

- Notes from APL Lab Manual

### Knot Theory

- A knot is a closed curve in space w/ no self intersections
- Trivial knot: a loop  $\rightarrow \text{---}$
- Non-trivial knots of one dimensional objects exist only in 3D
- Knots are denoted as  $C_k$

$C$  = minimum number of intersections when projecting knot onto a plane

$k_C$  = a cardinal number to distinguish between topologically different knots w/ the same  $C$

- In the experiment, we use a ball chain of hollow spheres connected by rods
- These can be treated as chemical bonds
- The balls are free to slide along the rods
- The chain displays diffuse behaviour while vibrating on the metal plate due to its random motion

- The chain is said to become uncrossed when the number of crossings goes from 3 to  $\geq 2$
- For a knot in the center of the chain, the average unknotting time is

$$T_{\text{avg}} = T_0 (N - N_0)^5$$

number of beads on  $\rightarrow$   $\leftarrow$  min number of beads in knot (const.)

- Basic Experiment
- Measure  $\delta$  for at least one set of experimental conditions w/ a trefoil (31) knot
- Use chains of same material & bead size, but different lengths
- Knot initially in middle of chain
- First choice: yellow brass chain w/ 2.4 mm bead diameter beads
- The dynamics of the boundary balls can vary from periodic to chaotic depending on freq./ amplitude of shaker
- Shaker has resonant freq.  $\approx 20$  Hz
- Cannot do sinusoidal motion for  $< 10$  Hz or large frequencies
- To find suitable conditions, look for a freq. 11-19 Hz that produces random chain motion
- Trefoil knot is asymmetric: one end passes under a loop and one end passes over
- This may cause the motion of the crossing points to be asymmetric. Note which end unknots each time
- Also examine ~~the~~ survival probability S3 from Ben-Naim et. al. and describe qualitatively how the unknottting process is affected by experimental conditions

- The survival probability of a knot is the probability that the knot still exists at time  $t$ , denoted by  $S(t, N)$
  - The exit time distribution is
- $$R(t, N) = -\frac{d}{dt} S(t, N)$$
- and  $T = \int dt t R(t, N)$
- Ben-Naim suggests that  $S(t, N) = f(z)$  w/  $z = t/T$
  - I'll have to read more about this later
  - I don't know how to measure this

### Data Analysis

- The motion should be random so we should take multiple ~~more~~ trials of for each length. For  $M$  trials,

$$\bar{T}_{\text{avg}} = \frac{1}{M} \sum_{j=1}^M T_{jN}$$

$$\sigma_T = \sqrt{\frac{1}{M} \sum_{j=1}^M (T_j - \bar{T}_{\text{avg}})^2}$$

- The uncertainty in the mean is

$$\sigma_{\text{avg}} = \frac{\sigma_T}{\sqrt{M}}$$

Fr., March 10

### Equipment

- The apparatus is an aluminum plate attached to a magnetically driven speaker, driven by a signal generator
- Generates sinusoidal oscillation
- Accelerometer at bottom of plate, accel. proportional to plate output voltage, measured by oscilloscope
- Make sure max accel. is constant

- Showed up and identified equipment
- Showed, speaker, signal generator, oscilloscope

- Turned on oscilloscope & freq generator, set freq. to 11 Hz. Left amp at 4 Vpp?

- Turned on speaker
- Started oscillating

→ Vpp is the peak-to-peak amplitude

- Oscilloscope varies from sinusoidal to just noise
- Do the speaker vol. knobs do anything?
- Two channels on speaker

- Is freq too small? No. It was just the auto range and small amplitude
- The knob on the speaker sets the amplitude

- What about the amplitude in the freq generator

- I'll just leave it at 4Vpp for now
- Talked w/ lab technician, both Vpp on the signal generator and speaker have knob set amplitude

- I will leave 1Vpp on freq generator since speaker has a lot of power

- I will be working w/ 7B chains (0.1 mm cm balls?)

- I cut off a length of 80 balls and placed on plate unknotted

Fri, March 10

## Parte PP

- PP amplitude a const  $1.29 \pm 0.01$  V on oscilloscope
- The chain tends to drift to side of plate closer to me for 3 trials. Fix legs
- Prof. John came in, we had a discussion about stochastic mech. study random walk of crossing points
- $N_0$  is the minimum number of beads required to make a knot. A constant, dependent on Cle and bead
- Take  $\sim 30$  trials for each set of conditions
- You want to make the experiment easy to redo. Mark center of knot, left end, and right end w/ sharpie
- For survival probability,  $T/T_{avg}$  for each set of conditions, and sort the array! ?.
- This is easier to do for lower amp and higher freq. 912 mV, 18 Hz
- Played w/ legs until staker can go for 10+ sec w/o noticeable drift
- Tied a Cle knot, looks like  $N_0 = 24 \pm 1$
- Minimum
- Cut a 44 N=49 chain. smaller than this should be very hard to knot
- Nevermind, too hard to knot.
- Start w/ N=80
- Back to

Fri, March 10

- Random mot<sup>1</sup> at  $13\text{Hz}$ ,  $\sim 1$  Volt pp osc.

• Tied a 31 knot on  $N=80$  chain

• Marked the center w/ red pen

- I tied the wrong knot initially

•  $N_0 = 19 \pm 1$  for trefoil

• Placed knot on center of staker and started it w/ stopwatch

• Let U denote under unknotted first and O denote over

$\uparrow$   
loop

U = passes under loop

O = passes over

<u><math>N=80</math> unknotting times</u>	$T(s)$	Unknotted side	$T(s)$	Unknotted side
11	11.14	O	5	U
18	18.5	U	4	O
9	9.09	U	6	U
24	23.75	O	8	U
6	5.56	U	26	O
18	18.37	U	7	U
61	22.21	O	6	U
3	7.79	O	10	O
7	U	14	O	
12	O	9	U	
7	U	47	U	
7	U	14	O	
5	O	77	O	
24	U	7	O	
25	O	7	O	

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## • Notes:

- It is hard to tell exactly when the knot does at this amplitude. Large uncertainty in  $T_s$ , and more likely that I overestimate  $T_s$  rather than underestimate. Usually I see extra  $I$  than  $\bar{I}$  for really long times ( $20s+$ ) It is possible that the chain drifts and interacts w/ walls of plate. This may affect results
- I placed chain in center of the shaker, w/ arms extending straight. Over to right
- Measured  $T_s$  w/ phone stopwatch

• Next chain:  $N=40$  120

• Once again, marked 0 end in black, center in red

• Repeat process

Table 2:

$T(s)$	Unknotted side	changed this to red + black sticker plus too
8	0	
24	0	
39	U	
27	0	
12	0	
26	U	
76	0	
15	0	
27	0	

→ Switched to  
stopwatch  
here

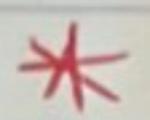
• Too much self crossing!

• Talked to Prof. John. I want just enough  
amplitude so that the knot moves around,  
but not so much that it

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self crosses. Throw away data on  $\bar{I} > 8$ 

- Start w/ the upper & lower bands of measurement & subdivide
- Take data until standard error becomes small
- Around 840 mV seems appropriate. Still 13 Hz



N=40 — Table 3

$T(s)$	Unknotted	$\bar{I}(s)$	Unknotted
11.43	U	5.22	U
3.93	U	6.85	0
9.47	U	4.25	U
13.47	0	12.66	0
6.31	U	6.19	U
2.34	U	4.38	U
9.90	0	3.00	U
3.09	0	6.28	U
6.69	U	4.68	U
3.97	U	3.65	U
		3.06	U
4.47	U	3.53	U
7.47	U	2.87	U
11.49	U	6.52	U
9.90	U	11.24	U
3.63	U		

Knot got stuck on edge ↗

• That was a lot better. Knot never flipped over so U and 0 remt sides remained the same throughout mot<sup>c</sup>

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- For the high end, I'll use  $N=120$

$T(s)$	Unknotted	Table 4: 1S unknotting times for $N=120$
21.53	U	w/ $V_{pp}=840 \text{ mV}$
53.40	U	
296.07	U	freq = 13 Hz
105.44	U	
352.32	U	
22.13	U	
123.53	U	• For both table 3 and 4,
40.91	O	the knots tend to
86.09	U	unknot from the side which
78.03	U	passes <u>under</u> the loop
48.91	U	
125.96	O	
123.69	U	• I put each data set (Tbl 3 & 4)
+063.72	U	in their own <del>data sets</del> and performed
49.44	U	excel files

data analysis as on pg. 3

- Now I can add data points and automatically update the  $T_{avg} \pm \sigma_{\text{standard}}$
- I want to ~~do~~  $\bar{T}$ . This results in  $\bar{T}_{avg} \pm \sigma_{\text{standard}}$  here  $\bar{T}$  means err/mean
- $\bar{T}_{avg}(N=40) = 6.2 \text{ s} \pm 0.6 \text{ s}$  ( $\% \text{ error} = 0.09$ )
- $\bar{T}_{avg}(N=120) = 120.116 \pm 23 \text{ s}$  ( $\% \text{ error} = 0.20$ )  $\leftarrow$  this was not right?
- I think it is reasonable to shoot for  $\% \text{ error} < 0.1$
- Since it drops  $\sqrt{\text{length of dataset}}$ , I need 4 times more trials to get the error in  $\bar{T}_{avg}(N=120)$  to be 0.1 percent
- 60 trials
- I think that's 30 trials for now, then study other  $N$ s before returning

Tues, March 14

- Arrived at lab and turned on all equipment
- Reset amplitude to  $840 \text{ Vpp}$  ( $1.100 \text{ Vpp}$  on signal generator)
- Oscilloscope  $\rightarrow$   $1 \text{ mV}$
- Freq to 13 Hz (actual range is  $840 - 856 \text{ Vpp}$ )

- Back to taking data.
- Trid loop in middle of  $N=120$  chain, w/ the side passing over the loop still marked in black sharpie
- Placed knot in center of shaker and started

$T(s)$	Unknotted	Table 5: 1S more unknotting times for $N=120$ w/ $V_{pp}=840 \text{ mV}$ freq = 13 Hz
19.72	O	
76.13	U	
33.50	O	
41.44	O	
2341	O	• A lot more O's today
58.28	O	• A lot more shorter times?
87.19	U	• A lot more self intersection?
27.16	U	
63.31	U	• The voltage on the oscilloscope
60.28	U	tends to vary by a bit. 10-20 mV
16.09	O	• Lots variation
32.66	U	• This time, it varied seemed like
21.12	U	$840 \text{ mV}$ was at the bottom of
17.28	U	the variation, not the center. I will take a few
49.78	U	more data points at a slightly lower $V_{pp}$ , w/ $840 \text{ mV}$ at center and see the difference

Tues, March 14<sup>th</sup>, 2023

$T$ (s)	unknotted	
19.28	U	Table 6: 15 unknotting times
150.93	O	For $N=120$ w/ $V_{pp} = 840 \text{ mV}$
47.04	U	and freq = 13 Hz
173.03	O	
155.47	U	Combined w/ table 4, <del>•</del> $T_{avg}(N=120) = 116 \pm 14 \text{ s}$
108.63	O	
32.13	O	• STD is 76 seconds
118.08	O	(10:43 AM)
158.53	O	$T_{avg}(N=120) = 100 \pm 14 \text{ s}$
49.28	U	(Mar 16, 3:06)
159.94	U	
33.78	U	
26.75	O	
56.25	O	
52.25	U	

- After 5 attempts, this seemed a lot more similar to the conditions I had last time

10:20

- No self intersection in the vibrating chain, and longer times

- \*  $V_{pp}$  on oscilloscope oscillates from 832 - 848 mV, centered at 840 mV. Occasionally varies as much as 824 - 856 mV. I will replicate this from now on
- Amp 1 = 1.094  $V_{pp}$  on signal generator. Use this if nobody turns knob on speaker.

Throw away table 5 :)

10:32

- Observation: suppose it takes about 115 s for MA to react to the unknotting.

Tues, March 14<sup>th</sup>

This would account for a bias in all of my measurements. This won't be a problem for large  $N$  w/ times of 1 minute +. But what about small  $N$ ? How can I account for this bias?

- I could shift my dataset by some constant value to attempt to improve my fit. Maybe try 15 or 0.5 s
- Consider this later in analysis phase

Time to take measurements for  $N = 80$

$T$ (s)	Unknotted	$T$ (s)	Unknotted	Table 7: 30
15.58	U	17.06	U	Unknottting times
8.00	U	13.21	U	for $N=80$ w/
19.13	U	6.65	U	$V_{pp} = 840 \text{ mV}$ and
12.46	U	35.28	O	freq ~ 13 Hz
18.72	U	28.13	U	
13.85	U	17.03	U	$T_{avg}(N=80) = 17 \pm 1 \text{ s}$
35.90	U	19.15	U	STD = 8 s
11.78	U	23.28	U	
9.88	U	11.88	U	
17.31	U	31.46	O	
22.38	U	11.50	U	
27.97	U	10.94	U	
15.56	U	10.97	U	
22.57	U	26.13	U	
23.13	O	13.75	U	

Tues, March 14<sup>th</sup>

- Next, repeat the process for  $N=60$

$T(s)$	Unknotted	$T(s)$	Unknotted	Table 8:30 unknitting times for $N=60$ w/ $V_{pp} = 840\text{mV}$ and $\text{Freq} = 13\text{Hz}$
14.91	U	8.72	U	
8.63	U	7.34	U	
6.12	U	18.16	U	
22.53	U	13.69	U	
10.56	U	21.06	U	$\text{Tang}(N=60) = 12 \pm 1\text{s}$
13.40	O	9.75	U	$\text{STD} = 7\text{s}$
23.18	O	9.65	U	
9.72	U	15.72	U	
7.75	U	8.28	U	
4.94	U	9.22	O	
10.81	U	4.85	U	
6.88	U	15.57	U	
10.56	U	24.25	O	
24.34	U	11.69	U	
38.47	O	18.18	U	

- Plotting the data I've found so far, does not appear quadratic for  $N < 80$ .
- I will investigate larger  $N$ s
- Maybe  $N = 100 \div 200$  range?
- In particular,  $N = 80$  seems to have a much smaller  $\text{Tang}$  than the model predicts.

Thurs. March 16<sup>th</sup>

- Last time, I found that  $N=60$  and  $N=80$  seemed to disagree w/ the model

-The model also predicts that  $\sigma/\text{Tang} \approx 0.63$ , independent of length. I found

•

$$N=40 \Rightarrow \sigma/\text{Tang} = 0.50$$

$$N=60 \Rightarrow \sigma/\text{Tang} = 0.61$$

$$N=80 \Rightarrow \sigma/\text{Tang} = 0.45$$

$$N=120 \Rightarrow \sigma/\text{Tang} = 0.66$$

- $N=40$  disagreement makes sense. I estimated there is  $\approx 1\text{sec}$  bias, which means  $\text{Tang}(N=40)$  is 16% bigger than it should be

- Why does  $N=80$  disagree? I will remeasure this now

• Turned on ~~newer~~ equipment. Set  $V_{pp}$  to 832-848mV

$T(s)$	Unknotted	$T(s)$	Unknotted	$T(s)$	Unknotted
43.12	U	11.59	U	18.03	U
70.62	U	15.72	U	38.56	U
63.37	O	21.19	U	28.03	U
53.78	U	100.16	U	17.32	U
136.15	U	72.97	U	17.56	U
116.13	U	15.03	U	30.85	U
21.06	U	38.16	O		
63.22	U	97.75	U		
28.72	U	18.72	U		
20.91	U	13.13	O		
32.75	U	25.75	U		
30.37	O	15.13	U		

Table 9: 30 unknitting times  
for  $N=80$

$$\text{Tang}(N=80) = 43 \pm 8\text{s}$$

$$\rightarrow 43 \pm 6\text{s}$$

(Mar 16, 306)

Thurs, Mar 16

- 12:30
- After just 5  $N=80$  trials, it is clear something in table 7 is wrong
  - It is possible I did not pull the knot tight enough. It seems that the knot spends a long time loosening before it can travel.
  - I will test this by pulling the knot until it is very small, but not tight (for  $N=80$ )
  - ~~First~~ Times: 13.63 sec, 26.94 sec
  - That definitely seems to be the culprit.  
~~To make sure today~~

- I have one trial I needed to discard because the knot got stuck in periodic behaviour after getting stuck on wall of shaker

- ~~#~~
- It is hard to get repeat the same conditions for this experiment
  - The motion is very ~~sensi~~ sensitive to amplitude, but the oscilloscope amplitude varies a lot
  - It also seems that the knot is easier to tie tight w/ time

Thurs, Mar ~~16~~ 16<sup>th</sup>

- Retry  $N=60$  as well then

T (s)	Unknotted
6.81	U
9.44	O
20.68	U
44.17.43	U
44.69	U

Table 10: ~~30~~<sup>5</sup> unknottting times for  $N=60$ .

This agrees w/ table 8

• Putting together w/ table 8,  
 $T_{avg}(N=60) = 12 \pm 4 s$

$14 \pm 15$

(Mar 16, 8:05)

- Now, move on to  $N=100$

T (s)	Unknotted
80.44	U
123.25	U
55.34	U
31.81	O
121.09	U
118.72	U
87.28	U
69.94	Y
35.84	Y
44.94	U
34.03	U
88.06	U
106.32	U
36.60	U
60.97	U

Table 10: 30 unknottting times for  $N=100$

$T_{avg}(N=100) = 54 \pm 6 s$

- I noticed some errors on excel sheet math, will go back and fix (Mar 16, 8:05)

Thurs, March 16<sup>th</sup>

- I believe my analysis at the beginning of pug 16 is wrong
- I only took 2 times to prove my hypothesis that the chain was not tied tightly enough. It ~~is~~ is likely that it was just statistical fluctuation. ~~So~~, I combined the data from tables 7 and 9 to get

$$T_{avg} (N=80) = \frac{80.6}{31 \pm 3} \text{ s}$$

- This seems to agree more w/ the model. I should take more measurements for N=120 as well then

Fri, March 17<sup>th</sup>

- Arrived at lab, turned on equipment
- Set freq to ~~13~~ 13 Hz, amp to ~840 mV VPP
- Did a test run to make sure the chain doesn't self intersect
- Now, get 30 more times for N=120

<u>T (s)</u>	<u>Unknotted</u>	<u>T (s)</u>	<u>Unknotted</u>	<u>Table 11: 30</u>
33.47	U	52.60	0	Unknotting times
114.22	U	35.44	0	For N=120
66.31	U	116.15	U	Combine w/ data
84.62	U	28.22	U	for table 1 & b,
75.72	0	91.31	U	
35.62	U	104.84	U	$T_{avg} (N=120) = 91 \pm 9$
116.78	U	80.57	0	s
107.35	U	18.12	0	
115.06	U	61.42	U	
wired $\rightarrow$ {	349.50	0	134.66	U
	12.59	U	66.44	U
	31.75	U	29.44	U
	42.25	0	95.15	U
	88.82	U	50.50	0
32.44	U	200.56	U	

- I threw away a trial because the knot flipped over 3 trials

Fri, March 17th

- seaborne distplot
- Talked w/ prof. John
- He said to plot histograms for each data point
- Survival probability is cumulative histogram. Plot length\\_arr\\_cntr against time
- Get one more datapoint,  $N=140$

$T(s)$	Unknotting	$T(s)$	Unknotting	$T(s)$	Unknotting
79.19	U	52.22	U	44.78	U
144.81	O	91.97	O	103.25	U
62.25	O	157.91	O	81.84	U
404.56	O	193.17	U	58.53	U
51.94	U	60.10	U	89.56	U
148.53	U	236.03	O	32.56	O
35.63	U	80.75	O	217.19	O
125.75	U	72.50	O	174.94	U
46.1819	U	210.68	U	36.59	U
20.97	U	72.22	O	67.31	U
32.50	O	186.22	O		
34.63	U	79.38	O		
58.56	U	606.78	U		
66.84	O	18.97	U		
56.09	U	42.75	U		
36.13	U	198.78	U		
63.64	U	190.03	O		
63.59	U	27.75	U		
28.10	U	24.04	U		
142.22	U	222.22	U		
		37.31	U		

Table 12: 50 unknotting times for  $N=140$

$$T_{avg}(N=140) = 108 \pm 15 \text{ s}$$

• 15 Os!! That's pretty

• strange

Sat, March 18th

### Summary and Analysis

- Below is a summary of my data for finding  $\delta$

Table 13

$N$ (Length)	Mean Unknotting Times (s)	Standard Deviation	Standard Err
40	6.2 s	3.0 s	0.6 s
60	14 s	7 s	1 s
80	31 s	27 s	3 s
100	59 s	31 s	6 s
120	91 s	71 s	9 s
140	109 s	106 s	16 s

• Note that tables 1, 2, 4, 5 were omitted for the acceleration amplitudes being too large

• I will fit this data w/

$$T_{avg} = T_0(N - N_0)^{\delta} + b$$

• Since I only have 6 data points, I will use  $N_0$  and  $b$  as known parameters

• Further, I said  $N_0 = 19$ . However, I counted the crossing points of the chain in this estimate. These should not be included.  $N_0$  should refer th. to the interior of the knot

• A more accurate estimate is  $N_0 = 16$

•  $b$  is used to account for the systematic error discussed in pages 12-13

• It takes time for me to notice the knot has opened and to stop the timer. Thus I tend to over estimate the unknotting time by about 1s. So I take  $b = 1$

Sat, March 18<sup>th</sup>

- With this, I can perform a least squares fit for  $\delta$  and  $T_0$  resulting in

$$\delta = 2.0 \pm 0.1$$

$$T_0 = (1.7 \pm 3) \cdot 10^{-3} \text{ s}$$

- This value of  $\delta$  agrees w/ theory. The goodness of fit:

$$\chi^2_{\text{red}} = 1.6$$

$$\text{CDF} = 17\%$$

- My results show that the model agrees w/ reality

- Plot below

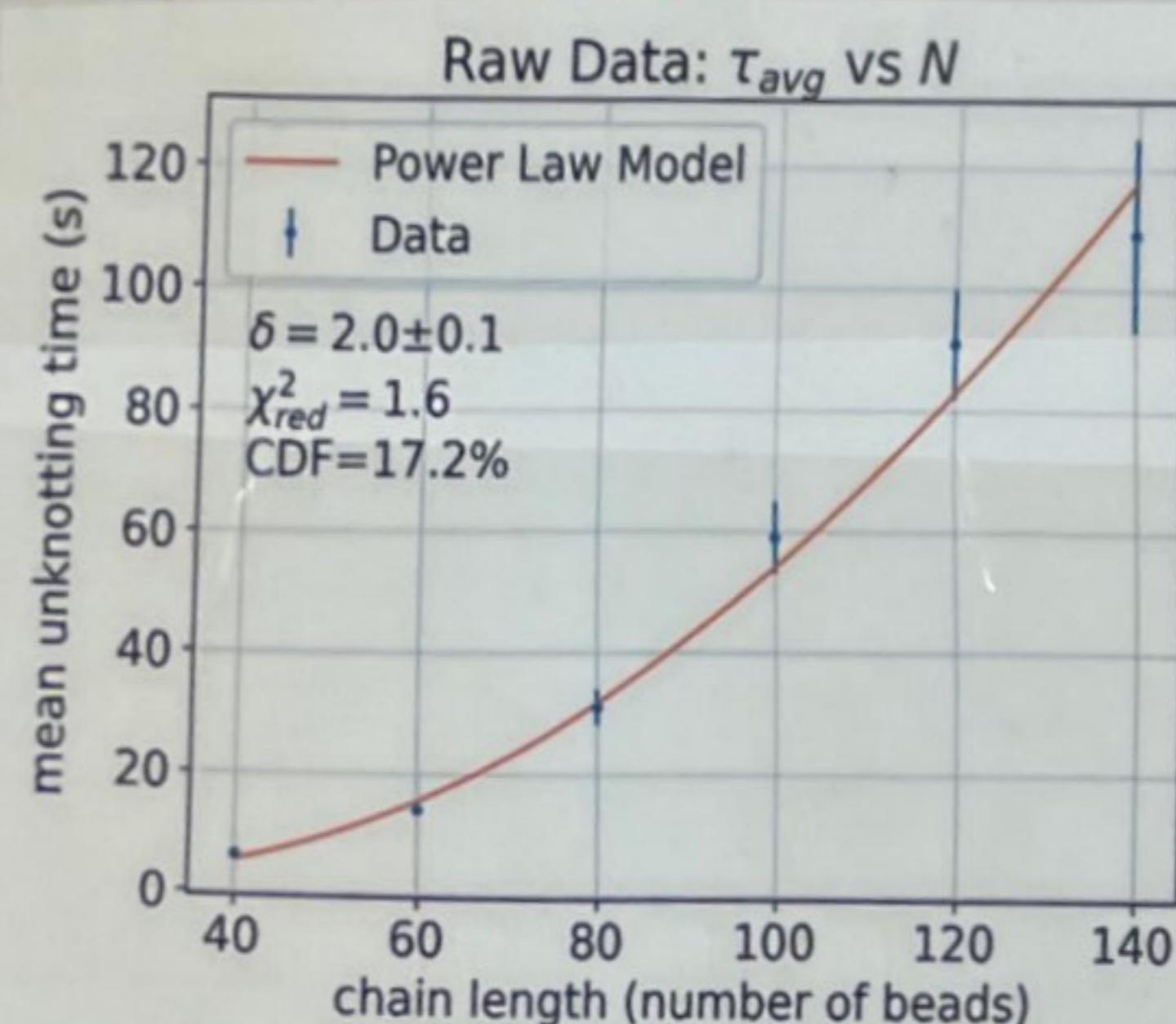


Fig 1: Average opening time vs  $N$  for Raw data

• Blue is data, orange is best fit

• According to Ben-Naim,  
 $T_0 = T_3/D$ , where  
 $T_3 = 0.056213$  is the theoretical, dimensionless mean

• Image generated using get-delta.py

exit time

•  $D$  is the diffusion constant / hopping rate. My result has  $D = 8 \pm 4 \text{ s}^{-1}$

• This makes sense. The chain was vibrating at 13 Hz, and did not go hop a bead during for a fraction of the oscillations, so having a hopping rate slightly lower than the freq. makes sense

22

Sat March 15<sup>th</sup>

- The survival probability  $S(t, N)$  can be measured like so: For a fixed length  $N$ , and for a time  $t$ , the empirical value of  $S(t, N)$  is the fraction of survival times in the data set greater than  $t$ .

- Plotting this against  $t/\tau_{\text{avg}}$  for each data set for different  $N$ s shows that they all follow the same characteristic curve.

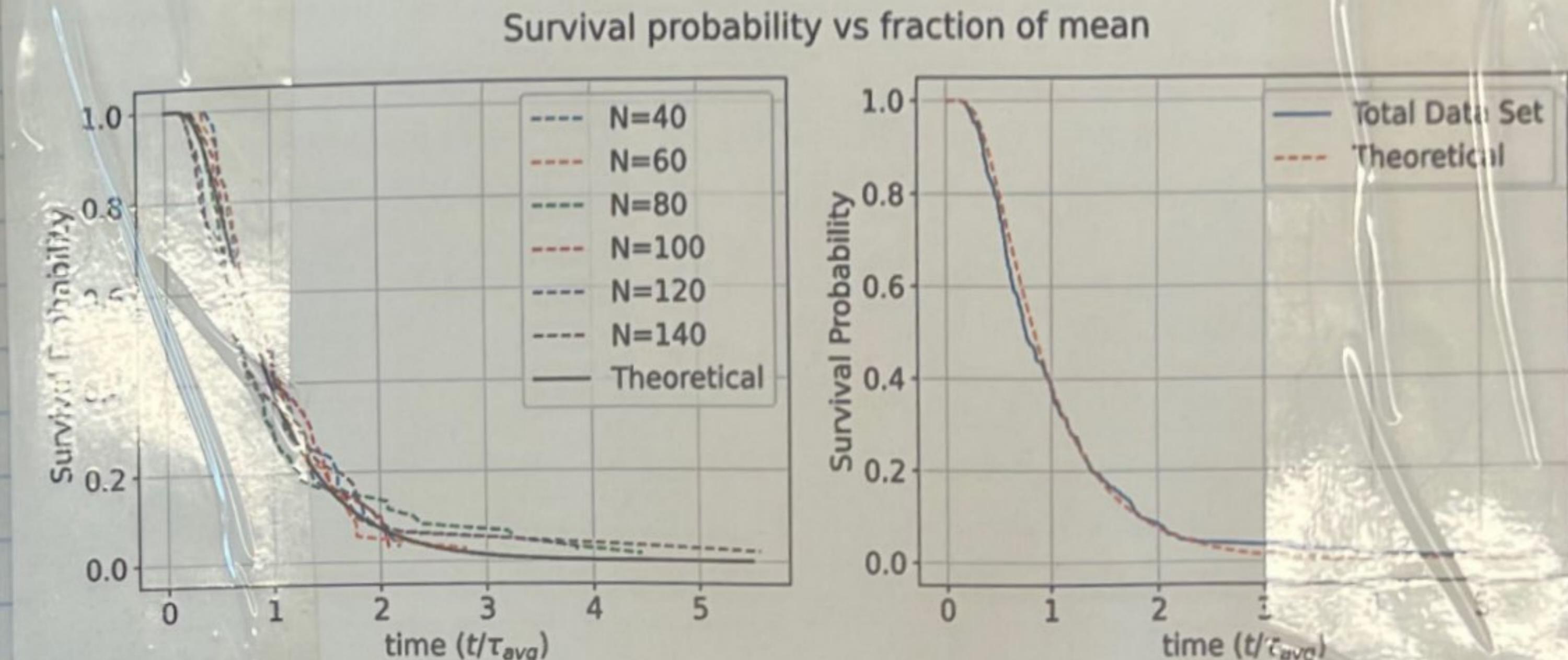


Fig 2: Survival probability vs  $t/\tau_{\text{avg}}$ . On left, we have the survival probability for each independent chain length and the theoretical curve. On the right, we have the survival probability computed from the entire data set

• Analysis on page 44

• Images generated using survival.py

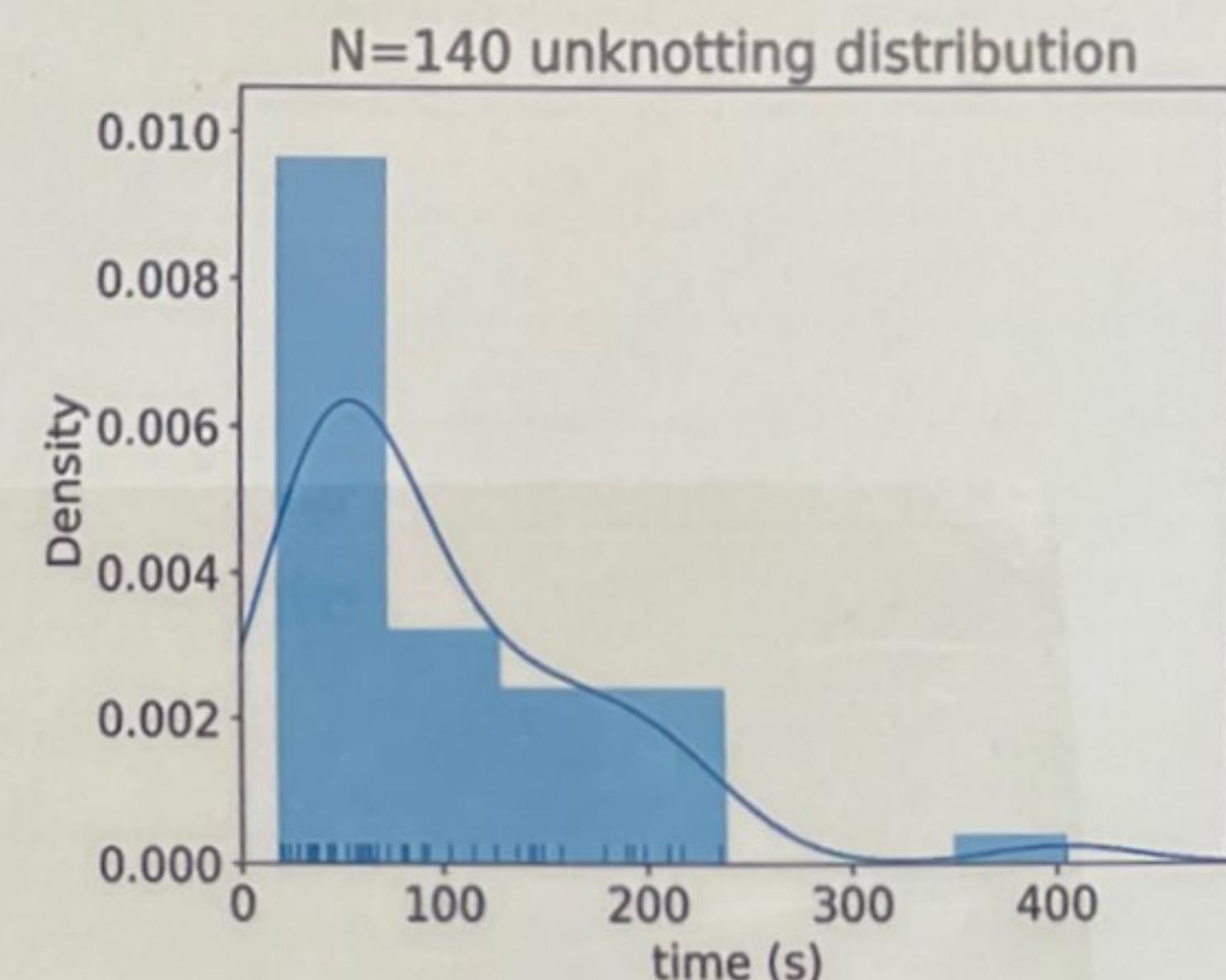
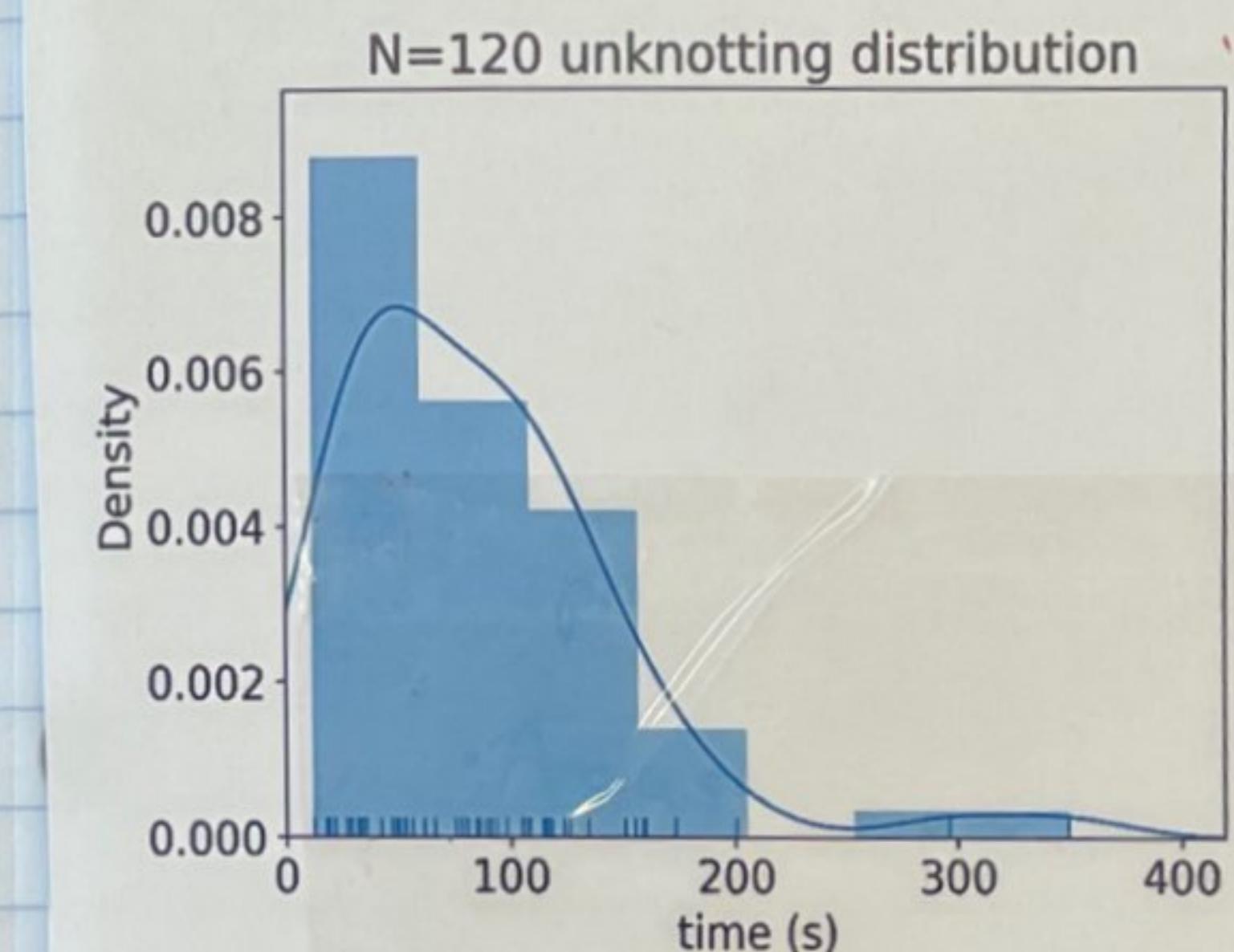
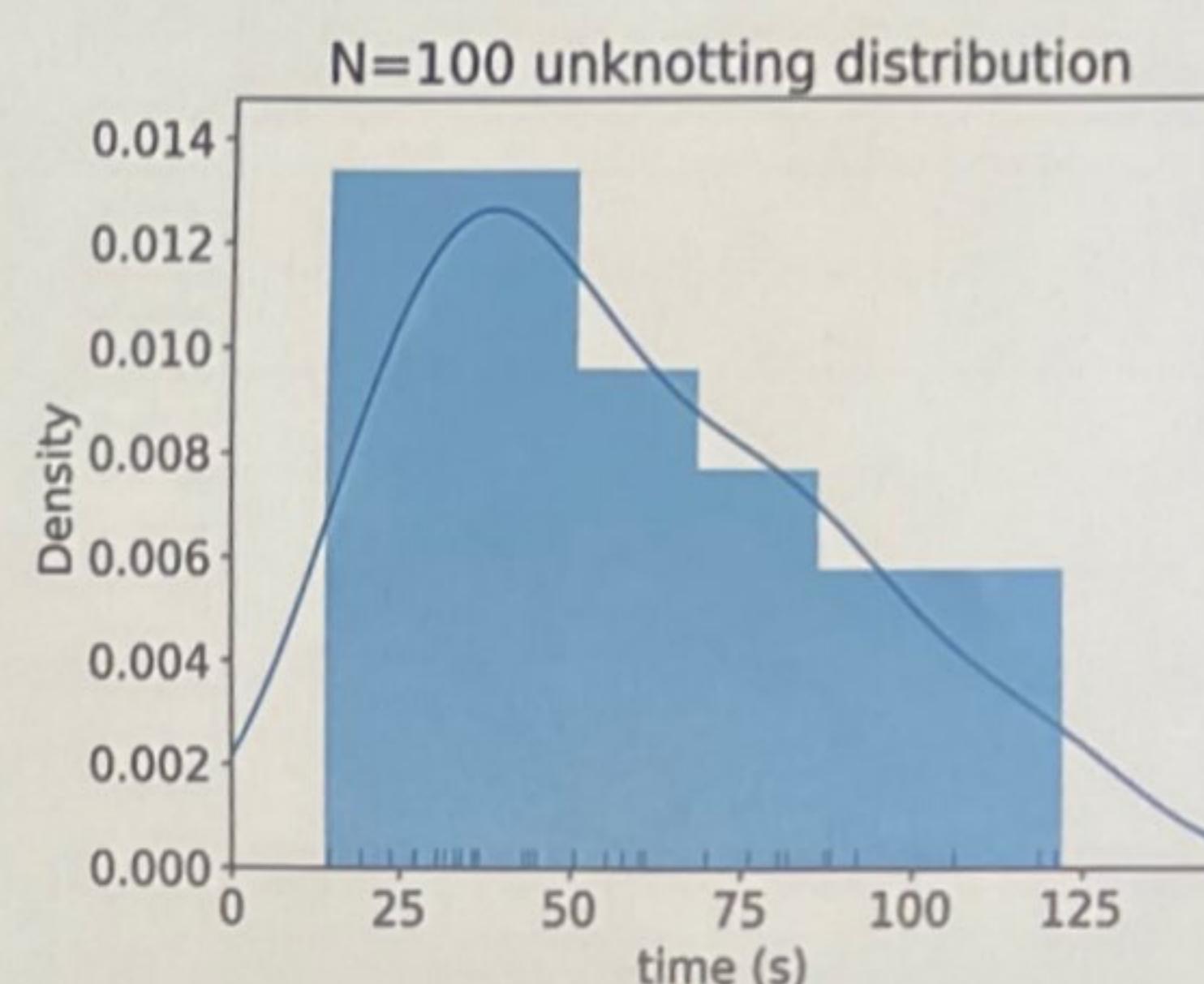
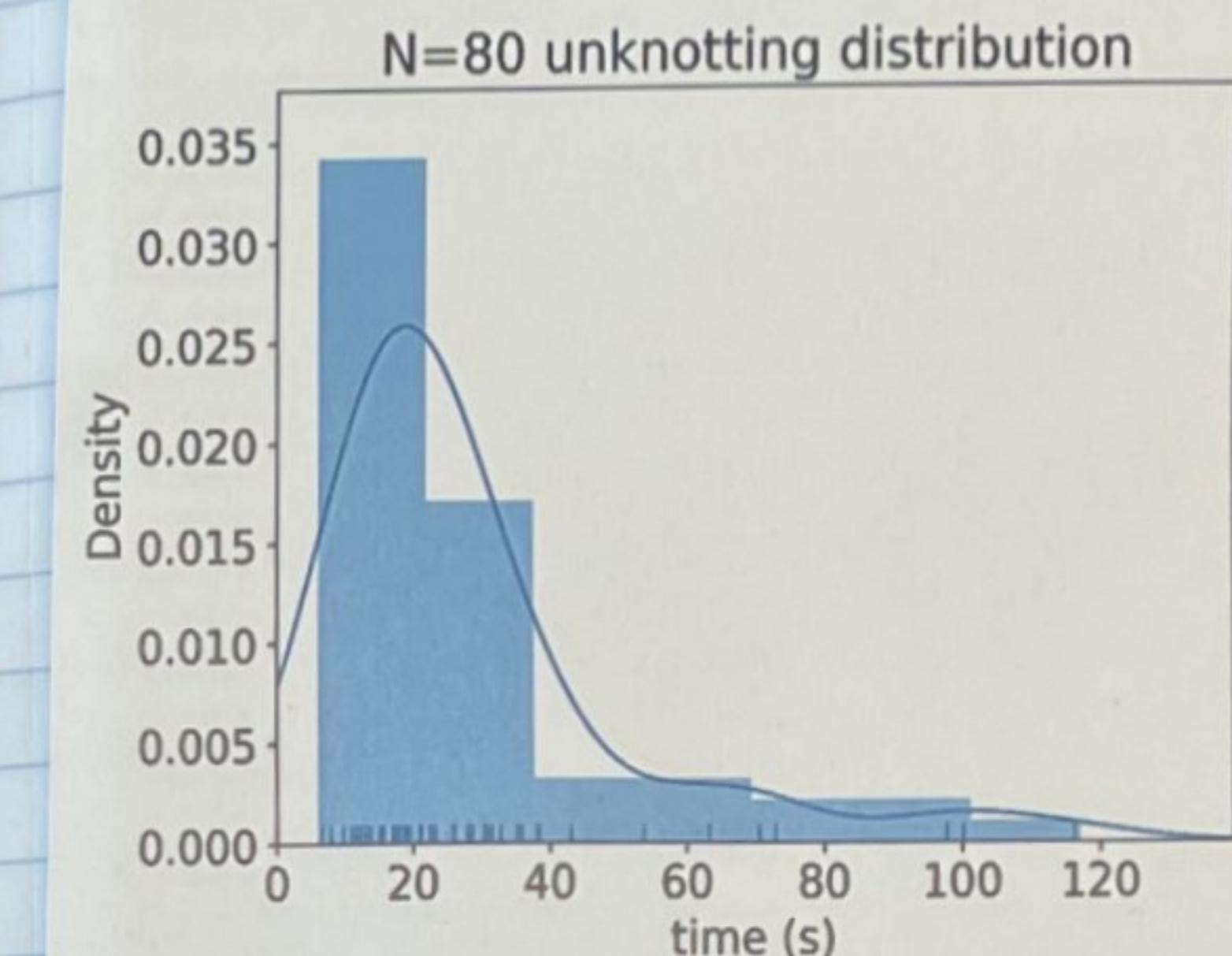
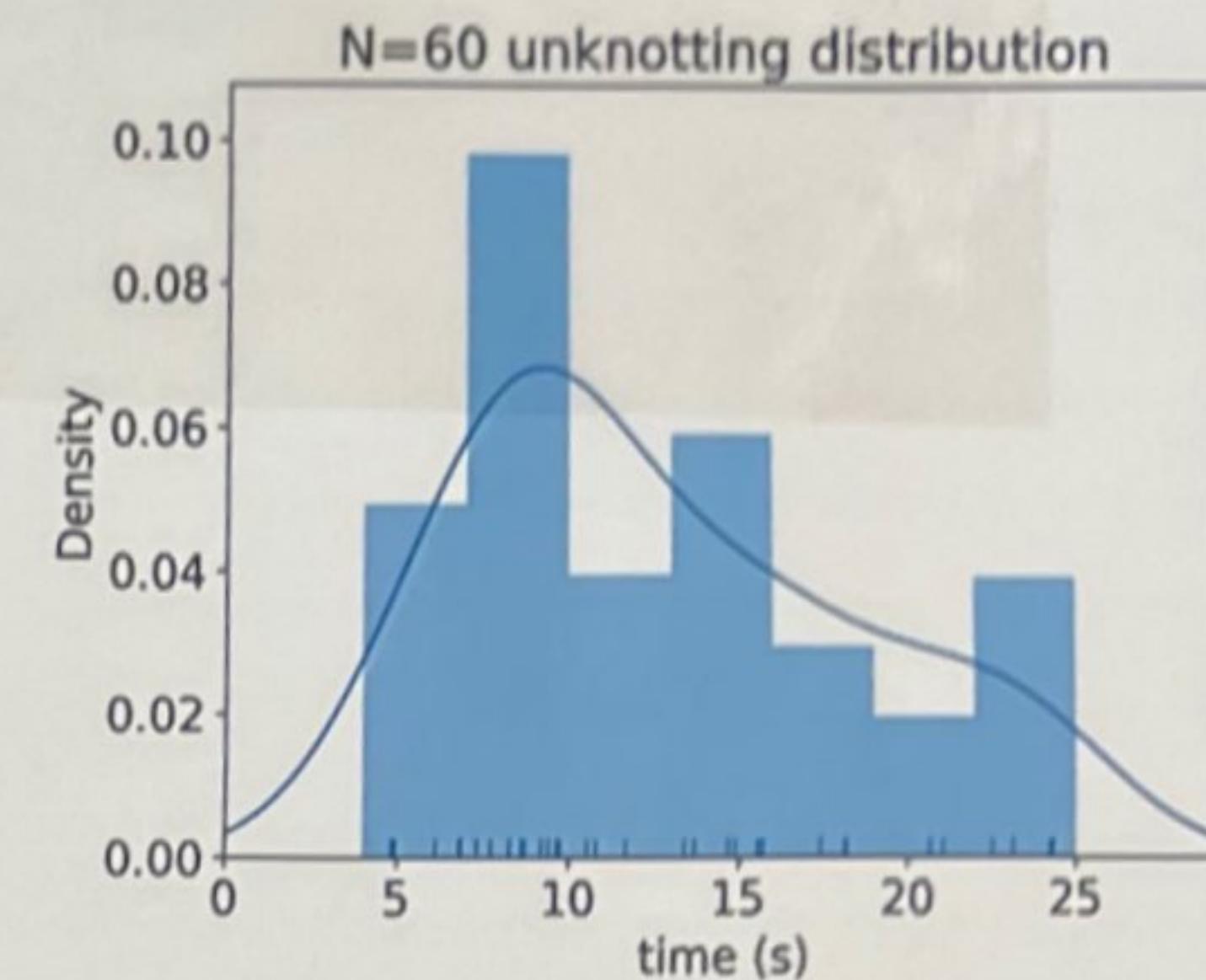
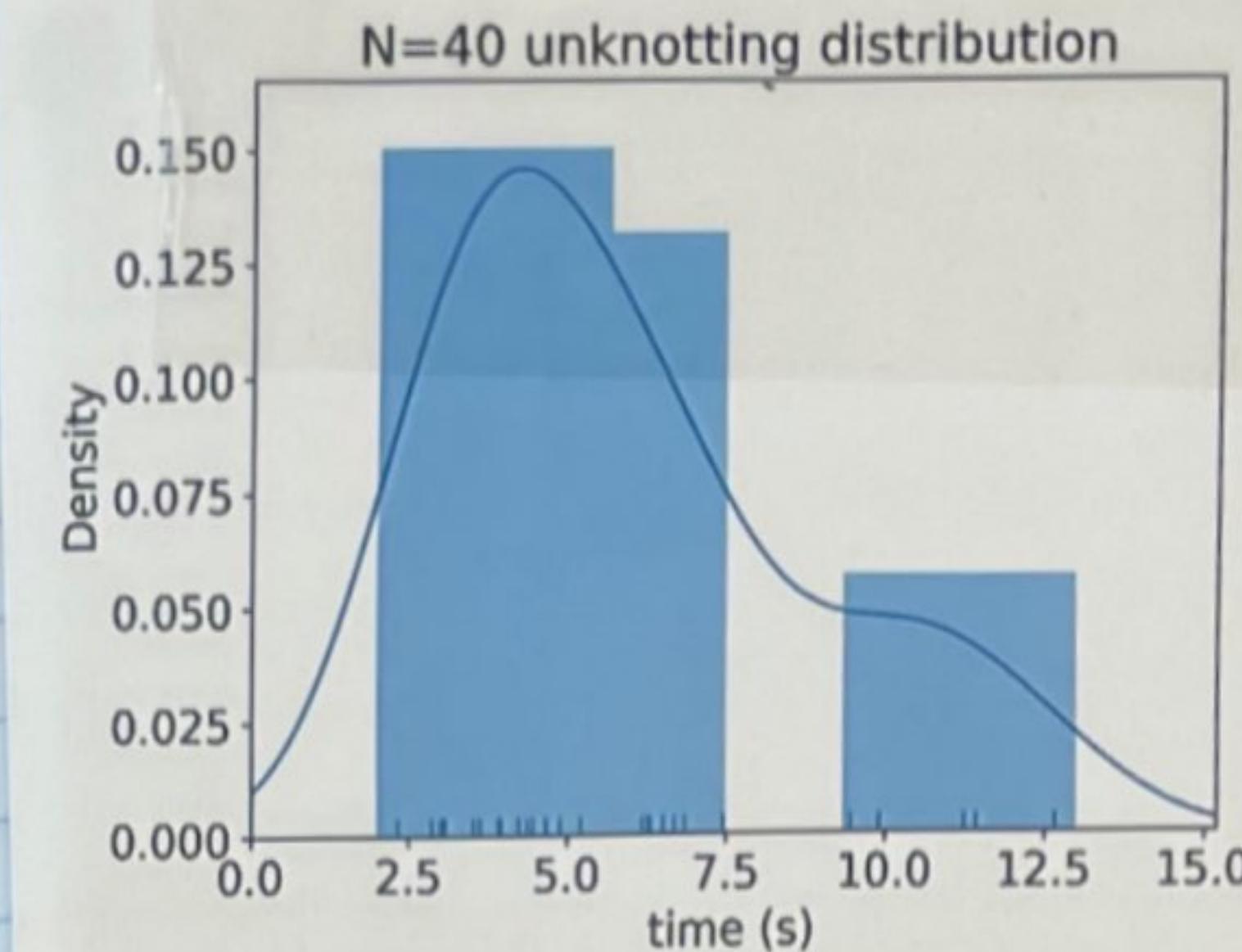
This page is wrong!!

24  
Sat, March 18<sup>th</sup>

- I mentioned on pg 19 that I discarded some trials because the knot flipped over. However, I did not do this for other trials.
- To study the effects of such points on the model (points w/ anomalously high unknotting times), I can plot a histogram for each data set and omit anomalous data points.
- I omitted the highest 3 data points for  $N=80, 120$
- Omitted highest data point for  $N=140$
- The result is a slightly worse fit.  
 $\left. \begin{array}{l} \delta = 1.9 \pm 0.1 \\ T_0 = (12 \pm 6) \cdot 10^{-8} \text{ s} \end{array} \right\} \chi^2_{\text{red}} = 2.8$   
 $\left. \begin{array}{l} CDF = 2.5\% \end{array} \right\}$
- I can conclude that these anomalous points are important to the distribution and should be included

Fig 3: Next page: The distributions of opening times of opening times for each chain length

- Note the Gaussian peaks w/ long tails
- A kernel density estimate & rug plot is included for each distribution
- Images generated using histograms.py



Sat, March 18<sup>th</sup>Sat, March 18<sup>th</sup>Important NotesQualitative Knot Behavior

- I found that the knot greatly preferred to open towards the side which passed under the loop. If the knot flipped, it tended to travel to the side which was now under the loop, which would increase the unknotting time.
- The knot tended to start by growing a bit from its natural minimal size, before all the crossing points began to travel towards the end of the chain which passed under the loop.
- For longer chains, the knot could spend a long time in this state, sometimes even tightening down to its smallest state again. When this happened, its random walk would come almost to a stop, greatly increasing its unknotting time.
- Occasionally, the crossing points would travel in opposite directions and the knot would grow slowly to a maximum size before opening.

Sat March 18<sup>th</sup>

- I made a mistake on pg 24
- When generating my histograms, I wanted to Sturge's Rule to plot my histogram. i.e.  
 $\text{num bins} = \lceil 1 + \log_2(\text{num data points}) \rceil$
- I then removed the anomalously large data points from the distribution. I did this by looking at the histograms and excluding those large times which did not come in clusters. i.e. The largest k for times. For each data set, this was

N	k	Mean (s)
40	5	$4.5 \pm 0.4$
60	0	$14 \pm 1$
80	8	$25 \pm 2$
100	4	$50 \pm 5$
120	3	$76 \pm 6$
140	1	$91 \pm 9$

The result was  
 $\delta = 2.01 \pm 0.07$        $\chi^2_{\text{red}} = 1.04$   
 $T_0 = (6 \pm 1) \cdot 10^{-3} \text{ s}$       CDF = 38.4%

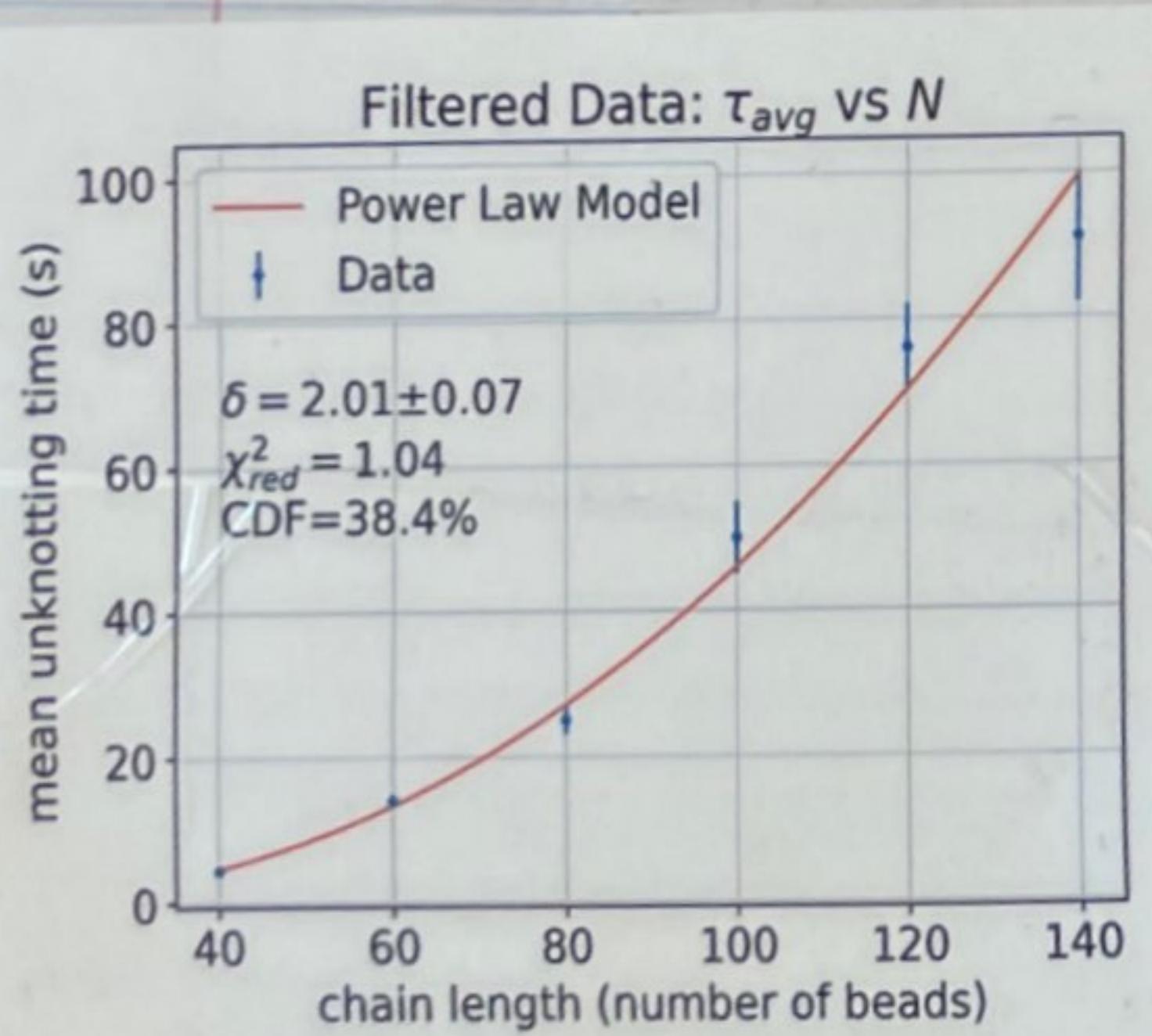


Fig 4: Average unknottedting time vs N, for the filtered data  
 - Image generated using get-delta.py  
 - The resulting diffusivity is  $D = 9 \pm 3 \text{ s}^{-1}$

- Removing the tail of the gaussian therefore improved my results
- The long tail mostly consisted of trials where the knot flipped, or the chain created a new self intersection. This violates Ben-Naim's assumptions, so it makes sense that the data improved

Mon  
Sun, March 20<sup>th</sup>

### Radius of Gyration:

- The radius of gyration of a chain of length N is

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

where  $\vec{r}_i$  is the position of the i<sup>th</sup> bead and  $\vec{R}_c$  given

by  $\vec{R}_c = \frac{1}{N} \sum_{i=1}^N \vec{r}_i$

is the chain's center of mass

- The maximum radius of gyration occurs when the chain is in a straight line and is equal to

$$R_{g,\max} = R_c = \frac{L}{2\sqrt{3}}$$

- Question: Does the radius of gyration approach a certain value  $R_g/R_{g,\max}$ ? If so, how does it depend on the physical properties of the chain and shaking process?

Tue, March 21<sup>st</sup>

- I will use the python code ~~real time ROG~~

~~Real Time - ROG~~

- No, code ~~Simple\_ROG~~ Simple ROG

which measures the ROG of a light chain on a dark background

- Start equipment w/  $V_{pp} = 840 \text{ mV}$  &  $\text{freq} = 13 \text{ Hz}$
- Use  $N = 120$ , 1mm YB chain for test video

- Nevermind, Forget all that

- A custom code will be developed which sends the video to grayscale, inverts it, uses a threshold value to determine which pixels are part of the chain, and then calculates the ROG for each frame

- Today I am using a webcam that films at 30 fps, so I will use freq = 15 Hz so the chain is at the same height each frame

- I want to investigate the dependence of <sup>asymptotic</sup> ROG on chain length
- Start w/  $N = 40$  in YB 1mm chain
- The chain keeps drifting out of frame
- At first, I tried to start the chain in a straight line (maximum ROG) but the transient motion takes a long time to end this way
- Regardless, for both max ROG start and a random initial condition, the final shape is



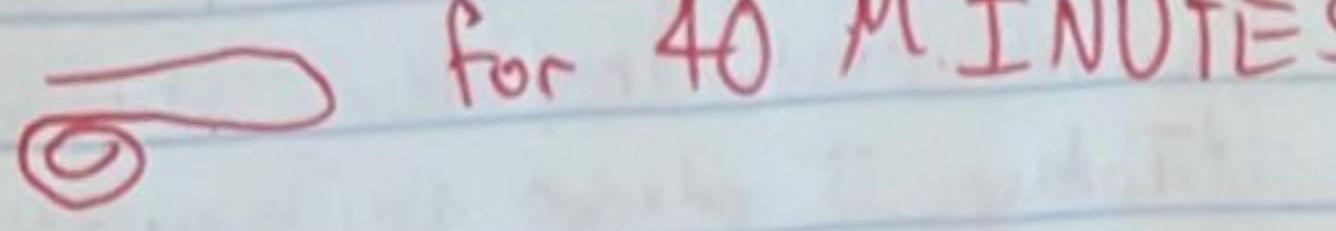
Tues, March 21st

- I will record each trial w/ for about a minute after transient ends
- I must cut new chains. The old ones are marked in black sharpie which could interfere w/ image software during thresholding
- Again, freq = 15 Hz, Amp = 840 mV & 32 mV
- For N=40, final shape C
- For N=60, final shape G
- For N=80, never settled into a final, stable state
  - Oh wait! Spiral S
  - Took several minutes to form
- The length of the transient ROG time seems to grow very quickly w/ chain length. If I can confirm that the final result is always a spiral, I can start the chain in a spiral position in the future to speed things along

Fri, March 24th

- Last time, plate was reflecting too much light which made thresholding difficult
- Today, I placed a black drop cloth and task light over the plate to reduce the reflected light and improve contrast between plate and chain
- I will also start chain in a compact, fixed form, randomly oriented to reduce time required for equilibrium
  - Start w/ N=40
    - Of course Vpp = 840 mV, Freq = 15 Hz
    - About 2 minutes like this A
    - Saved to trial 1.mp4
    - Next, N=60
    - About 2 minutes of footage like this P
    - Saved to trial 2.mp4
    - There seems to be a double image of the chain in the video
    - From its compactified pos<sup>c</sup>, equilibrium almost instantly
  - Next, N=80
    - After 10 mins, still no equilibrium
    - I had to throw away this time because it takes up too much space
    - Restart w/ random, compact orientation
    - Final spiral S
    - Saved to trial 3.mp4

Fri, March 24<sup>th</sup>

- N=100 next
- Stuck like this 

This  
was  
for  
N=120

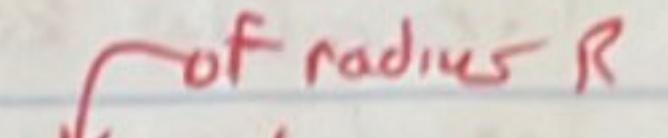
- Saved to trial 4.mp4
  - The chain spiraled, but w/ a twist, and then opened again before re-spiraling
  - After 47 minutes, we got a good spiral
  - ~~•~~ Saved to trial 5
  - These first 5 trials serve as evidence that the long term behaviour is a ~~loose~~ spiral. I will use this to as justification to start future trials in a spiral formation to save time
- loose* ↗

- Loose spiral for N=140. That still resulted in over 20 mins time because the spiral had slight deformities and unraveled
- Saved to ~~N=100~~ trial 6
- Camera frame has height 1080 and width 1920
- Took an image of a sticker triangle on shaker to get pixel to cm conversion
- Conversion rate: 22.7 cm / 1080 px
- I got this by putting the image in an image tracker, setting the cm scale using the triangle, and then measuring the height of the screen image, which I know to be 1080 px

Fri, March 24<sup>th</sup>

- A rough model for what is going on:

- The chain wants to spiral into a disk and fill its area

- The radius of gyration of a solid disk  is (using  $R_g$  as the ~~per~~ root mean square distance from center of mass)

$$\begin{aligned} R_g &= \sqrt{\frac{1}{\pi R^2} \int_0^{2\pi} \int_0^R r^2 (r dr d\theta) } \\ &= \sqrt{\frac{2\pi}{\pi R^2} \frac{R^4}{4}} \\ &= \frac{R}{\sqrt{2}} \end{aligned}$$

- Now, the area of the circle is filled by N radius a beads as so

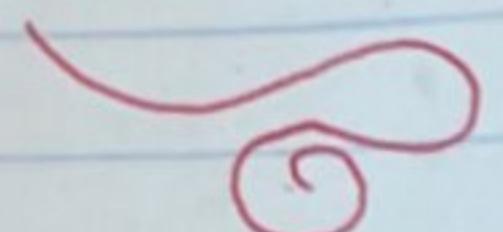
$$\begin{aligned} \pi R^2 &= \pi a^2 \cdot N \\ \Rightarrow 2\pi R_g^2 &= \pi a^2 \cdot N \\ \Rightarrow R_g &= a \sqrt{\frac{N}{2}} \quad ** \end{aligned}$$

- I should expect  $R_g \propto N^{1/2}$  for any bead size
- This model assumes large N

Fr., March 24<sup>th</sup>

Early analysis:

- I converted each video trial 1-6 to a folder of strides images, 1 frame every 2 seconds
- Calculated ROG in each image
- Took the last minute of footage for (30 frames) for each trial, when the chain is at equilibrium and plotted mean rog vs N, w/ standard error in the mean as y-error
- Trial 4 is clearly an outlier. The ROG is way too big and the final shape was something like



- I need to redo this trial

Tues., March 28<sup>th</sup>

- Turned on equipment. freq = 15hz, Amp = 840mV Vpp

- Put black drop cloth back over shaker.
- Redo N=100, but start chain in a loose spiral to save time

- It appears that the equilibrium ROG decreases until N=80
- It is possible I did not give N=40, 60 enough time as they were very loose spirals

- Computer froze as soon as video ended. Data may be lost :/

- I connected the camera to my laptop instead, the old PC is no good

- Since I hadn't touched the chain, I recorded a short 30 sec video again to get the equilibrium ROG data for N=100

- Saved to trial 7\_discarded

- Video too short, need to start over, I will do this after N=60

- For N=60, started in a tight, perfect spiral and it opened up again

- Saved to trial 7

After plotting, ROG seems to be increasing at the end of video. Not enough time to loosen

- N=100 again, in a tight spiral this time

- Saved to trial 8

†

- Cut N=50, put in a spiral and it opened!

- Saved to trial 9

Tues, March 28<sup>th</sup>

- Cut N=55 and it opened after a couple minutes

- Saved to trial 10

- The point where spirals can form is  $\approx 60$  balls

After, I will do  $N=160$

- Redo N=100. After plotting ROG vs time, I saw trial 8 had an increasing ROG still, not equilibrium

- The chain expanded to a very loose spiral and remained in that position

- Saved to trial 11

- Now repeat for  $N=160$

- I started this trial in a spiral formation but it unraveled. I think it was ~~too~~ trying to start a double spiral at this length. Did not have time to see the final result

39

Fri, March 31<sup>st</sup>

- Repeat  $N=160$ , but w/ a <sup>random</sup> compactified initial  $\rho_0$ : instead of a spiral (10:00 AM)

- Did not have time to finish this either

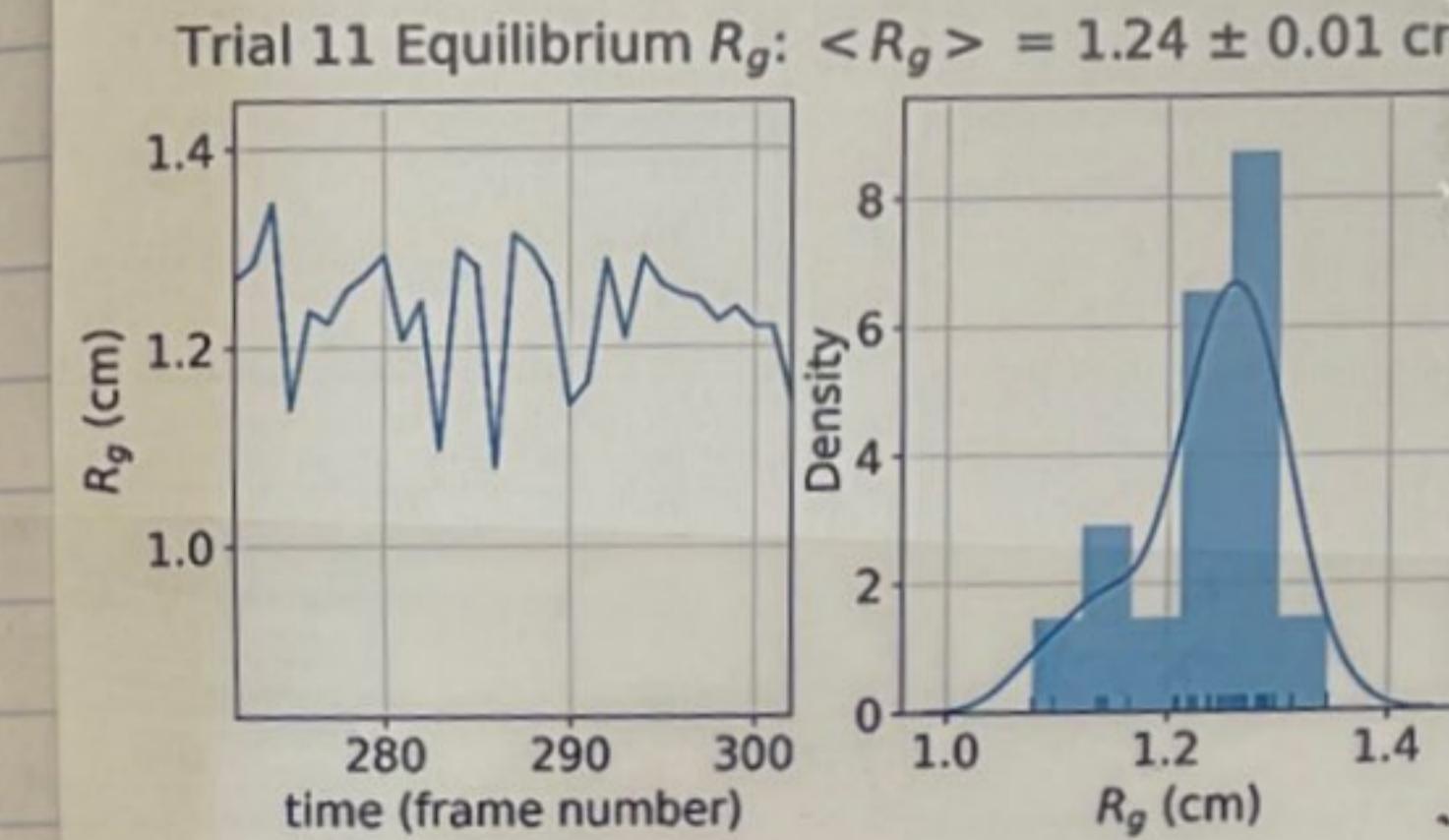
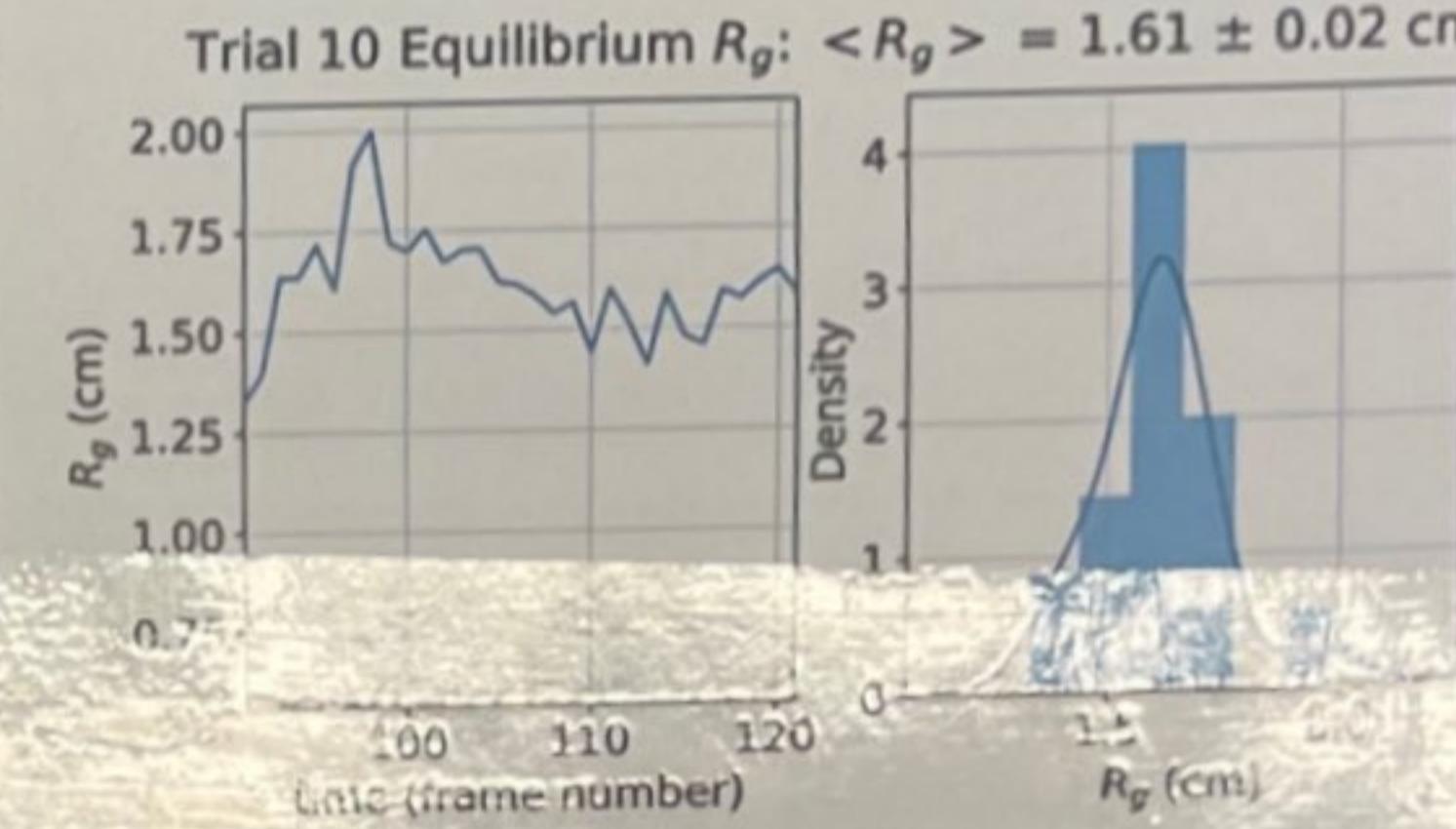
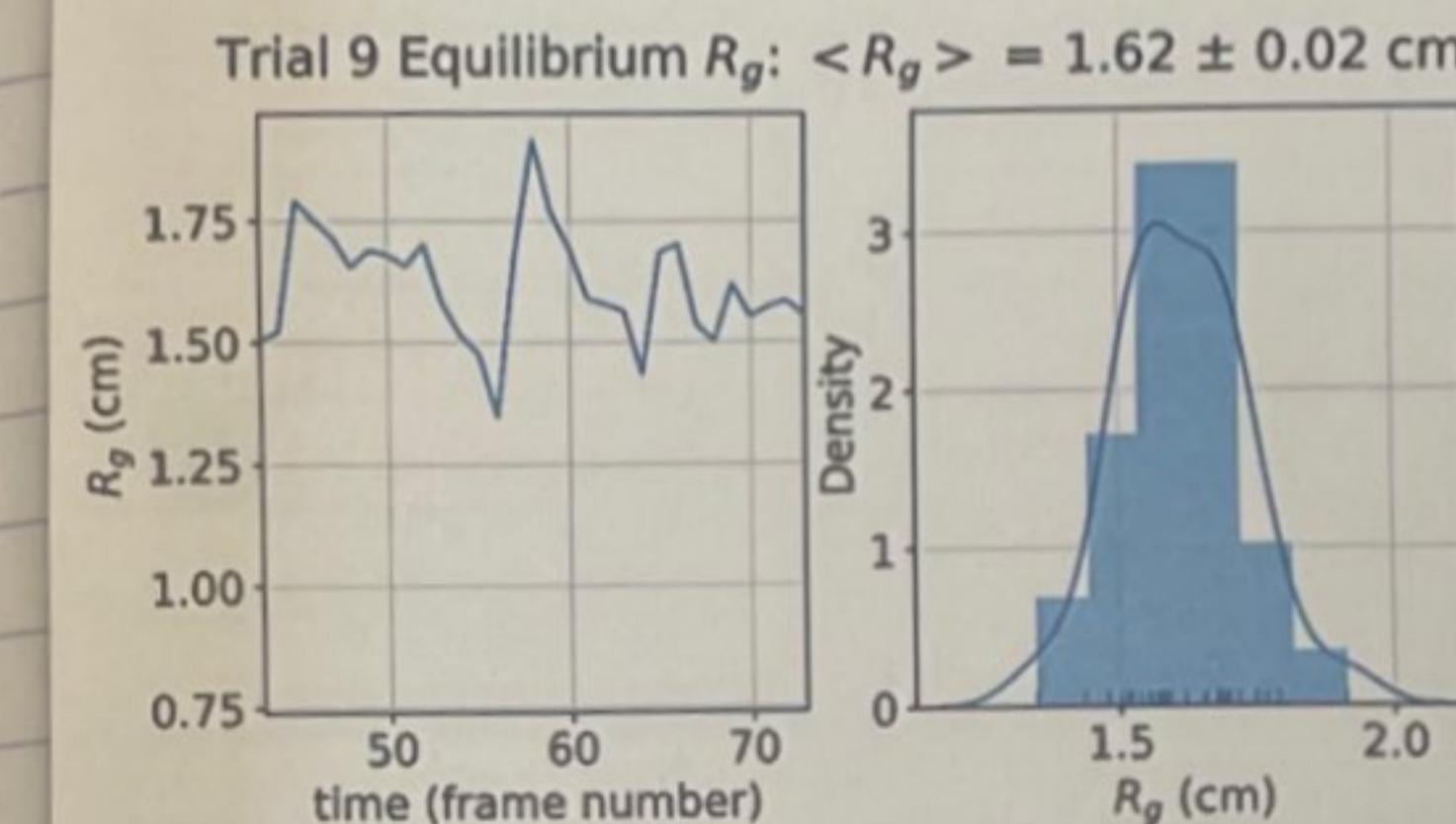
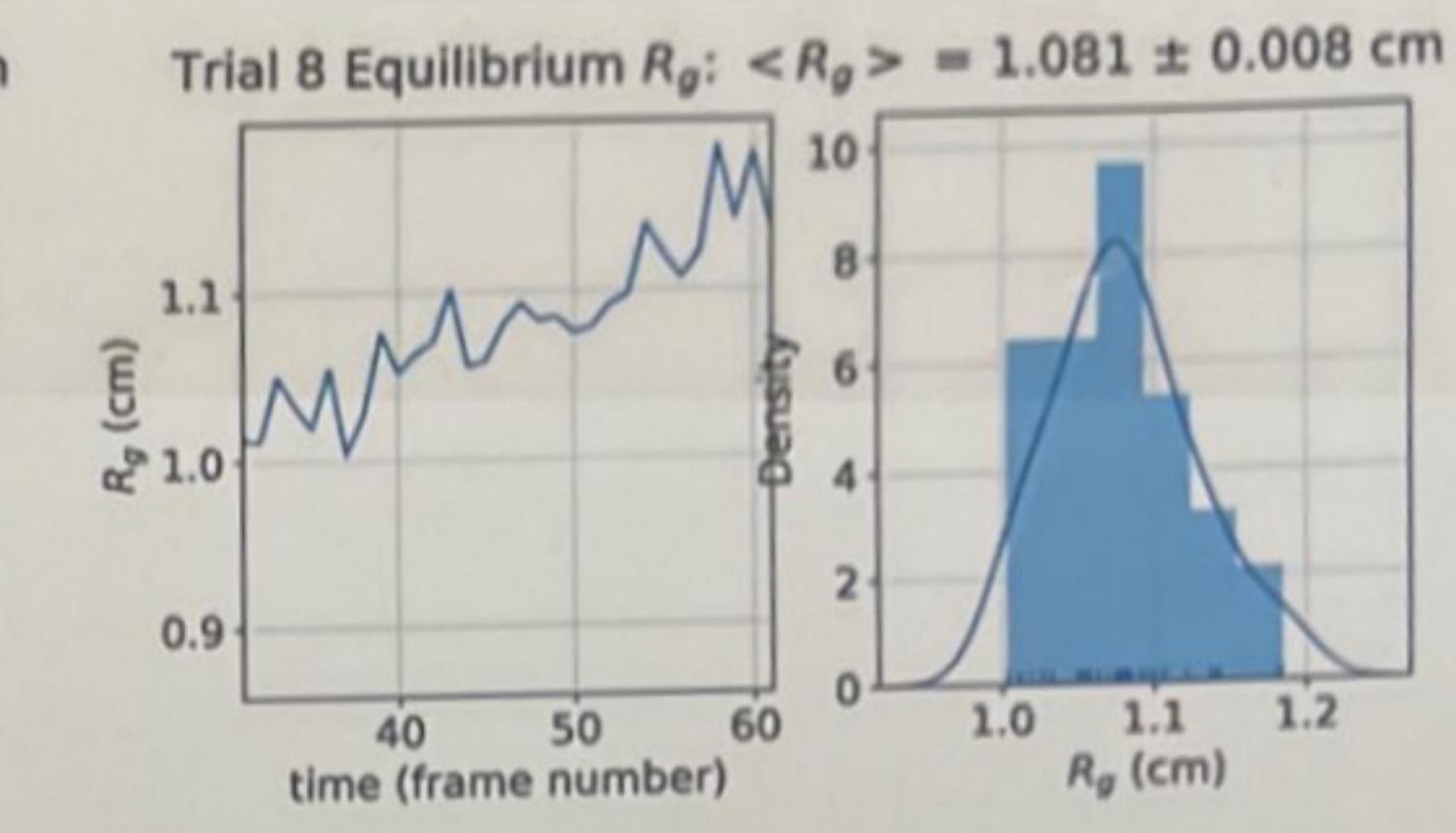
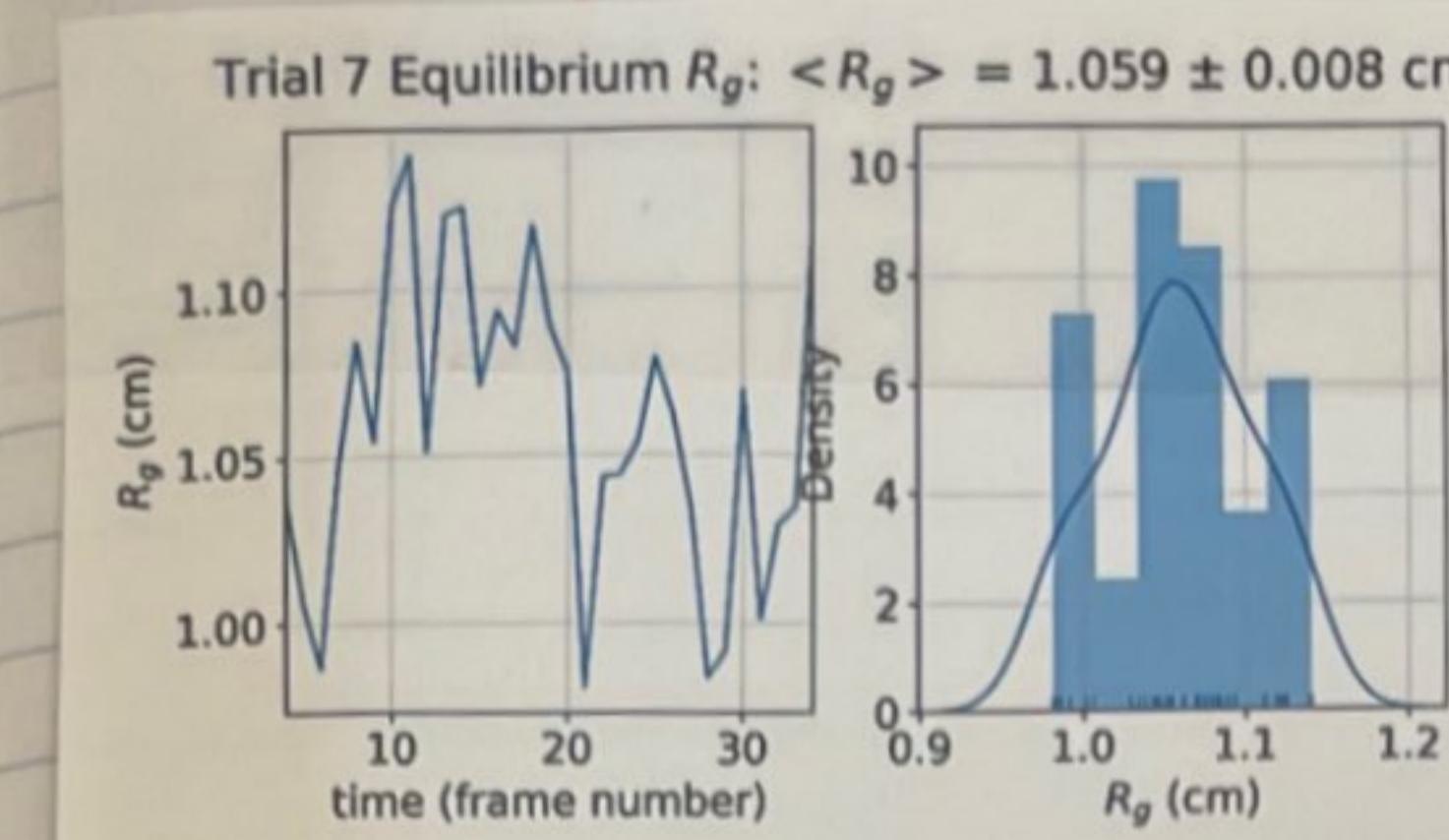
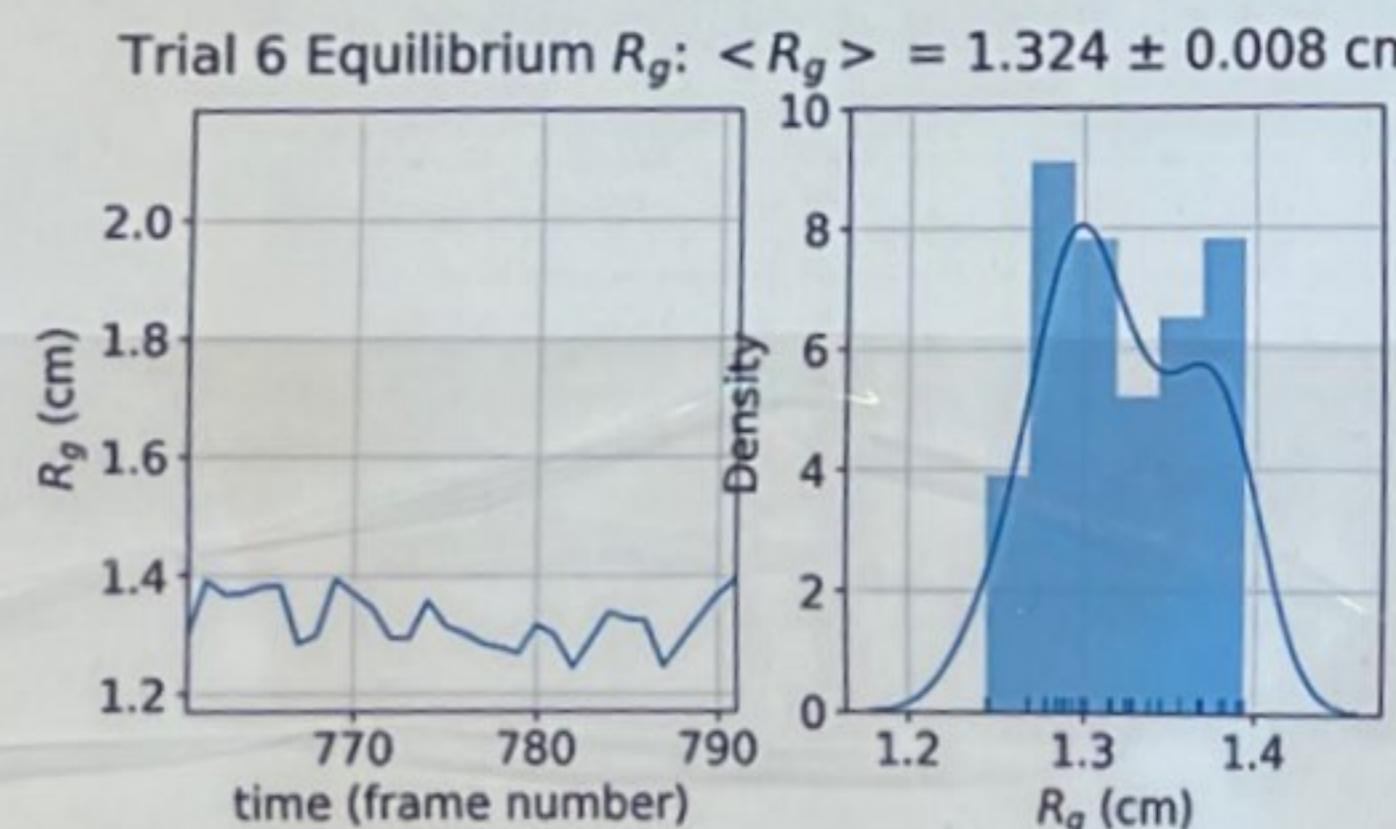
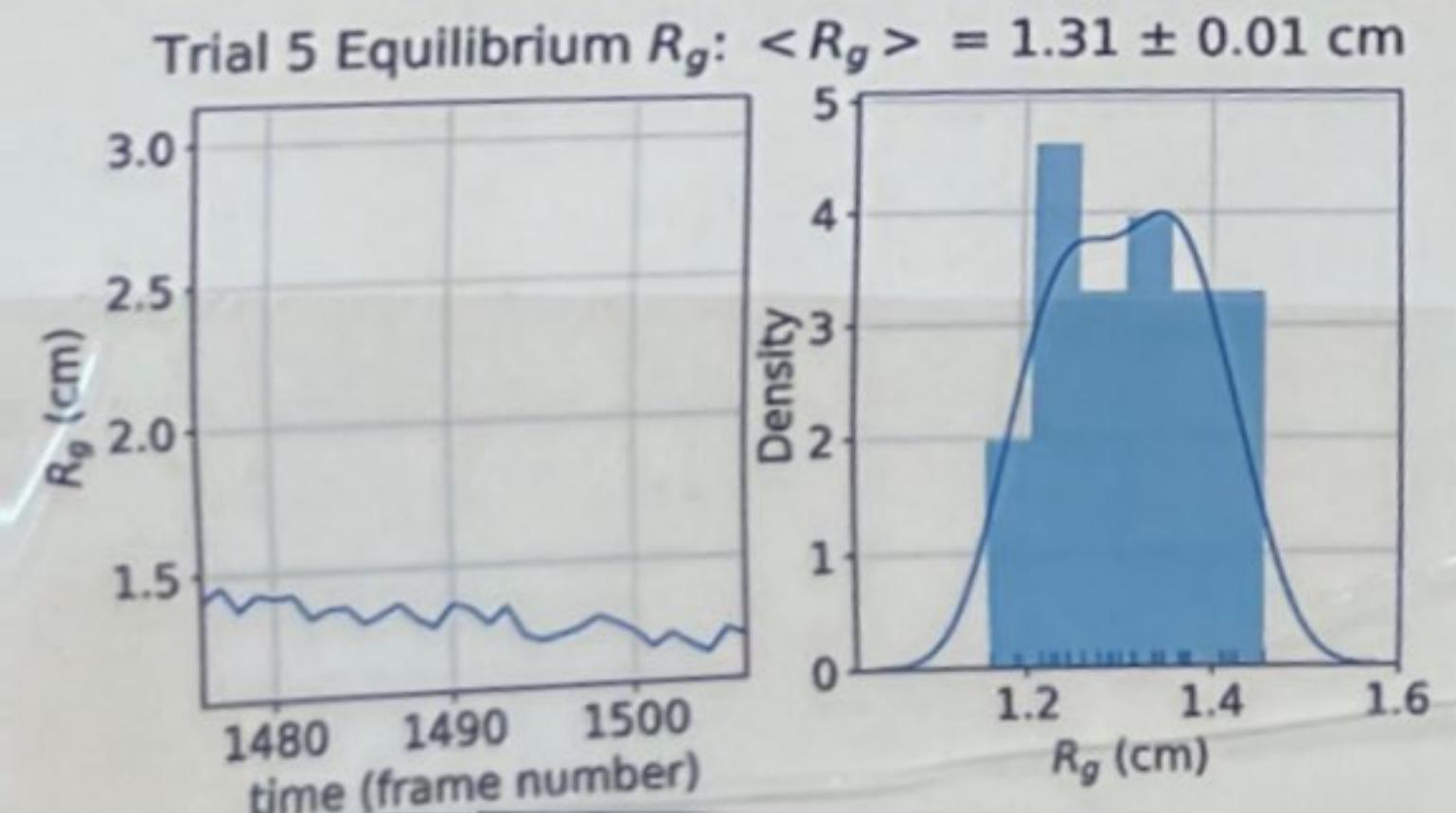
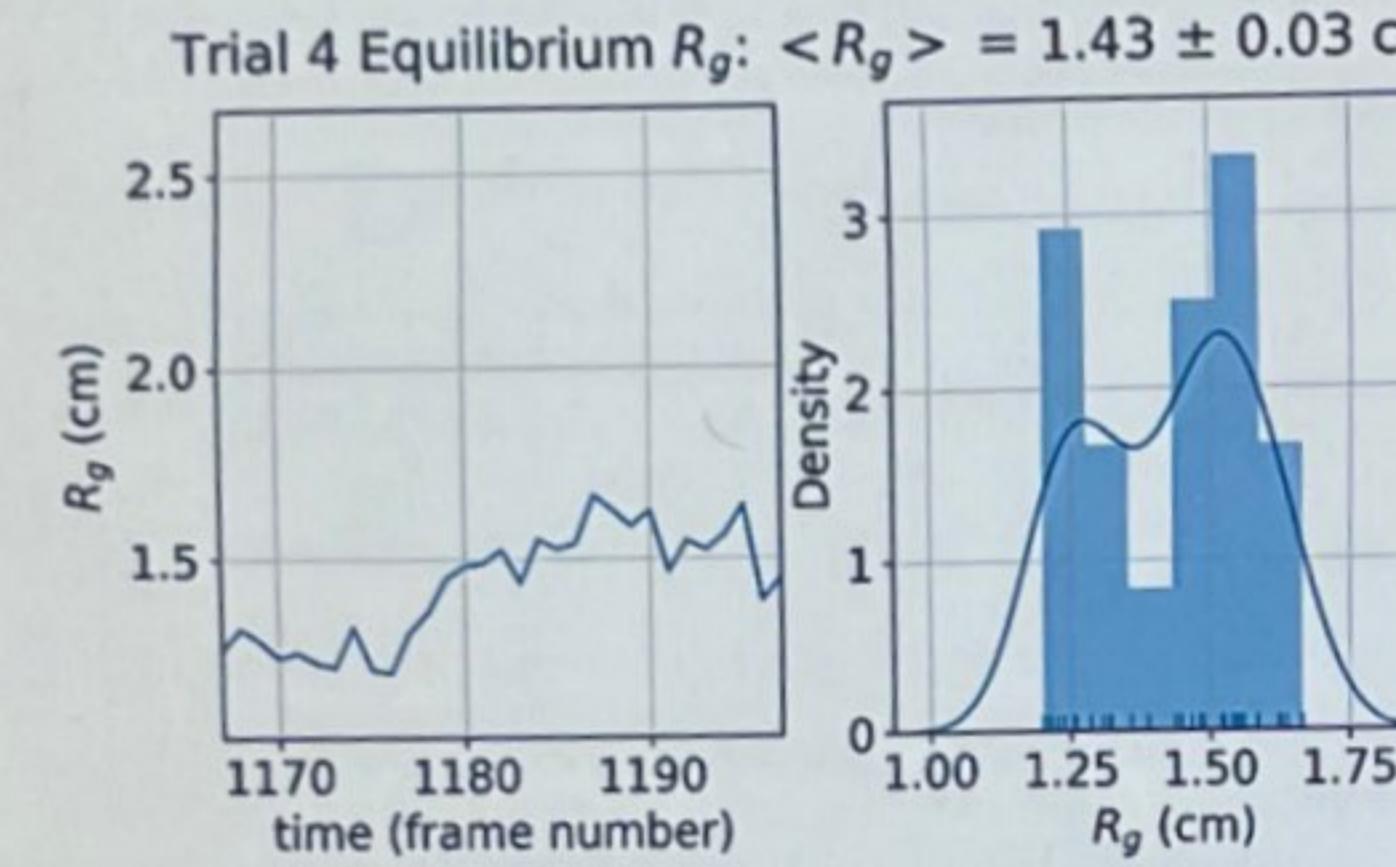
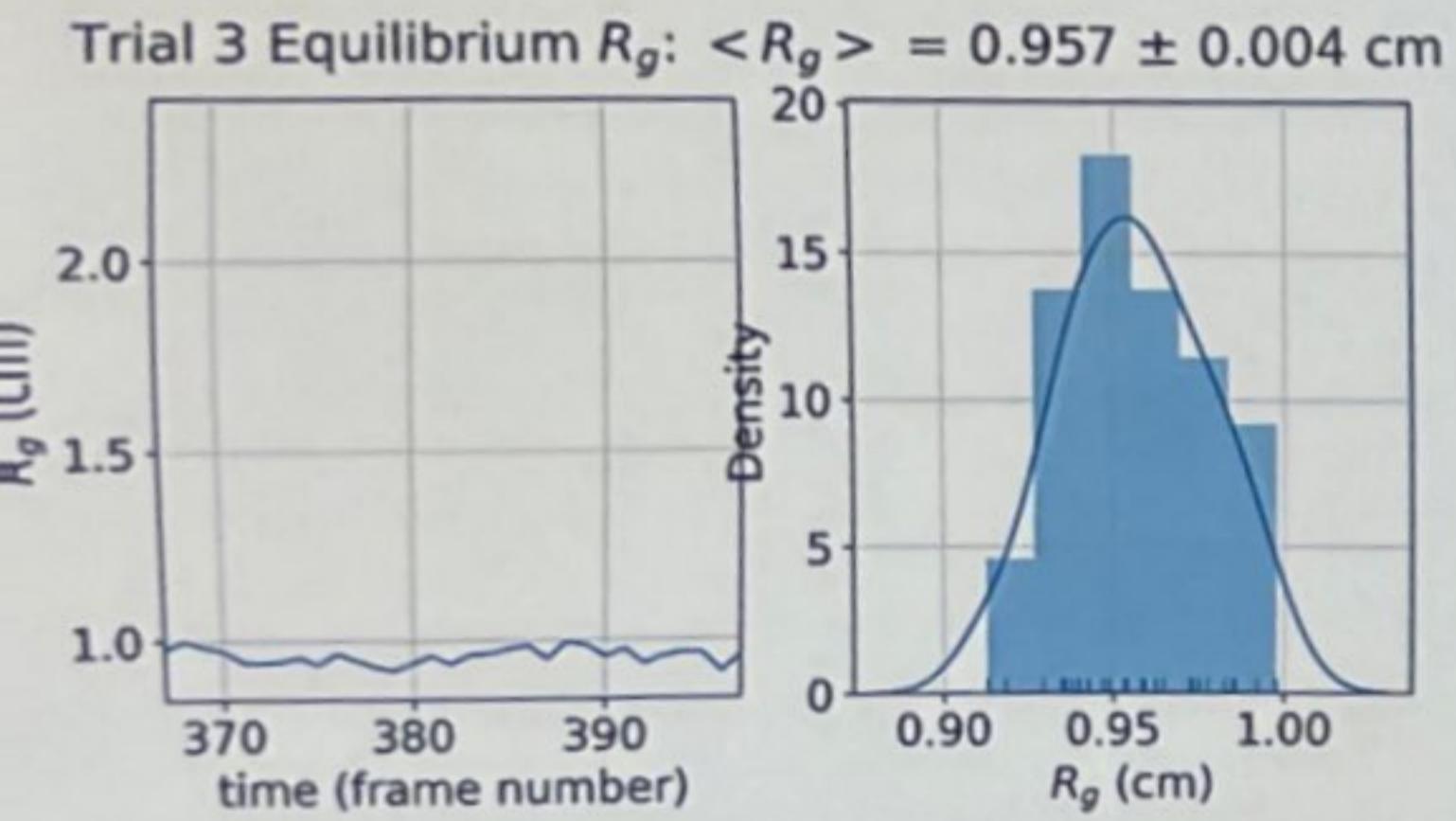
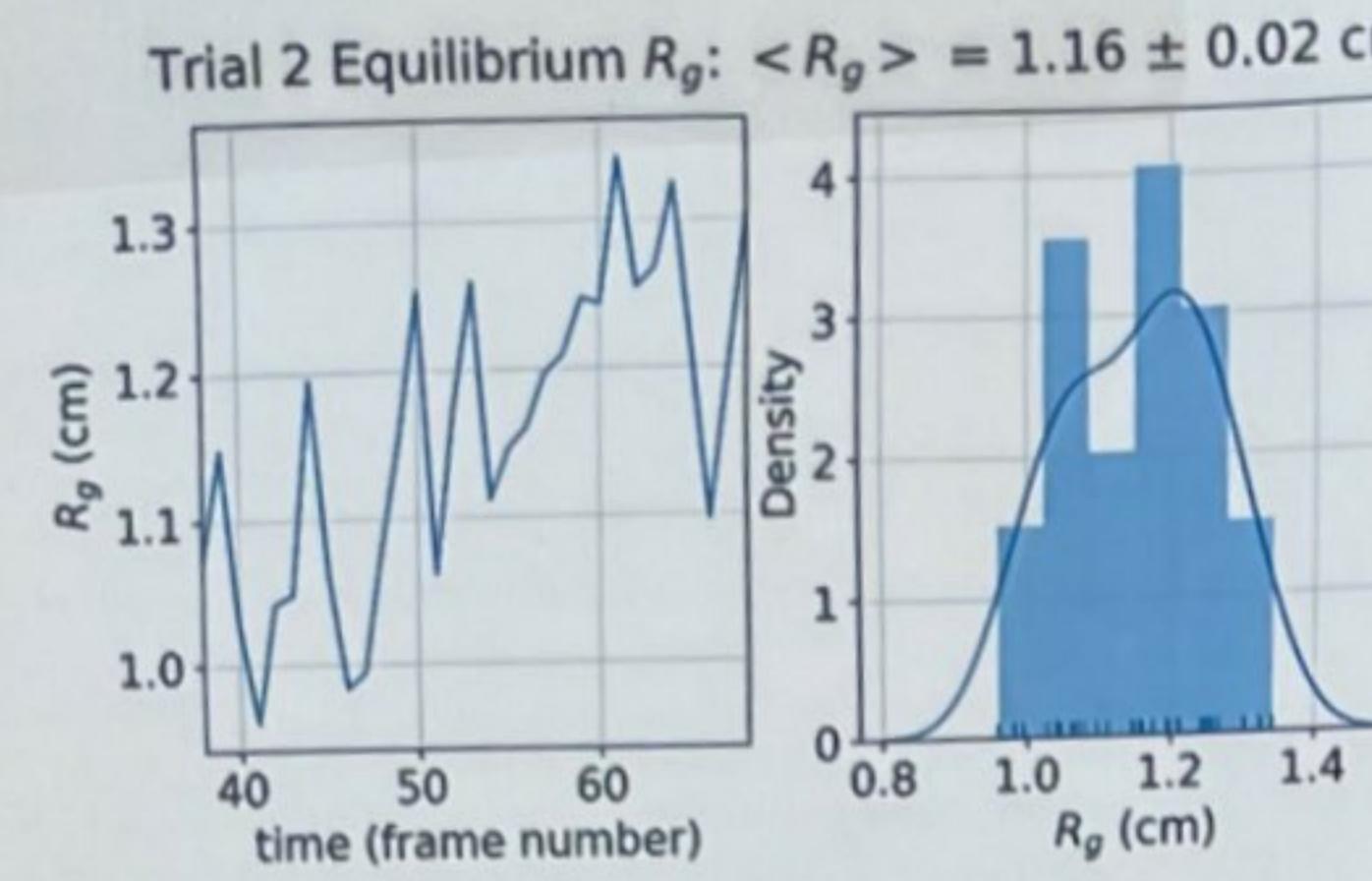
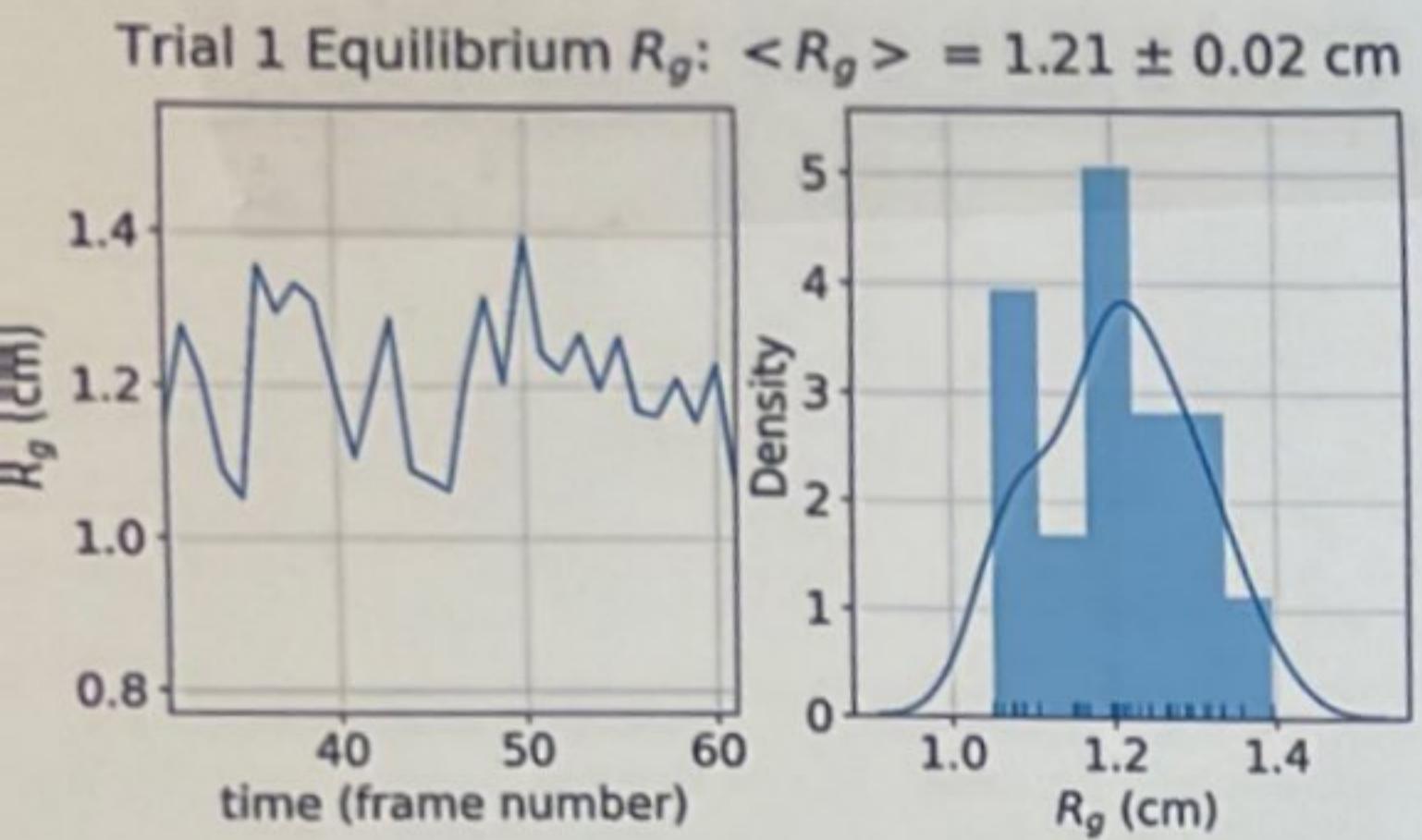


Fig 5: The last 60 seconds of each ROG trial, and the corresponding ROG distributions  
 -Trials 2, 4, 8 were discarded and not used in the analysis  
 • Images generated using plot-rog.py

NEXT  
PAGE

NEXT  
PAGE

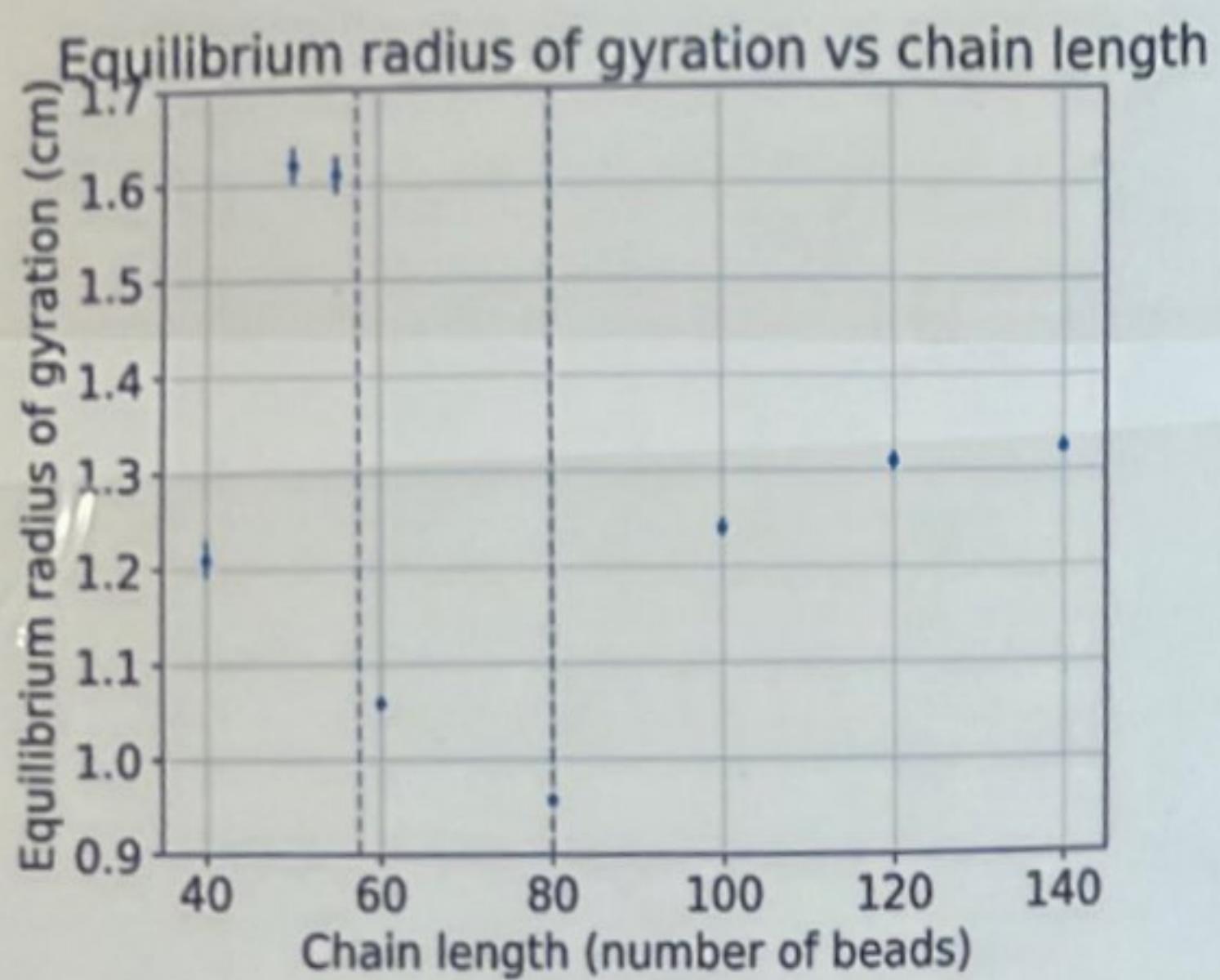


Fig 6: Equilibrium radius of gyration vs  $N$ . Each data point is the mean radius of gyration over the last 60 seconds of chain motion in a given trial. The error bars are given by the standard error in the mean.

The three black lines separate the three regimes of equilibrium motion.  
fit-Rg.py for more plotting

- The equilibrium radius of gyration seemed to fall into 3 regimes

#### Regime 1: $N < 60$

- This regime saw chains too short to form natural spirals
- These chains preferred an equilibrium U shape, and as a result, were much more inclined to have larger variations in equilibrium  $R_g$  due to having a more flexible shape than a spiral. Hence the large error bars when compared to other regimes
- This regime naturally saw a large increase in  $R_g$  w/ chain length
- The chain links have a maximum bending angle. For short chains, most of the links must be near this maximum bend to produce a spiral, which is a very unlikely state for the system to find itself in

- Even when starting in a spiral, chains in this regime would just open, as seen in trial 9

#### Regime 2: $60 < N < 80$

- This regime saw chains forming loose spirals
- Increasing  $N$  saw the mass of the outer loops of chain increase ~~w/ this~~
- This made it less likely for the spiral to open in fast random motion, and meant that for larger  $N$ , the chain would be more likely to seek to fill its area
- The result is  $R_g$  decreasing w/  $N$

#### Regime 3: $N > 80$

- This regime saw area filling spirals
- The large mass of the outer loops would trap the inner loops in an decreasing space until the area was full
- Because the spirals could no longer tighten, the radius of gyration had to grow with  $N$ . This regime behaves according to the model I described on page 35, and appears to grow as  $R_g \propto \sqrt{N}$
- More data is needed to perform an appropriate fit

- Investigation for  $N = 160$  saw that the spiral was opened. The chain's motion continued for hours w/ no equilibrium. This suggests a fourth regime, perhaps the

### Analysis of Survival Probability:

- The Kolmogorov Smirnov Test can be used to determine if two data sets come from the same distribution

- The `scipy.stats.kstest`, given two arrays A and B tests the following null-hypothesis:  
The distributions A and B are identical

Because the p-value is the probability that the null hypothesis is true, we actually want a p-value close to 1

- Running `ktest` on each distribution ~~pair~~ on page 23, results in p-value 1.0 for every pair
- This is evidence that every distribution there actually comes from the same curve

Then, the statistics of opening times can be analyzed w/o considering chain length by rescaling the mean times for each chain to unity

- Summary and abstract in ~~KNOT-Abstract~~  
KNOT-Abstract-And-Summary.pdf