First Passage in High Dimensions

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E. Ben-Naim and P.L. Krapivsky, J. Phys. A **43**, 495007 & 495008 (2010)

Talk, publications available from: http://cnls.lanl.gov/~ebn

University of Maryland, September 7, 2011

Plan

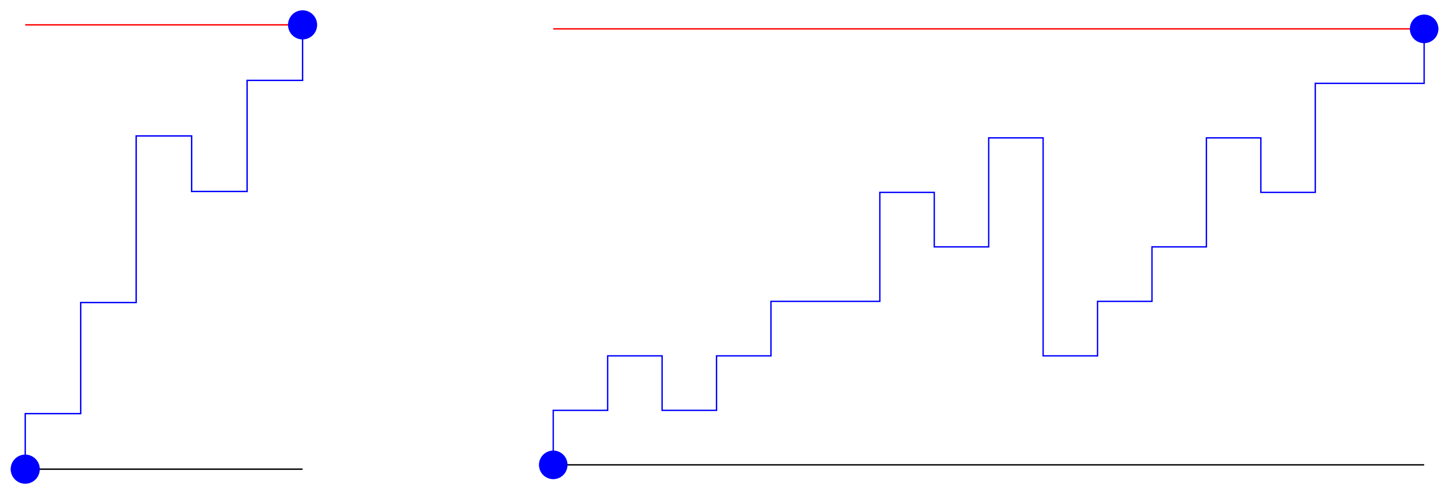
I. First Passage 101

II. Ordering of Diffusing Particles

III. Mixing of Diffusing Particles

Part I:
First Passage 101

First-Passage Processes



- Process by which a fluctuating quantity reaches a threshold for the first time.
- **First-passage probability:** for the random variable to reach the threshold as a function of time.
- **Total probability**: that threshold is ever reached. May or may not equal 1.
- **First-passage time**: the mean duration of the first-passage process. Can be finite or infinite.

S. Redner, A Guide to First-Passage Processes, 2001

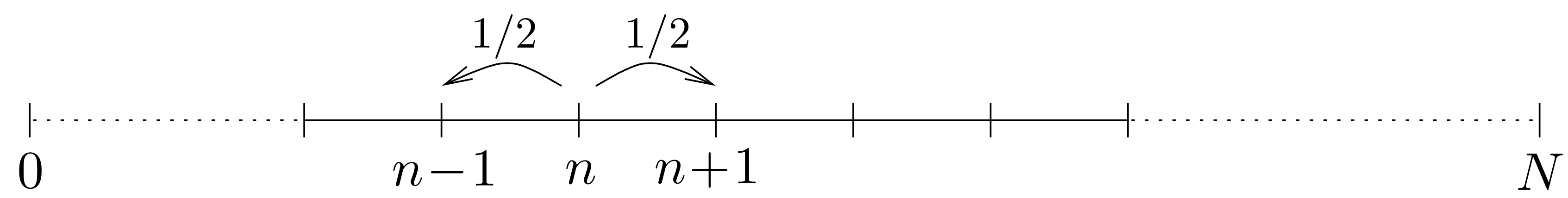
Relevance

- Economics: specify stock orders, define bear/bull markets
- Politics: redistricting
- Geophysics: earthquakes, avalanches
- Biological Physics: transport in channels, translocation
- Polymer Physics: <u>dynamics of knots</u>
- Population dynamics: epidemic outbreaks

Connections

- Electrostatics
- Heat conduction
- Probability theory
- Quantum Mechanics
- Diffusion-limited aggregation

Gambler Ruin Problem



- You versus casino. Fair coin. Your wealth = n, Casino = N-n
- Game ends with ruin. What is your winning probability E_n ?
- Winning probability satisfies discrete Laplace equation

$$E_n = \frac{E_{n-1} + E_{n+1}}{2} \qquad \nabla^2 E = 0$$

- Boundary conditions are crucial

$$E_0 = 0 \qquad \text{and} \qquad E_N = 1$$

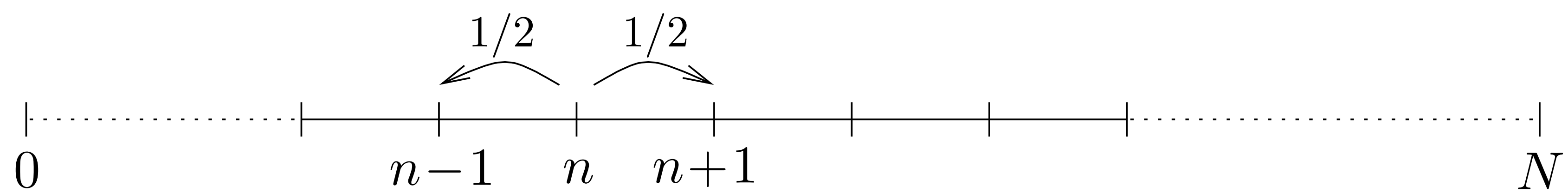
- Winning probability is proportional to your wealth

$$E_n = \frac{n}{N}$$

Feller 1968

First-passage probability satisfies a simple equation

First-Passage Time



- Average duration of game is T_n
- Duration satisfies discrete Poisson equation

$$T_n = \frac{T_{n-1}}{2} + \frac{T_{n+1}}{2} + 1 \qquad D\nabla^2 T = -1$$

- Boundary conditions: $T_0 = T_N = 0$
- Duration is quadratic

$$T_n = n(N-n)$$

- Small wealth = short game, big wealth = long game

$$T_n \sim \begin{cases} N & n = \mathcal{O}(1) \\ N^2 & n = \mathcal{O}(N) \end{cases} \qquad \begin{aligned} D\nabla^2(T_+E_+) &= -E_+ \\ D\nabla^2(T_-E_-) &= -E_- \end{aligned}$$

First-passage time satisfies a simple equation

Brute Force Approach

- Start with time-dependent diffusion equation

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

- Impose <u>absorbing</u> boundary conditions & initial conditions

$$P(x,t)\big|_{x=0} = P(x,t)\big|_{x=N} = 0 \quad \text{and} \quad P(x,t=0) = \delta(x-n)$$

- Obtain full time-dependent solution

$$P(x,t) = \frac{2}{N}\sum_{l\geq 1} \sin\frac{l\pi x}{N}\sin\frac{l\pi n}{N} e^{-(l\pi)^2 Dt/N^2}$$

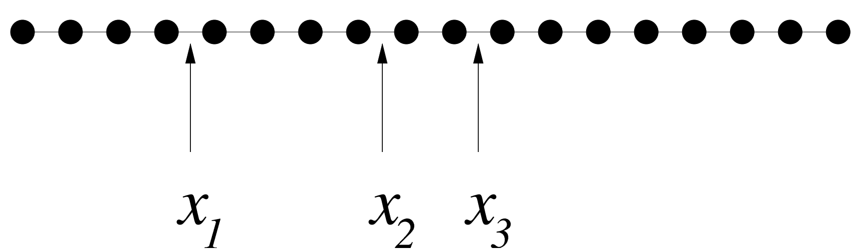
- Integrate flux to calculate winning probability and duration

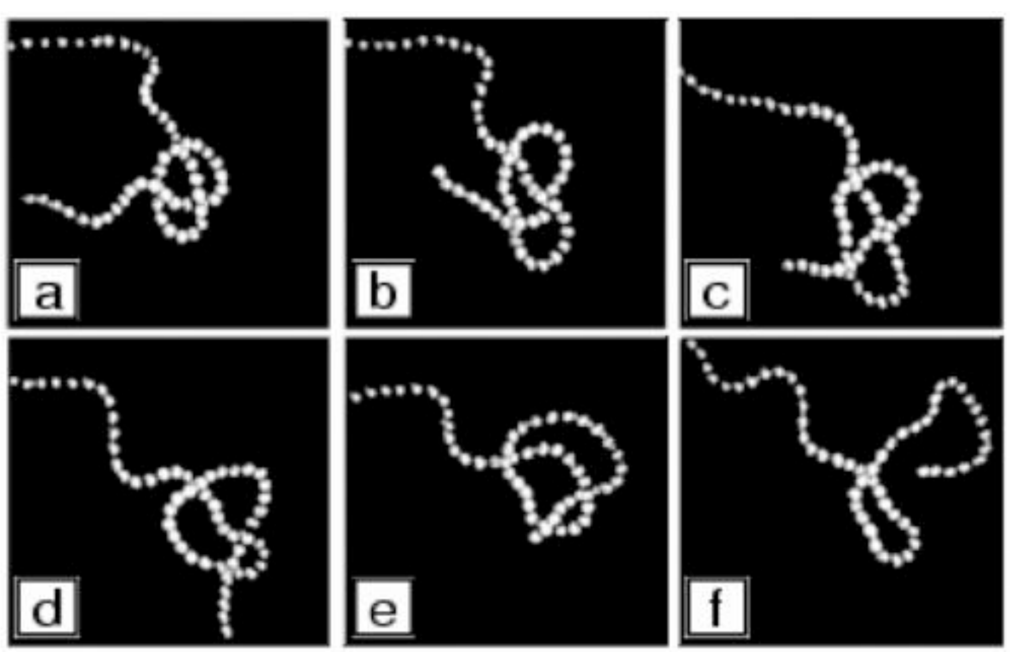
$$E_n = -\int_0^\infty dt\, D\frac{\partial P(x,t)}{\partial x}\Big|_{x=N} \quad \Longrightarrow \quad E_n = \frac{n}{N}$$

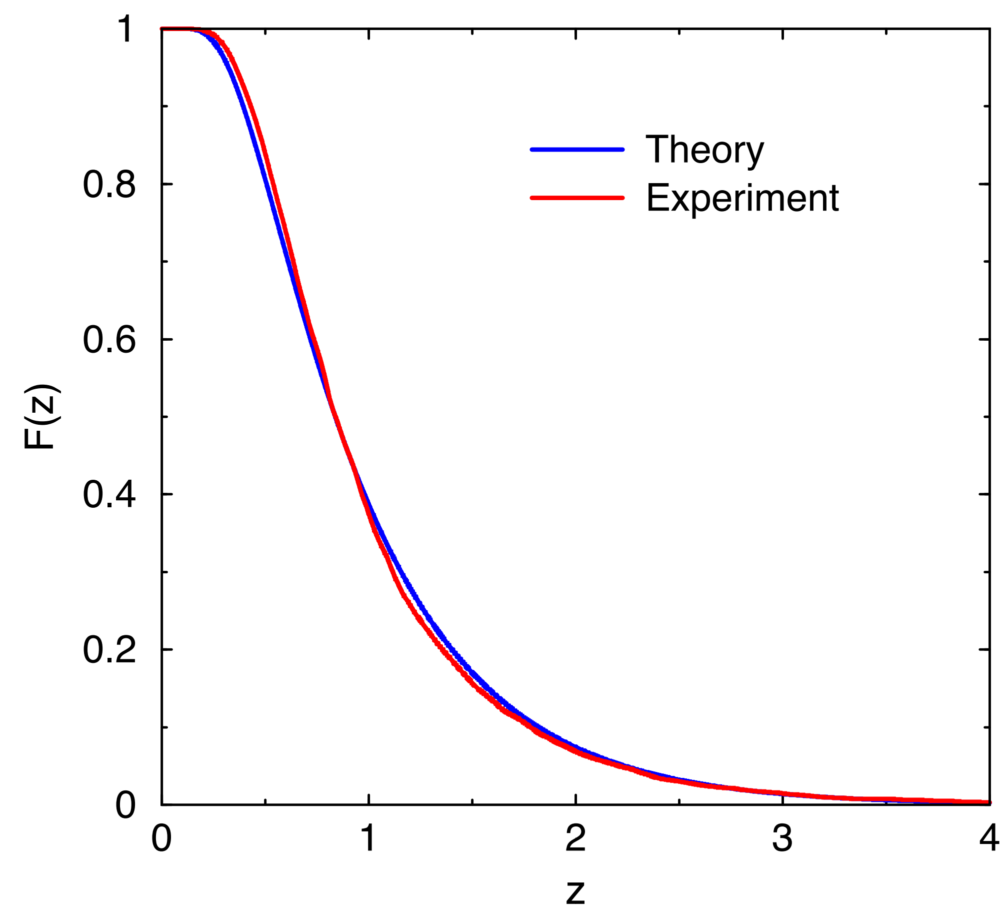
Lesson: focus on quantity of interest

Knots in Vibrated Granular Polymers

- Represent knot by three random walks (with exclusion)
- Solve gambler ruin problem in three dimensions







$$\sigma_{\rm exp} = 0.62 \pm 0.01$$

$$\sigma_{\rm theory} = 0.63047$$

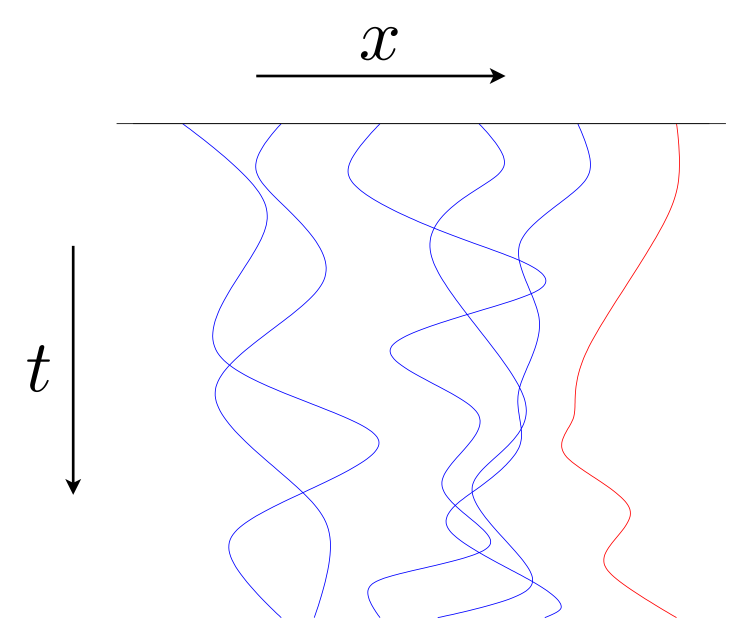
EB, Daya, Vorobieff, Ecke, PRL (2001); Maryland 2001

Part II:
Ordering of Diffusing Particles

The capture problem

- System: N independent diffusing particles in one dimension
- What is the probability that original leader maintains the lead?
- N Diffusing particles

$$\frac{\partial \varphi_i(x,t)}{\partial t} = D\nabla^2 \varphi_i(x,t)$$



- Initial conditions

$$x_N(0) < x_{N-1}(0) < \cdots < x_2(0) < x_1(0)$$

- Survival probability $S(t)$=probability "lamb" survives "lions" until t
- Independent of initial conditions, power-law asymptotic behavior

$$S(t) \sim t^{-\beta} \qquad \text{as} \qquad t \to \infty$$

Lebowitz 82
Fisher 84
Bramson 91
Redner 96
benAvraham 02
Grassberger 03

- Monte Carlo: nontrivial exponents that depend on N

N	2	3	4	5	6	10
$\beta(N)$	$1/2$	$3/4$	0.913	1.032	1.11	1.37

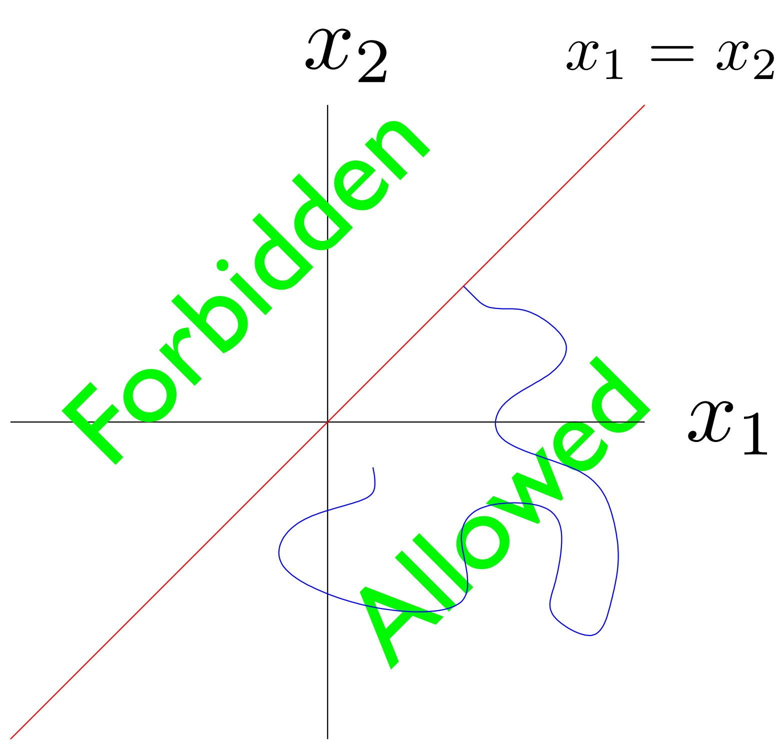
No theoretical computation of exponents

Two Particles

- We need the probability that two particles do not meet
- Map <u>two one-dimensional</u> walks onto <u>one two-dimensional</u> walk
- Space is divided into allowed and forbidden regions
- Boundary separating the two regions is absorbing
- Coordinate $x_1 - x_2$ performs one-dimensional random walk
- Survival probability decays as power-law

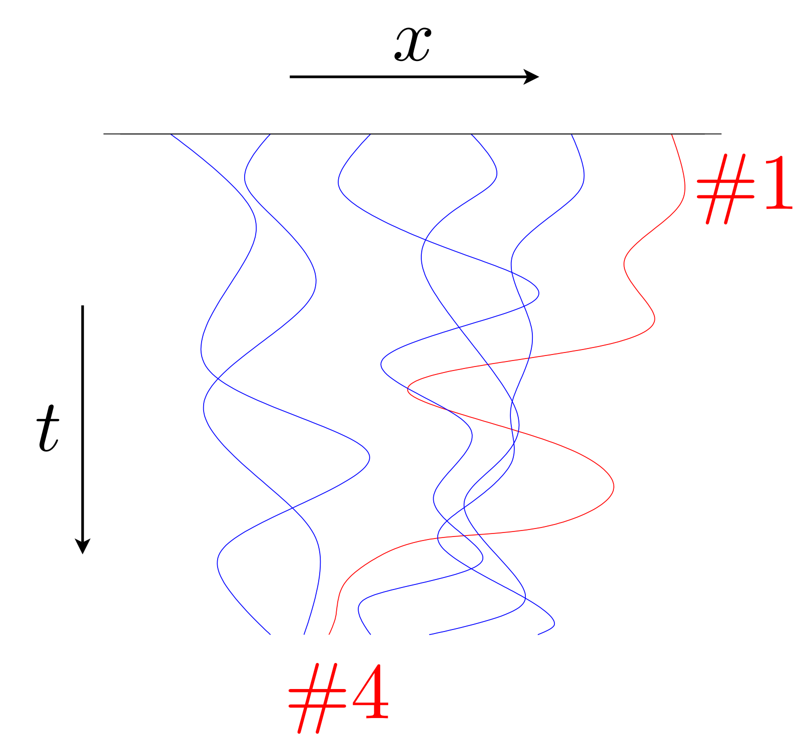
$$S_1(t) \sim t^{-1/2}$$

- In general, map N one-dimensional walk onto one walk in N dimension with complex boundary conditions



Order Statistics

- Generalize the capture problem: $S_m(t)$ is the probability that the leader does not fall below rank m until time t Lindenberg 01
- $S_1(t)$ is the probability that leader maintains the lead
- $S_{N-1}(t)$ is the probability that leader never becomes laggard
- Power-law asymptotic behavior is generic



$$S_m(t) \sim t^{-\beta_m(N)}$$

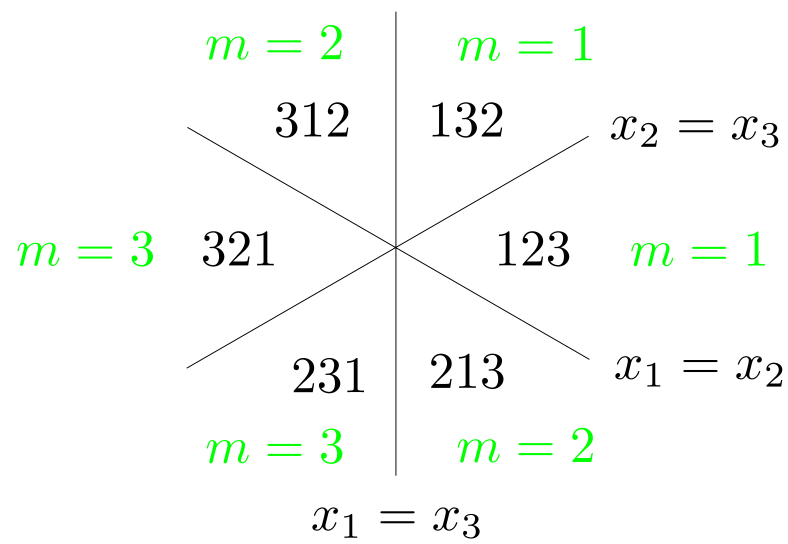
- Spectrum of first-passage exponents

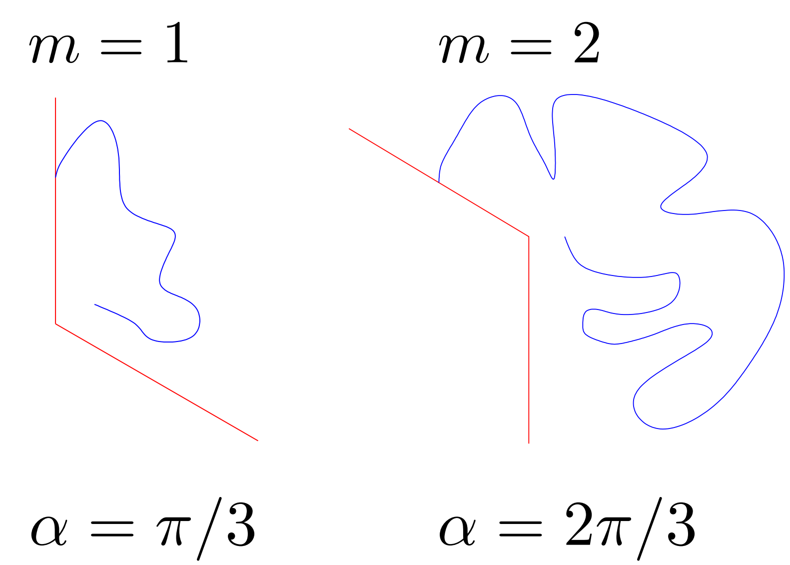
$$\beta_1(N) > \beta_2(N) > \cdots > \beta_{N-1}(N)$$

Can't solve the problem? Make it bigger!

Three Particles

- Diffusion in three dimensions; now, allowed regions are wedges





- Survival probability in wedge with opening angle $0<\alpha<\pi$

$$S(t)\sim t^{-\pi/(4\alpha)}$$

Spitzer 58
Fisher 84

- Survival probabilities decay as power-law with time

$$S_1\sim t^{-3/4} \quad \text{and} \quad S_2\sim t^{-3/8}$$

- Indeed, a family of nontrivial first-passage exponents

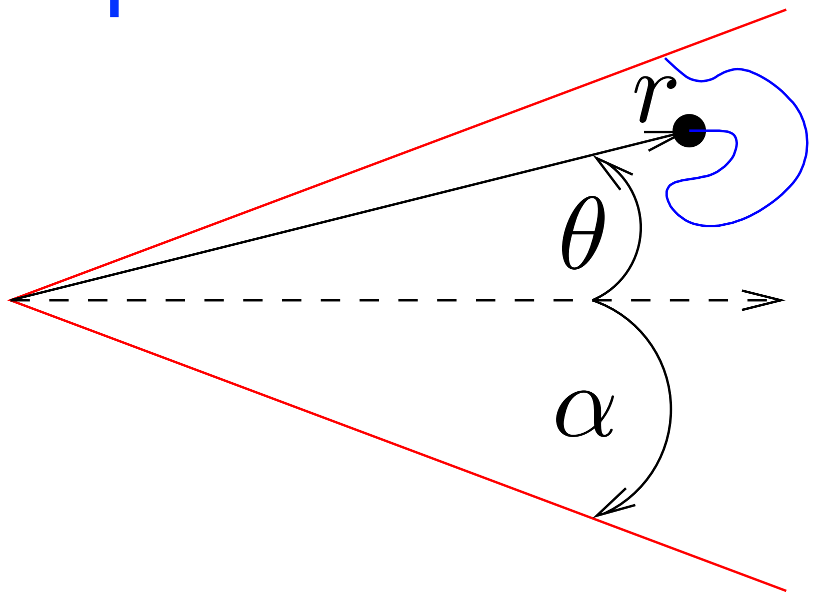
$$S_m\sim t^{-\beta_m} \qquad \text{with} \qquad \beta_1>\beta_2>\cdots>\beta_{N-1}$$

Large spectrum of first-passage exponents

First Passage in a Wedge

- Survival probability obeys the diffusion equation

$$\frac{\partial S(r,\theta,t)}{\partial t} = D\nabla^2 S(r,\theta,t)$$



- Focus on long-time limit

$$S(r,\theta,t) \simeq \Phi(r,\theta)\,t^{-\beta}$$

- Amplitude obeys Laplace's equation

$$\nabla^2\Phi(r,\theta) = 0$$

- Use dimensional analysis

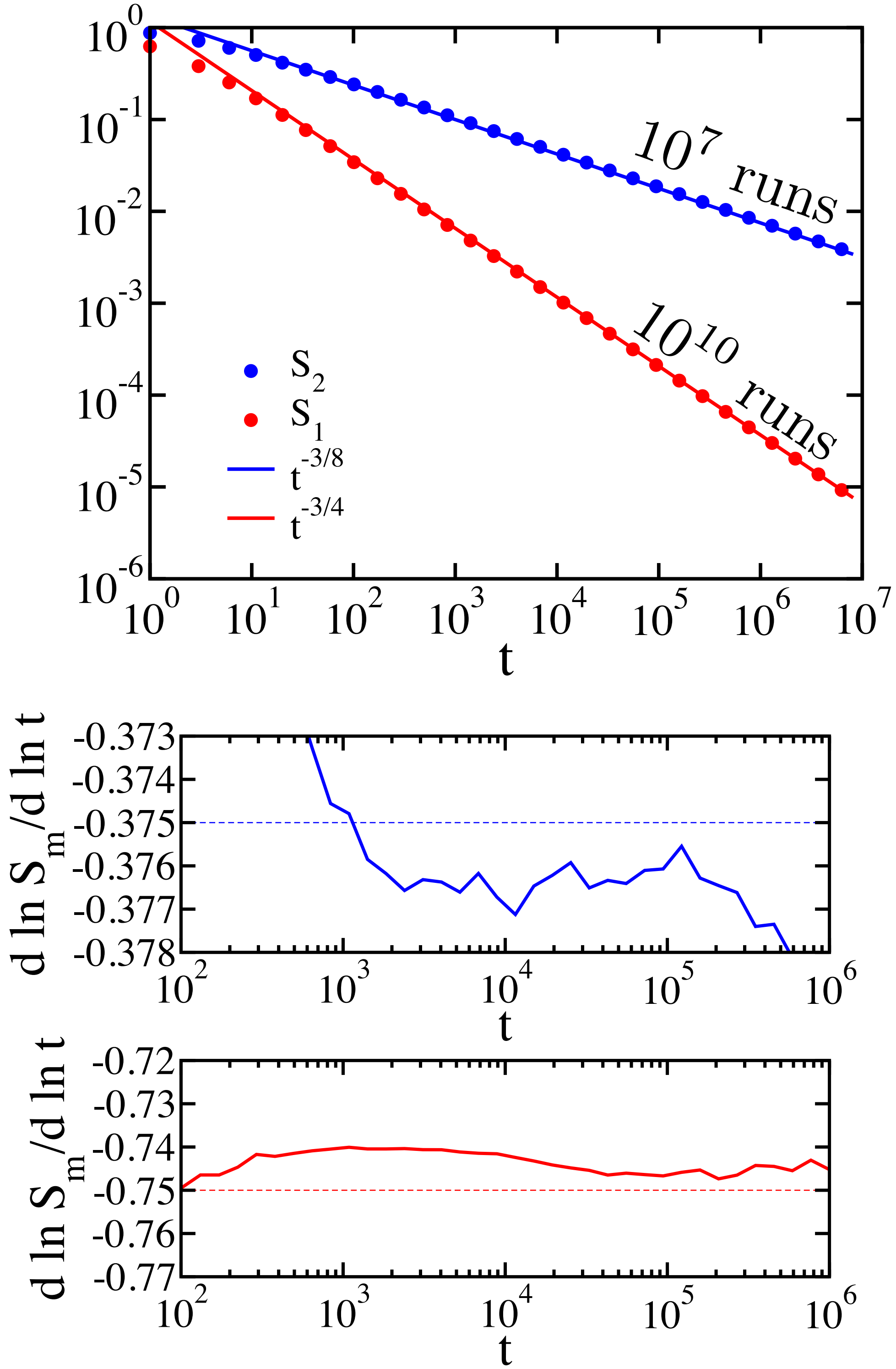
$$\Phi(r,\theta) \sim (r^2/D)^\beta \psi(\theta) \quad\Longrightarrow\quad \psi_{\theta\theta} + (2\beta)^2\psi = 0$$

- Enforce boundary condition $S|_{\theta=\alpha} = \Phi|_{\theta=\alpha} = \psi|_{\theta=\alpha}$
- Lowest eigenvalue is the relevant one

$$\psi_2(\theta) = \cos(2\beta\theta) \quad\Longrightarrow\quad \beta = \frac{\pi}{4\alpha}$$

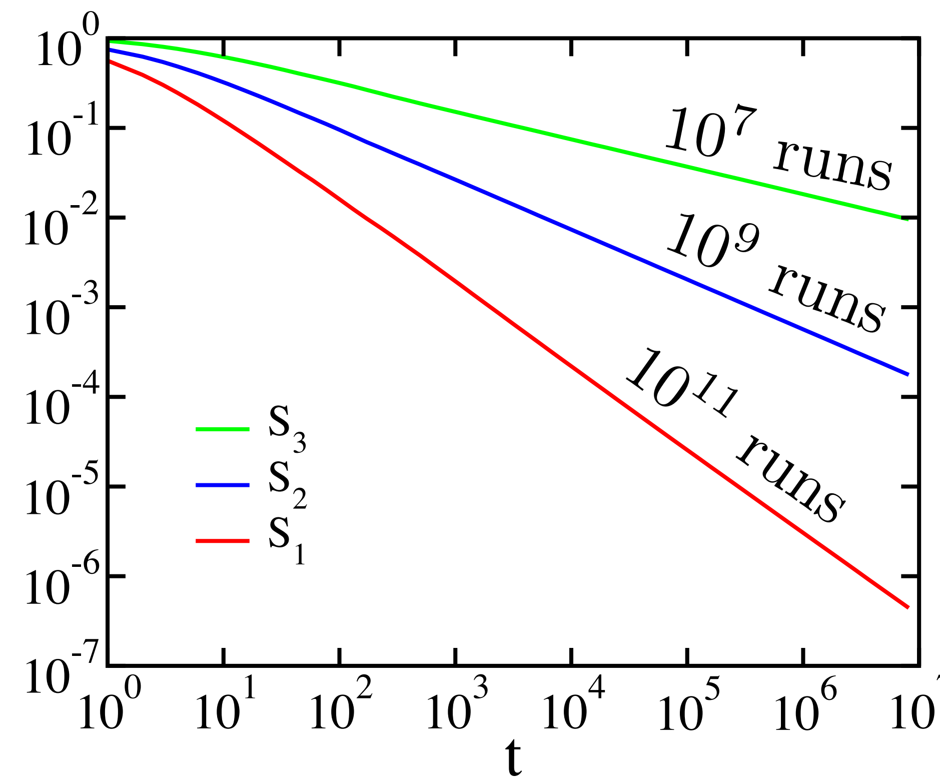
Monte Carlo Simulations

3 particles



confirm wedge theory results

4 particles



$$\beta_1 = 0.913$$

$$\beta_2 = 0.556$$

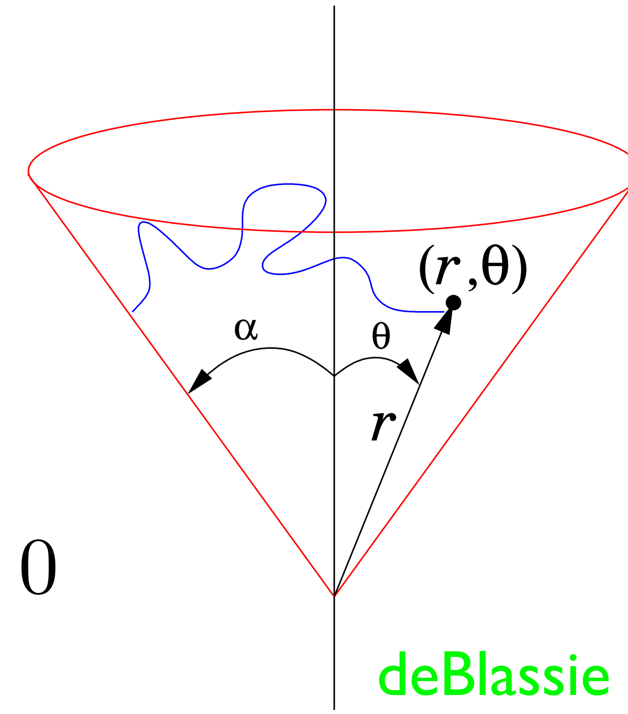
$$\beta_3 = 0.306$$

as expected, there are
3 nontrivial exponents

Kinetics of First Passage in a Cone

- Repeat wedge calculation step by step

$$S(r,\theta,t) \sim \psi(\theta)(Dt/r^2)^{-\beta}$$



deBlassie 88

- Angular function obeys Poisson-like equation

$$\frac{1}{(\sin\theta)^{d-2}}\frac{d}{d\theta}\left[(\sin\theta)^{d-2}\frac{d\psi}{d\theta}\right] + 2\beta(2\beta+d-2)\psi = 0$$

- Solution in terms of associated Legendre functions

$$\psi_d(\theta) = \begin{cases} (\sin\theta)^{-\delta} P^{\delta}_{2\beta+\delta}(\cos\theta) & d \text{ odd}, \\ (\sin\theta)^{-\delta} Q^{\delta}_{2\beta+\delta}(\cos\theta) & d \text{ even} \end{cases} \qquad \delta = \frac{d-3}{2}$$

- Enforce boundary condition, choose lowest eigenvalue

$$P^{\delta}_{2\beta+\delta}(\cos\alpha) = 0 \qquad d \text{ odd},$$
$$Q^{\delta}_{2\beta+\delta}(\cos\alpha) = 0 \qquad d \text{ even}.$$

Exponent is nontrivial root of Legendre function

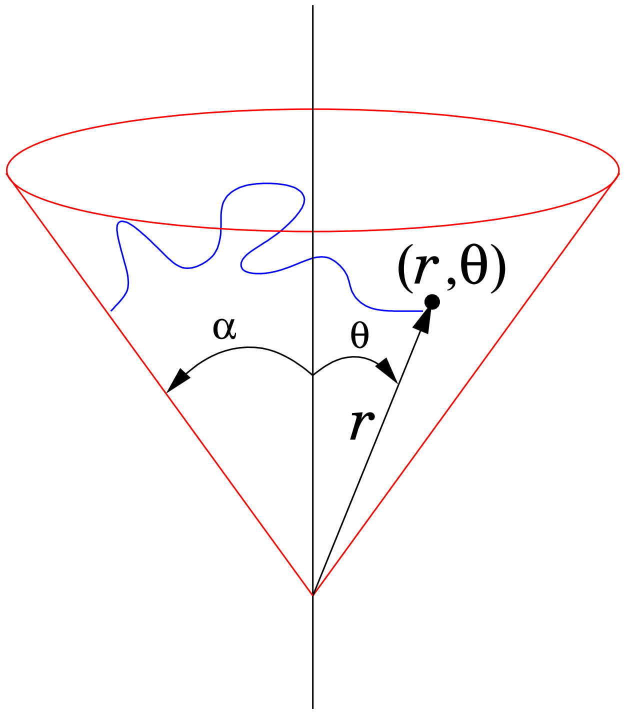
Additional Results

- Explicit results in 2d and 4d

$$\beta_2(\alpha) = \frac{\pi}{4\alpha} \quad \text{and} \quad \beta_4(\alpha) = \frac{\pi - \alpha}{2\alpha}$$

- Root of ordinary Legendre function in 3d

$$P_{2\beta}(\cos\alpha) = 0$$



- Flat cone is equivalent to one-dimension

$$\beta_d(\alpha = \pi/2) = 1/2$$

- First-passage time obeys Poisson's equation

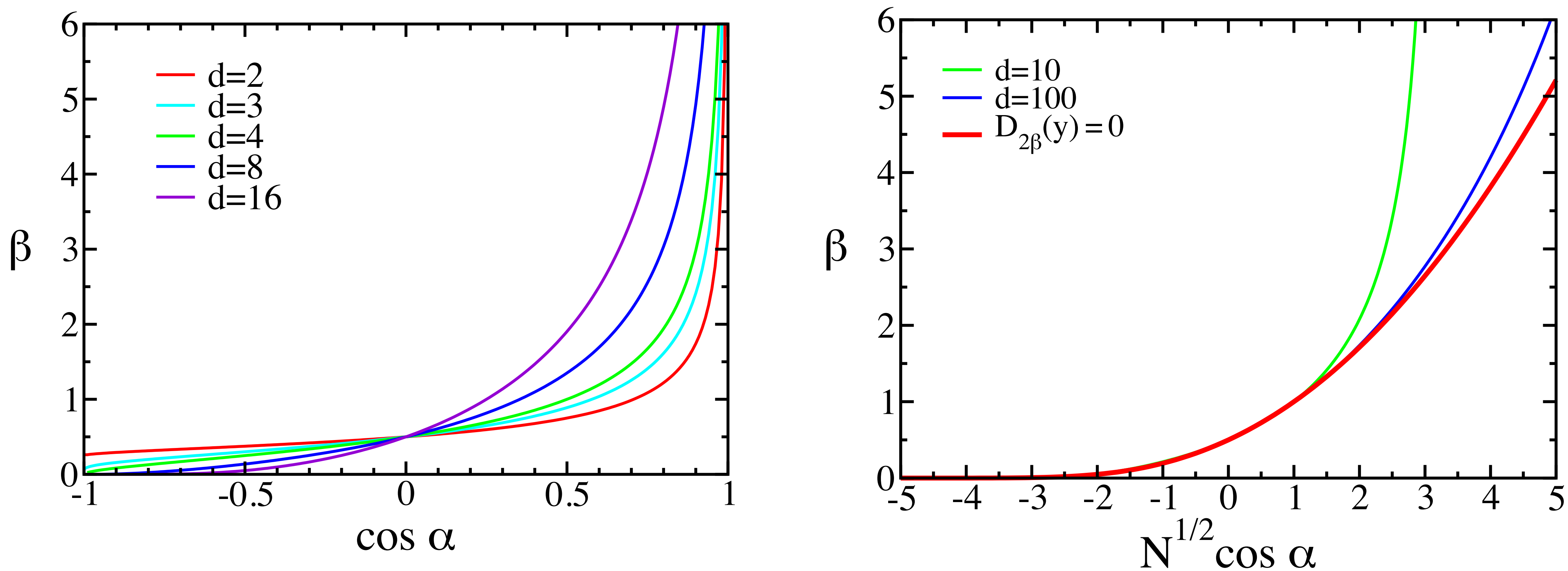
$$D\nabla^2 T(r,\theta) = -1$$

- First-passage time (when finite)

$$T(r,\theta) = \frac{r^2}{2D}\,\frac{\cos^2\theta - \cos^2\alpha}{d\cos^2\alpha - 1}$$

$\alpha < \cos^{-1}(1/\sqrt{d})$

High Dimensions



- Exponent varies sharply for opening angles near $\pi/2$
- Universal behavior in high dimensions

$$\beta_d(\alpha) \to \beta(\sqrt{N}\cos\alpha)$$

- Scaling function is smallest root of parabolic cylinder function

$$D_{2\beta}(y) = 0$$

Exponent is function of one scaling variable, not two

Asymptotic Analysis

- Limiting behavior of scaling function

$$\beta(y) \simeq \begin{cases} \sqrt{y^2/8\pi}\, \exp\left(-y^2/2\right) & y \to -\infty, \\ y^2/8 & y \to \infty. \end{cases}$$

- Thin cones: exponent diverges

$$\beta_d(\alpha) \simeq B_d \alpha^{-1} \quad \text{with} \quad J_\delta(2B_d) = 0$$

- Wide cones: exponent vanishes when $d \geq 3$

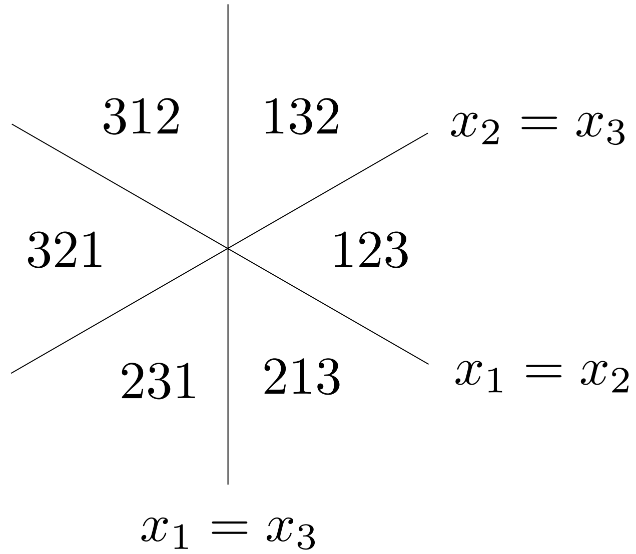
$$\beta_d(\alpha) \simeq A_d\,(\pi - \alpha)^{d-3} \quad \text{with} \quad A_d = \tfrac{1}{2} B\left(\tfrac{1}{2}, \tfrac{d-3}{2}\right)$$

- A needle is reached with certainty only when $d < 3$
- Large dimensions

$$\beta_d(\alpha) \simeq \begin{cases} \frac{d}{4}\left(\frac{1}{\sin\alpha} - 1\right) & \alpha < \pi/2, \\ C(\sin\alpha)^d & \alpha > \pi/2. \end{cases}$$

Diffusion in High Dimensions

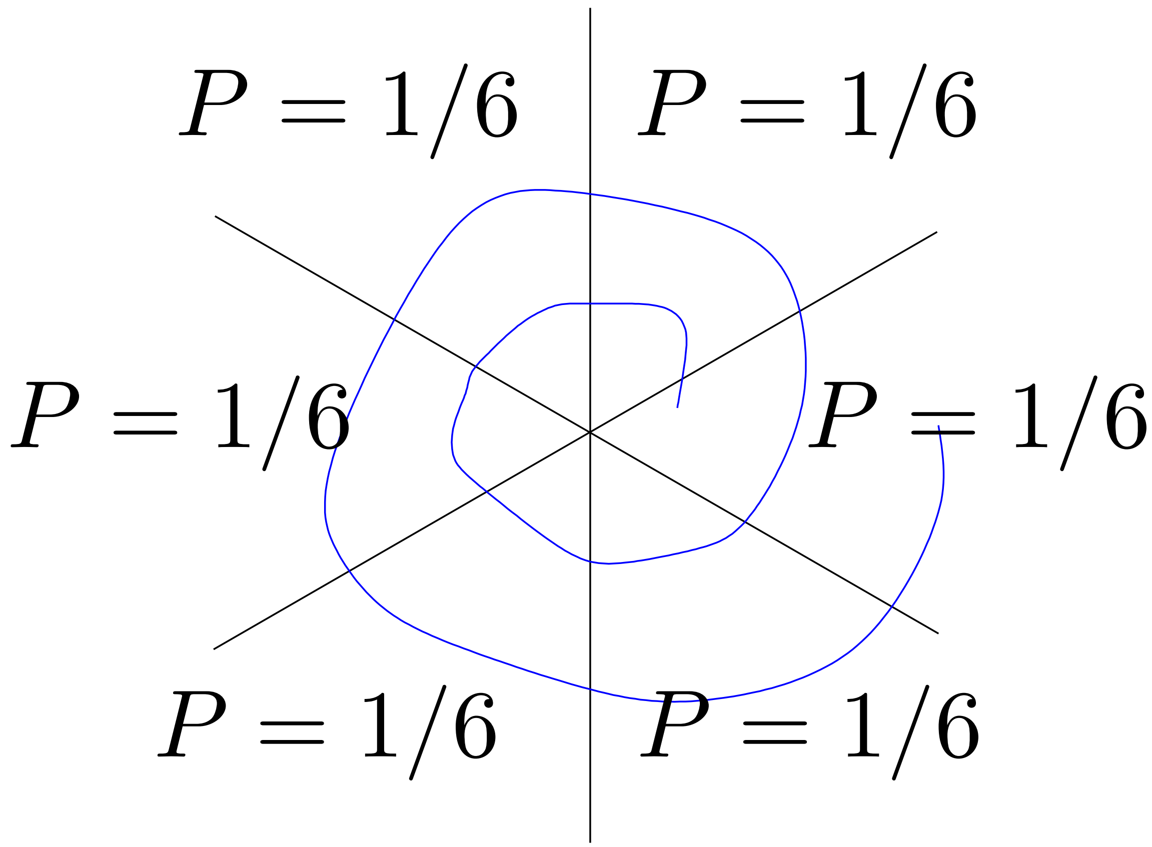
- In general, map N one-dimensional walk onto one walk in N dimension with complex boundary conditions

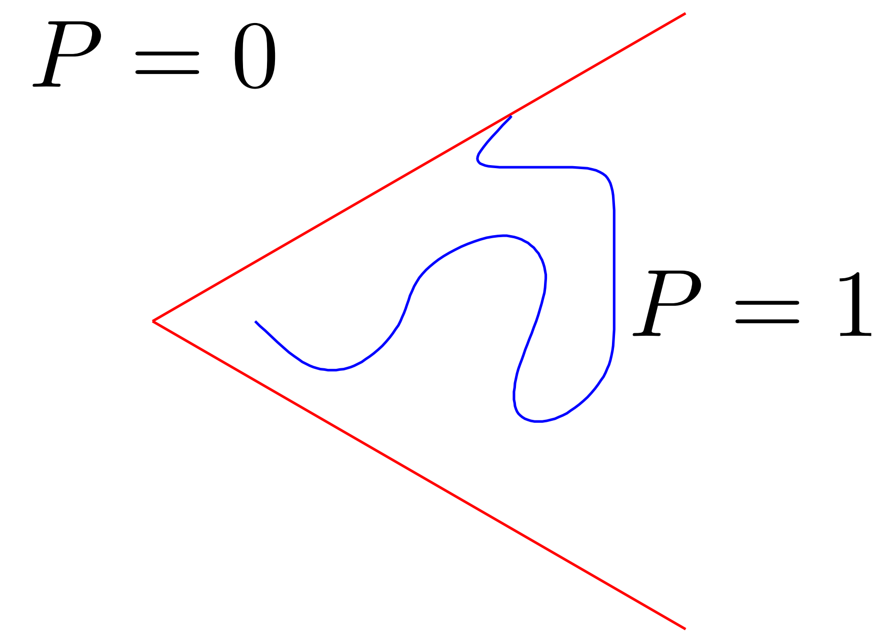


- There are $\binom{N}{2} = \frac{N(N-1)}{2}$ planes of the type $x_i = x_j$
- These planes divide space into $N!$ "chambers"
- Particle order is unique to each chamber
- The absorbing boundary encloses multiple chambers
- We do not know the shape of the allowed region
- However, we do know the volume of the allowed region
- Equilibrium distribution of particle order

$$V_m = \frac{m}{N}$$

Equilibrium versus Nonequilibrium



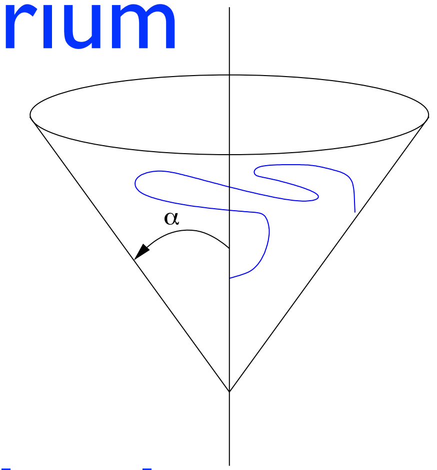


- Diffusion is an ergodic process
- Wait long enough and initial order is completely forgotten
- Equilibrium distribution: each chamber has weight $P = 1/N!$

First passage as a nonequilibrium process

Cone Approximation

- Fractional volume of allowed region given by equilibrium distribution of particle order



$$V_m(N) = \frac{m}{N}$$

- Replace allowed region with cone of same fractional volume

$$V(\alpha) = \frac{\int_0^\alpha d\theta\,(\sin\theta)^{N-3}}{\int_0^\pi d\theta\,(\sin\theta)^{N-3}}$$

$$d\Omega \propto \sin^{d-2}\theta\, d\theta$$
$$d = N-1$$

- Use analytically known exponent for first passage in cone

$$Q^{\gamma}_{2\beta+\gamma}(\cos\alpha) = 0 \qquad N \text{ odd},$$
$$P^{\gamma}_{2\beta+\gamma}(\cos\alpha) = 0 \qquad N \text{ even}.$$

$$\gamma = \frac{N-4}{2}$$

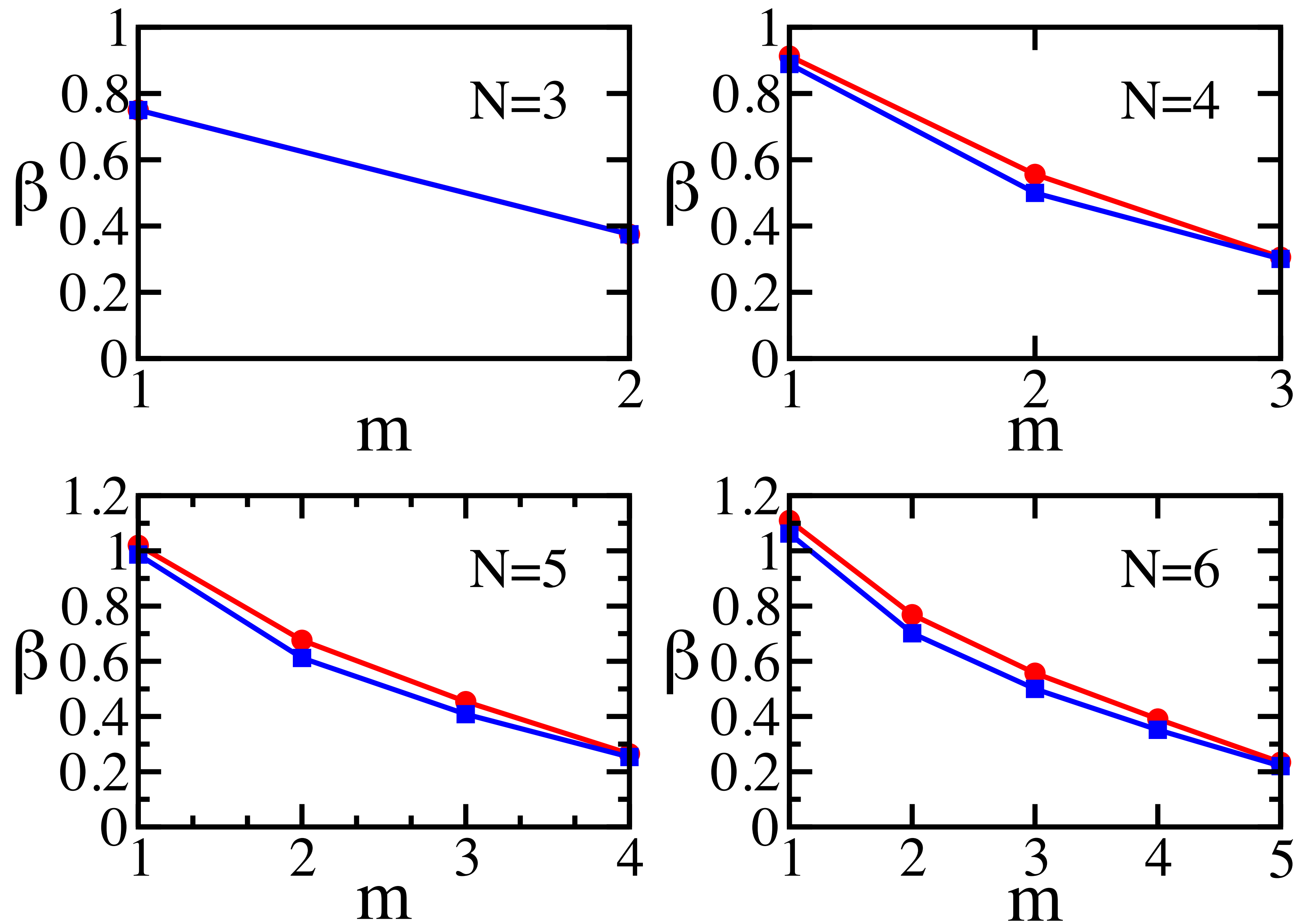
- Good approximation for four particles

m	1	2	3
V_m	1/4	1/2	3/4
β_m^{cone}	0.888644	1/2	0.300754
β_m	0.913	0.556	0.306

Small Number of Particles

- By construction, cone approximation is exact for $N=3$
- Cone approximation gives a formal lower bound

Rayleigh 1877
Faber-Krahn theorem



Excellent, consistent approximation!

Very Large Number of Particles ($N \to \infty$)

- Equilibrium distribution is simple

$$V_m = \frac{m}{N}$$

- Volume of cone is also given by error function

$$V(\alpha, N) \to \frac{1}{2} + \frac{1}{2}\,\mathrm{erf}\left(\frac{-y}{\sqrt{2}}\right) \qquad \text{with} \qquad y = (\cos\alpha)\sqrt{N}$$

- First-passage exponent has the scaling form

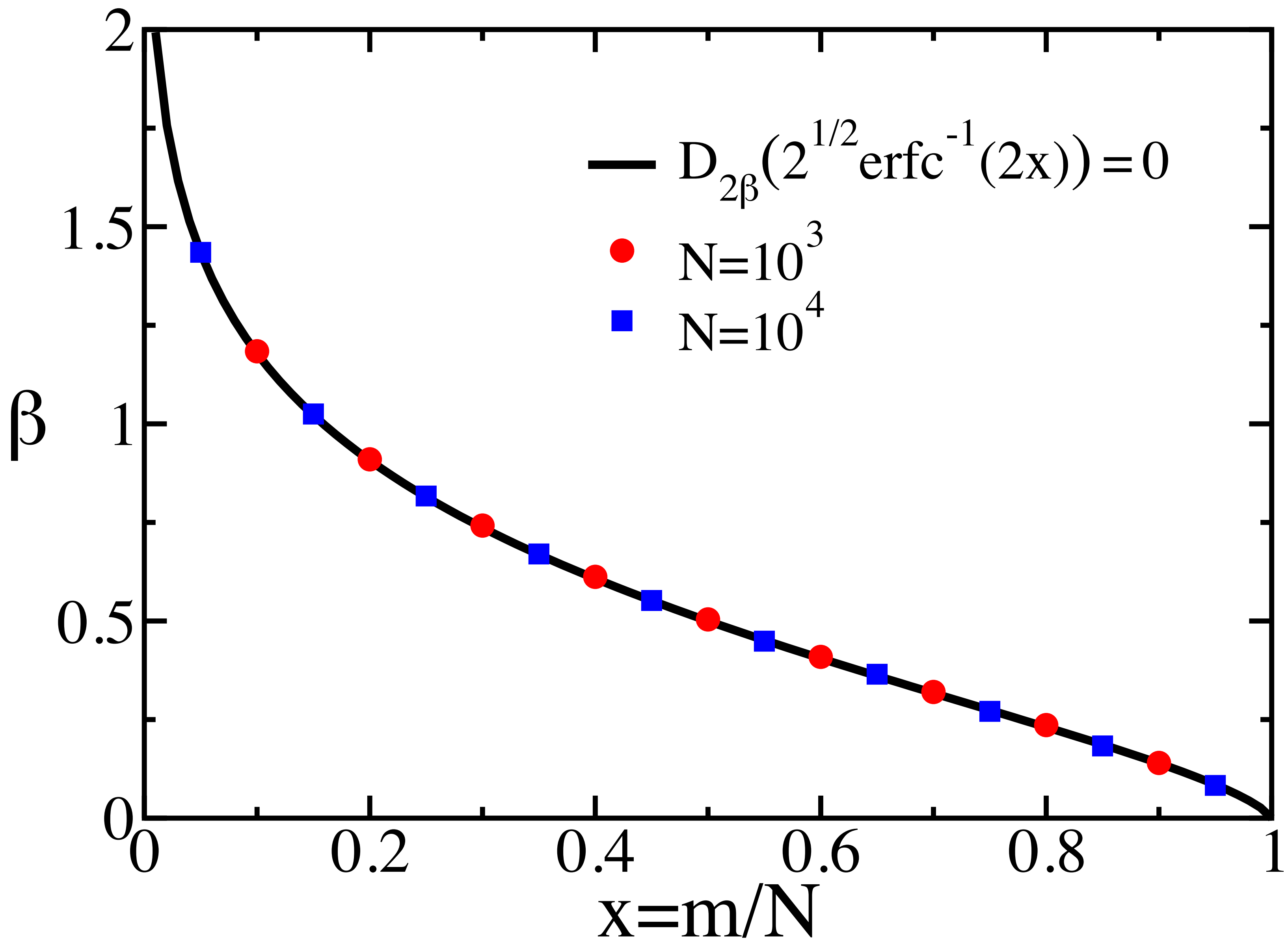
$$\beta_m(N) \to \beta(x) \quad \text{with} \quad x = m/N$$

- Scaling function is root of equation involving parabolic cylinder function

$$D_{2\beta}\left(\sqrt{2}\,\mathrm{erfc}^{-1}(2x)\right) = 0$$

Scaling law for scaling exponents!

Simulation Results

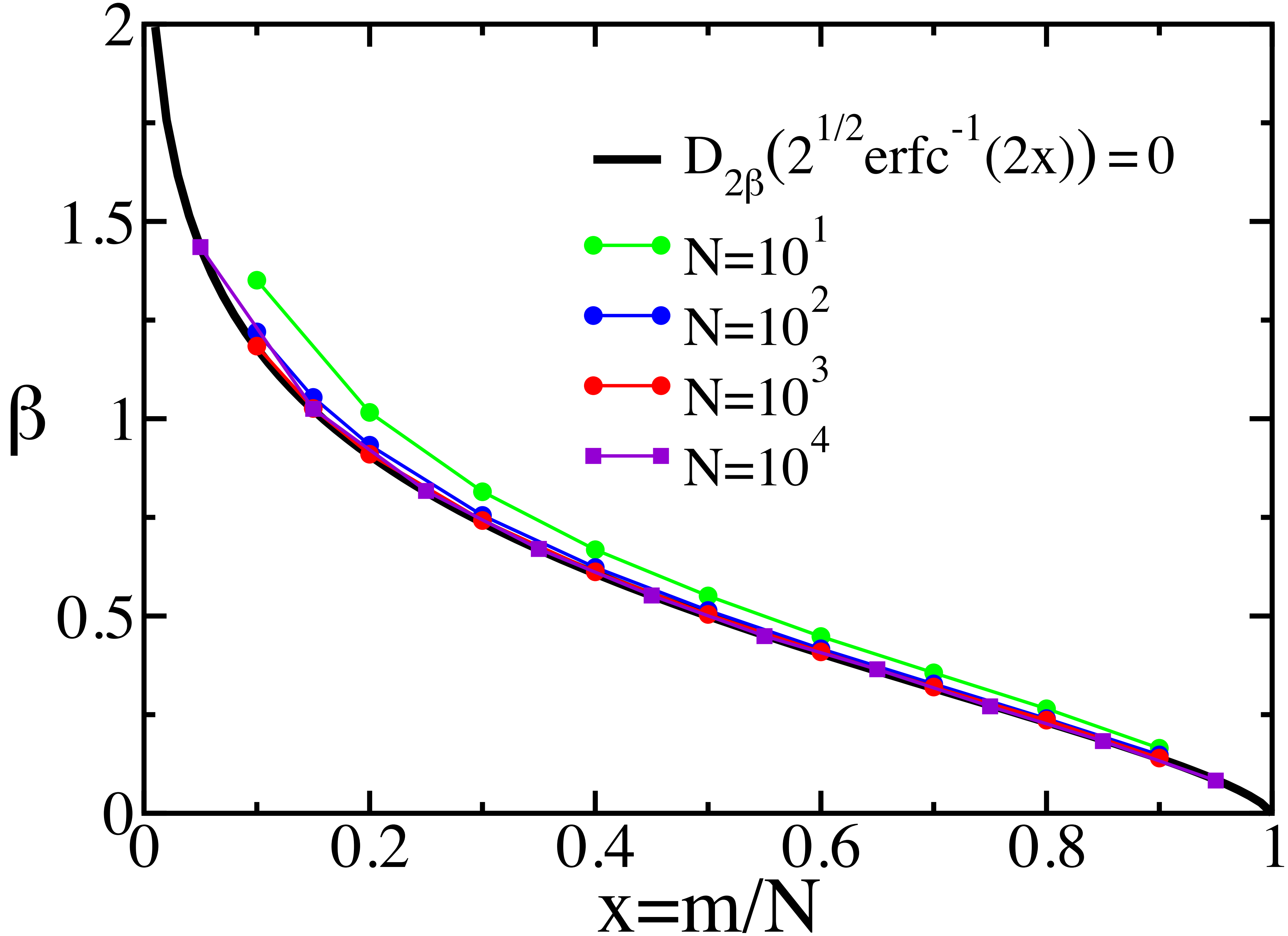


Numerical simulation of diffusion in 10,000 dimensions!

Only 10 measurements confirm scaling function!

Cone approximation is asymptotically exact!

Convergence



Scaling function converges quickly

Is spherical one as a limiting shape?

Small Number of Particles

N	β_1^{cone}	β_1
3	$3/4$	$3/4$
4	0.888644	0.91
5	0.986694	1.02
6	1.062297	1.11
7	1.123652	1.19
8	1.175189	1.27
9	1.219569	1.33
10	1.258510	1.37

N	$\beta_{N-1}^{\text{cone}}$	β_{N-1}
2	$1/2$	$1/2$
3	$3/8$	$3/8$
4	0.300754	0.306
5	0.253371	0.265
6	0.220490	0.234
7	0.196216	0.212
8	0.177469	0.190
9	0.162496	0.178
10	0.150221	0.165

Decent approximation for the exponents even for small number of particles

Extreme Exponents

- Extremal behavior of first-passage exponents

$$\beta(x) \simeq \begin{cases} \frac{1}{4}\ln\frac{1}{2x} & x \to 0 \\ (1-x)\ln\frac{1}{2(1-x)} & x \to 1 \end{cases}$$

- Probability leader never loses the lead (capture problem)

$$\beta_1 \simeq \frac{1}{4}\ln N$$

- Probability leader never becomes last (laggard problem)

$$\beta_{N-1} \simeq \frac{1}{N}\ln N$$

- Both agree with previous heuristic arguments

Krapivsky 02

Extremal exponents can not be measured directly

Indirect measurement via exact scaling function

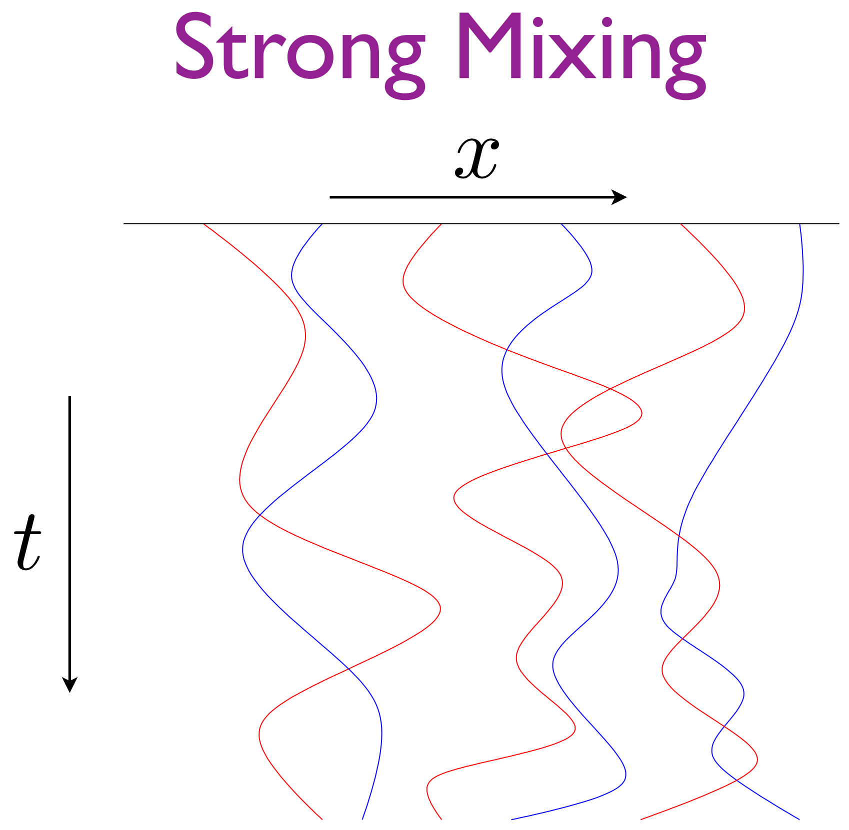
Summary

- First-passage kinetics are rich
- Family of first-passage exponents
- Cone approximation gives good estimates for exponents
- Exponents follow a scaling behavior in high dimensions
- Cone approximation yields the exact scaling function
- Combine equilibrium distribution and geometry to obtain exact or approximate nonequilibrium behavior, namely, first-passage kinetics

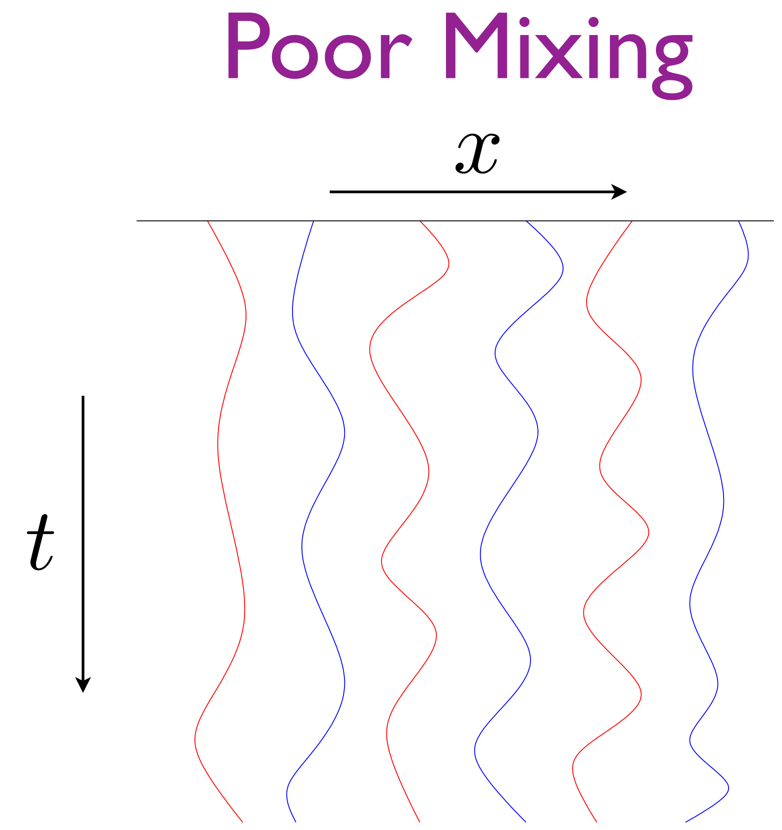
Part III:
Mixing of Diffusing Particles

Diffusion in One Dimension

- Mixing: well-studied in fluids, granular media, not in diffusion
- **System:** N independent random walks in one dimension



trajectories cross many times



trajectories rarely cross

How to quantify mixing of diffusing particles?

The Inversion Number

- Measures how "scrambled" a list of numbers is
- Used for ranking, sorting, recommending (books, songs, movies)
  - I rank: 1234, you rank 3142
  - There are three inversions: {1,3}, {2,3}, {2,4}
- Definition: The inversion number m equals the number of pairs that are inverted = out of sort
- Bounds:

$$0 \leq m \leq \frac{N(N-1)}{2}$$

McMahon 1913

Random Walks and Inversion Number

- Initial conditions: particles are ordered

$$x_1(0) < x_2(0) < \cdots < x_{N-1}(0) < x_N(0)$$

- Each particle is an independent random walk

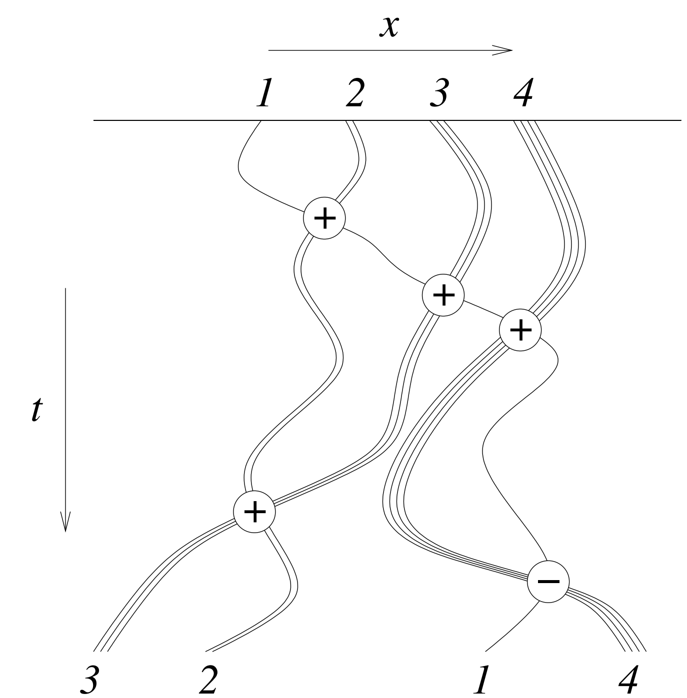
$$x \to \begin{cases} x-1 & \text{with probability } 1/2 \\ x+1 & \text{with probability } 1/2 \end{cases}$$

- Inversion number

$$m(t) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \Theta\big(x_i(t) - x_j(t)\big)$$

- Strong mixing: large inversion number
- Weak mixing: small inversion number persists

Space-time representation



$m(0) = 0$

$m(t) = 3$

Trajectory crossing = "collision"

Collision have + or - "charge"

Inversion number = sum of charges

Inversion number is a natural measure of mixing

Equilibrium Distribution

- Diffusion is ergodic, order is completely random when $t \to \infty$
- Every permutation occurs with the same weight $1/N!$
- Probability $P_m(N)$ of inversion number m for N particles

$$(P_0, P_1, \ldots, P_M) = \frac{1}{N!} \times \begin{cases} (1) & N = 1, \\ (1,1) & N = 2, \\ (1,2,2,1) & N = 3, \\ (1,3,5,6,5,3,1) & N = 4. \end{cases}$$

- Recursion equation

$$P_m(N) = \frac{1}{N} \sum_{l=0}^{N-1} P_{m-l}(N-1)$$

- Generating Function

$$\sum_{m=0}^{M} P_m(N) s^m = \frac{1}{N!} \prod_{n=1}^{N} (1 + s + s^2 + \cdots + s^{n-1})$$

Knuth 1998

Equilibrium Properties

- Average inversion number scales quadratically with N

$$\langle m \rangle = \frac{N(N-1)}{4}$$

- Variance scales cubically with N

$$\sigma^2 = \frac{N(N-1)(2N+5)}{72}$$

- Asymptotic distribution is Gaussian

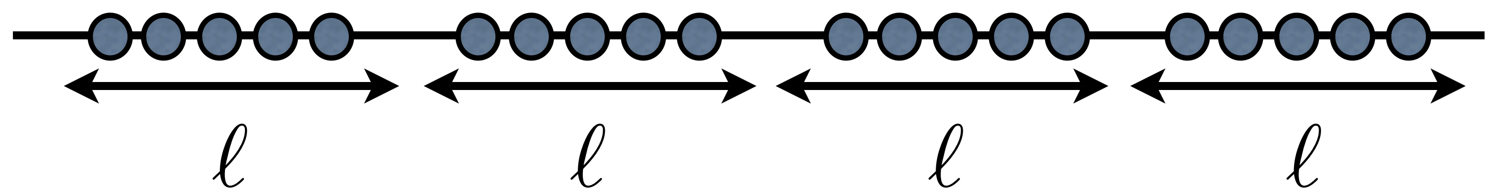
$$P_m(N) \simeq \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(m-\langle m \rangle)^2}{2\sigma^2}\right]$$

- Large fluctuations

$$m - N^2/4 \sim N^{3/2}$$

Feller 1968

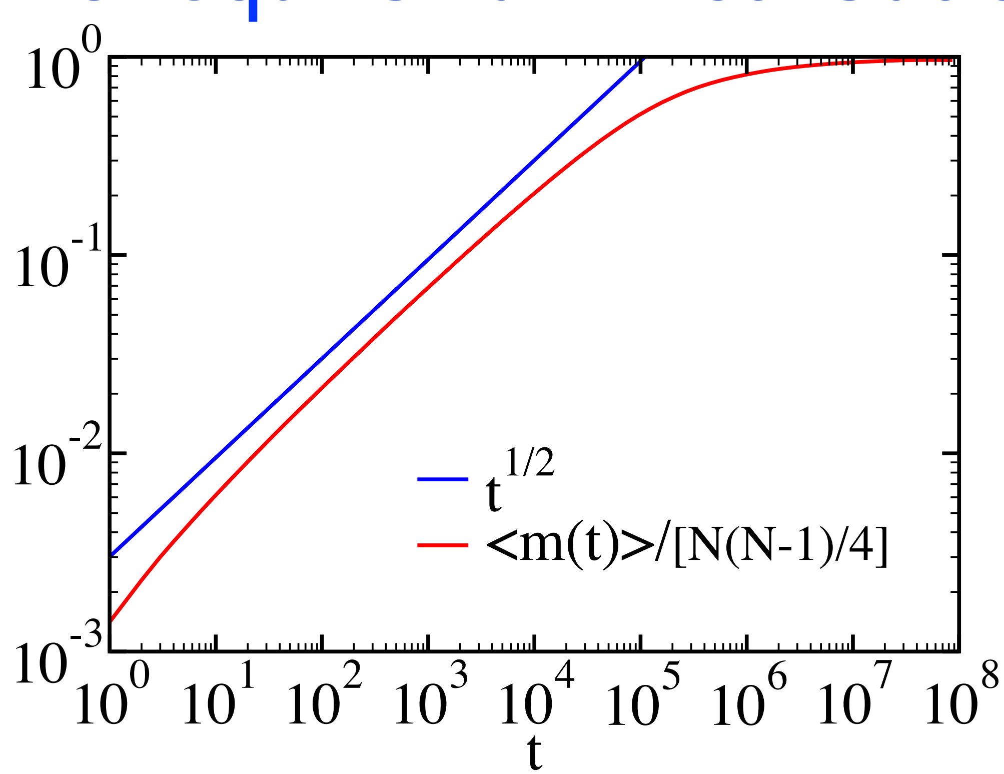
Transient Behavior

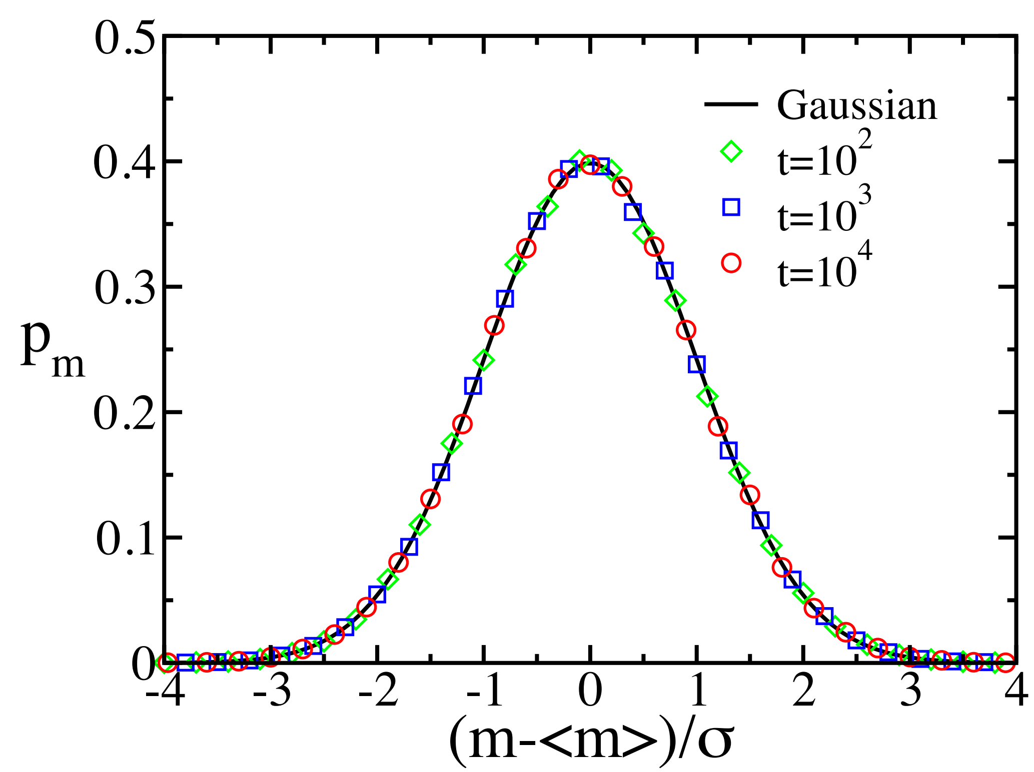


- Assume particles well mixed on a growing length scale
- Use equilibrium result for the sub-system $\langle m \rangle / N \sim \ell$
- Length scale must be diffusive $\ell \sim \sqrt{t}$

$$\langle m(t) \rangle \sim N\sqrt{t} \qquad \text{when} \qquad t \ll N^2$$

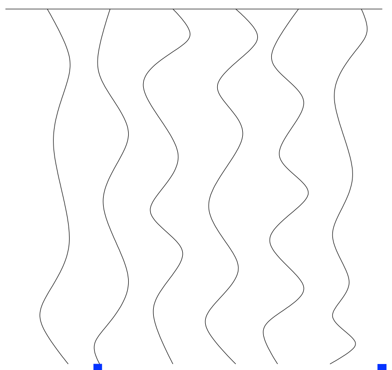
- Equilibrium behavior reached after a transient regime
- Nonequilibrium distribution is Gaussian as well





First-Passage Kinetics

- Survival probability $S_m(t)$ that inversion number $< m$ until time t



1. Probability there are no crossing

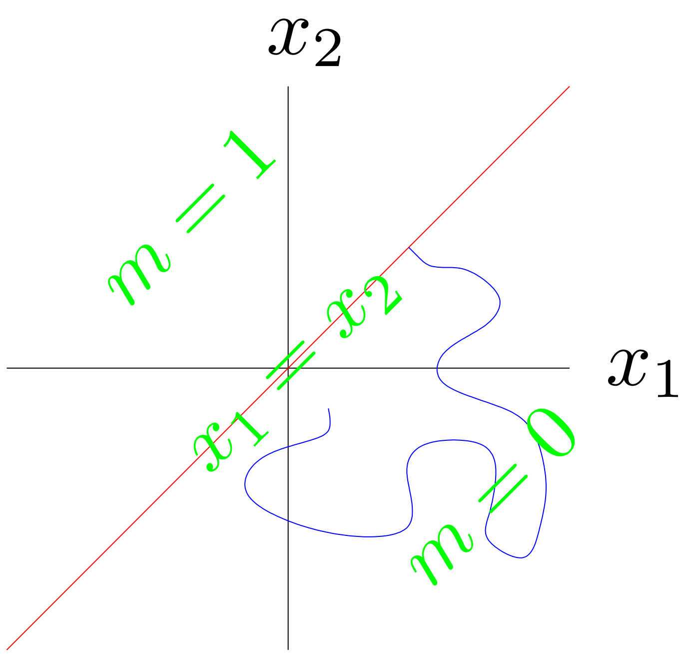
Fisher 1984

$$S_1(t) \sim t^{-N(N-1)/4}$$

2. Two-particles: coordinate $x_1 - x_2$ performs a random walk

$$S_1(t) \sim t^{-1/2}$$

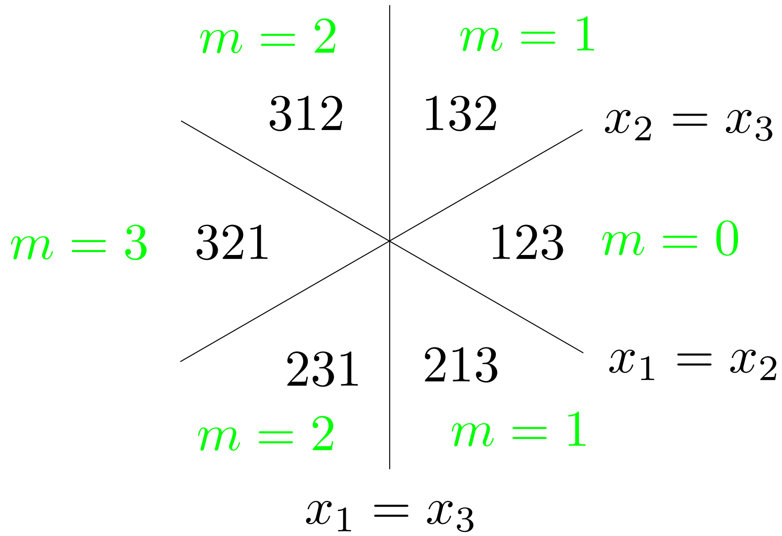
- Map N *1*-dimensional walks to *1* walk in N dimensions
  - Allowed region: inversion number $< m$
  - Forbidden region: inversion number $\geq m$
- Boundary is absorbing

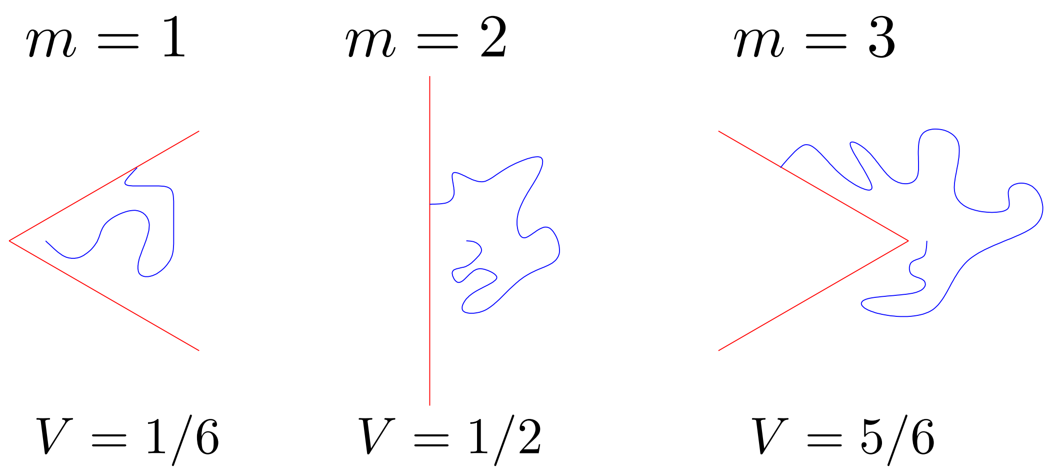


Problem reduces to diffusion in N dimensions in presence of complex absorbing boundary

Three Particles

- Diffusion in three dimensions; Allowed regions are wedges





- Survival probability in wedge with "fractional volume" $0 < V < 1$

$$S(t) \sim t^{-1/(4V)}$$

- Survival probabilities decay as power-law with time

$$S_1 \sim t^{-3/2}, \qquad S_2 \sim t^{-1/2}, \qquad S_3 \sim t^{-3/10}$$

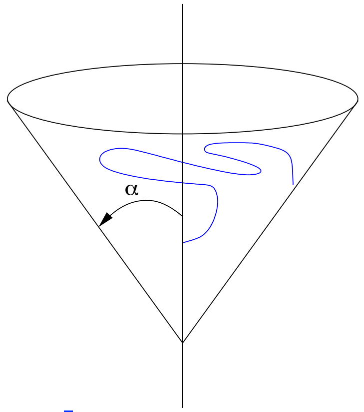
- In general, a series of nontrivial first-passage exponents

$$S_m \sim t^{-\beta_m} \qquad \text{with} \qquad \beta_1 > \beta_2 > \cdots > \beta_{N(N-1)/2}$$

Huge spectrum of first-passage exponents

Cone Approximation

- Fractional volume of allowed region given by equilibrium distribution of inversion number



$$V_m(N) = \sum_{l=0}^{m-1} P_l(N)$$

- Replace allowed region with cone of same fractional volume

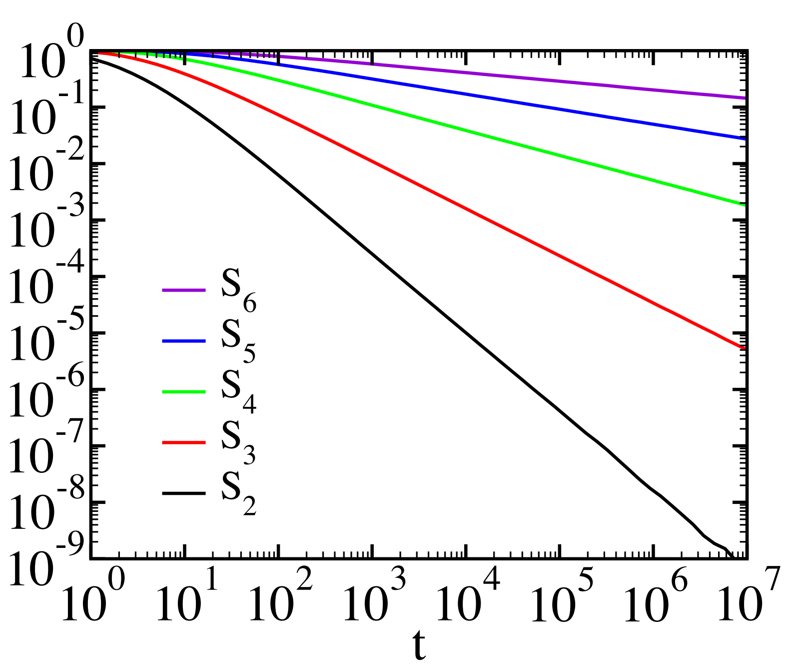
$$V(\alpha) = \frac{\int_0^\alpha d\theta\,(\sin\theta)^{N-3}}{\int_0^\pi d\theta\,(\sin\theta)^{N-3}}$$

- Use analytically known exponent for first-passage in cone

$$Q^{\gamma}_{2\beta+\gamma}(\cos\alpha) = 0 \qquad N \text{ odd},$$
$$P^{\gamma}_{2\beta+\gamma}(\cos\alpha) = 0 \qquad N \text{ even}.$$
$$\gamma = \frac{N-4}{2}$$

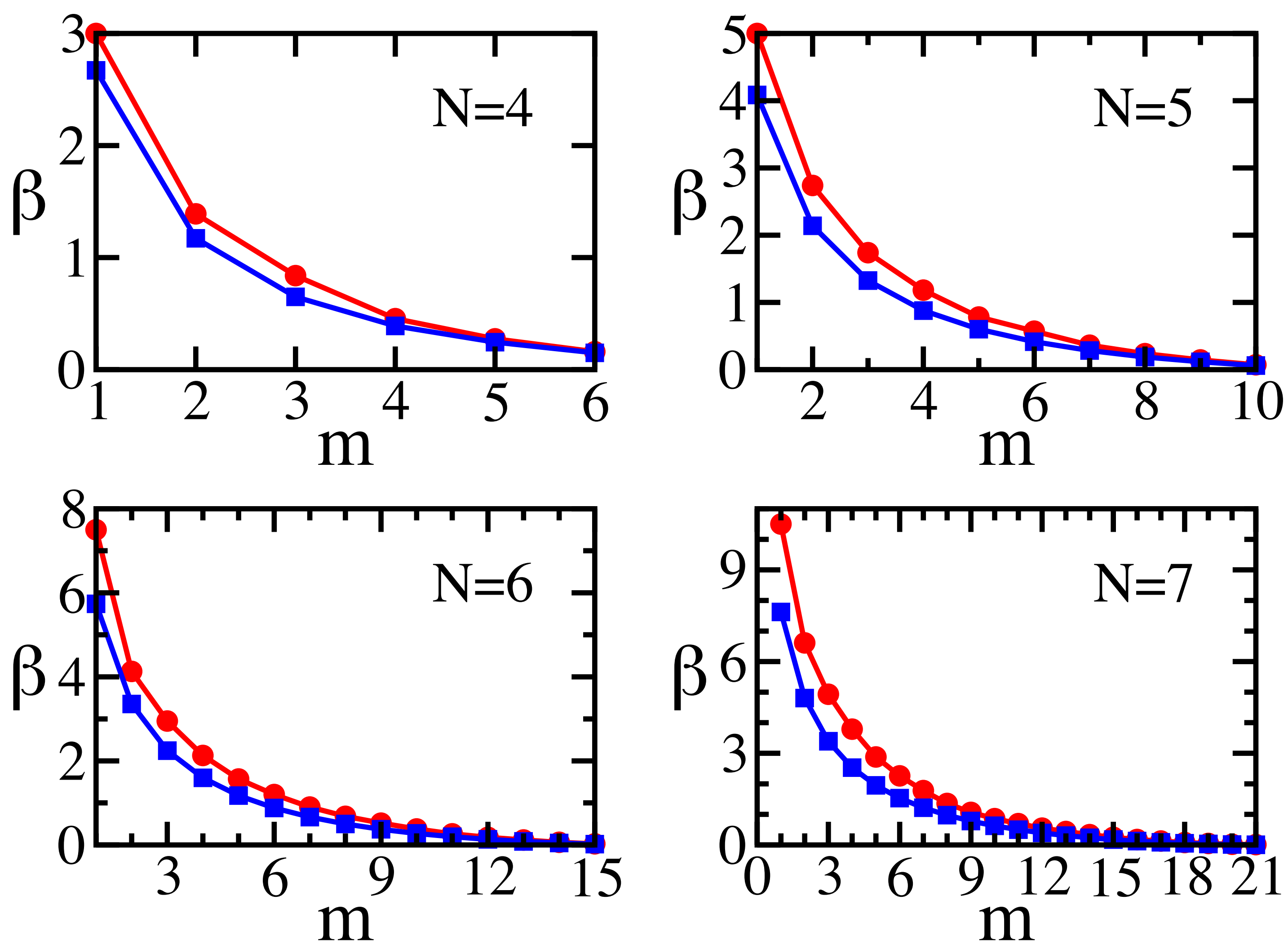
- Good approximation for four particles

m	1	2	3	4	5	6
V_m	$\frac{1}{24}$	$\frac{1}{6}$	$\frac{3}{8}$	$\frac{5}{8}$	$\frac{5}{6}$	$\frac{23}{24}$
α_m	0.41113	0.84106	1.31811	1.82347	2.30052	2.73045
β_m^{cone}	2.67100	1.17208	0.64975	0.39047	0.24517	0.14988
β_m	3	1.39	0.839	0.455	0.275	0.160



Small Number of Particles

- By construction, cone approximation is exact for N=3
- Cone approximation produces close estimates for first-passage exponents when the number of particles is small
- Cone approximation gives a formal lower bound



Very Large Number of Particles ($N \to \infty$)

- Gaussian equilibrium distribution implies

$$V_m(N) \to \frac{1}{2} + \frac{1}{2}\,\mathrm{erf}\left(\frac{z}{\sqrt{2}}\right) \qquad \text{with} \qquad z = \frac{m - \langle m \rangle}{\sigma}$$

- Volume of cone is also given by error function

$$V(\alpha, N) \to \frac{1}{2} + \frac{1}{2}\,\mathrm{erf}\left(\frac{-y}{\sqrt{2}}\right) \qquad \text{with} \qquad y = (\cos\alpha)\sqrt{N}$$

- First-passage exponent has the scaling form

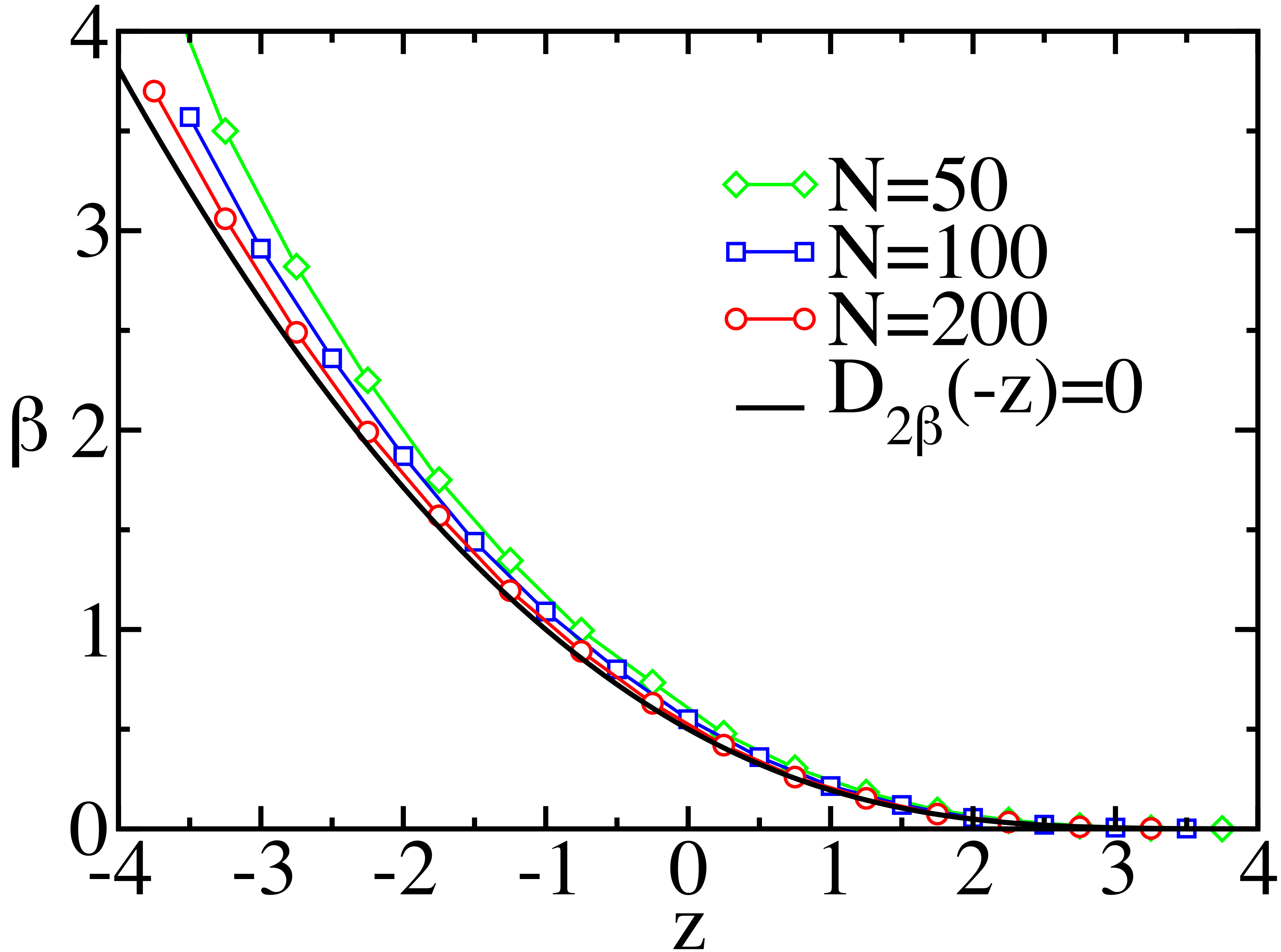
$$\beta_m(N) \to \beta(z) \quad \text{with} \quad z = \frac{m - \langle m \rangle}{\sigma}$$

- Scaling function is root of equation involving parabolic cylinder function

$$D_{2\beta}(-z) = 0$$

Scaling exponents have scaling behavior!

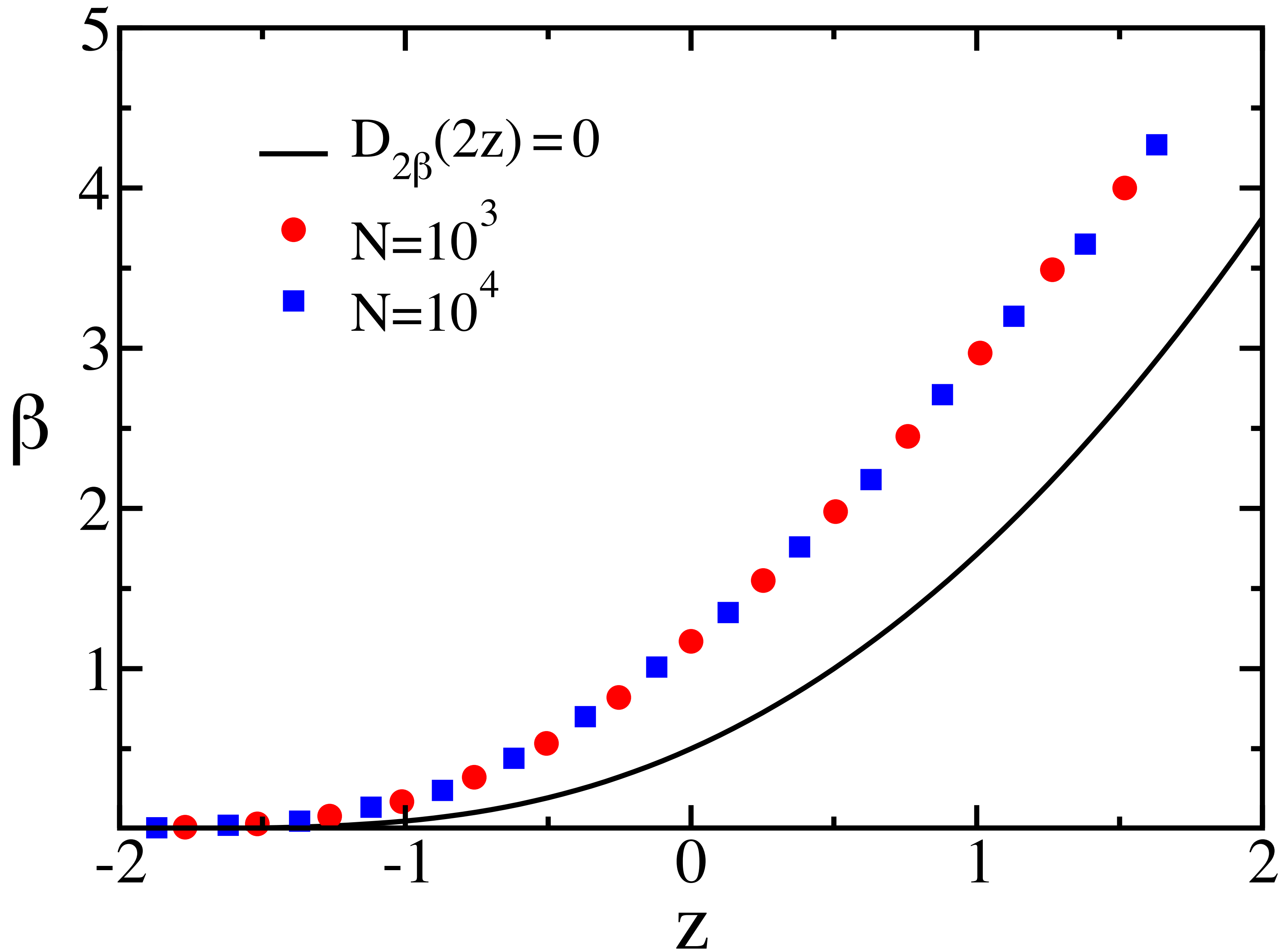
Simulation Results



Cone approximation is asymptotically exact!

Summary

- Inversion number as a measure for mixing
- Distribution of inversion number is Gaussian
- First-passage kinetics are rich
- Large spectrum of first-passage exponents
- Cone approximation gives good estimates for exponents
- Exponents follow a scaling behavior
- Cone approximation yields the exact scaling function
- Use inversion number to quantify mixing in 2 & 3 dimensions



Counter example: cone is not limiting shape

Outlook

- Heterogeneous Diffusion
- Fractional Diffusion — Metzler 11
- Accelerated Monte Carlo methods — Livermore Group (Donev) 09
- Scaling occurs in general
- Cone approach is not always asymptotically exact
- Geometric proof for exactness
- Limiting shapes in general

Publications

1. E. Ben-Naim,
   Phys. Rev. E **82**, 061103 (2010).

2. E. Ben-Naim and P.L. Krapivsky,
   J. Phys. A **43**, 495008 (2010).

3. E. Ben-Naim and P.L. Krapivsky,
   J. Phys. A **43**, 495007 (2010).

4. T. Antal, E. Ben-Naim, and P.L. Krapivsky,
   J. Stat. Mech. P07009 (2010)