

ADVANCED UNDERGRADUATE LABORATORY

KNOTS

Knots and topological transformations in vibrating chains

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Introduction

String-like objects such as DNA, RNA, or polymer macromolecules often form knots or otherwise become entangled. The thermal motion and vibration of such molecules can untie existing knots or cause new knots to form. Such processes help determine the macroscopic properties of materials such as gels and plastics, and can have dramatic effects at the microscopic level, e.g. a knotted DNA molecule cannot replicate, preventing cell division in both normal and cancerous cells. Understanding these knotting processes is crucial in understanding many biophysical processes¹ or the structural properties of many materials, but it is very difficult to study these processes directly.

In this experiment you will study the dynamics of knots in granular chains vibrating on a plate. The vibrating metal plate can be driven at varying frequencies and amplitudes, and various chains (the type used to hold drain plugs) are also provided. Using this equipment you may explore how the unknotting time (τ) of the chain depends on different parameters such as:

- Length of chain
- Frequency of vibration
- Amplitude of the plate
- Mass of chain
- Number of knots
- Type of knot

You may also examine the statistics of the unknotting process, and other aspects of the shaker and its dynamical relation with a chain on its surface. In addition to unknotting, it is also possible to study the formation of knots. For both knotting and unknotting, you may compare your experimental results with the predictions of theoretical models.

Spiral formation, structure and dynamics can be also be studied with the same chains as a function of the driving frequency and amplitude.

As the fundamental equipment in this experiment is very simple and easy to use, the challenge is in the planning and analysis stages. Feel free to use your imagination, explore ideas of your own, or focus your efforts on doing one part very well.

Knot Theory

Mathematical knot theory defines a knot as a closed curve in space that does not intersect itself. Nontrivial knots of one-dimensional objects only exist in three spatial dimensions, which may in fact explain why our universe actually has three dimensions.²

In our experiment, we use notation of the knots theory keeping in mind that our knots belong to an open curve created by a ball-chain. Knots are denoted as C_k where C is the minimal number of self-crossings displayed when the knot is projected into a plane, and k a cardinal index used to distinguish between topologically different knots with the same C . The simplest knot with three intersections, or trefoil, is



Figure 1: Trefoil (or $C_k=31$) knot.

denoted as 31; the knot with five intersections is denoted as 51, and so on. Bao, Lee & Quake³ report tying several such complex knots into DNA molecules with optical tweezers and then watching the process of unknotting. [There is an “Optical tweezers” experiment in the Advanced Physics Lab].

The ball chain in our experiment consists of hollow metal spheres connected through rods that can be treated as chemical bonds. Two adjacent beads can freely slide along the connective rod coming in touch with each other or becoming separated by the distance equal to the rod length. The interaction of the chain as it is vibrating on a metal plate is largely due to the kinetic energy of its random motion. Such diffusive behaviour is particularly characteristic of particles that have high random velocities (e.g. air). The beads interact via a hard-core repulsion, with the rods acting as dissipative non-linear springs. The beads and the plate interact via dissipative inelastic collisions, which implies that the kinetic energy of the chain is not conserved, and it is only motion of the plate that keeps the system in continuous motion. Ben-Naim *et al.*⁴ suggest that unknotting is a kind of diffusive process in which the chain crossings move in a random walk. The chain is said to become unknotted when the number of crossings goes from 3 to 2 (see Figure 2). For one knot in the center of a chain, the average unknotting time (τ_{avg}) may be related to the length of the chain (parameterized by N) by a power-law of the form:

$$\tau_{avg} = \tau_0(N - N_0)^\delta \tag{1}$$

where N is the number of beads in the chain, N_0 is the minimum number of beads contained in a knot (a constant), τ_0 is a constant with dimensions of time, and δ is a dimensionless constant. In this model, the ratio of the standard deviation to the average unknotting times is constant independent of the chain length, with a value of 0.63047 for a trefoil knot.

If the crossing points within a knot random walk along the length of the chain, their average displacement may be expected to grow in proportion to the square root of the number of steps. If the number of steps increases linearly with time, and the distance a crossing point must travel to untie the knot is proportional to $N - N_0$, you might expect $\delta = 2$.

Apparatus

The shaker is an aluminium plate securely attached to a magnetically driven SP10 Sub-Woofers speaker, driven by a signal/frequency generator through a power amplifier. The plate is anodized to create a deep black background for obtaining good images of chains on the plate. The signal generator sends a (normally sinusoidal) voltage through the amplifier to the speaker, causing the plate to oscillate vertically.

After being in use for some time, it was realized that the original black plate has different coefficients of restitution at different locations. This can be seen by comparing how high a ball bearing bounces when dropped from the same height near the centre and the edge of the black plate. This may affect how the chains bounce, so several bare (gray, unanodized) aluminium disks were machined to just fit into the shaker plates. These make the coefficient of restitution much more uniform, at the cost of reducing the dynamic range accessible since the extra mass of the disks reduces the maximum shaking



Figure 2: Trefoil knot just after unknotting.

amplitude. In addition, the top surfaces of these disks have a gentle spherical concave surface that keeps the chain near the centre of the disk, eliminating problems caused when the chain migrates to the edge of the plate and the outer wall interferes with the unknotting process. (Note: 1 of the 3 available plates is disks on both surfaces.) When using these plates, **DO NOT USE DOUBLE-SIDED TAPE OR GLUE TO ATTACH THE ALUMINUM DISKS TO THE BLACK SURFACE**. A few cubic centimetres of water poured onto the black surface before inserting the concave plate (flat side down) will hold the plate quite adequately. (You may wish to calculate the total force due to air pressure holding the bare plate to the black surface.) The plate can easily be removed by pulling up on one side to let some air in under the plate.

An MMA 1220 accelerometer is attached to the bottom of the plate; the acceleration of the plate is proportional to the accelerometer output voltage which can be measured with an oscilloscope. The sensitivity of accelerometer can be found in the MMA 1220 accelerometer specifications available on the Knots experiment webpage. This accelerometer should be used to ensure that the peak acceleration is constant for a series of unknotting measurements, and also provides the information for studying how unknotting depends on acceleration.

Basic measurements of unknotting times are most quickly made using a stop-watch. Two devices are also available to record images and video: A Logitech webcam and Casio EX-FC100 digital camera that can record up to 1000 frames per second (fps) in a video mode. To watch images taken by Logitech camera, click on the desktop icon “Knots Experiment”. Choose the option Webcam Gallery and click a “Take Photo/Video” button. You will see an image taken by the Logitech digital camera. You may choose Photo or Video option to the left. The Casio high-speed camera requires good illumination of the chain on the plate, so you will perhaps need to add lights; videos taken at greater than 240 fps are not likely to be useful.

Safety Reminders

- Do not stick your fingers or other objects inside the moving parts of the sub-woofer.
- Do not touch the sub-woofer power connectors when the amplifier is on.
- Turn down the power level before switching on the power amplifier, to avoid potential damage to you or the shaker. Immediately turn down or turn off the amplifier if the shaker starts making loud or unusual noises or movements.
- You **must** consult with the supervising professor **before** vibrating **any** material. (e.g. liquid nitrogen, sugar, baby powder, ...) that is not provided with the experiment.

NOTE: This is not a complete list of all hazards; we cannot warn against every possible dangerous stupidity, e.g. opening plugged-in electrical equipment, juggling cryostats, Experimenters must constantly use common sense to assess and avoid risks, e.g. if you spill liquid on the floor it will become slippery, sharp edges may cut you, If you are unsure whether something is safe, ask the supervising professor, the lab technologist, or the lab coordinator. If an accident or incident happens, you must let us know. More safety information is available at <http://www.ehs.utoronto.ca/resources.htm>.

Basic Experiment

You should measure δ for at least one set of experimental conditions with a trefoil (i.e. 31) knot. Use a number of chains of same material and bead size, but of different lengths. A good first choice is a

yellow brass (YB) chain with 2.4 mm diameter beads. The knot must be initially at the middle of the chain!

A bouncing ball on a vertically oscillating plate will change from periodic to chaotic behaviour, depending on the frequency and amplitude of the plate vibrations,⁵ so one should expect the dynamics of the bouncing chain to depend on the frequency and amplitude of the shaker. The shaker itself has natural resonant frequencies (~20 Hz), and all does not generate perfect sinusoidal oscillations at low frequencies (~10 Hz) or large driving amplitudes. The speed and randomness of the crossing-point movements may depend non-trivially on the frequency and amplitude. To find suitable conditions for unknotting, make several test measurements of unknotting time of several chains for frequencies in range 11Hz – 19 Hz that appear to produce random motion of the chain.

The two ends of a chain in a trefoil knot lying on the plate are not symmetric, i.e. one passes over a loop and the other passes under a loop (See Figure 1). This asymmetry, or possible intrinsic asymmetry in the manufacture of the chain, may cause the movement of the different crossing points to be asymmetric or otherwise differ. It is worth noting any characteristics of the unknotting process that might reveal such asymmetries, e.g. recording which end unknots (in Figure 2, the unknotting occurred at the end that had passed on top of the loop).

In addition to studying measuring the dependence of the mean unknotting time on chain length, also examine the survival probability S_3 for the trefoil as discussed by Ben-Naim et al.⁴, and describe qualitatively how the details of unknotting process is affected by the various experimental conditions.

Once you have analyzed this first basic set of unknotting measurements, **you are expected to pursue one or more of the Options listed later in this write-up**, or follow an idea of your own devising.

Data Analysis

The unknotting process is a random one, meaning that the unknotting time varies from measurement to measurement, even for the same chain under exactly the same conditions. Assume that for a single set of experimental conditions such as chain length, frequency, etc., you take M measurements of unknotting time, which you call τ_j , where $j=1$ to M . The average unknotting time is

$$\tau_{avg} = \frac{1}{M} \sum_{j=1}^M \tau_j \quad (2)$$

and the standard deviation is

$$\sigma_\tau = \sqrt{\frac{1}{M} \sum_{j=1}^M (\tau_j - \tau_{avg})^2} \quad (3)$$

If the unknotting time distribution were Gaussian, for each measurement you would expect the observed unknotting time to be between $(\tau_{avg} + \sigma_\tau)$ and $(\tau_{avg} - \sigma_\tau)$ 68% of the time (see Bevington and Robinson Chapter 3)⁶. The distribution of individual unknotting times is, however, not expected to be Gaussian, but to have a median unknotting time less than the average. Qualitatively this is simply because the standard deviation is a large fraction of the mean, and there is a lower limit on the unknotting time but no upper limit.

Even if the individual measurements have a non-Gaussian distribution, as long as this distribution has a finite mean and standard deviation then by the Central Limit Theorem⁷ the variation of the average of many individual measurements should be close to Gaussian. The error or uncertainty on the average (σ_{avg}) will be less than the standard deviation (σ_{τ}) of individual measurements. If σ_{τ} is assumed to be a constant for every measurement, the uncertainty in the mean is

$$\sigma_{avg} = \frac{\sigma_{\tau}}{\sqrt{M}} \tag{4}$$

Therefore, as you increase the number of measurements, M, your measurement of the average unknotting time, $\tau_{avg} \pm \sigma_{avg}$ becomes more precise.

Options: You are expected to pursue one or more of the following Options, or follow an idea of your own devising.

Option 1: How universal is the model?

How good is the model of Ben-Naim¹ at describing the unknotting of all chains? As time permits, measure the unknotting of a variety of sets of different types of chains, e.g. sets with other bead sizes, materials, or knots and measure τ_{avg} for each chain of the set. For other knot types, e.g. the Ck=51 knot shown in Figure 3 or a simple CK=11 crossing of Figure 4, you can use/modify python programs available on experiment web page to calculate the survival probabilities from Ben-Naim formulas (3) and (4) or by Monte Carlo simulation.

Can you verify or disprove the claim of Ben-Naim et al that “knot survival probability follows a universal scaling function which is independent of chain length” and kind of a knot in the middle of a chain? Does it fail in extreme cases, e.g. for very short or very long chains?

Number of Knots

You may wish to explore what happens if more than one simple knot, side-by-side, is used. For multiple knots, how does average unknotting time vary with number of knots? Do you expect the Ben-Naim model to apply?

Option 2: Other Knotting Investigations

Frequency

You may examine how the unknotting time varies with respect to changes in frequency while other parameters are fixed. Try to see what are the maximum and minimum frequency limits that will generate unknotting. Some possible questions are

- How does the mean unknotting time and standard deviation vary with frequency?
- How would you describe the movement of the knot when outside the frequencies where unknotting occurs?

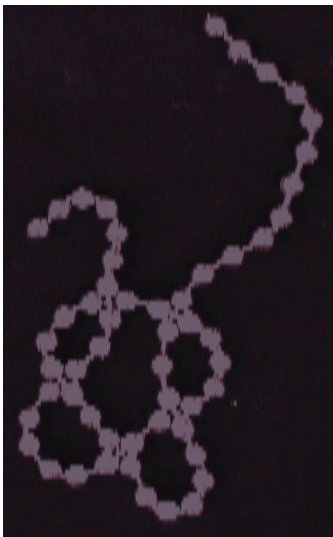


Figure 3: Ck=51 knot.



Figure 4: The simplest “knot”: a single crossing (or Ck=11) knot.

- Do your results depend on the size of the individual beads?

Amplitude, Mass

Similar investigations are possible for the variation of unknotting time with respect to the amplitude of oscillation of the plate and the linear density of the chain.

- Chains of different individual bead masses are provided. How does bead mass relate to unknotting time? What about chain density, in grams per centimetre? Does the difference in spacing between beads influence unknotting time?
- As the amplitude of shaking increases, how is unknotting time affected? Is the amplitude best parameterized in terms of distance the plate travels, plate speed or plate acceleration? All of these relate to frequency in different ways. For example, if A is the distance amplitude of the plate's motion, and the plate moves up and down in a sine-wave pattern (does it?) then the maximum speed is $A \cdot \omega$ and the maximum acceleration is $A \cdot \omega^2$.

Adding a long-range potential

The configurations of polymers in solvents are affected by long-range forces between the polymer strands. Similar forces can be created for a beaded-chain by the surface tension of a thin layer of water on the plate.⁸ How do such forces affect the unknotting time? How does the effect depend on the thickness of the layer of water?

Knotting (re-knotting)

A vibrated unknotted chain may sometimes form a knot spontaneously. Knotting times are much, much longer than unknotting times, so the number of observations you can make is likely to be small or even just one. Try to follow the experiment conditions and use a similar chain as reported by Hickford,⁹ As soon as the knot appears, the process of unknotting starts, so in order not to miss the small lifetime of the knot, you should take video while observing the knotting chain. Compare your results with those presented in diagrams 2, 3 and 5 of Hickford. Can you draw a diagram like Fig.3 of the reference?

Other questions

- It may have been assumed that number of beads in the chain is a better parameter than the physical length in centimetres. Is this true? How do measured parameters such as τ_0 and δ differ if you use the chain length outside the knot ($x-x_0$) rather than number of beads outside the knot, $(N-N_0)$?
- Once you have explored the parameters that you found interesting, is it possible to link them all together and make a general "formula" for the unknotting time?

Option 3: Radius of Gyration of an Unknotted Chain

When studying DNA and other polymers, it important to know how much space a strand takes up at various times. The radius of gyration is one way of parameterizing the "size" of a chain. It is a scalar quantity with units of length, defined as

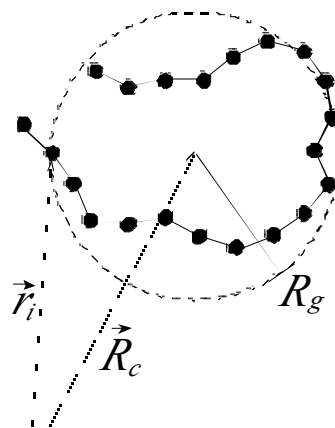


Figure 5: Graphical definition of quantities used in determining radius of gyration, R_g .

$$R_g = \sqrt{\frac{1}{N} \sum_{i=1}^N (\vec{r}_i - \vec{R}_c)^2} \quad (5)$$

where N is the number of beads in the chain, and each bead is specified by an integer, i (see Figure 5.)

To find the vector position of center of gravity R_c , simply take some reference point as an origin and draw vectors to each bead, the average of these over N will give you the center of gravity.

$$\vec{R}_c = \frac{1}{N} \sum_{i=1}^N \vec{r}_i \quad (6)$$

On the course website there is RealTime_ROG Python code (http://www.physics.utoronto.ca/~phy326/knot/RealTime_ROG.zip) that allows you to use a webcam to measure the radius of gyration of a light-coloured chain against a dark, circular background in real time. Plotting the radius of gyration for different configurations versus will show you how the radius of gyration changes over time. The maximum radius of gyration is when the chain is in a perfectly straight line, in which case it can be shown that $R_{g,\max} = \frac{L}{2\sqrt{3}}$, where L is the length of the chain. Does the radius of gyration of a chain approach a certain value of $R_g/R_{g,\max}$? If so, how does this value depend on the various physical properties of the chain and shaking process?

Option 4: Dynamics of the plate and spontaneous spirals

There is an accelerometer attached to the fluid shaker, which allows you to measure the instantaneous acceleration of the plate, or plot it versus time on the oscilloscope. The basic function of the accelerometer is to produce an output voltage that is proportional to the acceleration.

- How do parameters such as τ_0 and δ vary with acceleration?
- What is the nature of the motion of the plate? Does it match the shape of the input signal? Can the plate respond accurately to a non-sinusoidal signal, e.g. square or sawtooth?
- Is there a phase shift between the oscillation of the plate and the input signal? What causes this?
- Compute a calibration for the accelerometer by measuring the physical distance amplitude for sinusoidal motion.
- Ecke *et al.*¹⁰ report that sufficiently long chains spontaneously organize into spirals for narrow range of accelerations and frequencies. Can you reproduce their “spontaneous spirals”? Edge effects can be a challenge.

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