Knots and Random Walks in Vibrated Granular Chains

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E. Ben-Naim, Z. Daya, P. Vorobieff, R. Ecke, Phys. Rev. Lett. **86**, 1414 (2001)

Plan

I Knots

II Vibrated knot experiment

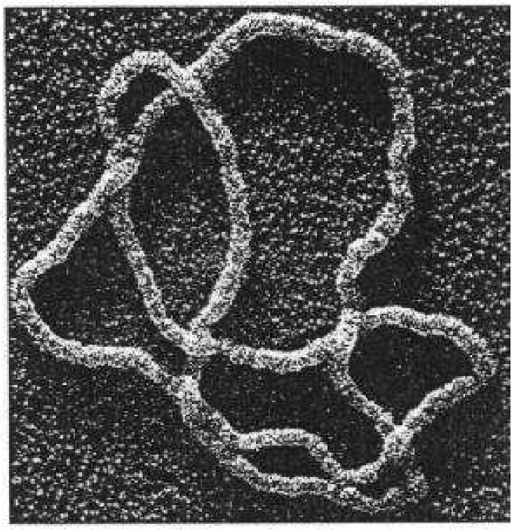
III Diffusion theory

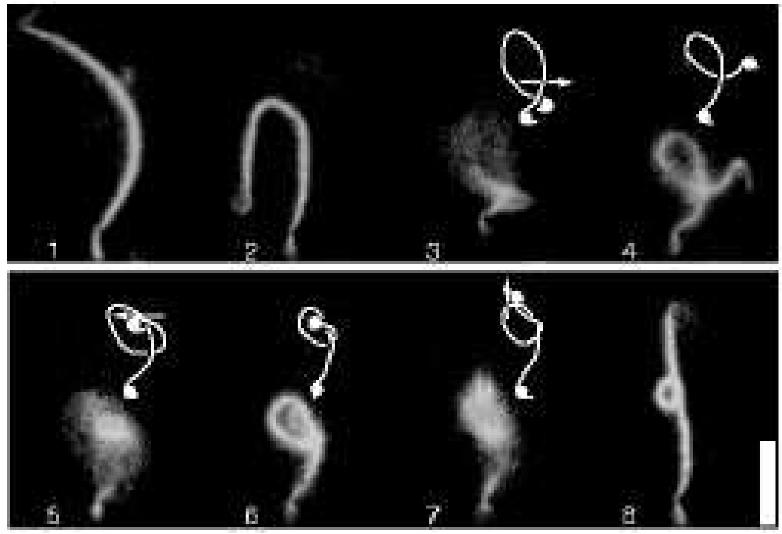
IV Experiment vs theory

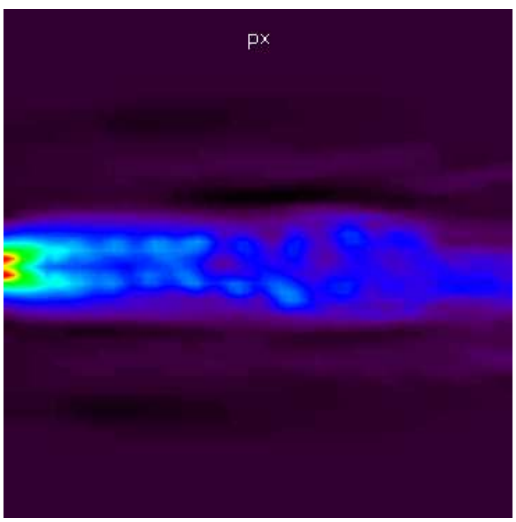
V First passage & adjoint equations

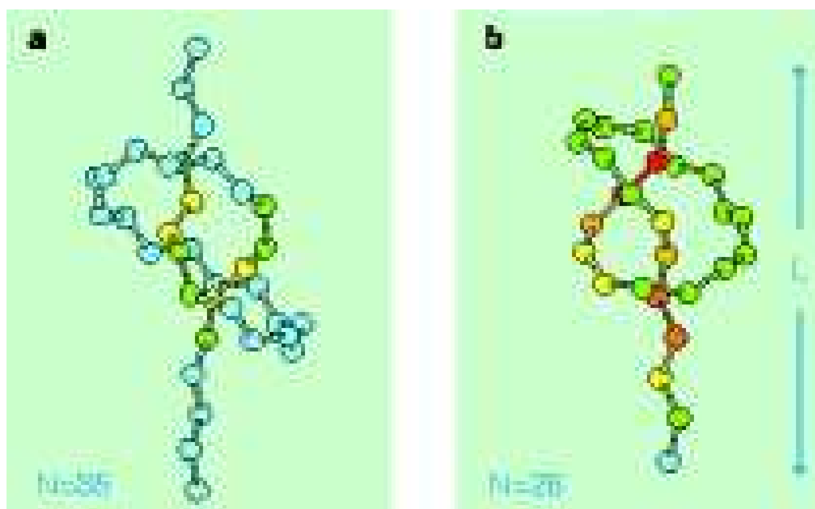
VI Conclusions & outlook

Knots in Physical Systems









Knots in DNA strands	Wang JMB 71
Tying a microtubule with optical twizzers	Itoh, Nature 99
Knotted jets in accretion disks (MHD)	F Thomsen 99
Strain on knot (MD)	Wasserman, Nature 99

Knots & Topological Constraints

- Knots happen — Whittington JCP 88

$$\text{probability(no knot)} \sim \exp(-N/N_0)$$

- Knots tighten ($T = \infty$) — Sommer JPA 92

$$n/N \to 0 \qquad when \qquad N \to \infty$$

- Reduce size of chain ($m =$ knot complexity)

$$R \sim N^\nu m^{-\alpha} \qquad \alpha = \nu - 1/3$$

- Reduce accessible phase space
- Large relaxation times — de Gennes, Edwards

$$\tau_{reptation} \sim N^3$$

- Weaken macromolecule
- Bio: affect chemistry, function

Granular Chains

Mechanical analog of bead-spring model

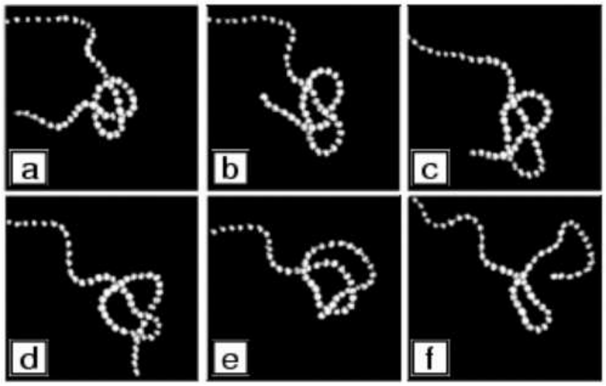
$$U(\{\mathbf{R}_i\}) = v_0 \sum_{i \neq j} \delta(\mathbf{R}_i - \mathbf{R}_j) + \frac{3}{2b^2} \sum_i (\mathbf{R}_i - \mathbf{R}_{i+1})^2$$

- Beads/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

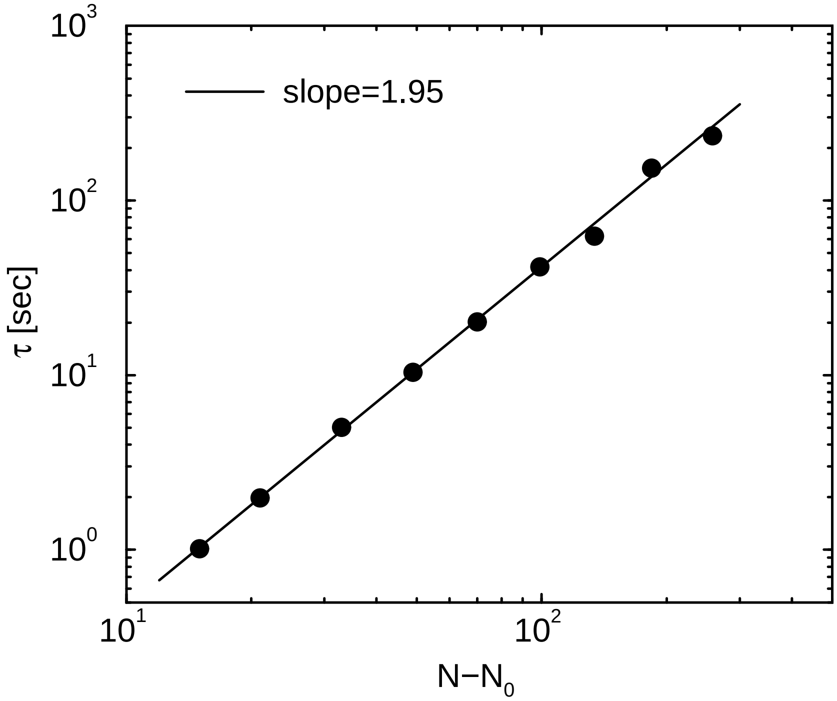


- $t = 0$: trefoil knot placed at chain center
- Parameters
  - — Number of monomers: $30 < N < 270$
  - — Minimal knot size: $N_0 = 15$
- Driving conditions
  - — Frequency: $\nu = 13Hz$
  - — Acceleration: $\Gamma = A\omega^2/g = 3.4$

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

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

$\boxed{\textbf{Opening time is diffusive}}$

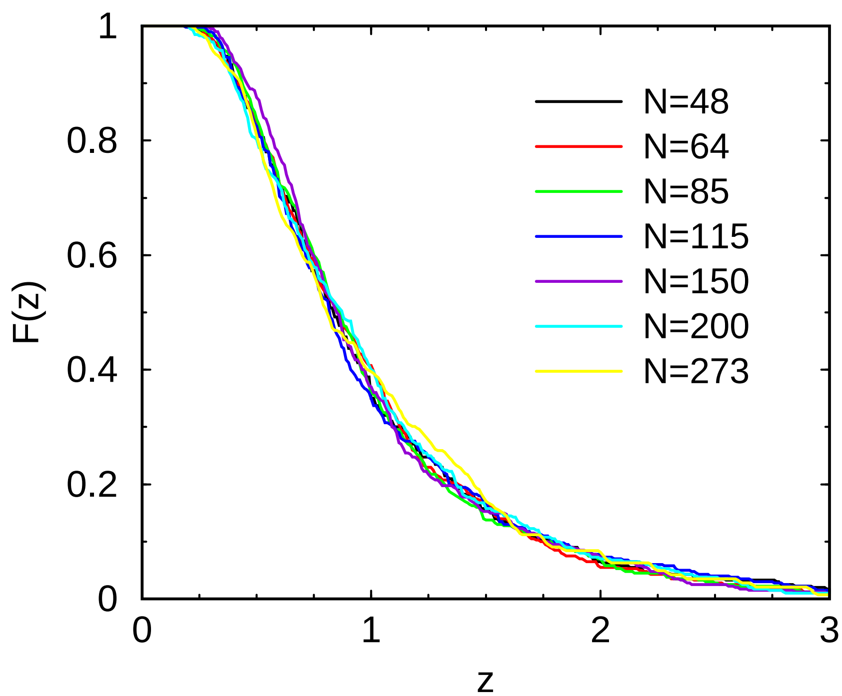
The Survival Probability

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

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

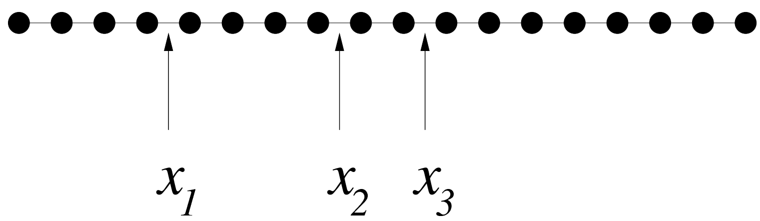
- $S(t, N)$ obeys scaling

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



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

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

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

3 walks in 1D $\equiv$ 1 walk in 3D

Product Solution

- Product of 1D solutions

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

- Boundary conditions (absorbing only)

$$p|_{x=0} = p|_{x=1} = 0$$

- Initial conditions

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

- Diffusion equation

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

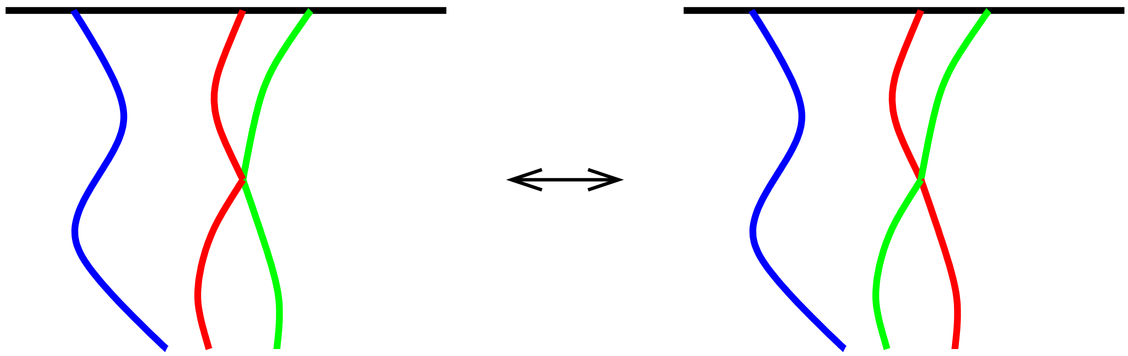
- 1 walk survival probability

$$s(t) = \int_0^1 dx\, p(x,t)$$

- 3 walks survival probability

$$S_3(t) = [s(t)]^3$$

Why does this work?



- Exchange identities of walkers when paths cross

- Reduce interacting particle problem to noninteracting particle problem

- Eliminate complicated geometry

- Reduced to one-dimensional problem

- Diffusive opening times

$$\langle\, t\,\rangle \simeq \tau_m \frac{(N-N_0)^2}{D} \qquad \tau_3 = 0.056213$$

The 1D problem

- Expansion in complete basis

$$p(x,t) = \sum_{n=1} a_n(x_0,t)\sin(n\pi x)$$

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

$$\frac{da}{dt} = -n^2\pi^2 a \quad \Rightarrow \quad a_n(x_0,t) = a_n(x_0,0)e^{-n^2\pi^2 t}$$

- Initial conditions $p(x,t=0) = \delta(x-x_0)$

$$a_n(x_0,0) = 2\int dx\, p(x,t=0)\sin(n\pi x) = 2\sin(n\pi x_0)$$

- The probability distribution

$$p(x,x_0,t) = 2\sum_{n=1} \sin(n\pi x_0)\sin(n\pi x)e^{-n^2\pi^2 t}$$

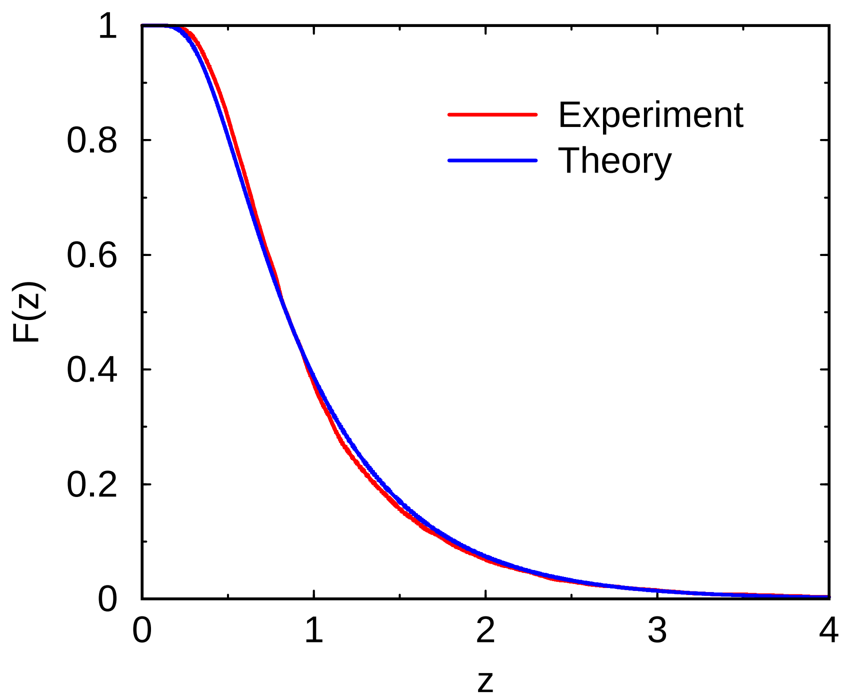
- The survival probability $s(t) = \int_0^1 dx\, p(x,t)$

$$s(t) = \frac{4}{\pi}\sum_{n\mathrm{odd}} \frac{\sin[n\pi x_0]}{n} e^{-n^2\pi^2 t}$$

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!

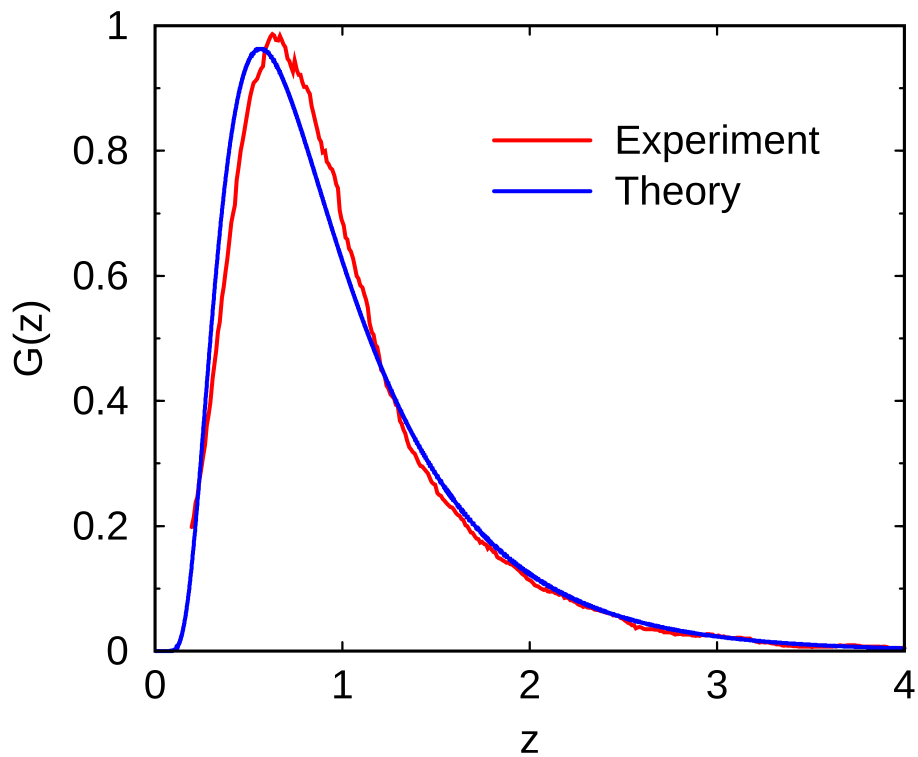
Excellent quantitative agreement

The Exit Time Probability

Scaling function

$$R(t,N) = \frac{1}{\tau}G(z) \qquad z = \frac{t}{\tau(N)}$$

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



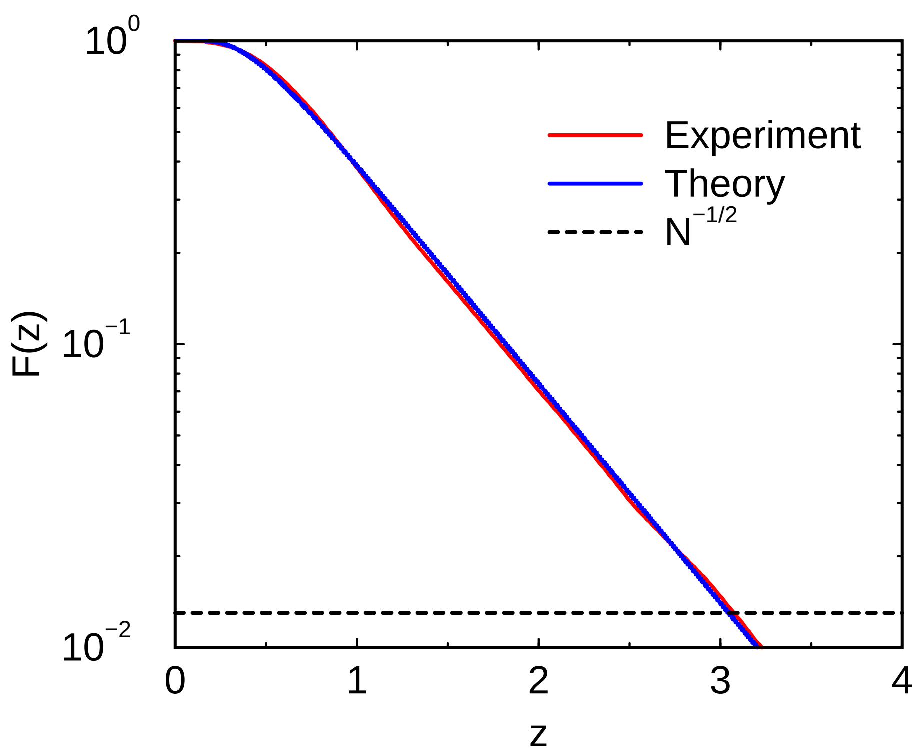
Large Exit Times

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

$$F(z) \sim e^{-\beta z} \qquad z \gg 1$$

- Decay coefficient $\beta = m\pi^2\tau_m$

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



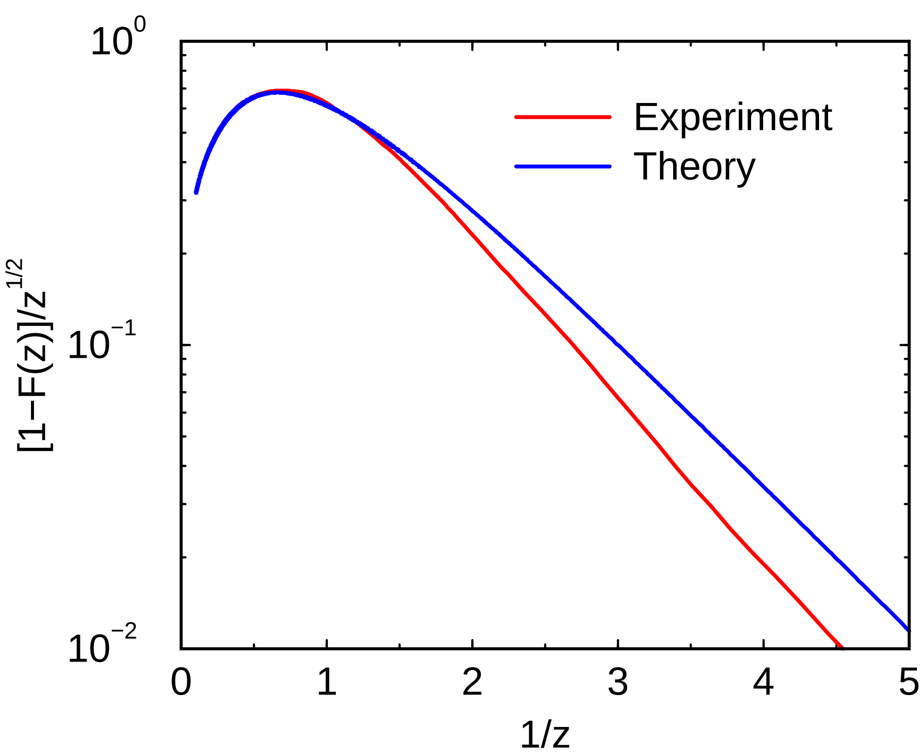
Small Exit Times

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

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

- Decay coefficient $\alpha = 1/16\tau_m$

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



Larger discrepancy

Short Times

- Use scaling form $S(t, N) \sim F\left(\frac{t}{N^2}\right)$
- Smallest exit time $t = \frac{N}{2}$, $1 - S \sim 2^{-N/2}$

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

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

Analytic Calculation

- Laplace transform of exact solution

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

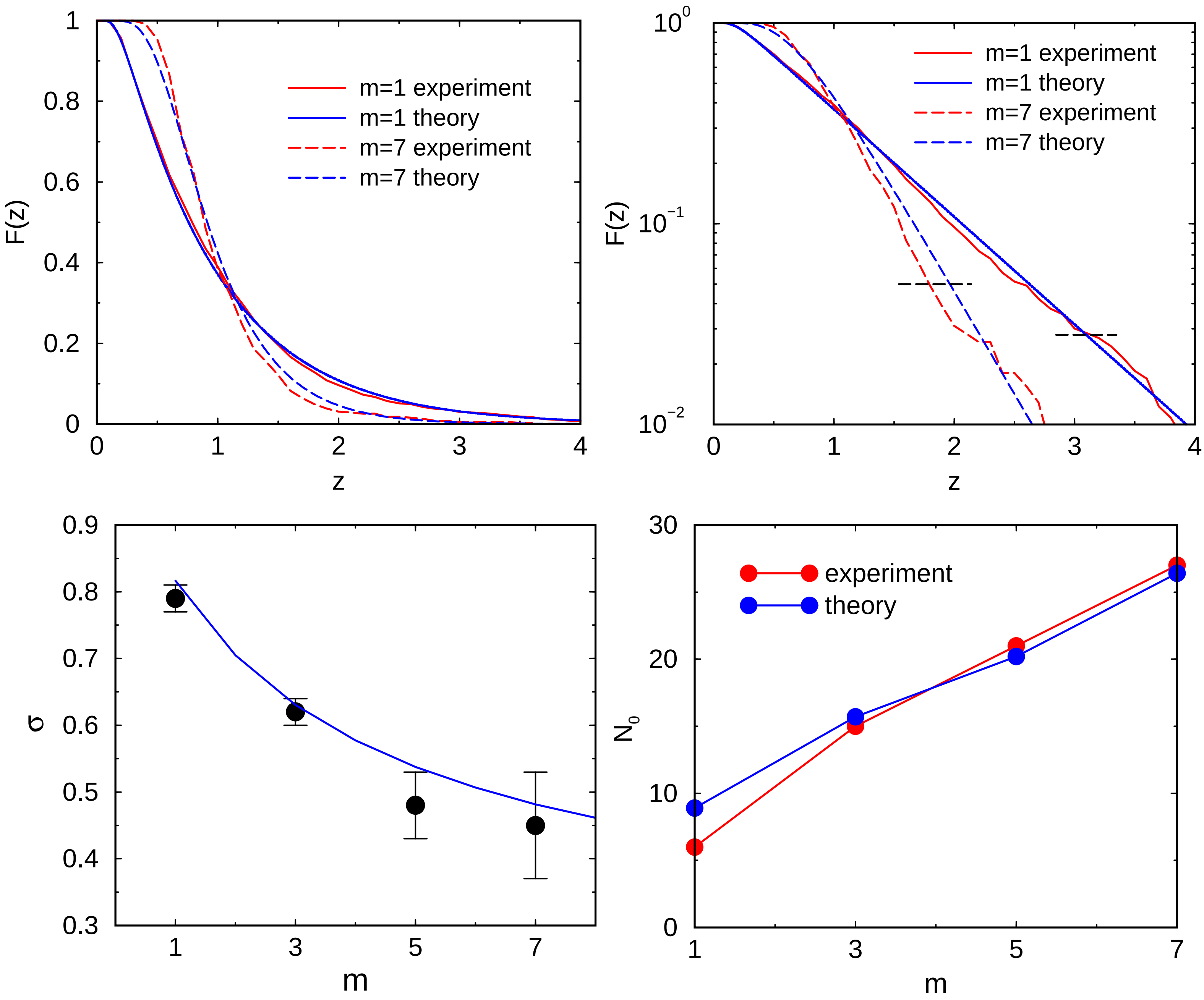
- Steepest descent

$$s(q) \sim e^{-\sqrt{q}/2} \sim \int dt\, e^{-qt - 1/16t} \quad q \to \infty$$

- Allows calculation of correction

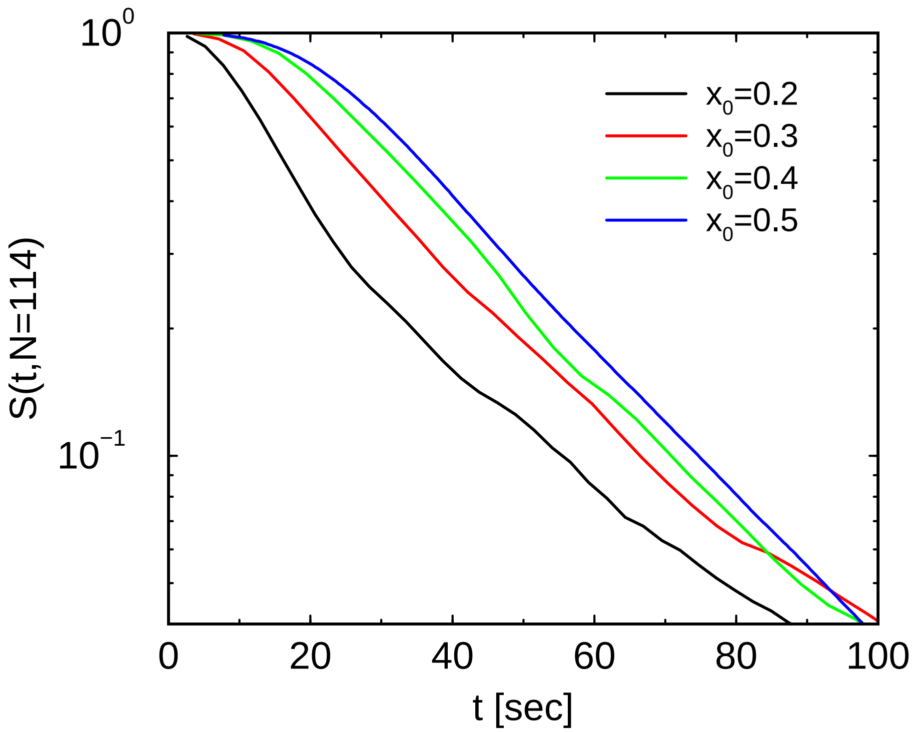
$$1 - F(z) \sim z^{1/2} e^{-\alpha/z} \quad z \to 0$$

Different knots ($m = 1, 3, 5, 7$)



Complex knots ($m \gg 1$): $\tau \sim \sigma \sim \frac{1}{\ln m}$

Off-Center Initial Conditions



- Survival probability: universal decay

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

- Eventually, initial conditions forgotten
- What is exit probability $E(x_0)$?
- What is exit time $T(x_0)$?

The First Passage Probability (1 walk)

- Straightforward calculation

$$E(x_0) = \int_0^\infty dt \partial_x p(x,t)\big|_{x=1} = \frac{2}{\pi}\sum_{n=1} (-1)^{n-1} \frac{\sin(n\pi x_0)}{n} = x_0$$

- Adjoint equation (discrete space)

$$E_n = \frac{1}{2}(E_{n-1} + E_{n+1}) \Rightarrow E_{n+1} - 2E_n + E_{n-1} = 0$$

- Electrostatic problem (continuous space)

$$\frac{\partial^2}{\partial^2 x_0} E(x_0) = 0$$

- Boundary conditions

$$E(0) = 0 \qquad E(1) = 1$$

- The gambler ruin problem

$$E(x_0) = x_0$$

The First Passage Time (1 walk)

- Straightforward calculation

$$T(x_0) = \int_0^{\infty} dt\, t\, \partial_x p(x,t)\big|_{x=1} = \frac{4}{\pi^3} \sum_{n\,\mathrm{odd}} \frac{\sin(n\pi x_0)}{n^3} = \frac{1}{2} x_0(1-x_0)$$

- Adjoint equation (discrete space)

$$T_n = \frac{1}{2}(T_{n-1}+T_{n+1}) + \frac{1}{D} \Rightarrow D(T_{n+1}-2T_n+T_{n-1}) = -1$$

- Electrostatic problem (continuous space)

$$D \frac{\partial^2}{\partial^2 x_0} T(x_0) = -1$$

- Boundary conditions

$$T(0) = T(1) = 0$$

- Solution

$$T(x_0) = \frac{1}{2D} x_0(1-x_0)$$

Derivation (continuum space)

- The Greens function $G(\mathbf{x}, \mathbf{x}', t) = \delta(\mathbf{x} - \mathbf{x}')$

$$D\nabla'^2 G(\mathbf{x}, \mathbf{x}') = D\nabla^2 G(\mathbf{x}, \mathbf{x}') = \frac{\partial}{\partial t} G(\mathbf{x}, \mathbf{x}', t)$$

- Survival probability & exit time

$$\begin{aligned} S(\mathbf{x}', t) &= \int d\mathbf{x} G(\mathbf{x}, \mathbf{x}', t) \\ T(\mathbf{x}') &= -\int_0^\infty dt\, t\, \frac{\partial}{\partial t} S(\mathbf{x}', t) \end{aligned}$$

- The adjoint equation

$$\begin{aligned} D\nabla'^2 T(\mathbf{x}') &= -D \int \int d\mathbf{x} dt\, t\, \frac{\partial}{\partial t} \nabla'^2 G(\mathbf{x}, \mathbf{x}', t) \\ &= -\int \int d\mathbf{x} dt\, t\, \frac{\partial^2}{\partial^2 t} G(\mathbf{x}, \mathbf{x}', t) \\ &= -\int dt\, t\, \frac{\partial^2}{\partial^2 t} S(\mathbf{x}', t) \\ &= \int dt \frac{\partial}{\partial t} S(\mathbf{x}', t) = S(\mathbf{x}', \infty) - S(\mathbf{x}', 0) \\ &= -1 \end{aligned}$$

The First Passage Time (d walks)

- The exit probability

$$\nabla^2 E(x, y, z) = 0$$

- The average exit time

$$\nabla^2 T(x, y, z) = -1$$

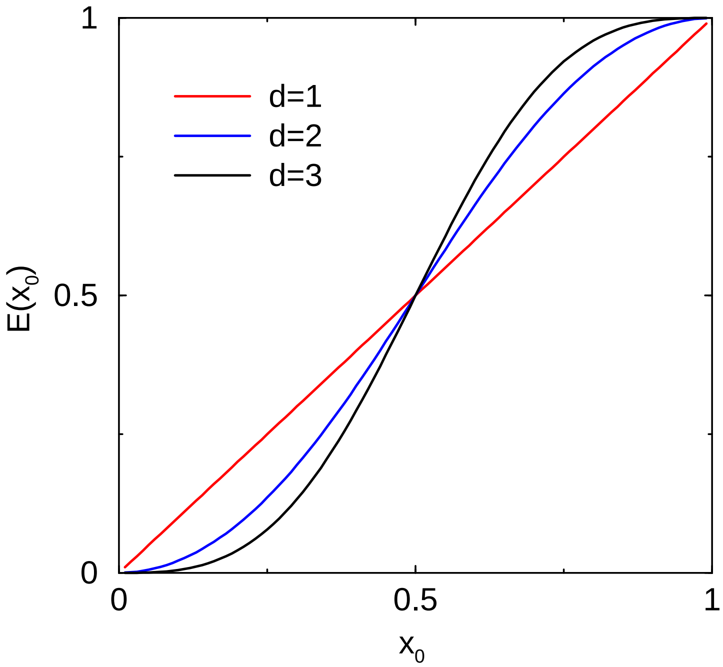
- Generally, d-sums

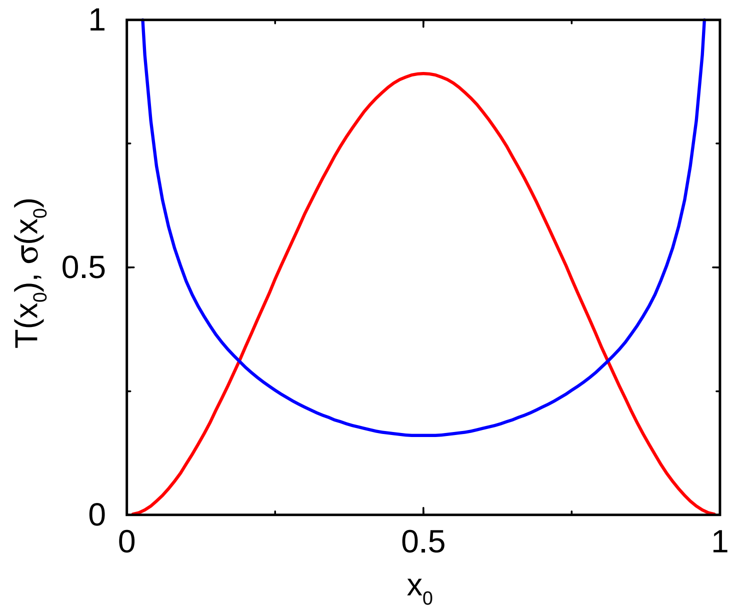
$$E(x_0) = \frac{d}{2}\left(\frac{4}{\pi}\right)^d \sum_{k_1=1}^{\infty}\sum_{k_2=0}^{\infty}\cdots\sum_{k_d=0}^{\infty} \frac{(-1)^{k_1-1} k_1 \sin[k_1 \pi x_0]}{k_1^2 + \sum_{i=2}^{d}(2k_i+1)^2} \prod_{i=2}^{d} \frac{\sin[(2k_i+1)\pi x_0]}{(2k_i+1)}$$

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

S. Redner, A guide to first passage processes (cambridge, 2001).

Predictions





- Good agreement for $S(t)$, $S_{\rm far}(t)$, $S_{\rm close}(t)$
- 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 (diffusive relaxation)

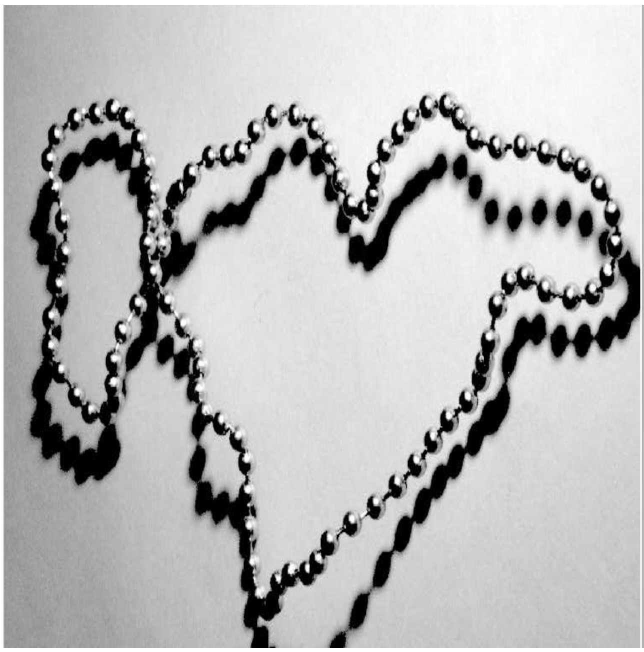
Outlook

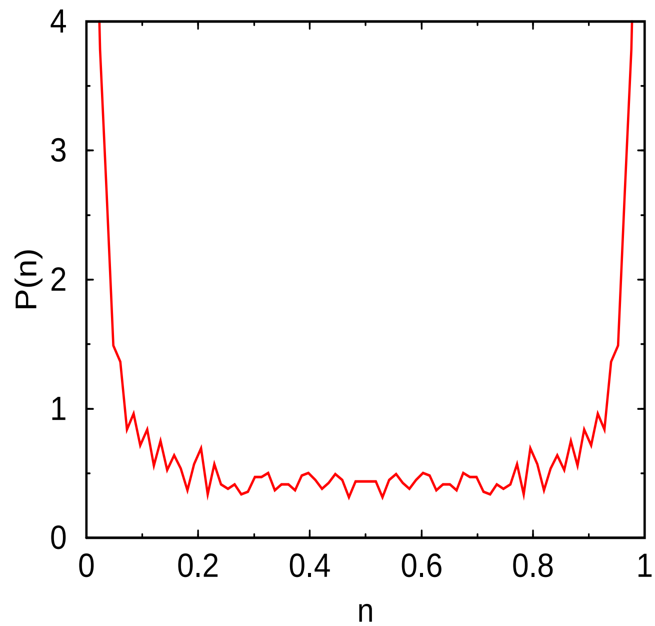
- Different knot types
- Correlation between crossing points

Many possibilities with granular chains

Entropic Tightening

with Matthew Hastings, Zahir Daya, Robert Ecke





- Equilibrium (counting states) prediction

$$P(n) \propto [n(N-n)]^{-d/2}$$

$$n/N \to 0 \qquad when \qquad N \to \infty$$

- Observed under nonequilibrium driving

Role of entropy?

Johnathan McKay

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