fig. 2. No knots were obtained for  $L < 0.46$  m, where [SI Movie 1](#) shows that the confinement and tumbling did not induce sufficient bending to allow knot formation. As  $L$  was increased from 0.46 to 1.5 m,  $P$  increased sharply. However, as  $L$  was increased from 1.5 to 6 m,  $P$  saturated at  $\approx 50\%$ . The photos and movies show that when the string is confined in the box, the finite stiffness of the string results in its tending to form a coil (not perfectly, but to some degree) with a radius similar to the box width. During and after tumbling, this coiled structure is preserved, often with some compression of its radius perpendicular to the rotation axis (Fig. 1 and [SI Movie 2](#)).

A series of additional experiments were done to investigate the effect of changing the experimental parameters, as summarized in Table 1. Tripling the agitation time caused a substantial increase in  $P$ , indicating that the knotting is kinetically limited. Decreasing the rotation rate by 3-fold while keeping the same number of rotations caused little change in  $P$ . [SI Movie 3](#) shows that effective agitation still occurs because the string is periodically carried upward along the box wall. A 3-fold increase in the rotation rate, on the other hand, caused a sharp decrease in  $P$ . [SI Movie 4](#) shows that in this case, the string tends to be flung against the walls of the box by centrifugal force, resulting in less tumbling motion.

Doubling the box width increased  $P$  slightly, but decreasing it by 33% caused  $P$  to drop sharply. [SI Movie 5](#) shows that the tumbling motion was reduced because the finite stiffness of the coiled string tends to wedge it more firmly against the walls of the box. We also did measurements with a stiffer string (see *Materials and Methods*) in the 0.15-m box and observed a substantial drop in  $P$ . Observations again revealed that the tumbling motion was reduced due to wedging of the string against the walls of the box. Conversely, measurements with a more flexible string found a substantial increase in  $P$ . With the longest length studied of this string (4.6 m),  $P$  reached 85%,

Author contributions: D.M.R. and D.E.S. designed research, performed research, analyzed data, and wrote the paper.

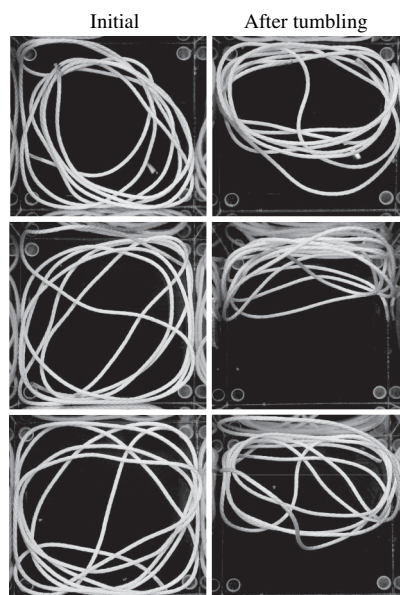
The authors declare no conflict of interest.

This article is a PNAS Direct Submission.

\*To whom correspondence may be addressed. E-mail: draymer@physics.ucsd.edu or des@physics.ucsd.edu.

This article contains supporting information online at [www.pnas.org/cgi/content/full/0611320104/DC1](http://www.pnas.org/cgi/content/full/0611320104/DC1).

© 2007 by The National Academy of Sciences of the USA



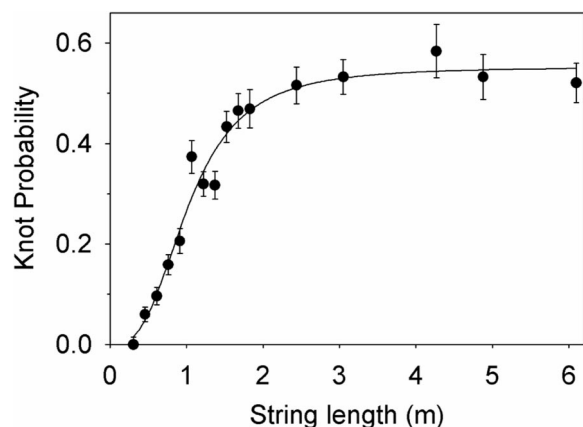
**Fig. 1.** Three examples of photos of the conformation of the string in the box before and after tumbling.

suggesting that  $P$  tends to 100% in the limit of long agitation time, long length, and high flexibility.

### Topological Analysis and Knot Classification

A string can be knotted in many possible ways, and a primary concern of knot theory is to formally distinguish and classify all possible knots. A measure of knot complexity is the number of minimum crossings that must occur when a knot is viewed as a two-dimensional projection (3). In the 1920s, J. Alexander (17) developed a way to classify most knots with up to nine crossings by showing that each knot could be associated with a specific polynomial that constituted a topological invariant. In 1985, V. Jones (18) discovered a new family of polynomials that constitute even stronger topological invariants.

A major effort of our study was to classify the observed knots by using the concept of polynomial invariants from knot theory. When a random knot formed, it was often in a nonsimple configuration, making identification virtually impossible. We therefore developed a computer algorithm for finding a knot's



**Fig. 2.** Measured probability of forming a knot versus string length. The line is a least-squares fit to a simple sigmoidal function  $N = N_0/(1 + (L/L_0)^b)$ , with  $N_0 = 0.55$ ,  $L_0 = 3.4$ , and  $b = -2.9$ .

Jones polynomial based on the skein theory approach introduced by L. Kauffman (3, 19).

This method involves enumerating all possible states of a diagram in which each crossing is “smoothed,” meaning cut out and reconnected in one of two possible ways:  $a = \times$  or  $b = \cup$ , resulting in  $|S|$  closed loops. All crossings were identified, as illustrated in Fig. 3, each being either “over” or “under” and having a writhe (3) (or “handedness”) of  $+1$  or  $-1$ . This information was input into a computer program that we developed. The Kauffman bracket polynomial, in the variable  $t$ , was then calculated as

$$-t^{-3w} \sum_S t^{(N_a - N_b)} (-t^2 - t^{-2})^{|S|-1}, \quad [1]$$

where the sum is over all possible states  $S$ ,  $N_a$ , and  $N_b$  are the numbers of each type of smoothing in a particular state, and  $w$  is the total writhe (3). The Jones polynomial is then obtained by the substitution  $t \rightarrow t^{-1/4}$  and compared with polynomials in the enumerated *Table of Knot Invariants*.<sup>†</sup>

Strikingly, we were able to identify  $\approx 96\%$  of all knots formed (1,007 of 1,127)<sup>‡</sup> as known prime knots having minimum crossing numbers ranging from 3 to 11. The prevalence of prime knots is rather surprising, because they are not the only possible type of knot. Computer simulations of random walks find an increasing fraction of nonprime “composite knots” with increasing length (14, 20). Here, only 120 of the knots were unclassifiable in 3,415 trials. Anecdotally, many of those were composite knots, such as pairs of  $3_1$  trefoils.

As shown in Fig. 4 *A* and *B*, the number of different types of knots observed (per number of trials) and the mean minimum crossing number  $c(K)$  increased sharply with increasing string length for  $L = 0.46$  to  $1.5$  m. However, for  $L > 1.5$  m, both quantities saturated, along with the total knot probability. Knots with  $c(K) = 3$  to 11 were observed and the mean  $c(K)$  increased from  $\approx 3$  to 6. As shown in Fig. 4C, all possible prime knots with  $c(K) = 3, 4, 5, 6$ , and 7 were observed. Above  $c(K) = 7$ , the fraction of possible knots observed dropped dramatically because the number of possible knots grows faster than exponentially, rapidly exceeding the number of experimental trials.

### Discussion

Although our experiments involve only mechanical motion of a one-dimensional object and occupation of a finite number of well defined topological states, the complexity introduced by knot formation raises a profound question: Can any theoretical framework, beside impractical brute-force calculation under Newton's laws, predict the formation of knots in our experiment?

Many computational studies have examined knotting of random walks. Although the conformations of our confined string are not just random walks (being more ordered), some similarities were observed. Specifically, computational studies find that the probability  $1 - P$  of not forming a knot decreases exponentially with random walk length (13, 14). In our experiments with the medium-stiffness string, we find the same trend for lengths ranging from  $L = 0.46$  to  $1.5$  m, but  $P$  approached a value of  $< 1$  as the length was increased further. As mentioned above, we attribute this to the finite agitation time.

In numerical studies of confined random walks (13, 20),  $P$  was found to increase with increasing confinement, and this effect has been proposed to explain the high probability of knotting of

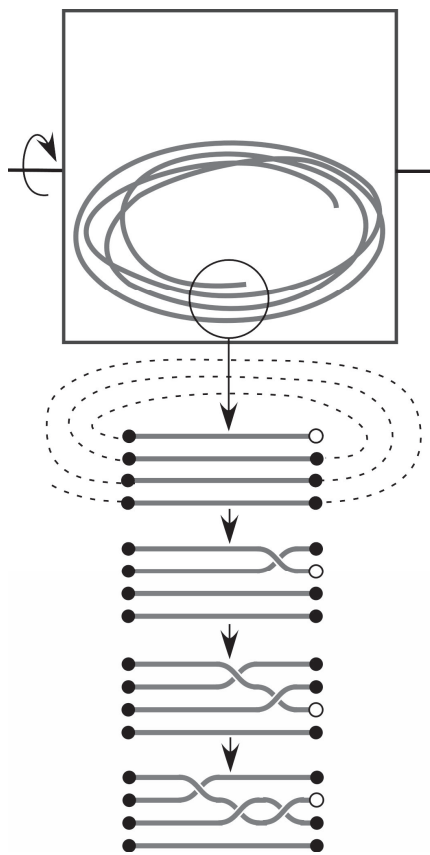
<sup>†</sup>Livingston, C., Cha, J. C., *Table of Knot Invariants* (Indiana University; [www.indiana.edu/~knotinfo](http://www.indiana.edu/~knotinfo)). Accessed December 2006.

<sup>‡</sup>In a small fraction of cases, the Jones polynomial alone did not determine the knot. In 6 cases the knot was distinguished by visual inspection, in 19 cases it was distinguished by calculating the Alexander polynomial, and in 7 cases it was distinguished by calculating the HOMFLY polynomial (3).







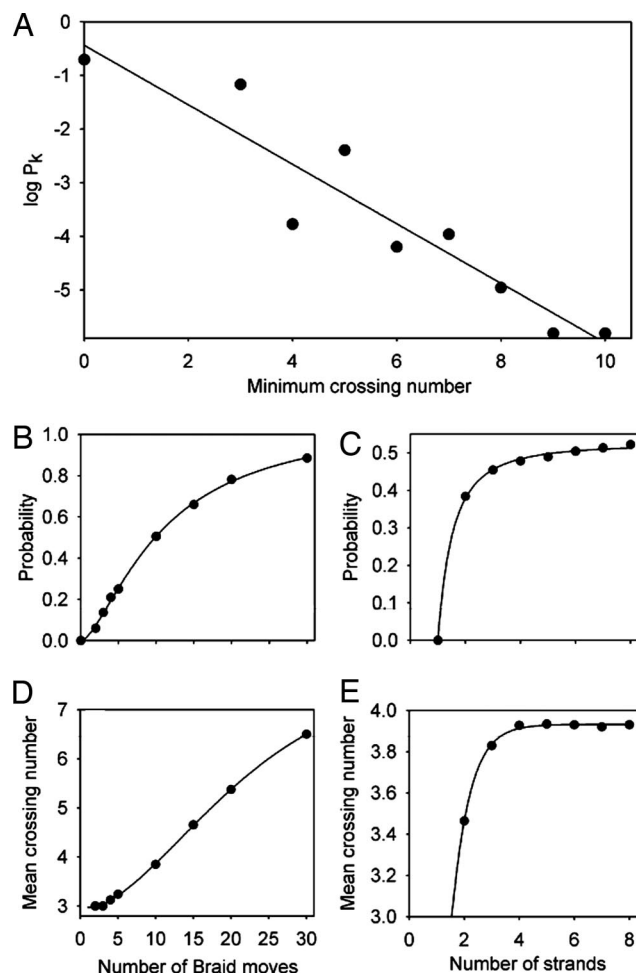


**Fig. 6.** Schematic illustration of the simplified model for knot formation. Because of its stiffness, the string tends to coil in the box, as seen in Fig. 1, causing a number of parallel string segments to lie parallel adjacent the end segment. As discussed in the text, we model knots as forming due to a random series of braid moves of the end segment among the adjacent segments (diagrams at bottom). The overall connectivity of the segments is indicated by the dashed line.

account for the occurrence of a threshold length for forming knots. A mathematical theorem proved by Milnor (28) states that the minimum curvature required to form a knot is  $4\pi$  versus  $2\pi$  for an unknotted closed loop. Similarly, to form a knot in our model, the string must have more than one coil, so that at least one segment lies adjacent to the string end. If we assume coils with a diameter equal to the width of the box ( $d$ ), the circumference is  $\pi d$ , or  $\approx 0.5$  m for the 0.15-m box, which is similar to the observed threshold length for forming knots (Fig. 2). For the 0.1-m box, the threshold also decreased to  $\approx 0.4$  m. At the opposite extreme, the longest strings correspond to having  $\approx 10$ –20 adjacent segments in our model.

We wrote a computer simulation that generated knots according to our model and determined their identities by calculating the Jones polynomials for the braid diagrams.<sup>8</sup> The model has only two adjustable parameters: the number of parallel segments ( $N_S$ ) and the number of braid moves ( $N_M$ ). Based on the considerations discussed above, we varied  $N_S$  from 2 to 20.  $N_M$  corresponds to “time” in our model, because we expect the number of braid moves to scale with agitation time in the experiment. The simulations show that the model can qualitatively account for several additional experimentally observed features.

<sup>8</sup>These calculations were done by using computer code in Bar-Natan, D., Morrison, S., et al., *The Mathematica Package KnotTheory* (University of Toronto; <http://katlas.math.toronto.edu>). Accessed July 2007.



**Fig. 7.** Predictions of the random braid move model discussed in the text. An ensemble of 1,000 conformations were generated for each condition and analyzed. (A) Distribution of minimum crossing numbers of knots generated with  $N_S = 10$  and  $N_M = 10$ , where  $P_K$  is the probability of forming a knot with minimum crossing number  $c(K)$ . (B) Probability of knotting  $P$  vs. number of random braid moves ( $N_M$ ) (proportional to agitation time) for  $N_S = 10$  segments (proportional to length). (C)  $P$  vs.  $N_S$  for  $N_M = 10$ . (D) Average minimum crossing number  $\langle c(K) \rangle$  vs.  $N_M$  for  $N_S = 10$  segments. (E)  $\langle c(K) \rangle$  vs.  $N_S$  for  $N_M = 10$ .

First, it predicts a broad distribution of knot types and complexities, as observed experimentally. For example, for  $N_S = 10$  and  $N_M = 10$ , the distribution (Fig. 7A) is similar to that observed experimentally with the long strings—knots ranging from crossing number 3 to 10 were observed with overall decreasing probability. The agreement was not perfect because, for example, the  $4_1$  knot had notably lower probability in the model, whereas  $5_1$  had notably lower probability in the experiment, but a similarly wide distribution of complexities were observed in both cases. Second, the model predicts that the overall probability of knotting  $P$  increases with time (i.e., with  $N_M$ ) and with string length ( $N_S$ ) (Fig. 7B and C), as observed in the experiment. Finally, it predicts that the average complexity of knots (average minimum crossing number) increases with time and string length (Fig. 7D and E), as observed.

## Materials and Methods

A computer-controlled microstepper motor spun the boxes, which were made of smooth acrylic plastic and purchased from Jule-Art. The boxes were cubic, of widths 0.1, 0.15, and 0.3 m. The string used in most experiments was solid #4 braided string (catalog no. 021008010030; Samson, Ferndale, WA), which had

a diameter of 3.2 mm, a density of 0.04 g/cm, and a flexural rigidity of  $3.1 \times 10^4$  dynes·cm<sup>2</sup>. In some experiments, a more flexible string was also used (nylon #18 twine) (catalog no. NST1814P; Lehigh Group, Macungie, PA), which had a diameter of 1.7 mm, a density of 0.0086 g/cm, and a flexural rigidity of 660 dynes·cm<sup>2</sup>. A stiffer rubber tubing was also used (catalog no. 141782AA; Fisher Scientific, Waltham, MA), which had a diameter of 8 mm, a density of 0.43 g/cm, and a flexural rigidity of  $3.9 \times 10^5$  dynes·cm<sup>2</sup>. The flexural rigidity was determined by cantilevering one end of the string off the edge of a table, such that the end deflected downward a small amount  $\Delta y$  due to the string bending under its own weight. According to the Euler

small displacement formula:  $\Delta y = mgL^3/(8EI)$ , where  $L$  is the length,  $mg$  is the weight, and  $EI$  is the flexural rigidity (29). In principle, tumbling in the plastic box may induce static electric charge in our string, which could influence the dynamics. However, no perturbation of a hanging string was observed when a second segment was brought into close proximity after tumbling, indicating that electrostatic repulsion effects are negligible compared with gravitational weights in our system.

We thank Parmis Bahrami and Joyce Luke for assistance with data collection.

1. Thomson W, Tait PG (1867) *Treatise on Natural Philosophy* (Oxford Univ Press, Oxford).
2. Simon J (2002) in *Physical Knots: Knotting, Linking, and Folding Geometric Objects in  $R^3$*  (American Mathematical Society, Providence, RI).
3. Adams CC (2004) *The Knot Book: An Elementary Introduction to the Mathematical Theory of Knots* (American Mathematical Society, Providence, RI).
4. Dean FB, Stasiak A, Koller T, Cozzarelli NR (1985) *J Biol Chem* 260:4975–4983.
5. Shaw SY, Wang JC (1993) *Science* 260:533–536.
6. Arsuaga J, Vázquez M, Trigueros S, Sumners D, Roca J (2002) *Proc Natl Acad Sci USA* 99:5373–5377.
7. Belmonte A, Shelley MJ, Eldakar ST, Wiggins CH (2001) *Phys Rev Lett* 87:114301.
8. Ben-Naim E, Daya ZA, Vorobieff P, Ecke RE (2001) *Phys Rev Lett* 86:1414–1417.
9. Hickford J, Jones R, duPont S, Eggers J (2006) *Phys Rev E* 74:052101.
10. Frisch HL, Wasserman E (1961) *J Am Chem Soc* 83:3789–3795.
11. Delbruck M (1962) *Proc Symp Appl Math* 14:55.
12. Frank-Kamenetskii MD, Lukashin AV, Vologodskii AV (1975) *Nature* 258:398–402.
13. Michels JPJ, Wiegel FW (1982) *Phys Lett A* 90:381–384.
14. Koniaris K, Muthukumar M (1991) *J Chem Phys* 95:2873–2881.
15. Sumners DW, Whittington SG (1988) *J Phys A Math Gen* 21:1689–1694.
16. Shimamura MK, Deguchi T (2002) *Phys Rev E* 66:040801.
17. Alexander JW (1928) *Trans Am Math Soc* 30:275–306.
18. Jones VFR (1985) *Bull Am Math Soc* 12:103–112.
19. Kauffman LH (1987) *Topology* 26:395–407.
20. Micheletti C, Marenduzzo D, Orlandini E, Sumners DW (2006) *J Chem Phys* 124:064903.
21. Goriely A (2005) in *Physical and Numerical Models in Knot Theory*, Series on Knots and Everything, eds Calvo JA, Millett KC, Rawdon EJ, Stasiak A (World Scientific, Singapore), Vol 36, pp 109–126.
22. Fukuhara S (1988) *A Fête of Topology: Papers Dedicated to Itiro Tamura*, eds Matsumoto Y, Mizutani T, Morita S (Academic, New York), pp 443–452.
23. O'Hara J (2003) *Energy of Knots and Conformal Geometry*, Series on Knots and Everything (World Scientific, Singapore), Vol 33.
24. Freedman MH, He ZX, Wang ZH (1994) *Ann Math* 139:1–50.
25. Kusner RB, Sullivan JM (1998) in *Ideal Knots*, eds Stasiak A, Katritch V, Kauffman LH (World Scientific, Singapore), p 315.
26. Belmonte A (2005) in *Physical and Numerical Models in Knot Theory*, Series on Knots and Everything, eds Calvo JA, Millett KC, Rawdon EJ, Stasiak A (World Scientific, Singapore), Vol 36, pp 65–74.
27. Alexander JW (1923) *Proc Natl Acad Sci USA* 9:93–95.
28. Milnor JW (1950) *Ann Math* 52:248–257.
29. Moore JH, Davis CC, Coplan MA (2002) *Building Scientific Apparatus* (Perseus, Cambridge, MA).