# Statistics of trefoil knot opening times in vibrated granular chains

**PHY424**
*April 3, 2023*
LUCAS PRATES

**Abstract**

This paper details my study of the opening times of trefoil knots in vertically vibrated granular chains. I find strong evidence of a quadradic relationship between the trefoil's mean opening time, $\tau_{\text{avg}}$, and the length of the granular chain, $N$. Additionally, I find quantitative evidence that the knot's survival time distribution $S(t, N)$ can be expressed as a function of a single parameter, $t/\tau_{avg}$.

## 1 Introduction

The thermal motion of filamentary objects such as DNA and polymer micromolecules can often lead to the formation and opening of knots. Understanding these processes can lead to an understanding of the macroscopic properties of materials like gels and plastics (Meluzzi et al., 2010). In particular, understanding how topological constraints such as knots affect the dynamics of these one dimensional filaments is crucial in understanding the flow and structural properties of the materials they componse. Unfortunately, such constraints are diffucult to observe and manipulate at such a scale (Ben-Naim et al., 2001).

Using a macroscopic analogy for such a system is a good first step towards understanding the dynamics of knots in one dimensional filaments, at a scale where the knots can be easily manipulated and observed. In this experiment, I create a simple analog by studying the dynamics of the trefoil knot in vertically vibrated ball chains.

In this paper, I seek to find a relationship between the chain length in number of balls, $N$, and the mean trefoil opening time, $\tau_{\text{avg}}$. Additionally, I study the survival probability $S(t, N)$, which is the probability that a knot in a length $N$ chain still exists at time $t$. This paper seeks to show that $S(t, N)$ can be expressed as a function of a single variable, $z = t/\tau_{\text{avg}}$.

## 2 Theory

Ben-Naim et al. (2001) models the motion of a trefoil knot with minimum size $N_0$ as the random walk of three independent point particles point particles which are not allowed to swap positions, along a one dimensional domain of size $N - N_0$, and identical diffusivity $D$. This essentially reduces to a three dimensional diffusion problem. By solving this diffusion problem with the appropriate assumptions, and intepreting the survival probability as the probability that the random walks remain confined to a finite domain, Ben-Naim et al. (2001) arrives at

$$S(t, N) = \left( \frac{4}{\pi} \sum_{k=0}^{\infty} \frac{\sin[(2k+1)\pi x_0]}{2k+1} e^{-(2k+1)^2 \pi^2 D t/(N-N_0)^2} \right)^3 \quad (1)$$

where $x_0$ is the knot's initial fractional position along the chain.

Now, let $R(t,N)$ be the exit time distribution for the chain. Then, $R(t,N)dt$ can be interpreted as the proportion of knots which open between $t$ and $t+dt$. The survival probability is the proportion of knots that remain unopened at time $t$. Then,

$$S(t,N) = 1 - \int_0^t R(\tilde{t},N)d\tilde{t} \implies R(t,N) = -\frac{\mathrm{d}S(t,N)}{\mathrm{d}t} \tag{2}$$

With this interpretation of the exit time distribution, the mean exit time can also be computed using

$$\tau_{\text{avg}} = \int_0^\infty tR(t,N)dt \tag{3}$$

Together with equations 1 and 2, 3 becomes

$$\tau_{\text{avg}} = \frac{\tau_3}{D}(N-N_0)^2 \tag{4}$$

where $\tau_3 = 0.056213$. Thus, this equation gives the relationship between $\tau_{\text{avg}}$ and $N$ which I seek to verify. Finally, the function $F(z)$ may be defined as

$$F(z) = \left(\frac{4}{\pi}\sum_{k=0}^{\infty}\frac{\sin[(2k+1)\pi x_0]}{2k+1}e^{-(2k+1)^2\pi^2\tau_3 z}\right)^3 \tag{5}$$

For $z = t/\tau_{\text{avg}}$, the survival probability can be expressed as $S(t,N) = F(z)$

# 3 Experimental techniques

## 3.1 Materials

In this experiment I studied the behaviour of 1mm diameter yellow brass ball chains. I cut the chains to the desired length $N$ using a set of pliers, and tied a trefoil knot in its center (note that this corresponds to $x_0 = 1/2$ in equation 1). For this to be easily repeatable, the center beads of each chain were marked with black sharpie. For the yellow brass ball chains used in this experiment, $N_0 = 16$. Figure 1 displays an example of a prepared chain.

Figure 1: A trefoil knot in the yellow brass chain. The knot is tied to its minimum size, with $N_0 = 16$ interior beads. The center of the chain is marked in black sharpie. Note the assymetry of the trefoil: the left arm passes under the loop while the right arm passes over.

The trefoil knot has a fundamental assymetry. One end of the knot must pass under the loop while the other passes over. To easily distinguish which end was which, I also marked the end which was to pass over the loop in black sharpie.

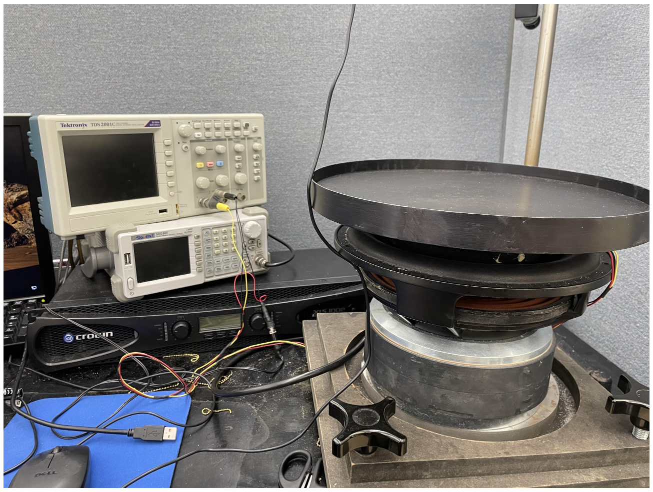

Figure 2: Pictured here is the alluminum shaker plate atop a speaker, driven by the power amplifier and signal generator. Atop the signal generator is the oscilloscope which reads the accelerometer volatge outputs. The accelerometer is located under the shaker plate.

The experimental apparatus, pictured in Figure 2 consisted of an alluminum plate attatched to a magnetically driven speaker, whose oscillations were determined by a signal generator. Attatched to the shaker plate was an accelerometer which sent a voltage proportional to shaker plate's acceleration to an oscilloscope. Since the shaker plate was driven sinusoidally, the accelerometer voltage reading was also proportional to the amplitude of the plate's motion. Thus, the oscilloscope voltage reading could be used as a measure of the plate amplitude.

### 3.2 Methods

For this experiment, it was critical that the chain's motion was random, but not so intense that the knot was allowed to flip or the chain to self-intersect, because such behaviours violate Ben-Naim's assumptions outlined in Section 2. I found that driving the plate at a frequency of $f = 13$Hz and peak to peak amplitude of $A = 840$mV worked well to satisfy these conditions. Although knot flipping and self-intersection was not completely eliminated, these parameters caused it to happen infrequently and also allowed for clear random motion of the chain. Additionally, any trials which saw the knot drift into the wall of the alluminum plate were discarded.

After preparing a length $N$ chain, I placed it on the center of the plate. For each trial, I started the signal generator and began a timer. I stopped the timer when the knot opened (that is, when one of the knot's arms passed through the loop). I then collected the final time. Since there was a lag of about 1 second between the knot opening and my stopping the stopwatch, I tended to overestimate the opening times. This caused a systematic bias which was accounted for in the analysis phase.

For each length of chain, I collected data until $d\tau_{\text{avg}}/\tau_{\text{avg}} \sim 0.1$, where $d\tau_{\text{avg}}$ is the standard error in the mean. This usually took about 30-60 datapoints. I took $40 \leq N \leq 140$ with increments of $20$. The lower bound was chosen based on the fact that $N_0 = 16$.

# 4 Analysis and discussion

## 4.1 Verifying the opening time power law

I performed a least squares fit on my raw data with

$$\tau_{\text{avg}} = \tau_0 (N - N_0)^{\delta} + b \tag{6}$$

for $\delta$ and $\tau_0$. I used the experimental value of $N_0 = 16$. I took $b = 1$s to account for the bias in my raw data where I over estimated the unknotting times. The fit resutled in best fit parameters $\delta = 2.0 \pm 0.1$ and, in combination with equation 4, diffusivity $D = 8 \pm 4\ \text{s}^{-1}$. The result is included in Figure 3.

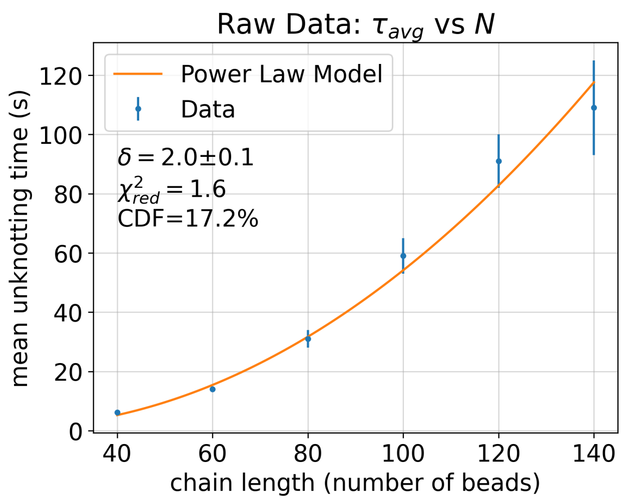


Figure 3: A plot of mean unknotting time vs the chain length. In blue is the raw data while the orange line is the best fit curve of the form of equation 6. The error bars are given by the standard error of the mean time.

To further improve my data, I plotted a histogram for the time distribution for each $N$, with the number of bins given by Sturge's Rule. Figure 4 contains an example of such a histogram for $N = 80$.

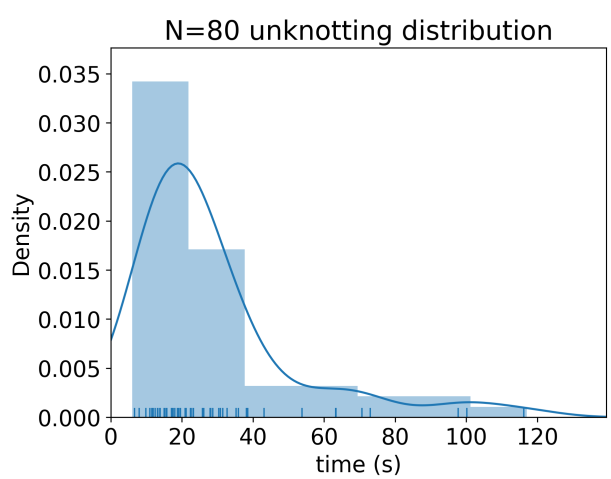


Figure 4: The unknotting time distribution for $N = 80$. A kernel density estimate and rug plot is included. Note that the distribution appears Gaussian, except for a long tail of anomalously long unknotting times.

I then filtered out the data points in each histogram which were anomalously large. The distribution of unknotting times is not Gaussian due to having a lower bound, but no upper bound. By suppressing these high unknotting times, we may get a Gaussian unknotting time distribution and improve the model's results. Furthermore, long unknotting times were typically occured in trials where the knot was flipped over or another intersection point was created. Such trials violate the assumptions outlined in Section 2 and thus cannot be described by the model. The result of fitting the filtered times with equation 6 is included in Figure 5. The cdf and reduced chi squared of this new fit indicatees an improvement of the model's ability to describe the behaviour of filtered data, and the resulting best fit parameters were $\delta = 2.01 \pm 0.07$ and diffusivity $D = 9 \pm 3\ \mathrm{s}^{-1}$. Finally, the knot tended to open towards the arm which passed under the loop with overwhelming frequency.

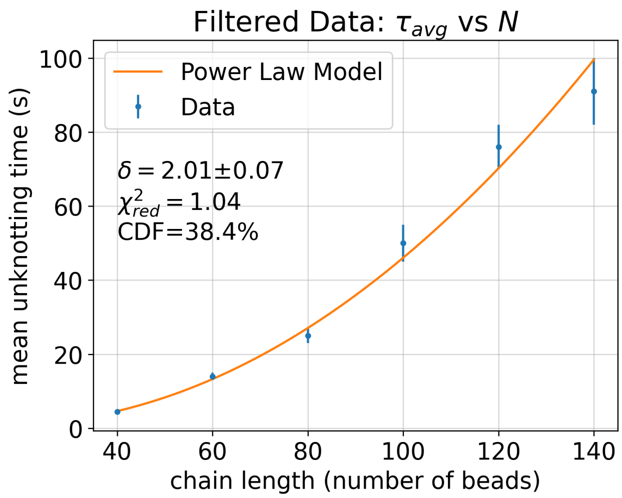


Figure 5: A plot of mean unknotting time vs the chain length. In blue is the filtered data while the orange line is the best fit curve of the form of equation 6.

## 4.2 Analysis of survival probability

Empirically, the survival probability $S(t, N)$ of a knot in a chain of length $N$ at time $t$ can be interpreted as the fraction of unknotting times $\tau$ in a given data set which satisfy $\tau > t$. Plotting this quantity against $t/\tau_{\mathrm{avg}}$ for each data set results in Figure 6.

To find a quanititative measure of the probability that the different survival probability curves come from the same distribution, I used the Komogorov Smirnov test. Given two sample populations, $A$ and $B$, this test returns a p-value for the following null hypothesis: $A$ and $B$ are given by identical distributions. The p-value gives the probability of obtaining the observed results given that the null hypothesis is true.

For each empirical distribution pair, the Komogorov Smirnov test resulted in a p-value of 1.0, meaning my data is exactly what one should expect to see if the null hypothesis is true. That is, each survival probability curve is given by the same distirbution.

By performing the Komogorov Smirnov test on the conglomerate data set and a thoeretical data set, obtained from applying $F(z)$ on all the empirically measured exit times, one arrives at a p-value of 0.367, which suggests a 36.7% chance of obtaining the observed curve if my empirical data set comes from the same distribution as the theoretical data set.

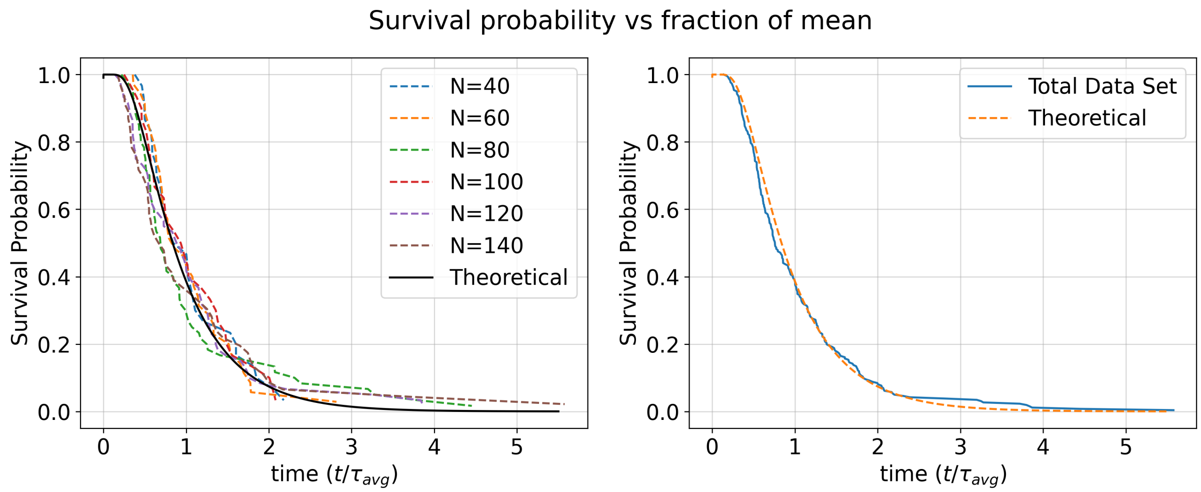


Figure 6: Left: The empirical survival probability $S(t, N)$ plotted against $t/\tau_{\text{avg}}$ for each of the six chain length data sets. Right: The empirical survival probability plotted against $t/\tau_{\text{avg}}$ for the conglomeration of each of the six chain length data sets. The theoretical curve is obtained using equation 5.

## 5 Conclusions

The dynamics of knots in one dimensional filaments are important in determining the macroscopic properties of the materials that these filaments comprise. This experiment was successful in studying a simple analog for such system: a trefoil knot in a macroscopic chain.

My final value of $\delta = 2.01 \pm 0.07$ agrees with equation 4. With a reduced chi squared of 1.04 and goodness of fit probability of 38.4%, I can conclude that Ben-Naim's model accurately predicts the opening times of the trefoil knot as a function of chain length.

The diffusivity $D$ can be interpreted as the knot's hopping rate accross the chain. A hopping rate of $D = 9 \pm 3\ \text{s}^{-1}$ is consistent with the oscillation frequency of $f = 13$ hz, because there was a significant fraction of oscillations where the chain would not hop over any beads.

When plotted against $z = t/\tau_{\text{avg}}$ as in Figure 6, the survival probability of the trefoil knot follows the same characteristic curve for each chain length $N$. This is evidence in favour of the prediction by Ben-Naim et al. (2001) that

$$S(t, N) = F(z)$$

In particular, the Komogorov Smirnov test provides strong evidence that the survival probability curves for each chain length come from the same distribution, as well as a 36.7% chance that my data would be obtained if the survival probability is indeed described by $F(z)$. This result is significant because it suggests that the statistics of trefoil knot opening times can be studied independently of the lengths of the chains in which they are embedded, simply by scaling the time scales by the mean exit time for that corresponding chain length.

## References

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