Knots and Random Walks in Vibrated Granular Chains

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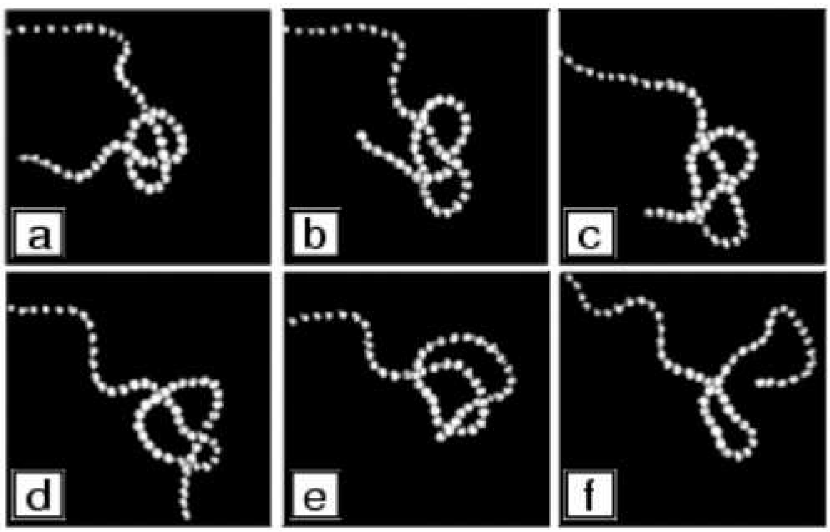

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Motivation

Topological constraints, entanglements:

- Reduce accessible phase space
- Involve large relaxation time scales
- Affect dynamics, flow

$$\eta \sim \tau \sim N^3$$

Relevance:

- Polymers: melts, rubber, gels
- DNA, biomolecules

Difficulties:

- Hard to observe directly
- Slow dynamics
- Finite size effects

Granular "Polymers"

Mechanical bead-spring:

$$U(\{\mathbf{R}_i\}) = v_0 \sum_{i \neq j} \delta(\mathbf{R}_i - \mathbf{R}_j) + \frac{3}{2b^2} \sum_i (\mathbf{R}_i - \mathbf{R}_{i+1})^2$$

- Beads interact via hard core repulsions
- Rods act as springs (nonlinear, dissipative)
- Inelastic collisions: bead-bead, bead-plate
- Vibrating plate supplies energy

Advantages:

- Number of "monomers" can be controlled
- Topological constraints: can be prepared, observed directly

Vibrated Knot Experiment

- $t = 0$: knot placed at chain center
- Parameters:

— Number of monomers: $30 < N < 270$
— Minimal knot size: $N_0 = 15$

- Driving conditions:

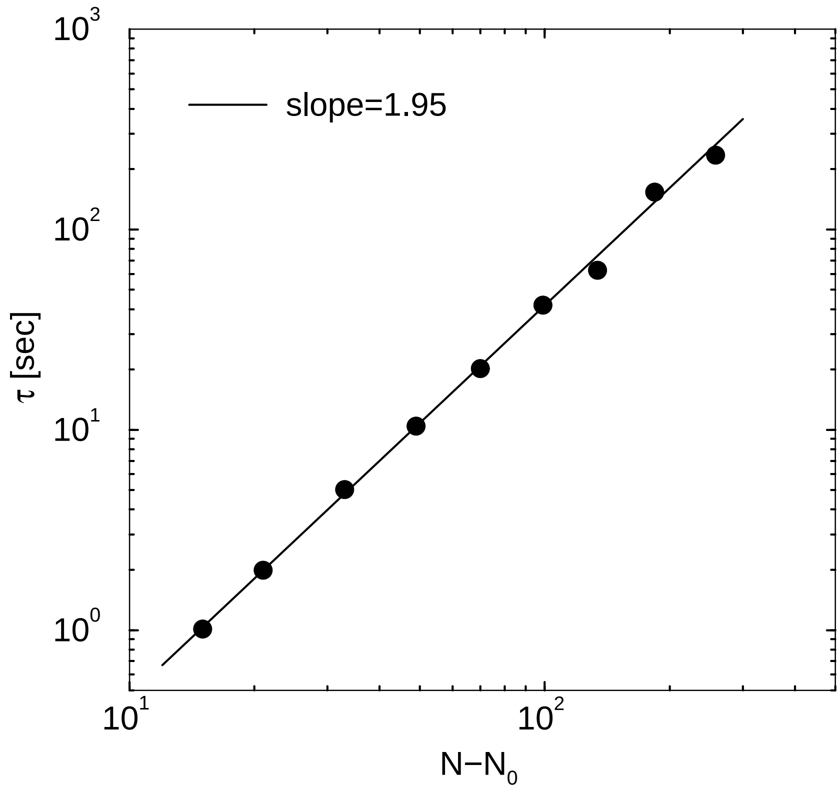
— Frequency: $\nu = 13Hz$
— Acceleration: $\Gamma = A\omega^2/g = 2.4$

- **Only measurement: opening time** t

Questions

1. Average opening time $\tau(N)$?
2. Survival probability $S(t, N)$?
   Distribution of opening times $R(t, N)$?

The Average Opening Time



$$\tau(N) \sim (N - N_0)^{\nu} \qquad \nu = 2.0 \pm 0.1$$

Opening time is diffusive

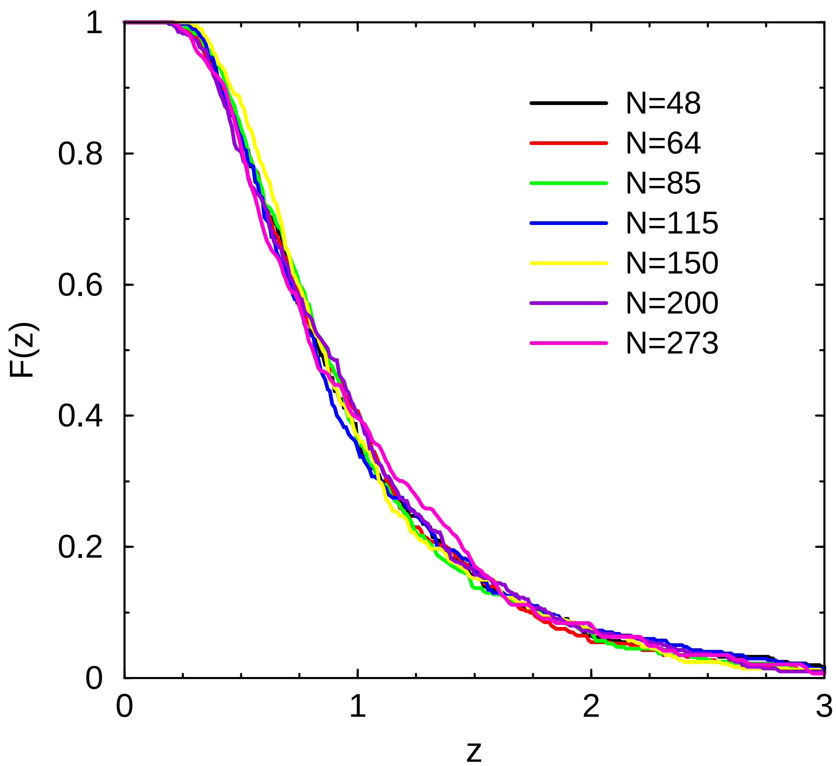
The Survival Probability

- $S(t, N)$ Probability knot "alive" at time t
- $R(t, N)$ Probability knot opens at time t

$$R(t, N) = -\frac{d}{dt} S(t, N)$$

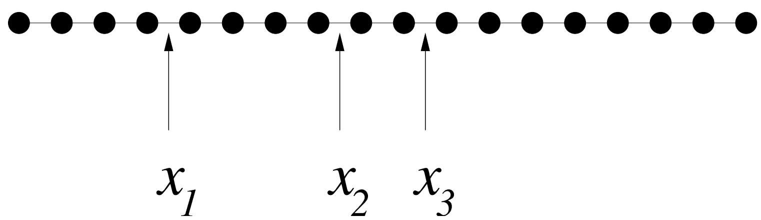
- $S(t, N)$ obeys scaling

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



$\boxed{\tau \text{ only relevant time scale}}$

Theoretical Model



Assumptions:

- Knot $\equiv$ 3 exclusion points
- Points hop randomly
- Points move independently (no correlation)
- Points are equivalent (size $= N_0/3$)

3 Random Walk Model:

- 1D walks with excluded volume interaction
- first point reaches boundary $\rightarrow$ knot opens

Diffusion in 3D

$$1<x_1<x_2<x_3<N-N_0 \quad \longrightarrow \quad 0<x<y<z<1$$

$$\frac{\partial}{\partial t}P(x,y,z,t) = \nabla^2 P(x,y,z,t)$$

- Boundary conditions

Absorbing: $P\big|_{x=0} = P\big|_{z=1} = 0$

Reflecting: $(\partial_x - \partial_y)P|_{x=y} = (\partial_y - \partial_z)P|_{y=z} = 0$

- Initial conditions $P\big|_{t=0}=\delta(x-x_0)\delta(y-x_0)\delta(z-x_0)$

- Survival probability

$$S_3(t) = \int_0^1 dx \int_x^1 dy \int_y^1 dz \; P(x,y,z,t)$$

$$\boxed{\textbf{3 walks in 1D} \equiv \textbf{1 walk in 3D}}$$

Product Solution

- Product of 1D solutions

$$P(x,y,z,t) = 3!p(x,t)p(y,t)p(z,t)$$

- 1D solution $p|_{x=0} = p|_{x=1} = 0 \quad p|_{t=0} = \delta(x-x_0)$

$$p_t(x,t) = p_{xx}(x,t)$$

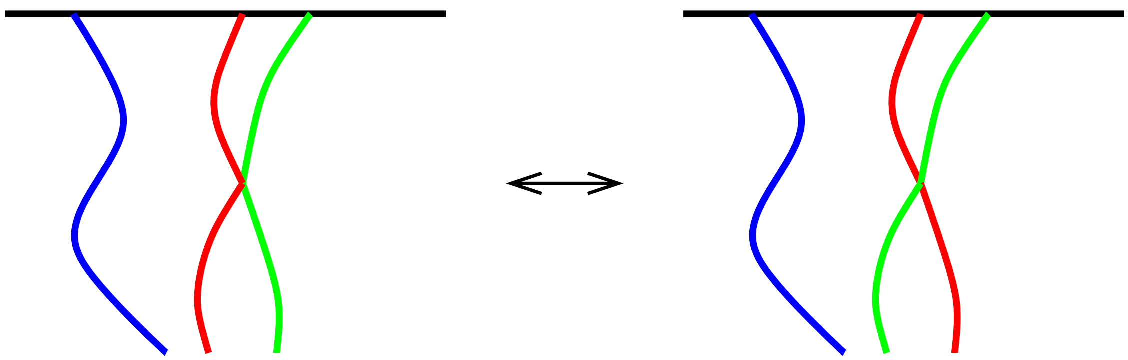
- m interacting walks survival probability

$$S_m(t) = [s(t)]^m$$

- 1 walk survival probability $s(t) = \int_0^1 dx\, p(x,t)$

$$s(t) = \frac{4}{\pi}\sum_{k=0}^{\infty}\frac{\sin[(2k+1)\pi x_0]}{2k+1}e^{-(2k+1)^2\pi^2 t}$$

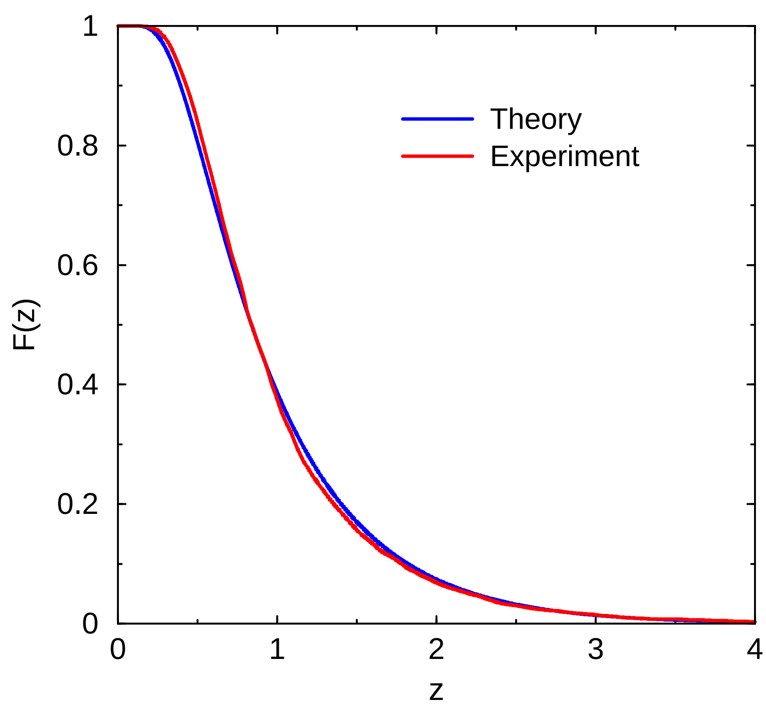
$$\boxed{\textbf{Reduced to noninteracting problem}}$$



Experiment vs. Theory

- Work with scaling variable $z = t/\tau$ $(\langle z \rangle = 1)$
- Combine different data sets (6000 pts)
- Fluctuations $\sigma^2 = \langle z^2 \rangle - \langle z \rangle^2$

$$\sigma_{\rm exp} = 0.62(1),\ \sigma_{\rm theory} = 0.63047\ (< 2\%)$$



No fitting parameters!

Excellent quantitative agreement

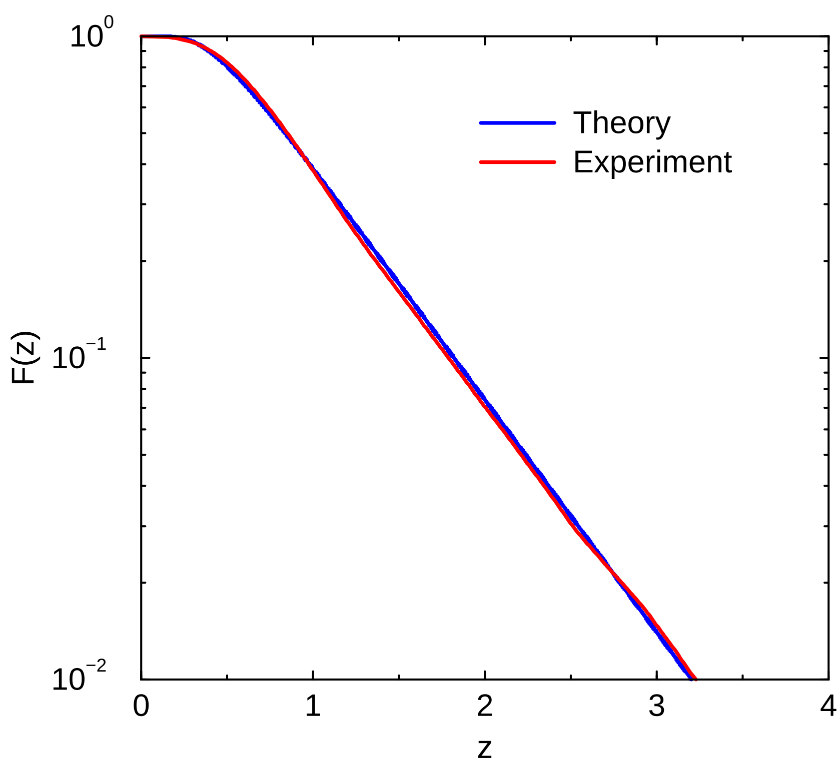
Large Exit Times

- Largest decay time dominates
- Large time tail is exponentially small

$$F(z) \sim e^{-\beta z} \qquad z \to \infty$$

- Decay coefficient

$$\beta_{\text{exp}} = 1.65(2) \qquad \beta_{\text{theory}} = 1.66440 \qquad (1\%)$$



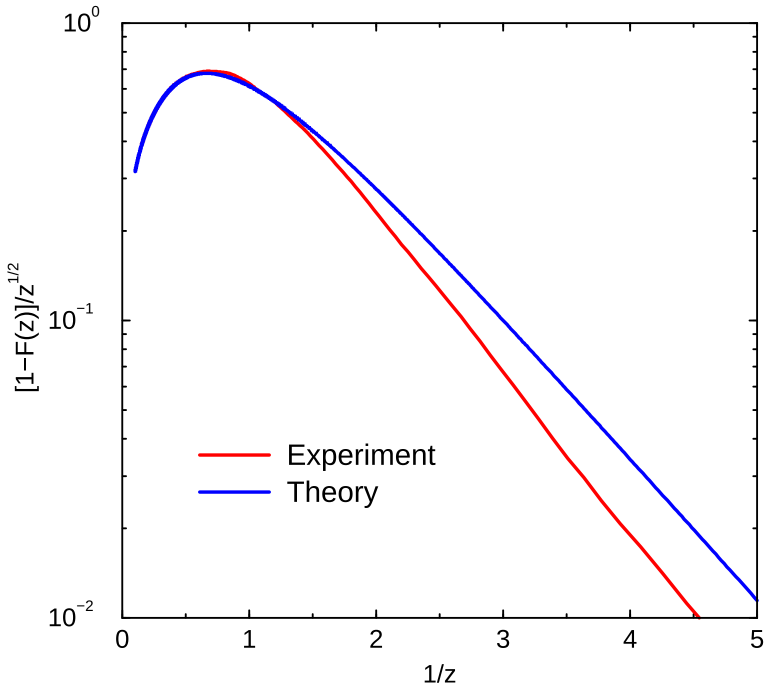
Small Exit Times

- Exponentially small (in $1/z$) tail

$$1 - F(z) \sim z^{1/2} e^{-\alpha/z} \qquad z \to 0$$

- Decay coefficient

$$\alpha_{\rm exp} = 1.2(1) \qquad \alpha_{\rm theory} = 1.11184 \qquad (10\%)$$



Larger discrepancy

Heuristic Argument (short times)

- Use scaling form

$$S(t,N) \sim F\left(\frac{t}{N^2}\right)$$

- Smallest exit time $t = \frac{N}{2}$, $1 - S \sim 2^{-N/2}$

$$1 - F\left(\frac{2}{N}\right) \sim e^{-\alpha N} \quad N \to \infty$$

$$1 - F(z) \sim e^{-\alpha/z} \quad z \to 0$$

Analytic Calculation

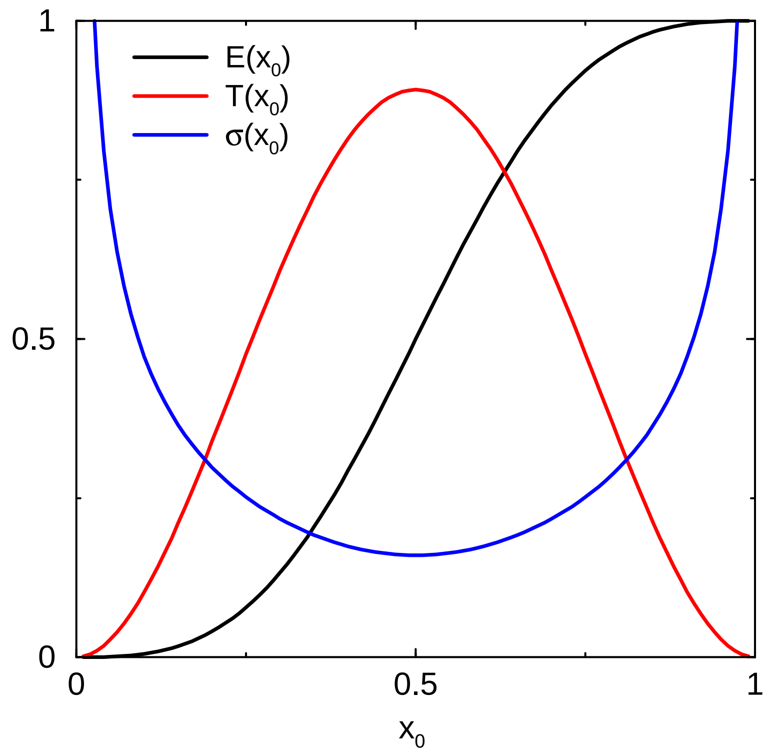
- Laplace transform of exact solution

$$s(q) = \int dt\, e^{-qt} s(t) = \frac{1}{\cosh(\sqrt{q}/2)}$$

- Steepest descent $s(q) \sim e^{-\sqrt{q}/2}$ as $q \to \infty$

$$1 - F(z) \sim z^{1/2} e^{-\alpha/z} \quad z \to 0$$

Off-Center knots = ruin problem



- Knot survival probability is equivalent to ruin problem with 3 players whose must maintan a heirarchy of assetts

- Average opening time $D\nabla^2 T(\mathbf{x}) = -1$

- Average opening probability $\nabla^2 E(\mathbf{x}) = 0$

Fluctuations diverge near boundary

Conclusions

- Knot governed by 3 exclusion points
- Exponential tails (large & small exit times)
- Macroscopic observables (t, $S(t)$) reveals details of a topological constraint

Predictive Power?

- $\tau(N) \simeq \tau_3 (N - N_0)^2 / D \Rightarrow N_0, D$
  $N_0 = 15.2$, $D = 11 Hz$
- $S(t)$ gives number of constraints m
  $m = 1$ for a small ring
- Off-center: ruin problem/ $\nabla^2 P = 0$
- Complicated constraints: $\tau, \sigma \sim 1/\ln m$
- Are the cross links correlated?
  no, beyond some correlation length ($\xi \cong 4$)

Granular Chains