Random Walks in a Vibrating Chain: A More Generalized Approach to Studying Asymmetric Unknotting

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In this experiment, a trefoil knot was tied in the center of chains made up of 3.9 mm diameter brass beads. When vibrated on a flat aluminum plate at a frequency of 17 Hz and accelerations of $2.6g - 3.5g$, the beads exhibit stochastic behavior, and given enough time, will unknot. Various lengths were tested, ranging from $N = 36$ to $N = 80$ beads. In a perfectly symmetric system, the unknotting time scales quadratically with the number of beads. Our experiment displays asymmetric behavior and shows that under certain circumstances, the unknotting time scales linearly.

I. INTRODUCTION

Knots are a common occurrence in nature, and are frequent in large molecular chains such as protein. Understanding how knots form and interact with various components is crucial in understanding protein structures and protein folding[1].

One method of modelling knots is via a chain consisting of brass beads separated by a thin rod. Adding rigidity to the structure, as opposed to using an extremely flexible material such as string, is a better model for large molecules, which can be tied into knots but also has limited flexibility. When the beads are tied into a trefoil knot, they are not in a very tight position. Therefore, perturbing the chain at certain frequencies and amplitudes can cause the knot to move around.

Ben-Naim et al. characterized the movement of this knot by considering how the crossing points moved. They observed that the crossing points move in a random pattern, and modelled them as a random walk. Given sufficient time, one of the crossing points will go off the end of the chain, effectively "unknotting" the chain. When considering small knots in very long chains, they were able to reduce the problem to a diffusion problem and both showed and observed that the average unknotting time scales as

$$\tau \sim (N - N_0)^2, \tag{1}$$

where N_0 is the number of beads in the knot[2].

A. Generalized Model

In this experiment, we generalize BenNaim's results by considering the case where the crossing points do not undergo a symmetric random walk, but instead an asymmetric random walk. Assume that for a given period of vibration, a given crossing point has a probability p to move to the right and a probability $1 - p$ to move to the left. We will also consider the right crossing point only. Using this model, the number of periods it takes for the right crossing point to go off the end of the chain is given by the recursive relationship,

$$T(x) = pT(x + 1) + (1 - p)T(x - 1) + 1 \tag{2}$$

Here, x is the location, representing the number of beads between the center bead and the crossing point, and $T(x)$ is the expected time it takes for the crossing point to go off the end of the chain if it starts at a position x. Note that this equation assumes that in each period, the crossing either, moves left and right, and doesn't stay in the same place. To resolve this, we can make the assumption that we can expect the crossing to move every M periods, and then redefine our time frame to be this new period. While there are some issues with this assumption, we shall see that it gives a good enough approximation. The general solution is

$$T(x) = A\left(\frac{1}{p} - 1\right)^x + B + \frac{x + p}{1 - 2p}, \tag{3}$$

where A and B are constants. We can consider the knot to be untied if $x = N/2$ (knot exits through right end) or $x = -N/2 + N_0$ (knot exits through right end). The boundary conditions of $T(0) = 0$ and $T(N - N_0) = 0$ then gives

$$T(x) = \frac{(N_0 - N)\kappa^{N/2+x} + \left(\frac{N}{2} - x\right)\kappa^{N_0} + (x + \frac{N}{2} - N_0)\kappa^N}{(2p - 1)(\kappa^N - \kappa^{N_0})}, \tag{4}$$

where $\kappa = \frac{1}{p} - 1$. If the knot is centered, then the number of beads between the center and the right crossing is exactly half the beads involved in the knot, $N_0/2$. Therefore, for a centered knot, the unknotting time is

$$T(-N_0/2) = \frac{N - N_0}{2(2p - 1)} \cdot \frac{\kappa^{N_0/2} - \kappa^{N/2}}{\kappa^{N_0/2} + \kappa^{N/2}}. \tag{5}$$

We can verify that

$$\lim_{p \to 1/2} T(-N_0/2) = (N - N_0)^2/4. \tag{6}$$

Let $p = 0.5 + \epsilon$ for $\epsilon \ll 1$. Then $\kappa \approx 1 - 4\epsilon$ and we have,

$$T(-N_0/2) = \frac{N - N_0}{4\epsilon} \cdot \frac{(1 + 2N_0\epsilon) - (1 + 2N\epsilon)}{(1 + 2N_0\epsilon) + (1 + 2N\epsilon)} \tag{7}$$

$$\approx -\frac{(N - N_0)^2}{4}, \tag{8}$$

where we made the assumption that $N \gg N_0$ and $N_0|\epsilon| \ll 1$, which supports equation 1. Without loss of generality, now consider the case where $p > 0.5$. If instead $p < 0.5$, due to symmetry it would behave the same as if $p \to 1-p$ (i.e. rotating 180°.) Then, $\kappa < 1$. In the limit where $N \gg N_0$, we obtain

$$f(N_0/2) \approx \frac{1}{6}(N - N_0) \cdot \left(1 - \kappa^{(N-N_0)/2}\right), \qquad (9)$$

which is a linear term and an exponential decay term. Therefore, for large N, we have a linear asymptotic behaviour,

$$f(N_0/2) \sim \frac{1}{6}(N - N_0). \qquad (10)$$

Using these assumptions, we can also predict

B. Knot Terminology

When tying a trefoil knot, an orientation can be assigned to the outer two crossing points. We will describe this orientation by considering the three crossings X_1, X_2, X_3. We define X_1 to be the *over-crossing* since the arc containing X_1 and the end of the chain goes over X_1. Similarly, we define X_2 to be the *under-crossing* since the arc containing X_2 and the end of the chain goes under X_2. The knot is untied when one of the crossings

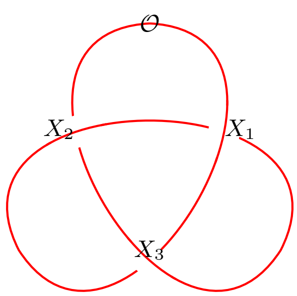

FIG. 1: The trefoil knot. In our experiment, instead of the knot forming a continuous loop, the end at $\mathcal{O}$ is open, and represents the two "ends" of the chain.

moves off the end of the chain. If X_1 moves off the end of the chain, we denote the run as a positive (+) run. If X_2 moves off the end of the chain, we denote the run as a negative (−) run. Through our experiment, we did not witness any cases where X_3 moves off the end of the chain, likely due to the bulkiness of the chain and physical collisions preventing it from happening. Because of this observation, the relative positions of X_1, X_2, X_3 will stay constant. Therefore, when we talk about the end of the chain with respect to a crossing X_i, we refer to the end that can be connected to X_i without passing any other crossings, and this is well-defined.

C. Direction of Movement

Using our assumptions, we can predict which direction the knot will untie in. Consider the crossing point X_2. In each step, suppose its probability of moving away from its endpoint and towards X_1 is $p > \frac{1}{2}$. The probability of a negative run is then given by the recursive form,

$$P(x) = (1-p)P(x-1) + pP(x+1),$$

where x is the number of beads between X_2 and the end of the chain. Solving this recursive formula and accounting for initial conditions, we obtain

$$P(n) = \left(\frac{1}{p} - 1\right)^n = \kappa^n. \qquad (11)$$

In reality, it is unlikely for systems to be exactly symmetric, especially when there is an asymmetry to how the knot was tied. By keeping track of this asymmetry our experiment is able to compare Ben-Naim's model to our more generalized model of the knot.

II. METHOD

The apparatus setup followed Professor David Bailey's instructions[3]. A frequency generator, whose signal is amplified through a power amplifier, is able to control the amplitude and frequency of an aluminum vibrating plate. This plate has an accelerometer attached to the bottom, which allows its acceleration data to be recorded. The base of the setup is connected to the table via four legs whose heights are adjustable via a knob. A lot of careful work was done to adjust the knobs such that the plate is level. This was tested by placing a chain in the center, and observing that the chain does not hit the edges. The frequency of the vibrating plate was set to 17 Hz

FIG. 2: A trefoil knot tied in a chain of $N = 50$ beads. An Allen key was used to consistently maintain $N_0 = 18$ beads in the knot.

and the amplitude, as measured in peak-to-peak voltage V_{pp} of the MMA 1220 accelerometer was varied between 1.5 V and 1.75 V. The chains consisted of 3.9 mm diameter brass beads, and the number of beads ranged from

$N = 36$ to $N = 80$. A trefoil knot was tied at the center, as shown in figure 2, and due to the stochastic nature of the experiment, each condition was run for 30 trials.

To maintain consistency, the knot was tied around an Allen key, in order to ensure the size of the knot stays the same. We estimate that the number of beads involved in the knot is $N_0 = 18 \pm 1$.

III. RESULTS AND DISCUSSION

A. Determining the Power Law

At $V_{pp} = 1.75$V, 30 trials were conducted for chains with $N = 36, 50, 65, 80, 90$ beads. The results are summarized in figure 3, and uncertainty in time is given by the standard error of all the trials. We see that we have a mostly linear fit, with $R^2 = 0.97$ and $\chi_r^2 = 2.8$. Since χ_r^2 is close to 1, the estimates for uncertainties are reasonable, though they may be slightly underestimated. The uncertainty in time comes from the standard error from all 30 trials. Note that for longer chains, this error becomes very large. We have observed trials finishing almost immediately in a few seconds to extending on for a minute.

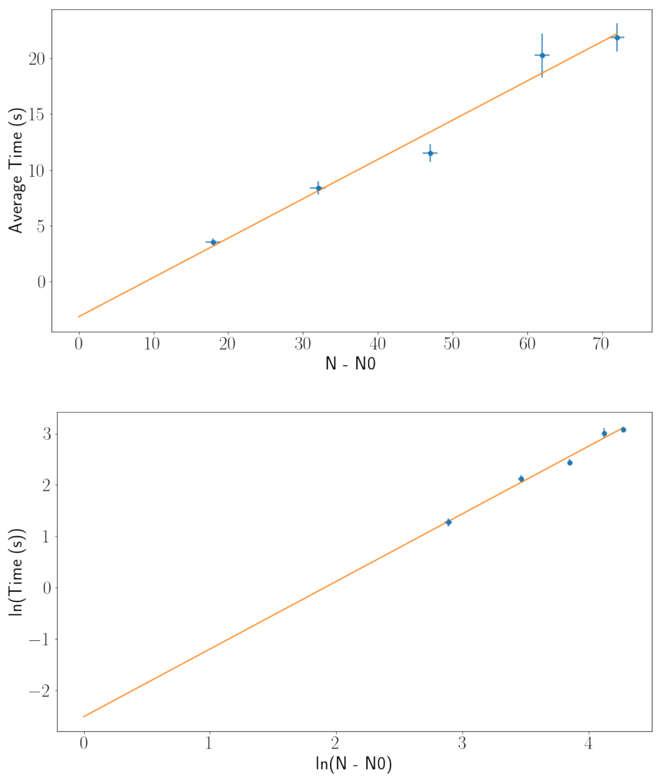

FIG. 3: (Top) The average time for the knot to untie as a function of the number of beads in the chain. The solid line is a linear fit to the data, with $R^2 = 0.97$. (Bottom) The natural log of the average time for the knot to untie as a function of the number of beads in the chain. The solid line is a linear fit to the data, with $R^2 = 0.99$.

We can also seek how closely our data can be described by a power law fit, i.e.

$$\tau = a(N - N_0)^{\delta}.$$

A δ value closer to 2 would suggest Ben-Naim's model is a better fit, but a δ value closer to 1 would suggest our generalized model, which predicts this linear behaviour, may be better. The natural log of both sides are plotted in figure 3, and we see that the data is well described by a linear fit, with $\delta = 1.3 \pm 0.2.$ and $a = 0.081 \pm 0.007$.

The uncertainty in δ was estimated using a heuristic upper bound and lower bound estimate by looking at how the data points can vary according to their uncertainties, i.e. we set

$$\Delta\delta = \frac{\delta_{\text{upper}} - \delta_{\text{lower}}}{2}. \tag{12}$$

The reason this was done was because the fit parameters predicted an uncertainty of only 0.09, which did not take the uncertainties into account. This value of δ does not agree with $\delta = 2$ and again agrees closer to our generalized model.

While the data is strictly not linear, it is closer to being linear then being quadratic. Our model predicts that the behaviour will be "almost" but not exactly linear, giving more credibility to our mathematical model.

B. Direction that the knot unties

At a voltage of $V_{pp} = 1.50$ V, the same experiment was done for a chain with beads of the same size and with $N = 60$ beads. However, the knot was placed off-center such that X_2 was placed closer to the end than X_1, making a negative run more likely. We define the setup ratio r to be

$$r \equiv \frac{\text{beads to the left of } X_2}{N}. \tag{13}$$

We tested r values of $8\%, 12\%, 17\%, 23\%, 35\%$. Using these values, we can rewrite equation 11 as

$$P(n) = \left(\frac{1}{p} - 1\right)^{rN}, \tag{14}$$

and fit our data to this equation, which is done in figure 4. Our fit gives $p = 53\%$, showing that just a small asymmetry in the knot can have a large effect on the direction of the run. To verify this result, we ran a Monte Carlo simulation of the trefoil knot untying via two asymmetric random walks. At four different values of p, thirty setup ratios were tested, and for each test, a total of 1000 trials were run. As shown in figure 5, the negative run probability decreases exponentially for all probabilities other than $p = 0.5$.

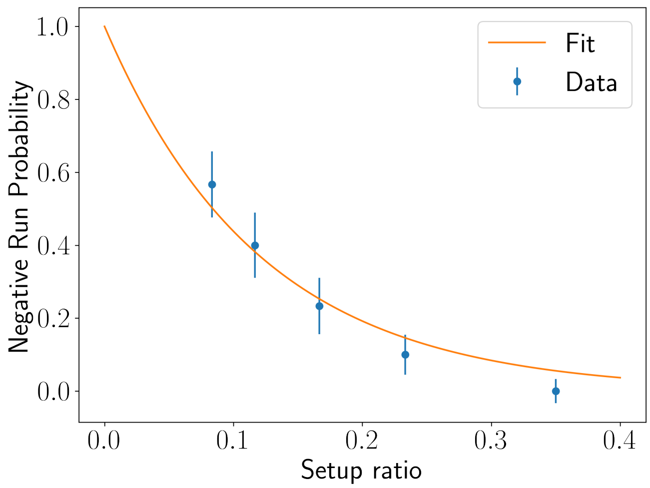

FIG. 4: The average time for the knot to untie as a function of the setup ratio r.

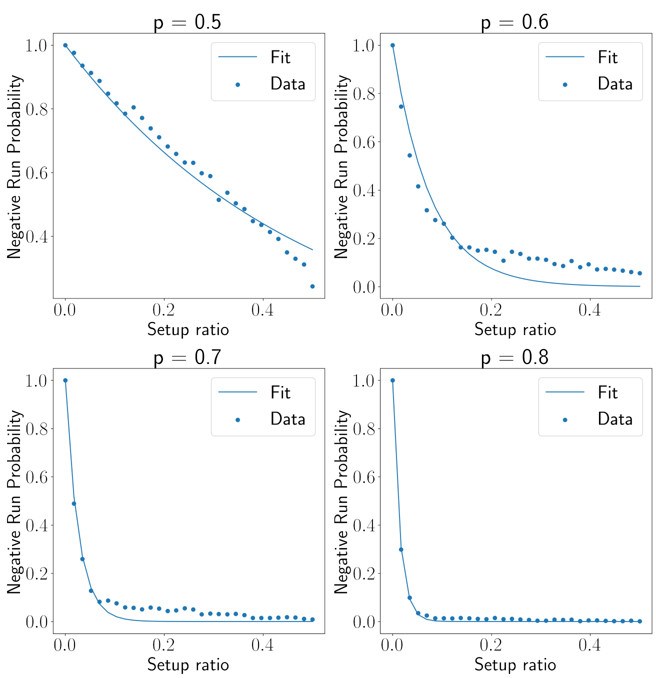

FIG. 5: The probability of a negative run as a function of the setup ratio r for four different values of p. The higher the p value, the steeper the graph.

The model isn't great, and we don't need the residuals plot to see that. Clearly the probability drops much quicker than our model anticipates, but it is still able to predict the exponential-like behavior. With more data points, we can make a better judgement of this model.

C. Discussion of Uncertainties

Because the behavior of the knot under vibrations is a stochastic process, the majority of the uncertainties come from simply not collecting enough data to make a definitive statement about averages. If we are to ensure the set-up procedure is always consistent, then each trial can take a considerable amount of time, and our data analysis has shown that 30 trials per condition is not enough to make conclusive justifications. In particular, if histograms were plotted for how long it took a center knot to untie, we see in figure 6 we do not get a smooth positive skew distribution. For experiments where there is a lower bound for the time it takes but no upper bound, the distribution of the total times is typically positively skewed. Qualitatively, the $N = 80$ case has a distribution

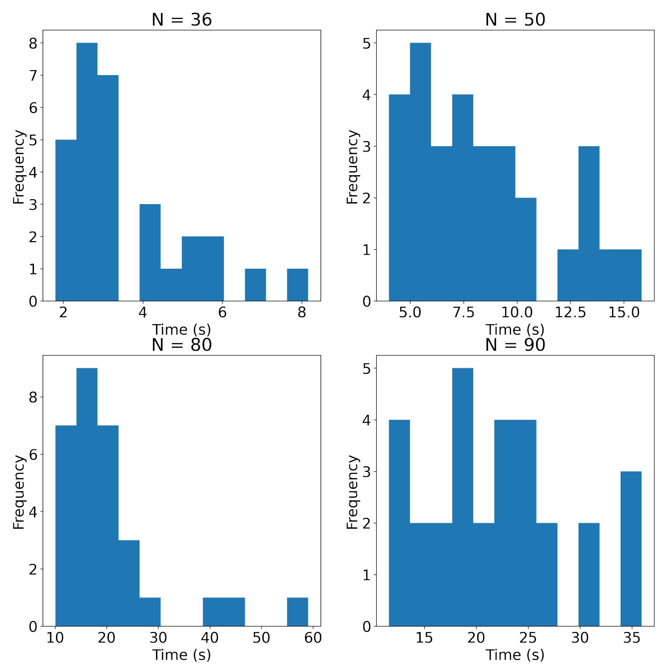

FIG. 6: Histograms of the time it took for the center knot to untie for $N = 36, 50, 80, 90$ beads. The $N = 65$ case was skipped but has visual similarity to the $N = 50$ case.

that is roughly smooth. Most of the trials fall between $t = 10$ s and $t = 25$ s, with a small tail extending to $t = 60$ s. However, the distribution for $N = 90$ looks very uniform. The average time it takes to unknot is greater, but no smooth skew-like shape can be found, as well as it has a limited range.

We accept that it is a possibility that the results and findings of our experiment is limited by the number of samples we've taken, and thus we expect that if we increase the number of trials to a point where the distributions in figure 6 become smooth, then we can make more definitive statements about the behavior of the knot.

IV. CONCLUSION

Our experiment shows that there are inherent flaws with the model first proposed by Ben-Naim when extending it to asymmetrical systems[2]. Even given a small asymmetry in the probability of each crossing point moving in a certain direction, it can lead to very different outcomes for the run. In our experiment, a power-law fit shows that the exponent is $\delta = 1.3 \pm 0.2$, which is closer to a linear fit than Ben-Naim's quadratic fit. Our model, which is more generalized, is able to predict the linear behavior we see in our experiment, as well as predict which direction the knot will untie in, but these predictions are not perfect, and we expect more data to be collected to make more definitive statements.

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[2] E. Ben-Naim, Z. A. Daya, P. Vorobieff, and R. E. Ecke. Knots and random walks in vibrated granular chains. *Physical Review Letters*, 86(8):1414–1417, February 2001.

[3] David Bailey. Knots and topological transformations in vibrating chains. September 2015.