Knots and Random Walks in Vibrated Granular Chains

Eli Ben-Naim
Los Alamos National Laboratory

Zahir Daya (Los Alamos)
Aaron Lauda (UC Riverside)
Peter Vorobieff (New Mexico)
Robert Ecke (Los Alamos)

Plan

I Knots

II Vibrated Knot Experiment

III Diffusion Theory

IV Experiment vs Theory

V Conclusions & Outlook
Knots in Physical Systems

- Knots in DNA strands
- Tying a microtubule with optical twizzers
- Knotted jets in accretion disks (MHD)
- Strain on knot (MD)

Wang JMB 71
Itoh, Nature 99
F Thomsen 99
Wasserman, Nature 99
Knots & Topological Constraints

- Knots happen
  \[ \text{probability (no knot)} \sim \exp(-N/N_0) \]
  Whittington JCP 88

- Knots tighten \((T = \infty)\)
  \[ n/N \to 0 \quad \text{when} \quad N \to \infty \]
  Sommer JPA 92

- Reduce size of chain \((m = \text{knot complexity})\)
  \[ R \sim N^{\nu}m^{-\alpha} \quad \alpha = \nu - 1/3 \]

- Reduce accessible phase space

- Large relaxation times
  \[ \tau_{\text{reptation}} \sim N^3 \]
  de Gennes, Edwards

- Weaken macromolecule

- Bio: affect chemistry, function
Granular Chains

Mechanical analog of bead-spring model

\[ U(\{R_i\}) = v_0 \sum_{i \neq j} \delta(R_i - R_j) + \frac{3}{2b^2} \sum_i (R_i - R_{i+1})^2 \]

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

Advantages

- Number of beads can be controlled
- Topological constraints: can be prepared, observed directly
Vibrated Knot Experiment

- $t = 0$: trefoil knot placed at chain center
- Parameters
  - Number of monomers: $30 < N < 270$
  - Minimal knot size: $N_0 = 15$
- Driving conditions
  - Frequency: $\nu = 13\, Hz$
  - Acceleration: $\Gamma = A\omega^2/g = 3.4$

Only measurement: opening time $t$

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

Average over 400 independent measurements

\[ \tau(N) \sim (N - N_0)^\nu \quad \nu = 2.0 \pm 0.1 \]

Opening time is diffusive
The Survival Probability

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

\[
S(t, N) = 1 - \int_0^t dt' R(t', N)
\]

- $S(t, N)$ obeys scaling

\[
S(t, N) = F(z) \quad z = \frac{t}{\tau(N)}
\]

$\tau$ 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

\[ 1 < x_1 < x_2 < x_3 < N - N_0 \quad \rightarrow \quad 0 < x < y < z < 1 \]

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

- **Boundary conditions**
  - **Absorbing:** \( P\big|_{x=0} = P\big|_{z=1} = 0 \)
  - **Reflecting:** \((\partial_x - \partial_y) P\big|_{x=y} = (\partial_y - \partial_z) P\big|_{y=z} = 0 \)

- **Initial conditions** \( P\big|_{t=0} = \delta(x-x_0)\delta(y-y_0)\delta(z-x_0) \)

- **Survival probability**

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

3 walks in 1D \( \equiv \) 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 case \( p|_{x=0} = p|_{x=1} = 0 \quad p|_{t=0} = \delta(x - x_0) \)
  \[ p_t(x, t) = p_{xx}(x, t) \]

- 1 walk survival probability \( s(t) = \int_0^1 dx \ p(x, t) \)
  \[ s(t) = \frac{4}{\pi} \sum_{k=0}^{\infty} \frac{\sin[(2k + 1)\pi x_0]}{2k + 1} e^{-\frac{(2k+1)^2\pi^2 t}{2}} \]

- \( m \) interacting walks survival probability
  \[ S_m(t) = [s(t)]^m \]

- Average opening time
  \[ \langle t \rangle \simeq \tau_m \frac{(N - N_0)^2}{D} \quad \tau_3 = 0.056213 \]

Reduced to noninteracting problem
Alternative Derivation

Exchange identities of walkers when paths cross
Experiment vs. Theory

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

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

No fitting parameters!

Excellent quantitative agreement
The Exit Time Probability

Scaling function

\[ R(t, N) = \frac{1}{\tau} G(z) \quad z = \frac{t}{\tau(N)} \]

\[ G(z) = -\frac{d}{dz} F(z) \]

![Graph showing the comparison between experimental and theoretical G(z) values.](image-url)
Large Exit Times

- Largest decay time dominates
- Large time tail is exponentially small
  \[ F(z) \sim e^{-\beta z} \quad z \gg 1 \]

- Decay coefficient \( \beta = m \pi^2 \tau_m \)
  \[ \beta_{\text{exp}} = 1.65(2) \quad \beta_{\text{theory}} = 1.66440 \quad (1\%) \]
Small Exit Times

- Exponentially small (in $1/z$) tail
  \[ 1 - F(z) \sim z^{1/2} e^{-\alpha / z} \quad z \ll 1 \]
- Decay coefficient $\alpha = 1/16\tau_m$
  \[ \alpha_{\text{exp}} = 1.2(1) \quad \alpha_{\text{theory}} = 1.11184 \quad (10\%) \]

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 \( s(t) + \) steepest descent
  \[
  1 - F(z) \sim z^{1/2} e^{-\alpha/z}
  \]

• Complex knots: \( e^{-1/t} \sim m^{-1} \)
  \[
  \tau \sim \sigma \sim \frac{1}{\ln m} \quad m \gg 1
  \]
Different knots ($m = 1, 3, 5, 7$)
Off-Center Initial Conditions

Decay coefficient independent of $x_0$

$$S_m(t) \simeq A(x_0)e^{-m\pi^2 t}$$

Eventually, initial conditions are forgotten
Knots Opening & the Gambler Ruin Problem

- The exit probability
  \[ \nabla^2 E(x_1, \ldots, x_d) = 0 \]

- Linear in 1D: \( E(x_0) = x_0 \)

- In general dimension \( d \equiv m \)
  \[ E(x_0) \sim (x_0)^d \quad x_0 \ll 1 \]

- The average exit time
  \[ D \nabla^2 T(x_1, \ldots, x_d) = -1 \]

- General solution

\[
E(x_0) = \frac{d}{2} \left( \frac{4}{\pi} \right)^d \sum_{k_1 = 1}^{\infty} \sum_{k_2 = 0}^{\infty} \ldots \sum_{k_d = 0}^{\infty} (-1)^{k_1 - 1} k_1 \sin[k_1 \pi x_0] \prod_{i=2}^{d} \frac{\sin[(2k_i + 1)\pi x_0]}{(2k_i + 1)}
\]

\[
T(x_0) = \frac{1}{\pi^2} \left( \frac{4}{\pi} \right)^d \sum_{k_1 = 0}^{\infty} \ldots \sum_{k_d = 0}^{\infty} \frac{1}{\sum_{i=1}^{d} (2k_i + 1)^2} \prod_{i=1}^{d} \frac{\sin[(2k_i + 1)\pi x_0]}{(2k_i + 1)}
\]

**Knot opening \equiv 3** gamblers ruin problem with fixed wealth hierarchy
Predictions

- Good agreement for $S(t)$, $S_{\text{far}}(t)$, $S_{\text{close}}(t)$
- Poor agreement for $E(x_0)$, $T(x_0)$
- Current data insufficient (600pts)

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
- Knot relaxation governed by number of crossing points
- Athermal driving, yet, effective degrees of freedom randomized

Outlook

- Different knot types
- Correlation between crossing points

Many possibilities with granular chains
Entropic Tightening
with Matthew Hastings, Zahir Daya, Robert Ecke

- Equilibrium (counting states) prediction
  \[ P(n) \propto [n(N - n)]^{-d/2} \]
  \[ n/N \to 0 \quad \text{when} \quad N \to \infty \]

- Observed under nonequilibrium driving

Role of entropy?
My soul is an entangled knot
Upon a liquid vortex wrought
The secret of its untying
In four-dimensional space is lying

J. C. Maxwell