

First-Passage Problems in Systems with Many Degrees of Freedom

Alan Bray

University of Manchester

27 June 2006

COWORKERS

- Bernard Derrida
- Claude Godrèche
- Satya Majumdar
- Clément Sire
- Stephen Cornell
- Joachim Krug
- Harald Kallabis
- George Ehrhardt
- Richard Blythe
- Panos Gonos
- Lucian Anton
- Richard Smith

OUTLINE

OUTLINE

- Introduction: What is a first-passage problem?

OUTLINE

- Introduction: What is a first-passage problem?
- Systems with few degrees of freedom:
 - ▶ The random walk

OUTLINE

- Introduction: What is a first-passage problem?
- Systems with few degrees of freedom:
 - ▶ The random walk
 - ▶ The random acceleration process

OUTLINE

- Introduction: What is a first-passage problem?
- Systems with few degrees of freedom:
 - ▶ The random walk
 - ▶ The random acceleration process
 - ▶ Generalizations; The “Windy Cliff” .

OUTLINE

- Introduction: What is a first-passage problem?
- Systems with few degrees of freedom:
 - ▶ The random walk
 - ▶ The random acceleration process
 - ▶ Generalizations; The “Windy Cliff” .
- Partial Survival

OUTLINE

- Introduction: What is a first-passage problem?
- Systems with few degrees of freedom:
 - ▶ The random walk
 - ▶ The random acceleration process
 - ▶ Generalizations; The “Windy Cliff” .
- Partial Survival
- Systems with infinitely many degrees of freedom:

OUTLINE

- Introduction: What is a first-passage problem?
- Systems with few degrees of freedom:
 - ▶ The random walk
 - ▶ The random acceleration process
 - ▶ Generalizations; The “Windy Cliff” .
- Partial Survival
- Systems with infinitely many degrees of freedom:
 - ▶ Diffusion

OUTLINE

- Introduction: What is a first-passage problem?
- Systems with few degrees of freedom:
 - ▶ The random walk
 - ▶ The random acceleration process
 - ▶ Generalizations; The “Windy Cliff” .
- Partial Survival
- Systems with infinitely many degrees of freedom:
 - ▶ Diffusion
 - ▶ Coarsening problems

OUTLINE

- Introduction: What is a first-passage problem?
- Systems with few degrees of freedom:
 - The random walk
 - The random acceleration process
 - Generalizations; The “Windy Cliff” .
- Partial Survival
- Systems with infinitely many degrees of freedom:
 - Diffusion
 - Coarsening problems
 - (Fluctuating Interfaces).

OUTLINE

- Introduction: What is a first-passage problem?
- Systems with few degrees of freedom:
 - The random walk
 - The random acceleration process
 - Generalizations; The “Windy Cliff” .
- Partial Survival
- Systems with infinitely many degrees of freedom:
 - Diffusion
 - Coarsening problems
 - (Fluctuating Interfaces).
 - Reaction-Diffusion Models: The Trapping Reaction

OUTLINE

- Introduction: What is a first-passage problem?
- Systems with few degrees of freedom:
 - The random walk
 - The random acceleration process
 - Generalizations; The “Windy Cliff” .
- Partial Survival
- Systems with infinitely many degrees of freedom:
 - Diffusion
 - Coarsening problems
 - (Fluctuating Interfaces).
 - Reaction-Diffusion Models: The Trapping Reaction
- Summary

Introduction: What is a first-passage problem?

Introduction: What is a first-passage problem?

- You are playing roulette at a (fair) roulette wheel. You start with $\pounds n$ and decide to quit when your capital *first* reaches either zero or $\pounds N$. What is the probability that you reach $\pounds N$?

Introduction: What is a first-passage problem?

- You are playing roulette at a (fair) roulette wheel. You start with $\pounds n$ and decide to quit when your capital *first* reaches either zero or $\pounds N$. What is the probability that you reach $\pounds N$? (Ans: n/N)

Introduction: What is a first-passage problem?

- You are playing roulette at a (fair) roulette wheel. You start with $\pounds n$ and decide to quit when your capital *first* reaches either zero or $\pounds N$. What is the probability that you reach $\pounds N$? (Ans: n/N)
- You decide to keep playing until all your money is gone (“completion”). What is the probability, $Q(t)$, that you are *still playing* after time t ?

Introduction: What is a first-passage problem?

- You are playing roulette at a (fair) roulette wheel. You start with $\pounds n$ and decide to quit when your capital *first* reaches either zero or $\pounds N$. What is the probability that you reach $\pounds N$? (Ans: n/N)
- You decide to keep playing until all your money is gone (“completion”). What is the probability, $Q(t)$, that you are *still playing* after time t ? (Ans: If you bet at a uniform rate, $Q(t) \propto 1/\sqrt{t}$).

Introduction: What is a first-passage problem?

- You are playing roulette at a (fair) roulette wheel. You start with $\pounds n$ and decide to quit when your capital *first* reaches either zero or $\pounds N$. What is the probability that you reach $\pounds N$? (Ans: n/N)
- You decide to keep playing until all your money is gone (“completion”). What is the probability, $Q(t)$, that you are *still playing* after time t ? (Ans: If you bet at a uniform rate, $Q(t) \propto 1/\sqrt{t}$).
- You are walking home from the pub on a cliff path, staggering randomly from side to side. What is the probability that you *arrive home safely*?

Introduction: What is a first-passage problem?

- You are playing roulette at a (fair) roulette wheel. You start with $\pounds n$ and decide to quit when your capital *first* reaches either zero or $\pounds N$. What is the probability that you reach $\pounds N$? (Ans: n/N)
- You decide to keep playing until all your money is gone (“completion”). What is the probability, $Q(t)$, that you are *still playing* after time t ? (Ans: If you bet at a uniform rate, $Q(t) \propto 1/\sqrt{t}$).
- You are walking home from the pub on a cliff path, staggering randomly from side to side. What is the probability that you *arrive home safely*?
- You are swimming in a pool of alligators. What is the probability density, $P(t)$, to be eaten (“for the first time”) at time t ? What is the probability, $Q(t)$, to survive until time t ? Note that these are basically the same question, since $P(t) = -dQ/dt$.

The Random Walk (N=1):

The Random Walk (N=1):

$$\dot{x} = \eta(t); \quad \langle \eta(t)\eta(t') \rangle = 2D\delta(t - t'),$$

with an *absorbing boundary* at $x = 0$.

The Random Walk (N=1):

$$\dot{x} = \eta(t); \quad \langle \eta(t)\eta(t') \rangle = 2D\delta(t - t'),$$

with an *absorbing boundary* at $x = 0$.

First-passage problem:

What is the probability, $Q(x, t)$, that a walker *starting* at $x > 0$ has not yet reached zero at time t ?

$$\frac{\partial Q}{\partial t} = D \frac{\partial^2 Q}{\partial x^2} \quad (\text{BFPE})$$

Boundary conditions: $Q(0, t) = 0$, $Q(\infty, t) = 1$, all t

Initial Condition: $Q(x, 0) = 1$, $x > 0$.

The Random Walk (N=1):

$$\dot{x} = \eta(t); \quad \langle \eta(t)\eta(t') \rangle = 2D\delta(t - t'),$$

with an *absorbing boundary* at $x = 0$.

First-passage problem:

What is the probability, $Q(x, t)$, that a walker *starting* at $x > 0$ has not yet reached zero at time t ?

$$\frac{\partial Q}{\partial t} = D \frac{\partial^2 Q}{\partial x^2} \quad (\text{BFPE})$$

Boundary conditions: $Q(0, t) = 0$, $Q(\infty, t) = 1$, all t

Initial Condition: $Q(x, 0) = 1$, $x > 0$.

Solution:

$$Q(x, t) = \text{erf} \left(\frac{x}{\sqrt{4Dt}} \right) \propto t^{-1/2}, \quad t \gg x^2/D$$

The Random Acceleration Process (N=2):

The Random Acceleration Process (N=2):

$$\ddot{x} = \eta(t), \quad \text{or} \quad \dot{x} = v; \quad \dot{v} = \eta(t)$$

The Random Acceleration Process (N=2):

$$\ddot{x} = \eta(t), \quad \text{or} \quad \dot{x} = v; \quad \dot{v} = \eta(t)$$

$Q(x, v, t)$ is the probability that a particle *starting* at $x > 0$ with velocity v has not yet reached the absorbing boundary at $x = 0$ at time t .

$$\frac{\partial Q}{\partial t} = D \frac{\partial^2 Q}{\partial v^2} + v \frac{\partial Q}{\partial x} \quad (\text{BFPE})$$

The Random Acceleration Process (N=2):

$$\ddot{x} = \eta(t), \quad \text{or} \quad \dot{x} = v; \quad \dot{v} = \eta(t)$$

$Q(x, v, t)$ is the probability that a particle *starting* at $x > 0$ with velocity v has not yet reached the absorbing boundary at $x = 0$ at time t .

$$\frac{\partial Q}{\partial t} = D \frac{\partial^2 Q}{\partial^2 v} + v \frac{\partial Q}{\partial x} \quad (\text{BFPE})$$

Boundary Condition: $Q(0, v, t) = 0$ for all $v < 0$ and all t .

$$Q(x, v, t) = F \left(\frac{x^{2/3}}{D^{1/3}t}, \frac{v^3}{Dx} \right) \underset{t \rightarrow \infty}{\sim} \left(\frac{x^{2/3}}{D^{1/3}t} \right)^\theta G \left(\frac{v^3}{Dx} \right)$$

Obtain second-order ordinary differential equation (Kümmer's equation) for $G(z)$ in which θ appears as a parameter. The boundary conditions fix the value of θ :

$$\theta = \frac{1}{4}$$

(McKean, Sinai, Burkhardt)

The Processes $d^n x/dt^n = \eta(t)$ ($N=n$):

The Processes $d^n x/dt^n = \eta(t)$ ($N=n$):

In each case, the survival probability (with an absorbing boundary at $x = 0$) decays asymptotically as $Q \sim t^{-\theta}$.

n	θ
1	1/2
2	1/4

The Processes $d^n x/dt^n = \eta(t)$ ($N=n$):

In each case, the survival probability (with an absorbing boundary at $x = 0$) decays asymptotically as $Q \sim t^{-\theta}$.

n	θ
1	1/2
2	1/4
3	0.2202
4	0.2096
5	0.2041
6	0.2008
∞	0.1875

The $n \rightarrow \infty$ limit is related to an entirely different problem – diffusion in two dimensions (see later).

All these processes are Gaussian, so everything, including the exponent θ , is determined by the two-time correlator, $C(t_1, t_2) = \langle x(t_1)x(t_2) \rangle$.

Higher Dimensions

Higher Dimensions

- The Random Walk: $\dot{\mathbf{x}} = \eta(t)$

$$\theta = (2 - d)/2, \quad d < 2$$

For dimensions $d > 2$ there is a non-zero probability that the walker never hits the absorbing region (borderline dimension signalling recurrence-transience transition of a random walker). The process is *recurrent* for $d < 2$, and *transient* for $d > 2$.

Higher Dimensions

- The Random Walk: $\dot{\mathbf{x}} = \eta(t)$

$$\theta = (2 - d)/2, \quad d < 2$$

For dimensions $d > 2$ there is a non-zero probability that the walker never hits the absorbing region (borderline dimension signalling recurrence-transience transition of a random walker). The process is *recurrent* for $d < 2$, and *transient* for $d > 2$.

- Random Acceleration: $\ddot{\mathbf{x}} = \eta(t)$

Is there a borderline dimension? If so, what is it?

The “Windy Cliff” (Redner and Krapivsky) ($N=2$)

The “Windy Cliff” (Redner and Krapivsky) (N=2)

The following class of *non-Gaussian* processes is also exactly soluble:

$$\begin{aligned}\dot{y} &= \eta(t) \\ \dot{x} &= \begin{cases} v_+ y^\alpha, & y > 0 \\ -v_- (-y)^\alpha, & y < 0 \end{cases}\end{aligned}$$

which corresponds to a particle diffusing (random walk) in the y direction under a deterministic (and asymmetric) “shear flow” in the x -direction. There is an absorbing boundary at $x = 0$.

The “Windy Cliff” (Redner and Krapivsky) (N=2)

The following class of *non-Gaussian* processes is also exactly soluble:

$$\begin{aligned}\dot{y} &= \eta(t) \\ \dot{x} &= \begin{cases} v_+ y^\alpha, & y > 0 \\ -v_- (-y)^\alpha, & y < 0 \end{cases}\end{aligned}$$

which corresponds to a particle diffusing (random walk) in the y direction under a deterministic (and asymmetric) “shear flow” in the x -direction. There is an absorbing boundary at $x = 0$.

Using the same method (after Burkhardt) as for the random acceleration problem (which corresponds to $\alpha = 1$ and $v_+ = v_-$) gives

$$\theta = \frac{1}{4} - \frac{1}{2\pi\beta} \tan^{-1} \left[\frac{\gamma - 1}{\gamma + 1} \tan \left(\frac{\pi\beta}{2} \right) \right] \quad (\text{AB} + \text{Gonos}(2004))$$

where $\gamma = (v_+/v_-)^\beta$ and $\beta = 1/(2 + \alpha)$.

For $v_+ = v_-$, the “universal” result $\theta = 1/4$ is obtained, independent of α .

PARTIAL SURVIVAL (Majumdar and AB, 1998)

PARTIAL SURVIVAL (Majumdar and AB, 1998)

We consider the probability $Q(p, t)$ for the process to survive to time t given that it survives each zero-crossing with probability p . It has the form

$$Q(p, t) = \sum_{n=0}^{\infty} p^n P_n(t) \sim t^{-\theta(p)}, \quad t \rightarrow \infty$$
$$\Rightarrow \ln Q(p, t) = \sum_{r=1}^{\infty} \frac{(\ln p)^r}{r!} \langle n^r \rangle_c \sim -\theta(p) \ln t, \quad (1)$$

relating $Q(p, t)$ to the *statistics of the number of crossings, n* , in time t .

PARTIAL SURVIVAL (Majumdar and AB, 1998)

We consider the probability $Q(p, t)$ for the process to survive to time t given that it survives each zero-crossing with probability p . It has the form

$$Q(p, t) = \sum_{n=0}^{\infty} p^n P_n(t) \sim t^{-\theta(p)}, \quad t \rightarrow \infty$$
$$\Rightarrow \ln Q(p, t) = \sum_{r=1}^{\infty} \frac{(\ln p)^r}{r!} \langle n^r \rangle_c \sim -\theta(p) \ln t, \quad (1)$$

relating $Q(p, t)$ to the *statistics of the number of crossings, n* , in time t .

Example: the generalised “windy cliff” –

PARTIAL SURVIVAL (Majumdar and AB, 1998)

We consider the probability $Q(p, t)$ for the process to survive to time t given that it survives each zero-crossing with probability p . It has the form

$$Q(p, t) = \sum_{n=0}^{\infty} p^n P_n(t) \sim t^{-\theta(p)}, \quad t \rightarrow \infty$$
$$\Rightarrow \ln Q(p, t) = \sum_{r=1}^{\infty} \frac{(\ln p)^r}{r!} \langle n^r \rangle_c \sim -\theta(p) \ln t, \quad (1)$$

relating $Q(p, t)$ to the *statistics of the number of crossings, n* , in time t .
Example: the generalised “windy cliff” –

$$\theta(p) = \frac{1}{4} - \frac{1}{2\pi\beta} \sin^{-1} \left(\sqrt{A} \sin \left(\frac{\pi\beta}{2} \right) \right), \quad \text{where}$$
$$A = \frac{2p^2 \cos^2 \left(\frac{\pi\beta}{2} \right) + 2 \sinh^2 \left(\frac{1}{2} \ln \gamma \right)}{\cos(\pi\beta) + \cosh(\ln \gamma)},$$

and $\gamma = (v_+/v_-)^\beta$, $\beta = 1/(2 + \alpha)$. (Majumdar and AB, 2006, in preparation)

"Persistence" in Spatially Extended Systems

“Persistence” in Spatially Extended Systems

“Simple” example: The Diffusion Equation

$$\frac{\partial \phi}{\partial t} = D \nabla^2 \phi$$

with random (white noise) initial conditions,

$$\langle \phi(\mathbf{x}, 0) \rangle = 0; \quad \langle \phi(\mathbf{x}, 0) \phi(\mathbf{x}', 0) \rangle = \Delta \delta^d(\mathbf{x} - \mathbf{x}')$$

“Persistence” in Spatially Extended Systems

“Simple” example: The Diffusion Equation

$$\frac{\partial \phi}{\partial t} = D \nabla^2 \phi$$

with random (white noise) initial conditions,

$$\langle \phi(\mathbf{x}, 0) \rangle = 0; \quad \langle \phi(\mathbf{x}, 0) \phi(\mathbf{x}', 0) \rangle = \Delta \delta^d(\mathbf{x} - \mathbf{x}')$$

The normalized one-point, two-time correlator is

$$C(t_1, t_2) = \frac{\langle \phi(\mathbf{x}, t_1) \phi(\mathbf{x}, t_2) \rangle}{[\langle \phi^2(\mathbf{x}, t_1) \rangle \langle \phi^2(\mathbf{x}, t_2) \rangle]^{1/2}} = \left(\frac{4t_1 t_2}{(t_1 + t_2)^2} \right)^{d/4} \quad (\text{scaling form})$$

“Persistence” in Spatially Extended Systems

“Simple” example: The Diffusion Equation

$$\frac{\partial \phi}{\partial t} = D \nabla^2 \phi$$

with random (white noise) initial conditions,

$$\langle \phi(\mathbf{x}, 0) \rangle = 0; \quad \langle \phi(\mathbf{x}, 0) \phi(\mathbf{x}', 0) \rangle = \Delta \delta^d(\mathbf{x} - \mathbf{x}')$$

The normalized one-point, two-time correlator is

$$C(t_1, t_2) = \frac{\langle \phi(\mathbf{x}, t_1) \phi(\mathbf{x}, t_2) \rangle}{[\langle \phi^2(\mathbf{x}, t_1) \rangle \langle \phi^2(\mathbf{x}, t_2) \rangle]^{1/2}} = \left(\frac{4t_1 t_2}{(t_1 + t_2)^2} \right)^{d/4} \quad (\text{scaling form})$$

Introduce a new time variable $T = \ln t$. Then $C(t_1, t_2) \rightarrow C(T)$, where $T = T_2 - T_1$ and

$$C(T) = \text{sech}^{d/2}(T/2) \quad (\text{Gaussian Stationary Process})$$

The Independent Interval Approximation (Majumdar et al.; Derrida et al.)

The Independent Interval Approximation (Majumdar et al.; Derrida et al.)

- $C(T)$ is the correlator of the GSP, $X(T) = \phi(\mathbf{x}, t) / \sqrt{\langle \phi^2(\mathbf{x}, t) \rangle}$.

The Independent Interval Approximation (Majumdar et al.; Derrida et al.)

- $C(T)$ is the correlator of the GSP, $X(T) = \phi(\mathbf{x}, t) / \sqrt{\langle \phi^2(\mathbf{x}, t) \rangle}$.
- We focus on the *zero crossings* of this process, and *assume* that the intervals between zero crossings are *independent random variables* with a known distribution, $P_{\text{int}}(T)$.

The Independent Interval Approximation (Majumdar et al.; Derrida et al.)

- $C(T)$ is the correlator of the GSP, $X(T) = \phi(\mathbf{x}, t) / \sqrt{\langle \phi^2(\mathbf{x}, t) \rangle}$.
- We focus on the *zero crossings* of this process, and *assume* that the intervals between zero crossings are *independent random variables* with a known distribution, $P_{\text{int}}(T)$.
- This distribution can be determined from the correlator of the *clipped* process, $\text{sgn } X(T)$, with correlator

$$A(T) = \langle \text{sgn } X(T) \text{sgn } X(0) \rangle = \frac{2}{\pi} \sin^{-1} C(T) \quad (\text{true for any GSP})$$

The Independent Interval Approximation (Majumdar et al.; Derrida et al.)

- $C(T)$ is the correlator of the GSP, $X(T) = \phi(\mathbf{x}, t) / \sqrt{\langle \phi^2(\mathbf{x}, t) \rangle}$.
- We focus on the *zero crossings* of this process, and *assume* that the intervals between zero crossings are *independent random variables* with a known distribution, $P_{\text{int}}(T)$.
- This distribution can be determined from the correlator of the *clipped* process, $\text{sgn } X(T)$, with correlator

$$A(T) = \langle \text{sgn } X(T) \text{sgn } X(0) \rangle = \frac{2}{\pi} \sin^{-1} C(T) \quad (\text{true for any GSP})$$

- The probability to have no crossings in time T is given, for large T , by the tail behavior, $P_{\text{int}}(T) \sim \exp(-\theta T) = t^{-\theta}$ for $T \rightarrow \infty$.

The Independent Interval Approximation (Majumdar et al.; Derrida et al.)

- $C(T)$ is the correlator of the GSP, $X(T) = \phi(\mathbf{x}, t) / \sqrt{\langle \phi^2(\mathbf{x}, t) \rangle}$.
- We focus on the *zero crossings* of this process, and *assume* that the intervals between zero crossings are *independent random variables* with a known distribution, $P_{\text{int}}(T)$.
- This distribution can be determined from the correlator of the *clipped* process, $\text{sgn} X(T)$, with correlator

$$A(T) = \langle \text{sgn} X(T) \text{sgn} X(0) \rangle = \frac{2}{\pi} \sin^{-1} C(T) \quad (\text{true for any GSP})$$

- The probability to have no crossings in time T is given, for large T , by the tail behavior, $P_{\text{int}}(T) \sim \exp(-\theta T) = t^{-\theta}$ for $T \rightarrow \infty$.
- The “persistence”, $Q(t) \sim t^{-\theta}$, is the fraction of space in which the field has not changed sign up to time t .
- This approach has recently been generalised to non-crossing of an arbitrary level (Sire, cond-mat/0606145).

Diffusive Persistence: Results

d	θ_{IIA}	θ^*
1	0.1203	0.1205
2	0.1862	0.1875
3	0.2358	0.2382

*From the “correlator expansion”
(Ehrhardt, AB, 2001; Ehrhardt, AB, Majumdar, 2004)

Diffusive Persistence: Results

d	θ_{IIA}	θ^*
1	0.1203	0.1205
2	0.1862	0.1875
3	0.2358	0.2382

*From the “correlator expansion”
(Ehrhardt, AB, 2001; Ehrhardt, AB, Majumdar, 2004)

Coarsening Dynamics of other Scalar Fields

- Two-dimensional Ising model at zero temperature ($\theta \approx 0.22$).
- Two-dimensional Ginzburg-Landau equation: $\partial_t \phi = \nabla^2 \phi + \phi - \phi^3$ ($\theta \approx 0.18$).
- One-dimensional Potts model (Derrida, Hakim, Pasquier, 1995):

$$\theta = -\frac{1}{8} + \frac{2}{\pi^2} \left[\cos^{-1} \left(\frac{2-q}{\sqrt{2q}} \right) \right]^2 \quad (q = \text{number of Potts states})$$

Structure of the Persistent Set

Structure of the Persistent Set

The three systems - diffusion, TDGL dynamics, and Ising dynamics all “coarsen” with a growing characteristic length scale $L(t) \sim t^{1/2}$. The persistent set is the set of points that have always been in same “phase” up to time t .

Structure of the Persistent Set

The three systems - diffusion, TDGL dynamics, and Ising dynamics all “coarsen” with a growing characteristic length scale $L(t) \sim t^{1/2}$. The persistent set is the set of points that have always been in same “phase” up to time t .

The probability that two points separated by r both belong to the persistent set has the form

$$P(r, t) = t^{-2\theta} f(r/t^{1/2})$$

where $f(x) \rightarrow \text{const.}$ for $x \gg 1$, and $f(x) \sim x^{-2\theta}$ for $x \ll 1$. In the latter regime

$$P(r, t) \sim t^{-\theta} r^{-2\theta}$$

Structure of the Persistent Set

The three systems - diffusion, TDGL dynamics, and Ising dynamics all “coarsen” with a growing characteristic length scale $L(t) \sim t^{1/2}$. The persistent set is the set of points that have always been in same “phase” up to time t .

The probability that two points separated by r both belong to the persistent set has the form

$$P(r, t) = t^{-2\theta} f(r/t^{1/2})$$

where $f(x) \rightarrow \text{const.}$ for $x \gg 1$, and $f(x) \sim x^{-2\theta}$ for $x \ll 1$. In the latter regime

$$P(r, t) \sim t^{-\theta} r^{-2\theta}$$

The probability for the second point to be in the set *given that the first point is in the set* is therefore

$$R(r, t) \sim r^{-2\theta} \quad (r \ll t^{1/2})$$

The set therefore has a fractal structure, on scales smaller than $t^{1/2}$, with fractal dimension

$$d_f = d - 2\theta$$

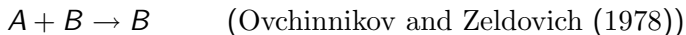
REACTION-DIFFUSION PROBLEMS: THE TRAPPING REACTION

REACTION-DIFFUSION PROBLEMS: THE TRAPPING REACTION



with different diffusion constants D_A, D_B .

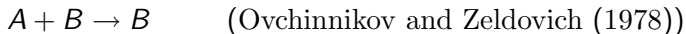
REACTION-DIFFUSION PROBLEMS: THE TRAPPING REACTION



with different diffusion constants D_A, D_B .

Define $Q(t)$ to be the fraction of A particles that survive till time t , which is also the probability that a randomly chosen A -particle survives till time t .

REACTION-DIFFUSION PROBLEMS: THE TRAPPING REACTION



with different diffusion constants D_A, D_B .

Define $Q(t)$ to be the fraction of A particles that survive till time t , which is also the probability that a randomly chosen A -particle survives till time t .

Rate equation approach:

$$\frac{dQ}{dt} = -\lambda\rho_B Q \Rightarrow Q(t) = \exp(-\lambda\rho_B t)$$

However, spatial fluctuations are important for $d \leq 2$ (reactions are diffusion-limited).

REACTION-DIFFUSION PROBLEMS: THE TRAPPING REACTION



with different diffusion constants D_A, D_B .

Define $Q(t)$ to be the fraction of A particles that survive till time t , which is also the probability that a randomly chosen A -particle survives till time t .

Rate equation approach:

$$\frac{dQ}{dt} = -\lambda \rho_B Q \Rightarrow Q(t) = \exp(-\lambda \rho_B t)$$

However, spatial fluctuations are important for $d \leq 2$ (reactions are diffusion-limited).

Exact asymptotic forms (Bramson and Lebowitz 1988):

$$Q(t) \sim \begin{cases} \exp(-\lambda_d t^{d/2}), & d < 2 \\ \exp(-\lambda_2 t / \ln t), & d = 2 \\ \exp(-\lambda_d t), & d > 2 \end{cases}$$

UPPER and LOWER BOUNDS ON $Q(t)$ (AB and Blythe (2002,2003))

The Upper Bound ($d=1$) ("*Pascal Principle*")

$$Q(t) \leq Q_U(t) = Q_{TAP}(t) = \exp\left(-\frac{4}{\sqrt{\pi}} \rho_B (D_B t)^{1/2}\right)$$

where $Q_{TAP}(t)$ is the result for the "Target Annihilation Problem", corresponding to $D_A = 0$ (static A -particle with mobile traps).

The Upper Bound ($d=1$) ("*Pascal Principle*")

$$Q(t) \leq Q_U(t) = Q_{TAP}(t) = \exp\left(-\frac{4}{\sqrt{\pi}} \rho_B (D_B t)^{1/2}\right)$$

where $Q_{TAP}(t)$ is the result for the "Target Annihilation Problem", corresponding to $D_A = 0$ (static A -particle with mobile traps).

For general dimensions $d \leq 2$ the results have the Bramson-Lebowitz forms

$$Q_U(t) = \begin{cases} \exp(-\lambda_d t^{d/2}), & d < 2 \\ \exp(-\lambda_2 t / \ln t), & d = 2 \end{cases}$$

with

$$\lambda_d = \begin{cases} \frac{2}{\pi d} \sin\left(\frac{\pi d}{2}\right) (4\pi D_B)^{d/2} \rho_B, & d < 2 \\ 4\pi D_B \rho_B, & d = 2 \end{cases}$$

THE PASCAL PRINCIPLE (Moreau et al; AB, Majumdar, Blythe, 2003)

THE PASCAL PRINCIPLE (Moreau et al; AB, Majumdar, Blythe, 2003)

“Tout le malheur des hommes vient d’une seule chose, qui est de ne savoir pas demeurer en repos, dans une chambre.”

(Pascal, Pensées, fragment 139 (1670)).

THE PASCAL PRINCIPLE (Moreau et al; AB, Majumdar, Blythe, 2003)

“Tout le malheur des hommes vient d’une seule chose, qui est de ne savoir pas demeurer en repos, dans une chambre.”

(Pascal, Pensées, fragment 139 (1670)).

“All the misfortune of man comes from the fact that he does not stay peacefully in his room.”

The Target Annihilation Problem (d=1)

The Target Annihilation Problem (d=1)

A B-particle (trap), starting at x , has not yet reached the target (located at $x = 0$) at time t with probability

$$q(t) = \operatorname{erf} \left(\frac{|x|}{\sqrt{4D_B t}} \right)$$

The Target Annihilation Problem (d=1)

A B-particle (trap), starting at x , has not yet reached the target (located at $x = 0$) at time t with probability

$$q(t) = \operatorname{erf} \left(\frac{|x|}{\sqrt{4D_B t}} \right)$$

Averaging over the initial position x , uniformly in the interval $(-L, L)$, gives

$$\bar{q} = 1 - \frac{1}{2L} \int_{-L}^L dx \operatorname{erfc} \left(\frac{|x|}{\sqrt{4D_B t}} \right) = 1 - \frac{1}{L} \frac{4}{\sqrt{\pi}} \sqrt{D_B t}$$

The Target Annihilation Problem (d=1)

A B-particle (trap), starting at x , has not yet reached the target (located at $x = 0$) at time t with probability

$$q(t) = \operatorname{erf} \left(\frac{|x|}{\sqrt{4D_B t}} \right)$$

Averaging over the initial position x , uniformly in the interval $(-L, L)$, gives

$$\bar{q} = 1 - \frac{1}{2L} \int_{-L}^L dx \operatorname{erfc} \left(\frac{|x|}{\sqrt{4D_B t}} \right) = 1 - \frac{1}{L} \frac{4}{\sqrt{\pi}} \sqrt{D_B t}$$

The probability that *none* of N traps has reached the target is

$$Q_{TAP}(t) = \left(1 - \frac{1}{L} \frac{4}{\sqrt{\pi}} \sqrt{D_B t} \right)^N \Rightarrow \exp \left(-\frac{4}{\sqrt{\pi}} \rho_B \sqrt{D_B t} \right)$$

(in the limit $N \rightarrow \infty$, $L \rightarrow \infty$ with $\rho_B = N/L$ fixed).

The Lower Bound ($d=1$)

The Lower Bound ($d=1$)

Create a fictitious box with edges at $x = \pm\ell/2$, and consider the subset of trajectories in which

- 1 There are no B-particles initially inside the box.
- 2 The A-particle stays in the box up to time t .
- 3 No B-particles enter the box up to time t .

The Lower Bound ($d=1$)

Create a fictitious box with edges at $x = \pm\ell/2$, and consider the subset of trajectories in which

- 1 There are no B-particles initially inside the box.
- 2 The A-particle stays in the box up to time t .
- 3 No B-particles enter the box up to time t .

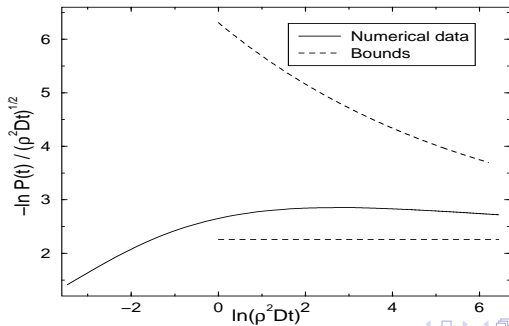
These trajectories are a subset of all trajectories for which the A-particle survives till time t , so

$$\begin{aligned} Q(t) \geq Q_L(t) &\sim \max_{\ell} \exp(-\rho_B \ell - \pi^2 D_{At}/\ell^2) Q_{TAP}(t) \\ &\sim \exp[-\text{const.}(\rho_B^2 D_{At})^{1/3}] Q_{TAP}(t) \end{aligned}$$

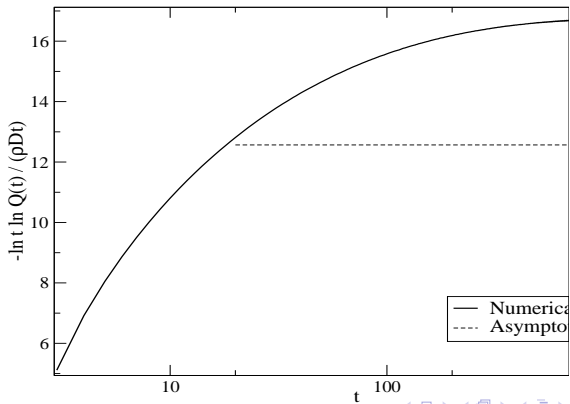
The prefactor is *subdominant* for $t \rightarrow \infty$:

$$Q_L(t) \sim \exp\left(-\frac{4}{\sqrt{\pi}} \rho_B (D_B t)^{1/2} - \text{const.}(\rho_B^2 D_{At})^{1/3}\right)$$

Compare with data from Mehra and Grassberger (2002):



In two dimensions (Mehra and Grassberger (2002)):



ELIMINATING THE B-PARTICLES (AB, Majumdar, Blythe (2003))

ELIMINATING THE B-PARTICLES (AB, Majumdar, Blythe (2003))

Consider the A and B particles to be *non-interacting* and consider events in which different B-particles hit the A-particle *for the first time*. These events are described by a *Poisson distribution* – the probability that the A-particle, *with a given trajectory* $z(t)$, has been hit by n different B-particles up to time t is

$$p_n = \frac{\mu^n}{n!} \exp(-\mu)$$

where $\mu = \mu[z(\tau)]$, $0 \leq \tau \leq t$, is a *functional* of the A-particle trajectory $z(t)$.

ELIMINATING THE B-PARTICLES (AB, Majumdar, Blythe (2003))

Consider the A and B particles to be *non-interacting* and consider events in which different B-particles hit the A-particle *for the first time*. These events are described by a *Poisson distribution* – the probability that the A-particle, *with a given trajectory* $z(t)$, has been hit by n different B-particles up to time t is

$$p_n = \frac{\mu^n}{n!} \exp(-\mu)$$

where $\mu = \mu[z(\tau)]$, $0 \leq \tau \leq t$, is a *functional* of the A-particle trajectory $z(t)$.

The probability of *no hits up to time* t is

$$Q(t) = \langle p_0(t) \rangle_z = \langle \exp(-\mu[z]) \rangle_z$$

where the average $\langle \dots \rangle_z$ is taken over all A-particle trajectories weighted with the usual Wiener measure.

To determine $\mu[z]$ we calculate, in two ways, the probability density for a B-particle to reach $z(t)$ at time t (in a *noninteracting* system):

$$\rho_B = \int_0^t dt' \dot{\mu}(t') G_B(z(t), t | z(t'), t')$$

where

$$G_B(z(t), t | z(t'), t') = \frac{1}{[4\pi D_B(t - t')]^{1/2}} \exp\left(-\frac{[z(t) - z(t')]^2}{4D_B(t - t')}\right)$$

is the B-particle diffusion propagator. For the target problem ($z(t) = 0$ for all t) this gives

$$\mu(t) = \mu_0(t) = \frac{4}{\sqrt{\pi}} \rho_B (D_B t)^{1/2}$$

as before.

PROOF OF THE PASCAL PRINCIPLE (AB, Majumdar, Blythe (2003); Moreau et al. (2003))

In general we can write $\mu[z] = \mu_0 + \mu_1[z]$. Then $\mu_1[z]$ satisfies the equation:

$$\mu_1[z] = \frac{1}{\pi} \int_0^t \frac{dt_1}{\sqrt{t-t_1}} \int_0^{t_1} \frac{dt_2}{\sqrt{t_1-t_2}} \dot{\mu}(t_2) K(t_1, t_2)$$

where

$$K(t_1, t_2) = 1 - \exp\left(\frac{-[z(t_1) - z(t_2)]^2}{4D_B(t_1 - t_2)}\right)$$

The obvious inequalities $K(t_1, t_2) \geq 0$ and $\dot{\mu}[z] \geq 0$ prove that

$$\mu_1[z] \geq 0 \Rightarrow \mu[z] \geq \mu_0$$

i.e. the “Pascal principle” is proved.

EXTENSIONS OF THE BASIC RESULT

EXTENSIONS OF THE BASIC RESULT

- Diffusion on a fractal space (Oshanin et al., 2003)
- Calculation of subleading (preasymptotic) terms in the trapping reaction for $D_A \ll D_B$ (Anton + AB, 2004)
- Trapping reaction with subdiffusive traps and particles (Yuste and Lindenberg, 2006)
- Some exact results in certain limits for the double trapping reaction, $A + B \rightarrow B$, $B + C \rightarrow C$ (AB + Smith, 2006): See Richard Smith's poster.

SUMMARY

SUMMARY

- ① First-passage problems are in general very difficult to solve, even in systems with few degrees of freedom.

SUMMARY

- ① First-passage problems are in general very difficult to solve, even in systems with few degrees of freedom.
- ② Exact results are available in a very small number of systems.

SUMMARY

- ① First-passage problems are in general very difficult to solve, even in systems with few degrees of freedom.
- ② Exact results are available in a very small number of systems.
 - ▶ The random walk ($N=1$); the random acceleration process ($N=2$); the “windy cliff” and its generalizations ($N=2$).

SUMMARY

- ① First-passage problems are in general very difficult to solve, even in systems with few degrees of freedom.
- ② Exact results are available in a very small number of systems.
 - ▶ The random walk ($N=1$); the random acceleration process ($N=2$); the “windy cliff” and its generalizations ($N=2$).
 - ▶ The one-dimensional Ising model with Glauber Dynamics.

SUMMARY

- 1 First-passage problems are in general very difficult to solve, even in systems with few degrees of freedom.
- 2 Exact results are available in a very small number of systems.
 - ▶ The random walk ($N=1$); the random acceleration process ($N=2$); the “windy cliff” and its generalizations ($N=2$).
 - ▶ The one-dimensional Ising model with Glauber Dynamics.
 - ▶ The asymptotics of the trapping reaction, $A + B \rightarrow B$, for $d \leq 2$.
 - ▶ The one-dimensional TDGL equation (AB, Derrida, Godreche, 1994).

EPILOGUE

I am sorry this talk has been so long, but I didn't have time to write a shorter one.

(After Pascal)