Mixing of Diffusing Particles

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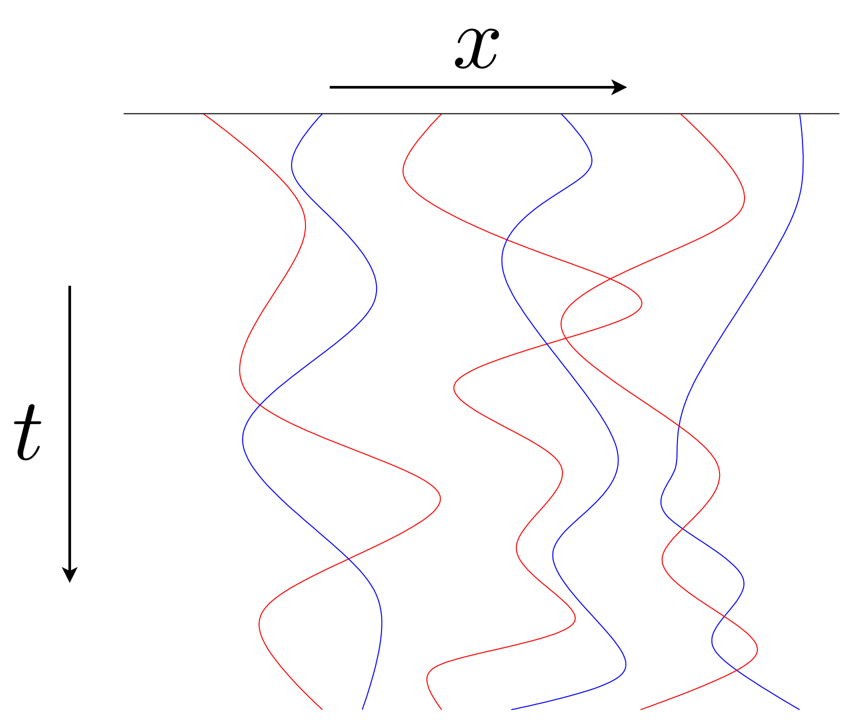
Diffusion in One Dimension

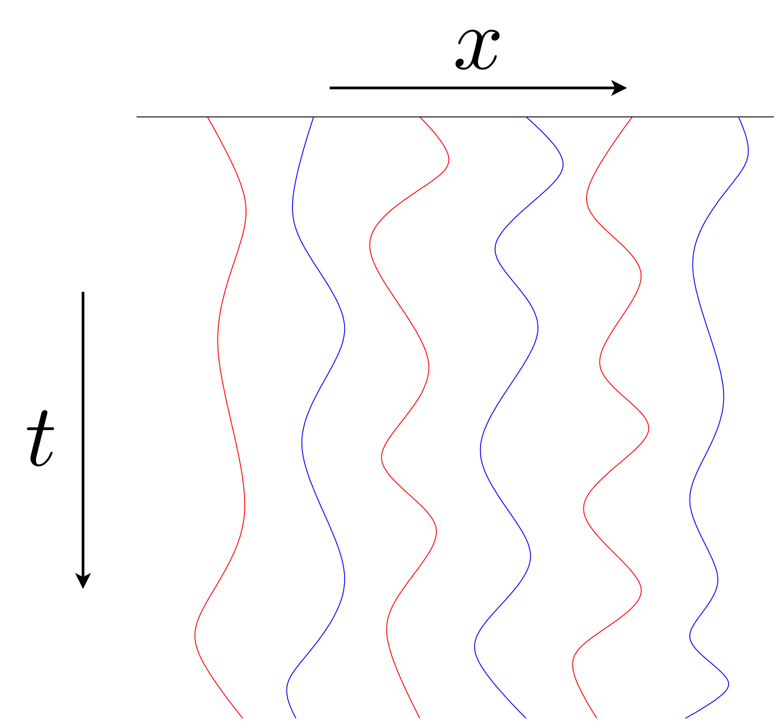
- Mixing: well-studied in fluids, granular media, not in <u>diffusion</u>
- **System:** N independent random walks in one dimension

Strong Mixing



trajectories cross many times

Poor Mixing



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

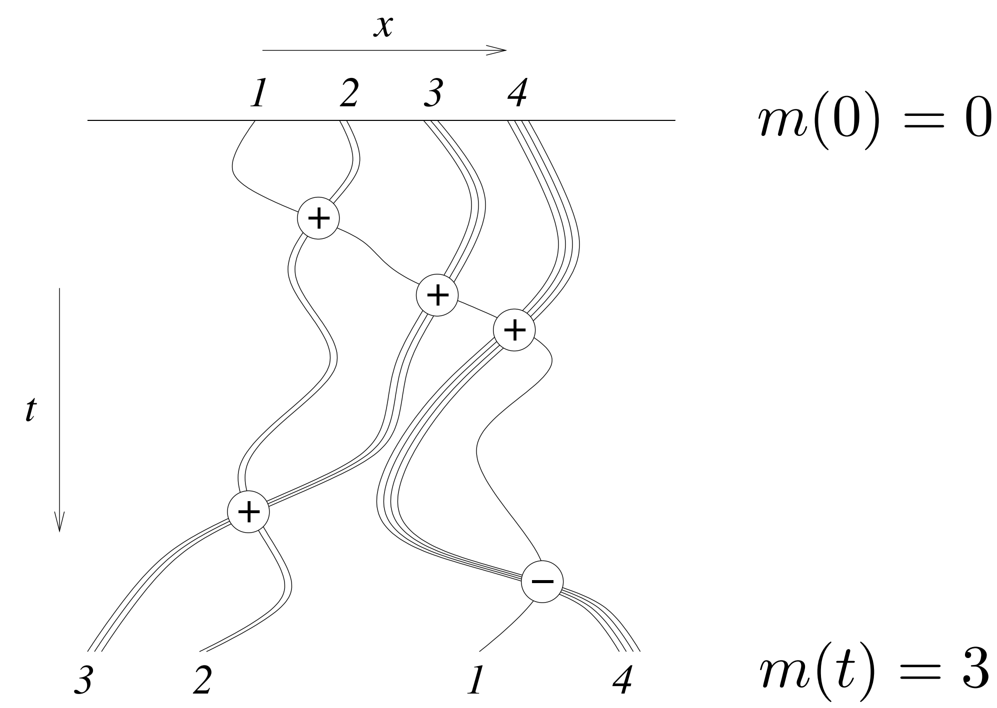
$$x \to \begin{cases} x-1 & \text{with probability } 1/2 \\ x+1 & \text{with probability } 1/2 \end{cases}$$

- 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



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

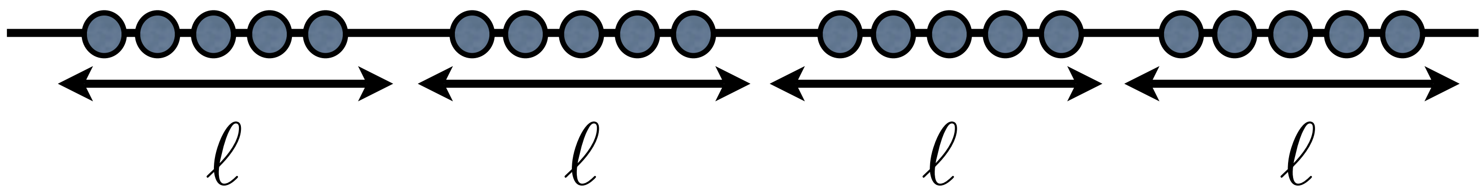
$$P_m(N) \simeq \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(m - \langle m \rangle)^2}{2\sigma^2}\right]$$

- Large fluctuations

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

Feller 1968

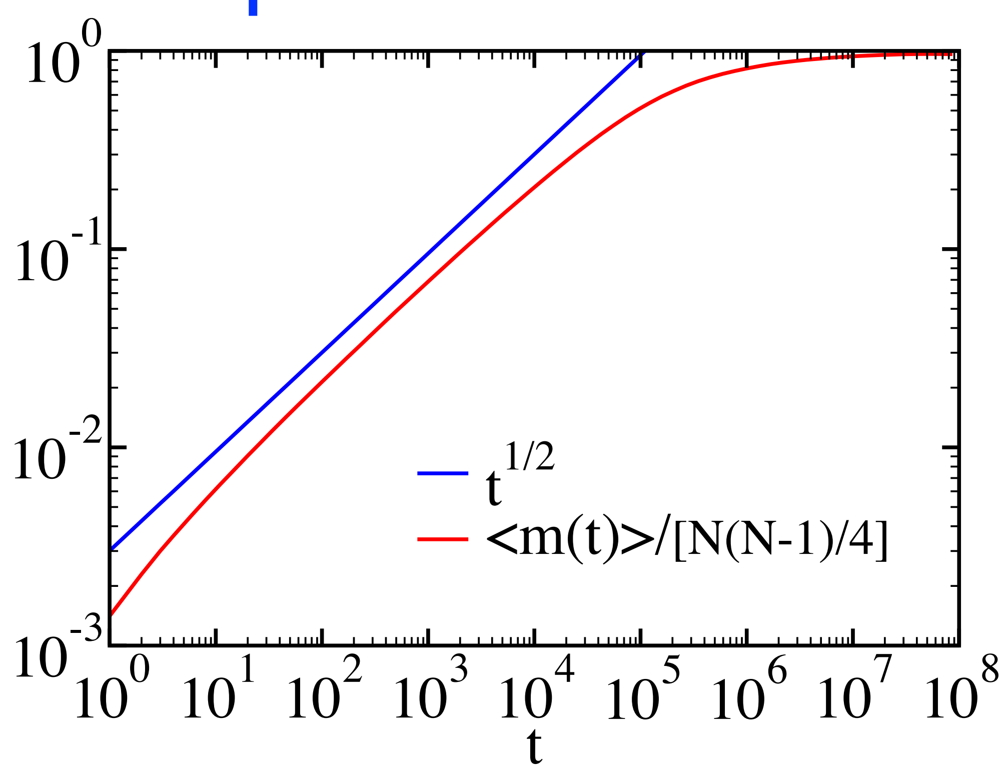
Transient Behavior

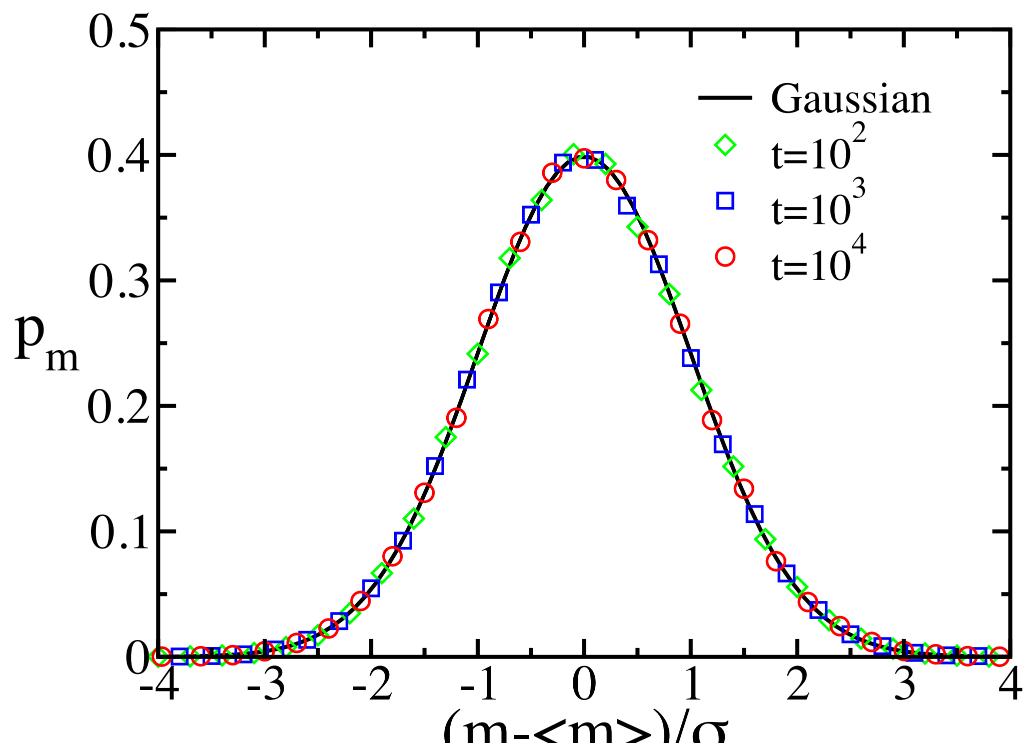


- Assume particles well mixed on a growing length scale
- Use equilibrium result for the sub-system $\langle m \rangle / N \sim \ell$
- Length scale must be diffusive $\ell \sim \sqrt{t}$

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

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

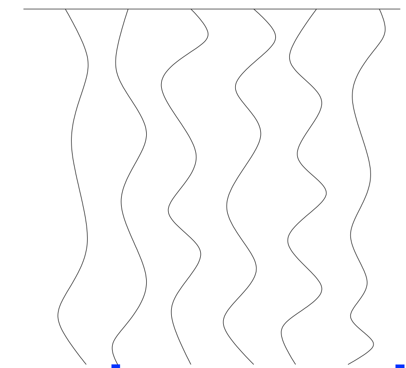




First-Passage Kinetics

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

1. Probability there are no crossing



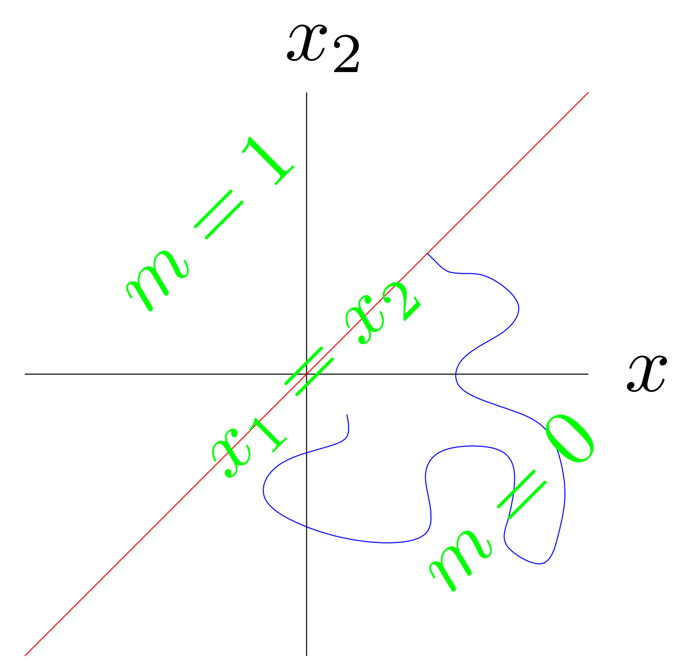
Fisher 1984

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

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

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

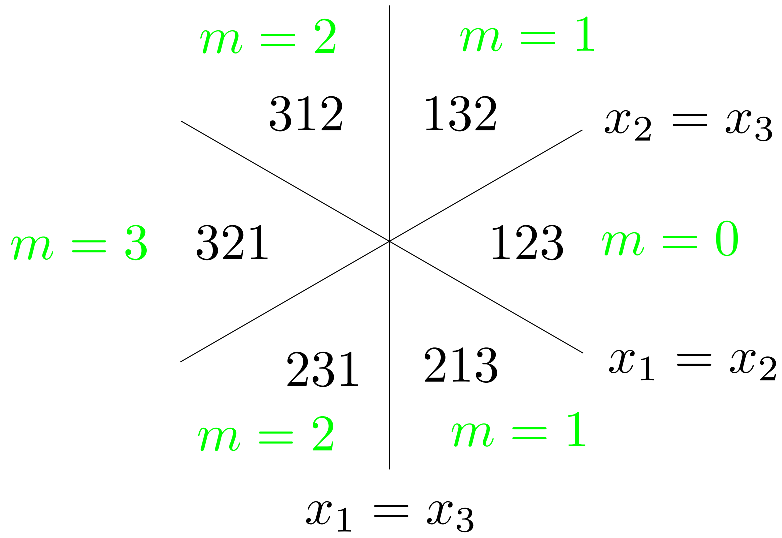
- Map N *1*-dimensional walks to *1* walk in N dimensions
  - Allowed region: inversion number $< m$
  - Forbidden region: inversion number $\geq m$
- Absorbing boundary condition

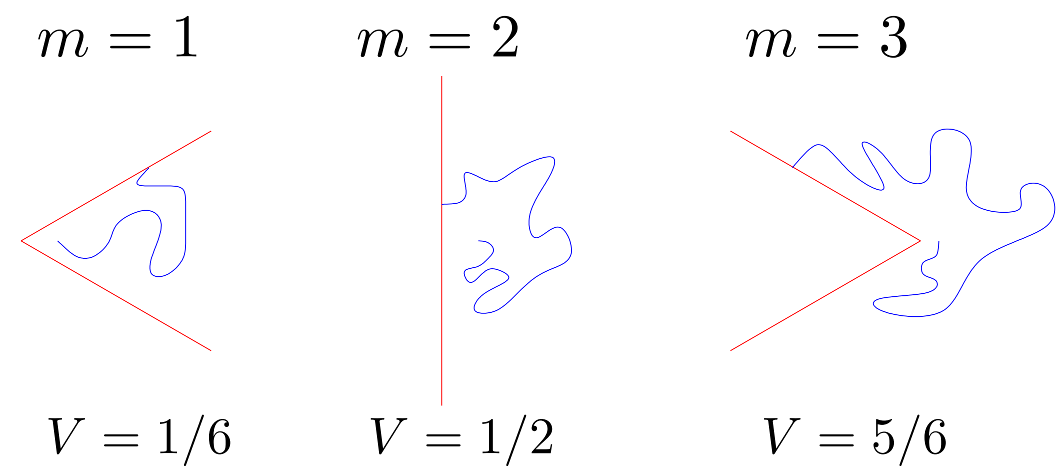


Problem reduces to diffusion in N dimensions in presence of complex absorbing boundary

Three particles

- Diffusion in three dimensions; Allowed regions are wedges





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

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

Redner 2001

- 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, the survival probabilities decay as power-law

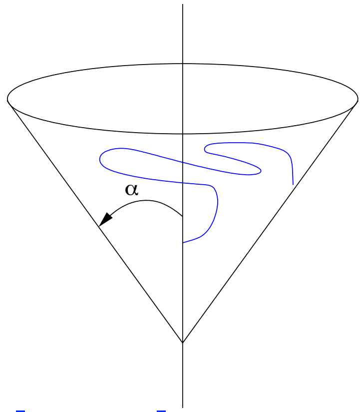
$$S_m\sim t^{-\beta_m} \qquad \text{with} \qquad \beta_1>\beta_2>\cdots>\beta_{N(N-1)/2}$$

Huge spectrum of first-passage exponents

Cone approximation

EB, Krapivsky 2010

- 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 with same fractional volume

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

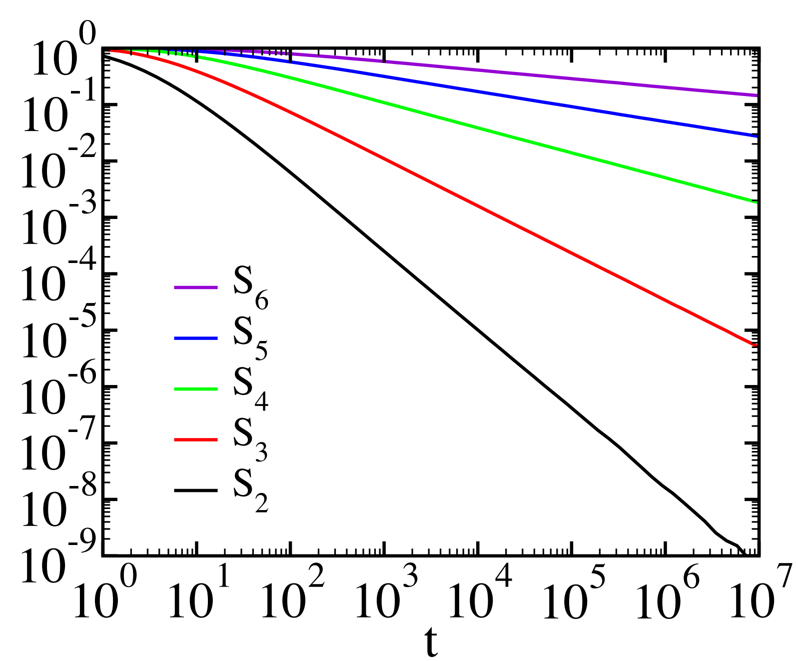
- Use analytically known exponent for first-passage in cone

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

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

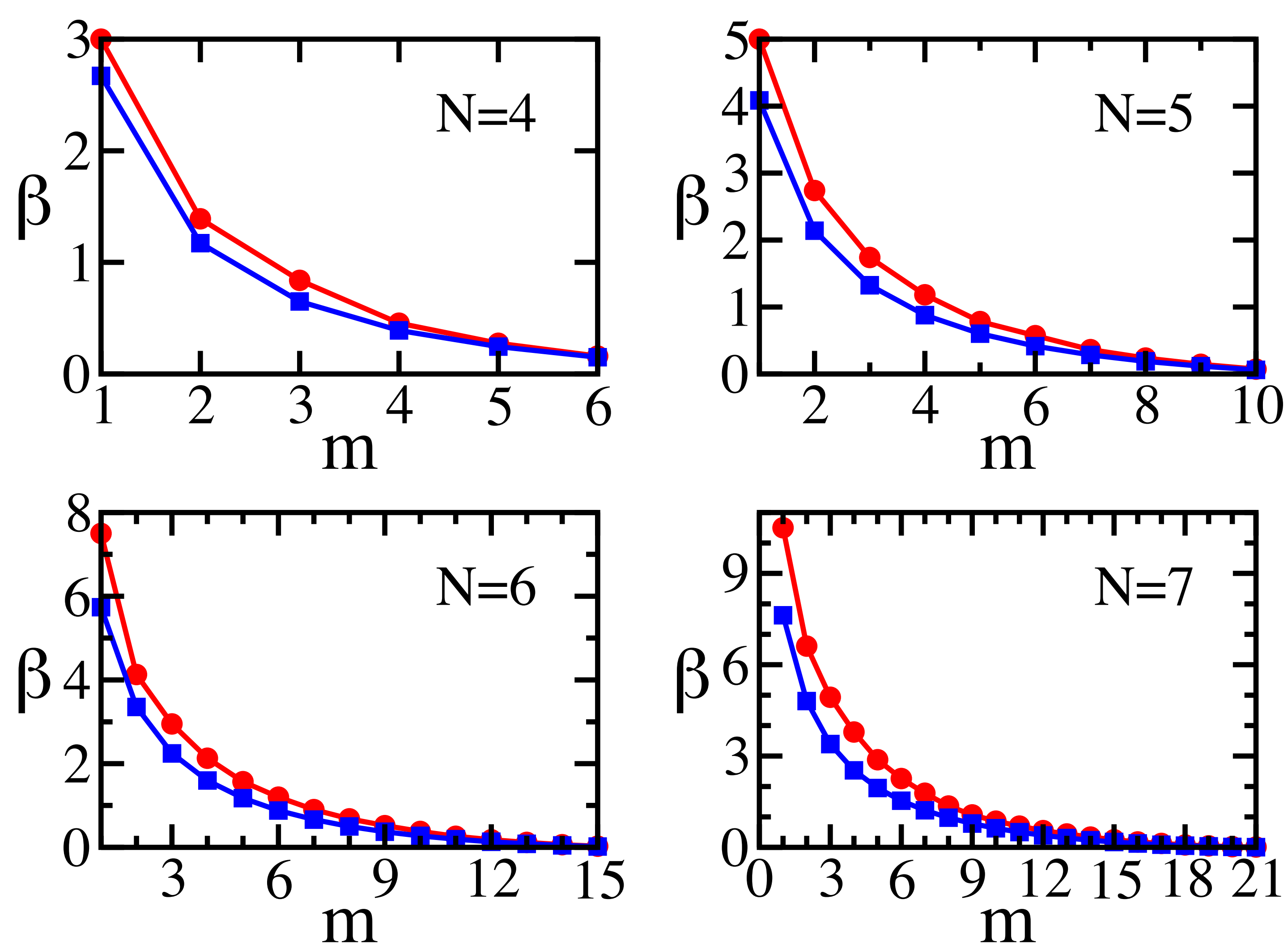
- Good approximation for four particles

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 EB, Krapivsky 2010

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

- First-passage exponent has the scaling form

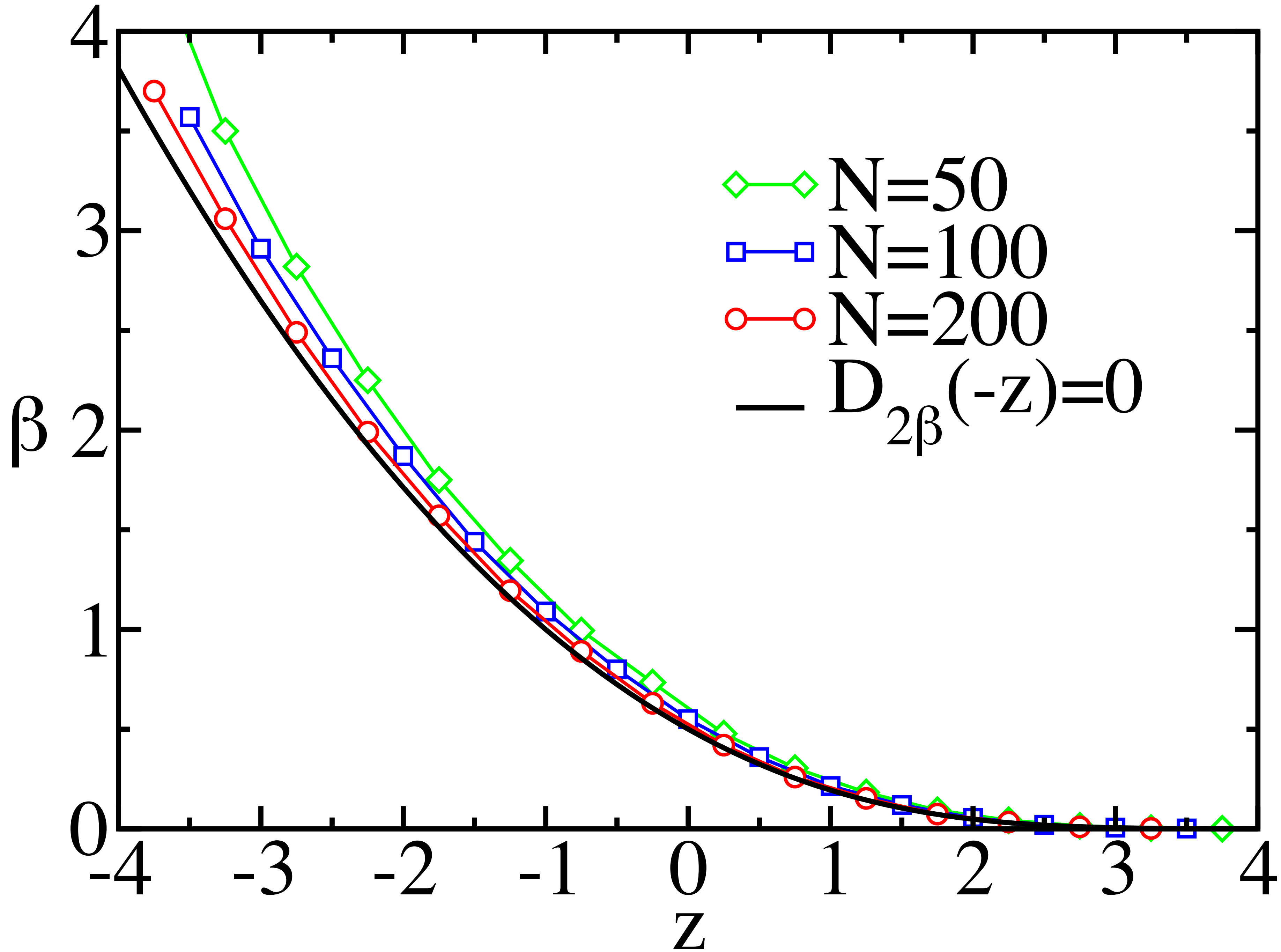
$$\beta_m(N) \to \beta(z) \quad \text{with} \quad z = \frac{m - \langle m \rangle}{\sigma}$$

- 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
- Geometric proof for exactness
- Use inversion number to quantify mixing in 2 & 3 dimensions