Knot Formation in Open and Closed Self-Avoiding Walks: an Empirical Comparative Study

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We describe an empirical study of the formation of knots in open and closed self-avoiding walks (SAWs), based on a simple model involving randomly agitated cords. The results suggest that the probability of a closed SAW remaining knot-free follows a similar scaling law to that for open-ended SAWs. In particular, the process of closing a given SAW prior to random agitation substantially increases the probability that it will be knot-free following agitation. The results point to a remedy for the well-known problem of tangling of cord, rope, headphone cables etc. The simple act of connecting the two free ends to each other, thus creating a loop, greatly reduces the risk of such tangling. Other implications, in particular for DNA storage in cells, are briefly discussed.

Background theory

The probability of a self-avoiding walk (SAW) remaining free of a knotted arc after N steps is bounded above by $P_o(N)$ where

$$P_o(N) \leq exp[-kN + o(N)] \quad k > 0 \qquad (1)$$

This well-known result, due to Sumners and Whittington (1988), suggests that the probability of a randomly agitated length of cord remaining knot-free will follow a similar relationship. Specifically, if L is the total length of the cord and L^* denotes the smallest length of cord capable of forming at least a 3_1 knot the probability of the cord remaining knot-free is expected to follow a relationship of the form

$$P_o(L) \leq \; exp[-k(L - L^*)] \quad L \geq L^* \qquad (2)$$

This functional form has been confirmed by many studies, both experimental (eg Hickford *et al* 2006) and computational (eg Deguchi & Tsurusaki 1997).

Consider now the case where the two free ends of such a cord are joined prior to agitation[1]. One would expect the probability of the resulting loop staying knot-free to be higher than the bound set by (2). Firstly, the process of looping reduces the maximal linear length available for knot formation from L to $L/2$. Secondly, the formation of knots in the looped cord is a more demanding phenomenon than in the free-ended case, requiring that $2n$ $(n = 1, 2, \ldots)$ arcs each of length S ($2L^* \leq S \leq L/2$) remain sufficiently close together to perform the spatial manoeuvres involved in knot formation.

This suggests that the probability of a *looped* cord remaining knot-free will follow a relationship analogous to (2), with

$$P_o(L)\,|_{loop} \;\leq\; exp[-k(L_{loop} - L^*_{loop})] \quad L_{loop} \geq L^*_{loop} \qquad (3)$$

where we now have

$$L_{loop} = \alpha L \;\text{ with } \alpha \leq 0.5$$

reflecting the fact that no more than L/2 of the original cord length can be sufficiently close together to form at least a 3_1 knot, while

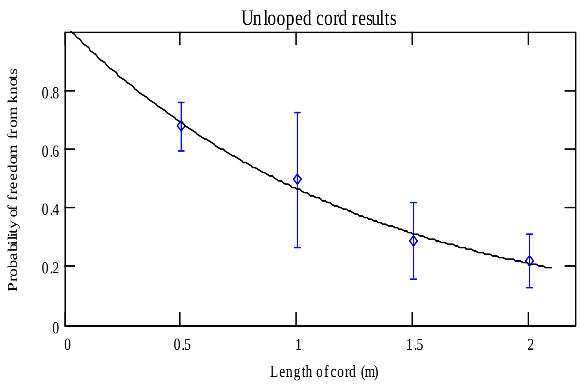
$$L^*_{loop} = \beta L^* \;\text{ with } \beta \geq 2$$

reflecting the fact that the loop requires a length of at least twice L* in order to form at least a 3_1 knot.

Experimental results

To investigate the validity of the relationships (2) and (3) above, we randomly agitated four cords of length L = 0.5, 1.0, 1.5 and 2 metres respectively, in both the free-ended and looped states. The cord was standard office parcel string, and the agitation done by hand for 10 seconds for a total of 5 sets of 20 trials for each of the four lengths in both the free-ended and looped states, giving a total of 400 trials for each state.

(a) Free-ended cord We found that the probability of a given length of cord with free ends remaining free of knots was well represented by a relationship of the general form given by (2), confirming previous research; see below (error bars are $\pm\, 1\sigma$):



A least-squares fit to the data gives:

$$P_o(L) = \; exp[-0.786(L - 0.03)] \qquad (4)$$

This functional dependence of knot freedom on length L implies that for the type of cord used, at least 0.03 m is required to generate at least a 3_1 knot, and that the probability of remaining knot-free halves for every 0.88 metres of length.

(b) Looped cord We found that the probability of looped cord remaining free of knots was also well-represented by the theoretical relationship given above:

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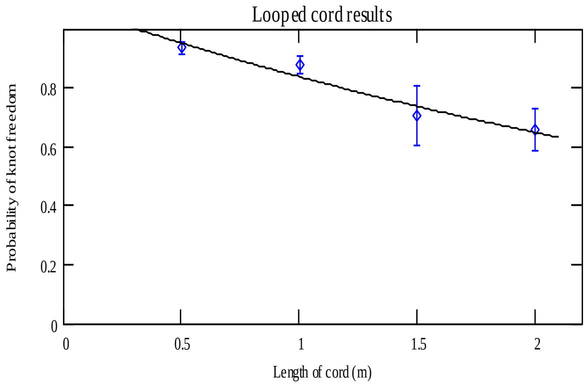
[1] In what follows, the concept of "knot formation in loops" refers specifically to knot formation in cord turned into a loop *prior to random agitation*. This is in contrast to the focus of much existing research, namely the formation of knots in SAWs *prior to the joining of their free ends*, leading to knots trapped *within* a looped SAW.



A least-squares fit to the data leads to

$$P_o(L)|_{loop} \; = \; exp[\,-0.255(L - \; 0.32)\,] \qquad (5)$$

As predicted, the probability of the looped cord remaining free of knots is considerably higher than for the free-ended cord for all measured L, and declines considerably more slowly, halving for every 2.7 metres in length. Furthermore, the minimal length required for the formation of even a simple knot is an order of magnitude greater than for the free-ended case, at 0.32 metres.

Re-casting the empirical relationship (5) into the canonical form (3), we find that the experimental values of α and β also agree with the predicted bounds given above. Specifically, we find that

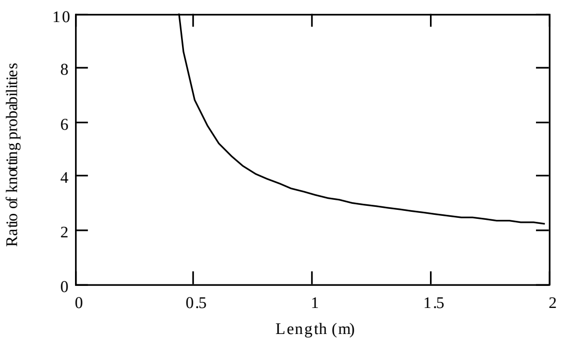
$$P_o(L)\,|_{loop} \; = \; exp[-0.786(L_{loop} - \; 0.104)\,] \qquad (6)$$

leading to $\alpha = 0.325$ and $\beta = 3.47$. Thus a length L of the cord used in these trials behaves as one of effective knottable length $0.325L$ when looped, with a greater amount of cord also being needed to form any form of knot.

This result suggests that looping a cord prior to random agitation produces a significant reduction in the risk of the cord becoming knotted. This benefit from looping is most clearly seen from the ratio R of the probabilities of forming *at least* one knot:

$$R(L) \equiv [1 - P_o(L)]/[1 - P_o(L)\,|_{loop}]. \qquad L > L^*_{loop} \qquad (7)$$

Inserting the empirical forms for $P_o(L)$ and $P_o(L)|_{loop}$ from (4) and (5) respectively leads to the following plot:



This shows that, for the cord used in this study, the act of looping reduces the risk of knotting *by at least an order of magnitude* for L up to ~ 0.5m, and by a factor of > 2 even for lengths up to 2m. The benefit of looping will be different for other materials with different stiffness, thickness etc., and in some cases may be even greater than shown here.

Discussion

The above results suggest that the knotting probability of looped cord follows a similar functional dependency on L as that of both real cord (Raymer & Smith 2007) and simulated SAWs (eg Deguchi & Tsurusaki 1997). As such, this study points to a simple way of combating the notorious problem of knotting in long lengths of cord, flex, rope etc first noted at least a century ago (Jerome, 1889). The effect on knotting probability of looping may also have a bearing on less “trivial” issues, such as the presence of loops in chromatin (eg Bohn, Heerman & van Driel 2007; Mateos-Langerak *et al* 2009).

A number of further questions suggest themselves for investigation:

Practical

- What are the effects of altering the stiffness of the cord ? Raymer & Smith found that, as intuition suggests, the probability of freedom from knotting increases with increasing stiffness of the cord. It seems reasonable to suspect that it will have an even more marked effect on looped SAWs, thus increasing the benefits of looping.
- How does the thickness of cord affect this probability ? Simulations show that knot-freedom increases with increasing thickness. Again, it seems reasonable to suspect that it will have an even more marked effect on looped SAWs.
- How does confining geometry/size affect knotting probability ? The results of Tesi *et al* (1994) involving SAPs suggest an effect on knotting probability for looped SAWs.

Theoretical

- How should the standard theory of knots and SAWs be extended to incorporate the knotting of loops ? Strictly, a mathematical knot is a closed curve embedded in R^3 , and thus cannot involve free ends. This mismatch with the everyday concept of knots is compounded in the case of knotted loops examined here, as one is now dealing with knots formed out of the trivial knot 0_1. However, the extension of the standard concepts may open up new areas for research: during the study reported here it was found that loops can form knots which appear similar, but not identical, to the “classical” knots such as the trefoil.
- Is it possible to put tighter theoretical bounds on the values of α and β, which relate properties of a looped SAW to that of its unlooped original ? Geometrical considerations of the knotting process suggest α and β are related and that their numerical values involve factors of order π .

Computational

- Can the model for the behaviour of looped cord proposed here be further investigated using numerical models used to study knotting in SAWs ? Such a model will require techniques for defining loop ends, and of identifying the different forms of knot that can form in such a loop.

Conclusion

The results presented here suggests that looping a cord prior to random agitation substantially increases the chances of the cord remaining knot-free. The functional form of the dependency of this probability on cord length L is similar to that of open-ended SAWs, and shows that the benefits of looping increase exponentially with L. As well as having obvious relevance to the commonplace nuisance of knots in headphone flex, rope, hose etc, the effect of looping may be of importance in other fields, notably cellular biology.

References

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