Knots and topological transformations in vibrating chains: Studying the relationships of the trefoil.*

Utkarsh Mali, John Ladan,† and Stephen Morris‡
Department of Physics, University of Toronto
60 St George St, Toronto, ON M5S 1A7, Canada

(Advanced Physics Lab)
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Objects like deoxyribonucleic acid (DNA) and ribonucleic acid (RNA) often form knots causing them to become entangled. Understanding their behaviour can help develop insight into emergent properties of complex structures. Our experiment aims to study properties associated with bead knotting. We then compare them with known results. In particular, we verify the power law relationship and survival probability. This is done by applying the central limit theorem on approximately Gaussian unknotting distributions. We then use postulate a model for amplitude variation data. After the experimental work, we verify the power law coefficient to be $\delta = 1.86 \pm 0.59$ (dimensionless units), this matches experimental predictions made by the Ben-Naim group $\delta_{BN} = 1.95 \pm 0.07$. The time-scaling factor was found to be $t_o = 0.0116 \pm 1.1 \times 10^{-5}$s. Subsequently, survival probability was also found to match known results. Finally, after attempting functional and distributive approaches, we fit a new model to amplitude variation data using the polynomial method. There is scope for more work on model selection. Understanding the role of these knots provides insight into complex structures such as DNA, RNA and polymers. Ultimately, studying the behavior of such vibrations will benefit the broader scientific community.

I. INTRODUCTION

The study of knots and braids have shown to provide deep insights into many physical systems. Knot theory is the mathematical study of the knots using both geometry and statistical methods [1]. Its study has lead to the development of many useful practical applications in biological science, physical chemistry and applied physics [2–5]

Understanding the nature of these behaviours is critical in understanding the underlying physics of the interactions. Understanding knot theory is important to the scientific community as it will open new avenues of research in many other fields. Typical knot systems, however, tend to be complex. In order to apply rigorous quantitative analysis, simplifications to the system are required. This will allow us to study these methods in greater detail.

Our goal in this experiment is to simplify a knotting system and apply statistical methods to study the knot properties, comparing them with known experimental results. We do this by using a pre-determined bead size of a known length and mass to represent a knotting string. We then apply a uniform known oscillation with a measurable acceleration, we expect that the string will unravel its knot. We then directly observe the behaviour and confirm observations with known laws from the literature [1].

Our first aim is to experimentally verify the power law and survival probabilities as measured in the literature [2, 6]. This is typically achieved by measuring the unknotting time. We then explore the relationship between the oscillation amplitude and the time taken to unknot. As a byproduct, we aim to search for the resonant frequency of the oscillations of the bead. Finally we explore the role of the average error propagation as a function of the number of times the knot flipped while vibrating.

II. METHODOLOGY

A. Experimental Setup

The experimental setup consists of an oscillating platform, an accelerometer and a power source. The power source and accelerometer are connected to an oscilloscope which displays both input and measured voltage. The oscillating platform is an aluminium plate driven by a SP10 sub-woofer speaker through the power amplifier. It has a smooth metallic plate which is slightly curved inwards to keep the beads at a central position. It is placed directly on the oscillating platform which drives the plate. A signal is sent from the signal generator through the amplifier to the sub-woofer. This causes vertical oscillations [7]. An accelerometer,a MMA 1220 Low G micro machined developed by Freescale Semiconductors, is connected to the sub-woofer which measures the realized oscillation amplitude. It is placed under the plate in an inverted position. It measures the acceleration as an output voltage which scales linearly with plate acceleration. The voltage that is measured which directly corresponds

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* An experiment from the Advanced Physics Undergraduate Lab
† Teaching Assistant
‡ Principal Investigator

to the acceleration of the plate. The beads were prepared from a yellow brass composite with a diameter of 2.4mm. The sole type of knot used in this experiment was the trefoil knot, the simplest known knot. During the experiment, oscillation frequencies vary from 10Hz to 20Hz. Outside of these values consistent unknotting was not observed.

B. Experimental Procedure

First, beads of fixed lengths were prepared. The diameter, composition and mass were all fixed. A wide range of lengths were needed to verify the power law relationship. The oscillation frequency was set to 15Hz, the tightest knot possible was 13 beads long $N_o = 13$, the thickness of the beads was measured to be $2.39mm \pm 0.02$, the driving amplitude was set at 3 volts (peak-peak) which corresponded to an accelerometer reading of $1.16V \pm 0.04$. When the bead strings were placed on the oscillating surface, the knots were always set to have a left skew (the left portion of the knot goes under the knot while the right potion of the know goes over the knot).

C. Data Measurements

In all our data, we measure the time taken for the trefoil knot to unknot. This measured time varies greatly. In order to approach the true time taken for a sample to unknot, we must take multiple measurements and then apply the central limit theorem (CLT). Applying central limit theorem would allow us to assume a Gaussian-distribution to the data which would allow us to easily measure its mean. By doing this, we assume that each drop is independent and identically distributed (idd). Studies have shown that a minimum sample size of 20-30 is required for the data distribution to be approximately Gaussian [8]. Following this we can find the average time taken to unknot.

$$t_{avg} = \frac{1}{N} \sum_{i=1}^{N} t_i \tag{1}$$

This can be used to measure the variance associated with the unknotting time.

$$\sigma_t = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left(t_i - t_{\text{avg}}\right)^2} \tag{2}$$

Since we assume the distribution is Gaussian distributed through the CLT, we are able to find the average mean uncertainty.

$$\sigma_{avg} = \frac{\sigma_t}{\sqrt{N}} \tag{3}$$

This will be used in all sections of the experiment to set error bounds on the unknotting time measurements. Henceforth a *measurement* will be assumed to be taking the mean value of 20-30 sample points.

D. Power Law

The first aim of this experiment was to verify the power law relationship. This relationship relates the length of the chain and the length of its tightest knot possible with the average time taken to unknot. It is one of the key results of knot theory and has been tested in many studies.

$$t_{avg} = t_o (N - N_o)^{\delta} \tag{4}$$

Here we define t_o a constant with dimension of time, and δ as a dimensionless constant. The former acts as a scaling factor while the latter represents the power-law relationship factor. In order to verify this relationship measurements were taken at varying lengths $N \in \{41, 51, 61, 71, 85, 124\}$. Both the number of flips and the bias direction of unknotting were also measured. In post-processing, we aim to apply a fitting function to derive the values of t_o and δ and compare them to known values [5].

E. Survival Probability

The survival probability represents the cumulative probability that a knot is likely to stay knotted or "survive". Recent literature has shown that the relationship between a specific length knot and its survival probability can be generalized by a scaling factor[4]. This can be formalized through an equation.

$$S(t, N) = F(z), z = \frac{t}{\tau} \tag{5}$$

The equation above implies that the scaling of every measurement taken from the power-law data should represent an identical curve under the universal scaling constant. This will be tested and further compared with known values.

F. Amplitude Relationship

The relationship between the amplitude of oscillations and the variation of unknotting time is one that has not been deeply studied. As the amplitude of oscillations increases, the acceleration of the plate increases. This increases the force applied to the bead while it is in contact with the surface of the plate. Here, the length of the beads are fixed to $N = 53$. The acceleration is the oscillation frequency of the plate with gravity. Since the oscilloscope is delivering a sinusoidal frequency of oscillation, we expect a sine dependence in the acceleration

[7].

$$A(t) = \frac{c\omega^2}{g} \sin t \tag{6}$$

The maximum amplitude of oscillation occurs when the phase ($\sin t$) maximizes A(t).

$$A_{max} = \frac{c\omega^2}{g} \tag{7}$$

This is directly measured from the inverted accelerometer. The inversion results in the gravity acting on the negative scale. As this is identical for all measurements, it will not be included in the analysis. The experimental aim is to develop a model that well encapsulates the data measured. This can then be used by other groups as prior information for subsequent work.

G. Error Relationship

The final goal of this experiment is to determine the relationship between the number of flips observed and the average central limit theorem variance associated with them. It is expected that the error should increase with the number of flips observed.

III. RESULTS

The first measurements were aimed at determining the relationship between number of beads and unknotting time. In, particular fitting the power law relationship.

Length (N)	t_{avg}	σ_{avg}	Num Trials
41	6.23	0.7	30
51	11.87	1.2	30
61	13.95	1.0	30
71	21.46	1.6	30
85	34.87	5.6	30
124	73.55	16.4	30

TABLE I. Tabular representation of relationship between varying length and time taken to unknot. An increase in bead length corresponds to an increase in unknotting time. There was a general upward trend in measurement variance with increase in length.

After numerical fitting, the parameters of the power law were estimated.

$$\delta = 1.86 \pm 0.59. \text{ (unitless)}$$
$$t_o = 0.0116 \pm 1.13 \times 10^{-5} \text{ (seconds)}$$

These values can be represented graphically using the power-law and data measured.

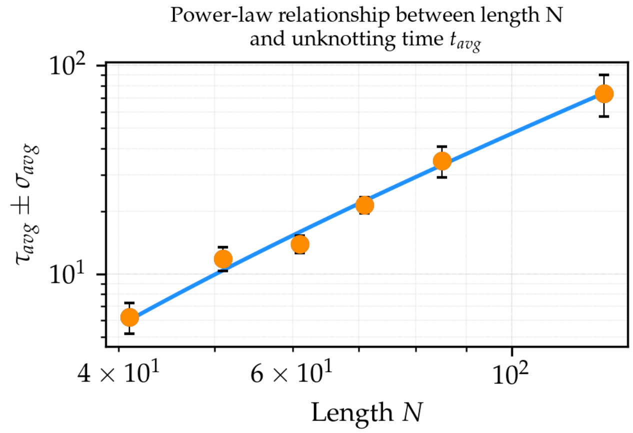

FIG. 1. Power-law relationship between number of beads and unknotting time. The relationship is linear in log-space. This matches theoretical expectations. The errors, while small were non-negligible for the longest bead length. They were measured to be the quadrature sum of the experimental variance with the power law fit.

We use the same data to compute both the survival probabilities $S(t, N)$ and the scaling factor. This is done according to section II E.

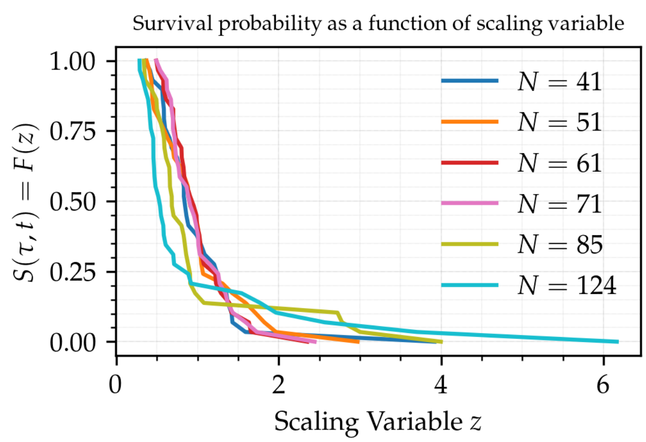

FIG. 2. Graphical representation of the probability that a knot survives as a function of scaling variable which is a function of time. Most curves follow a representative curve matching theoretical expectations.

The values of survival probability can be directly compared with other works [5]. There is good agreement between cites works and ours.

The second set of measurements vary the amplitude of oscillations (through acceleration) and measures the change in time taken to unknot. The goal of this section was to devise a model which succinctly describes the behaviour that can be used in future studies. The results can be seen in the table below.

Amplitude (V)	t_{avg}	σ_{avg}	Num Trials
1.16	11.14	1.0	20
1.34	14.62	2.1	20
1.48	22.55	3.7	20
1.64	19.30	2.5	20
1.76	17.28	2.4	20

TABLE II. Tabular representation of the relationship between the amplitude/acceleration of the plate and the average time taken to unknot. Fewer trials were taken as the data was already observed to look approximately Gaussian.

The results above were then used to generate potential models which would succinctly describe the amplitude behaviour. First, a Poisson distribution was used attempting to well represent the data. This however, could not be done due to the integer requirement of the factorial function in the distribution. Following this, a generalized Beta distribution was attempted. This would eliminate the factorial and allow floats. This requires a (0,1) normalization. However, the value of gamma in the beta distribution was un-normalizeable. The third approach was to use a functional skewed Gaussian of the following form. $t_{avg} = a(x-c)e^{-b(x-d)}$. While this attempt was able to give a model fit to the data, the results were clearly under fitted. This lead to the final approach of using a polynomial fit. This can be seen below.

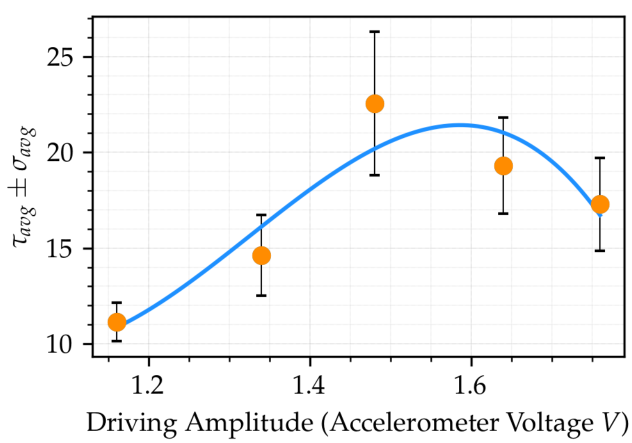

FIG. 3. Graphical representation of the relationship between the driving amplitude measured by the accelerometer and the average unknotting time.

The slightly larger error bars are associated with fewer trials taken before analysis. As before, the bias and flips were measured but have been omitted from the analysis. The final values of the 3rd degree polynomial were as follows.

$$t_{avg}(x) = 646x^3 + -823x^2 + 349x - 162 \tag{8}$$

This equation is unlikely to generalize. It does, however, fit the constraints of our model well.

The final section of analysis involves the average error associated with each measurement as a function of the number of flips taken. This was initially not an experiment objective but quickly became one once the group observed that the amount of flips tends to affect the unknotting time. This was formalized through root mean squared error analysis. $\frac{1}{N}\sqrt{\sum_{i=o}^{N}(x_i-\mu)^2}$. Below, the root mean squared error is plotted as a function of the number of flips.

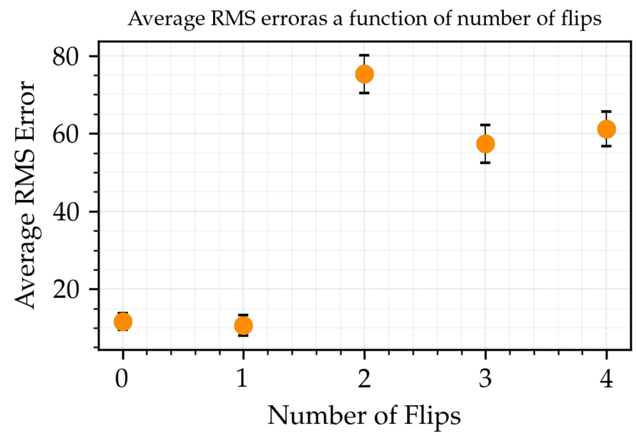

FIG. 4. Graphical representation of the relationship between the mean squared errors of each measurement and the number of times a specific data sample flipped. As expected, the errors increased with the flip frequency.

The root mean squared errors were computed between individual data points and their mean. This was then sorted by number of flips. This was done in order to preserve the scale of an error for each data point, otherwise larger length errors will dominate the data.

IV. DISCUSSION

The results clearly indicate that the behaviour of the beads matched the theoretical predictions. This includes the power-law relationship, survival probability. Furthermore, the results also indicate scope for developing new models, such as the amplitude to unknotting time dependence and the error as a function of flips relationship.

Firstly, the power law dependence was found to power parameter $\delta = 1.86 \pm 0.59$. Recent literature has computed this value to be $\delta_{BN} = 1.95 \pm 0.07$ [5]. The matching values indicate that the power-law relationship was successfully predicted. Furthermore, the straight line in Figure 1 represents a power scale relationship. The error bars observed arise from combining both the systematic uncertainty with the statistical uncertainty. Most points lie withing 1σ or 68% difference to the mean. The longer the string the longer the knot needs to travel before it un-knots itself.

Following this, we examine the survival probabilities associated with the length-unknotting time measurements. Our computed values of $S(t, N)$ represent the probability of the bead string being knotted. Our data seen in Figure 2 matches previous work [6]. While the values of the scaling factor typically end at 3. Our group measured readings varying from 2.3 to 6 with the typical value being 3. This matches the theoretical predictions. In conclusion, the beads length does not affect its survival probability $S(t, N)$. This factor will ultimately allow us to use collect multiple measurements for a single analysis decreasing the variance.

The third relationship studies the amplitude dependence on the unknotting time. It was observed that as the amplitude increased, so did the unknotting time. However, once the driving amplitude was set beyond 3.5V, the unknotting time started to decrease again. Our group expected a strictly decreasing amount of time taken with amplitude of oscillations. At very low amplitudes the beads were found to oscillate just enough to unknot quickly. As the amplitude of oscillations increased, the beads had enough time to shift both towards and away from unknotting. This increased the average time taken to unknot. Ultimately, the beads were vibrating rapidly. This resulted in the knots shifting multiple beads at a time which increased the rate of unknotting. This behaviour represents the sharp drop in unknotting time at large oscillations. Our model is over fit and will be difficult to generalize. This is due to the restrictive nature of the polynomial function. More work is needed to understanding this behaviour better. As a physical example, certain frequencies might promote polymer generation or DNA disentanglement.

The final source of analysis studied the errors on each measurement. The increasing errors as a function of flips represent the extra distance traveled by a single knot once it flips. As a simple example, a knot might be at the end of a bead-string (thus about to unknot), however, once a flip occurs the knot would have to traverse the entire length of the bead-string. As a result one would expect a larger error with an increased number of flips. This was confirmed through observation and analysis. Larger values of flips result in larger error bars since they are less likely to occur, as a result, there are fewer data points containing them. The implication of this suggests that rare events could occur in which polymers or DNA takes substantially large amount of time to unknot. The uncertainty associated with this will increase with complexity.

V. CONCLUSION

The ultimate goal of the experiment was to explore the relationship between unknotting time of beads and other dependent factors such as bead-length and oscillation amplitude. The central limit theorem was used to collapse highly variable data into measurable data with known variance. The power-law relationship was verified with the power parameter measured to be $\delta = 1.86 \pm 0.59$ (dimensionless) matching previous literature in which $\delta = 1.95 \pm 0.07$. Following this, the cumulative probability of a sample survival $S(t, N)$ was found to be consistent with theoretical models. Subsequently, a model for the amplitude-unknotting time relationship was derived fitting our data, but is unlikely to generalize well. More work is needed in this region. Finally, the errors associated with each measurement were compared against the number of times a flip was observed in the data. High flip frequencies corresponded to a larger root-mean-squared error suggesting. Our analysis confirms work done by academic peers [5]. This opens new avenues of research for future work. It has important significance to both biological and chemical systems.

[1] K. Murasugi, Knot theory and its applications (Academic, Boston, 1996).

[2] K. Koniaris and M. Muthukumar, Knottedness in ring polymers, Phys. Rev. Lett. **66**, 2211 (1991).

[3] S. W. Smith, C. K. Hall, and B. D. Freeman, Molecular dynamics study of entangled hard-chain fluids, The Journal of chemical physics **104**, 5616 (1996).

[4] S. R. Quake, Topological effects of knots in polymers, Phys. Rev. Lett. **73**, 3317 (1994).

[5] E. Ben-Naim, G. S. Grest, T. A. Witten, and A. R. C. Baljon, Individual entanglements in a simulated polymer melt, Phys. Rev. E **53**, 1816 (1996).

[6] E. Ben-Naim, Z. A. Daya, P. Vorobieff, and R. E. Ecke, Knots and random walks in vibrated granular chains, Phys. Rev. Lett. **86**, 1414 (2001).

[7] J. H. David Bailey, N. Krasnopolskaia and S. Satar, Advanced undergraduate laboratory: Knots, University of Toronto Public (2015).

[8] S. G. Kwak and J. H. Kim, Central limit theorem: the cornerstone of modern statistics, Korean journal of anesthesiology **70**, 144 (2017).