Diffusion in a slowly varying potential

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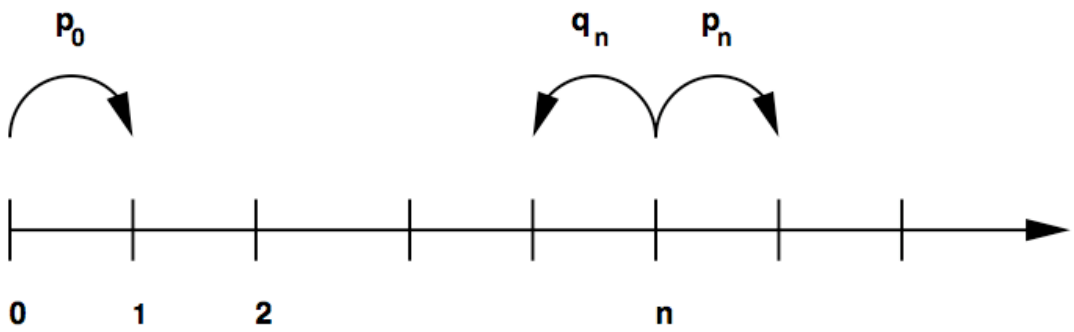
- Motivations
- Logarithmic potential: Scaling behaviour and mean first passage time
- Algebraic potential: Logarithmic speed in the presence of disorder

1. Model and Motivations

Model: Random walk on N_0 with asymptotically vanishing bias



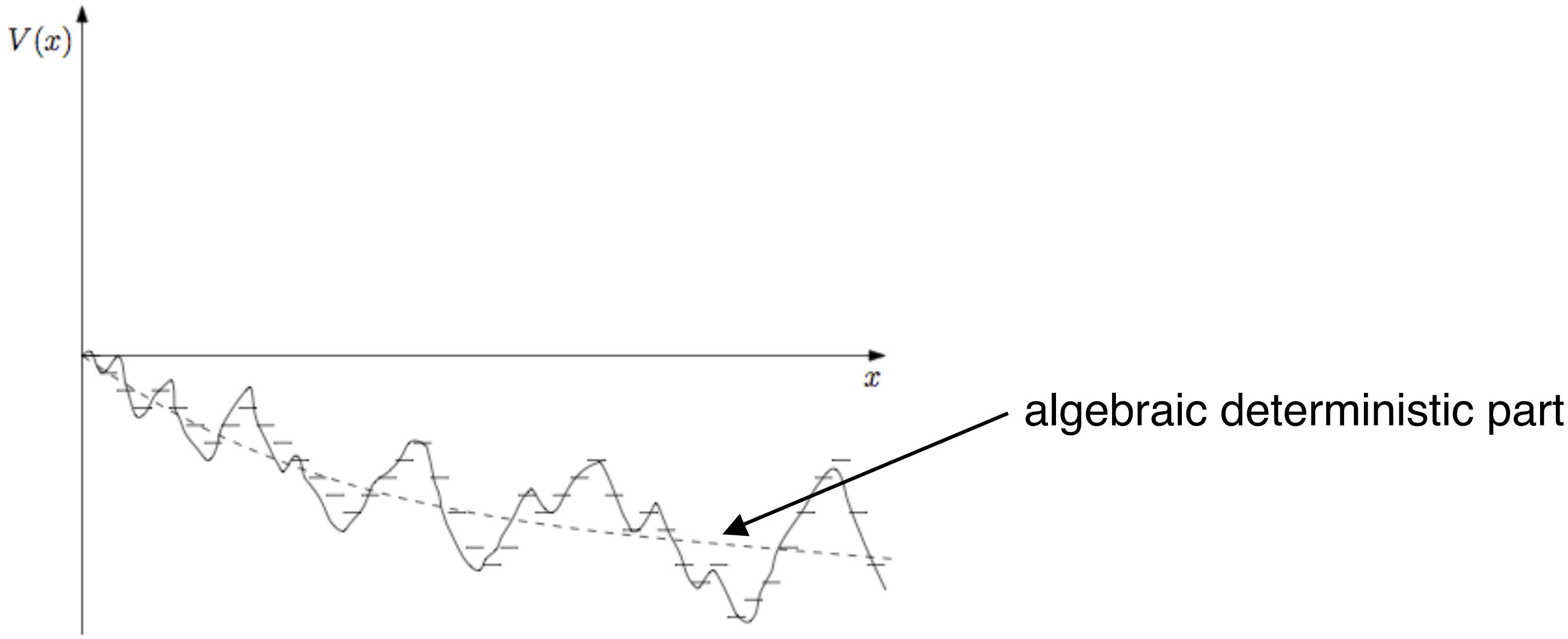
A) Ordered model: $p_n = 1$, $q_n = \exp(-b/n^{\alpha}) \approx 1 - b/n^{\alpha} + \ldots$

(Diffusion in power law potential $V(n) \sim n^{1-\alpha}$, $\alpha > 0$)

B) Disordered model: $p_n = 1$, $q_n = \exp(\omega_n - b/n^{\alpha})$, $\langle\omega_n\rangle=0$

(power law potential + Sinai disorder)

Potential (b>0):



Master equation for probability distribution:

$d/dt\ P(n,t) = P(n-1,t) + q_{n+1}\ P(n+1,t) - (1+q_n)\ P(n,t) \quad (n>0)$

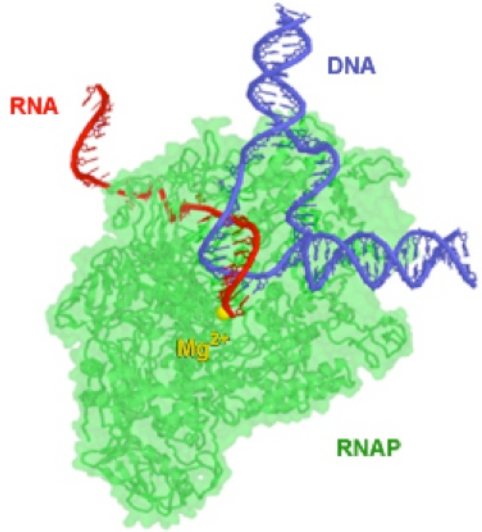
$d/dt\ P(0,t) = P(1,t) - q_0\ P(0,t)$

Motivations: 1) Dynamics of DNA denaturation:

- ❑ DNA unzips through action of molecular motors for various biological purposes

  ➔ creation of “bubbles” of single-stranded DNA

  bubble-size n(t) is a random variable



- ❑ Unzipping also through thermal activation ➔ DNA denaturation at high T (70...100 °C)

- ❑ Poland-Scheraga free energy

$$\mathcal{F}_n = an + b\ln n + c_0$$

a*n	free energy of unzipping	all in units of k_BT
b ln(n)	entropic contribution from number of bubble configurations	
c_0	free energy of bubble initiation	

DNA denaturation as a phase transition:

Equilibrium: bubble size distribution $P_n \approx \exp(-F_n)$

$a > 0$: exponentially small probability of big bubbles

$a < 0$: big bubbles preferred ➔ denaturation into two single-stranded DNA

$a = 0$: denaturation transition, log potential, power law distribution n^{-b} of bubble sizes

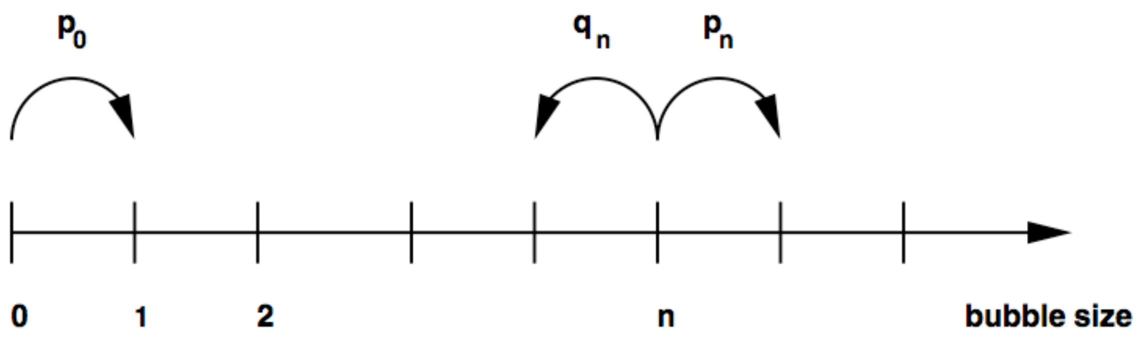
$b > 2$: finite mean bubble size at transition ➔ discontinuous (first order) transition

>> Controversial <<

Correspondence to condensation transition:

- power law distribution of random variable
- infinite mean bubble size for $b<2$ = infinite capacity to hold particles

Random walk model for bubble dynamics:

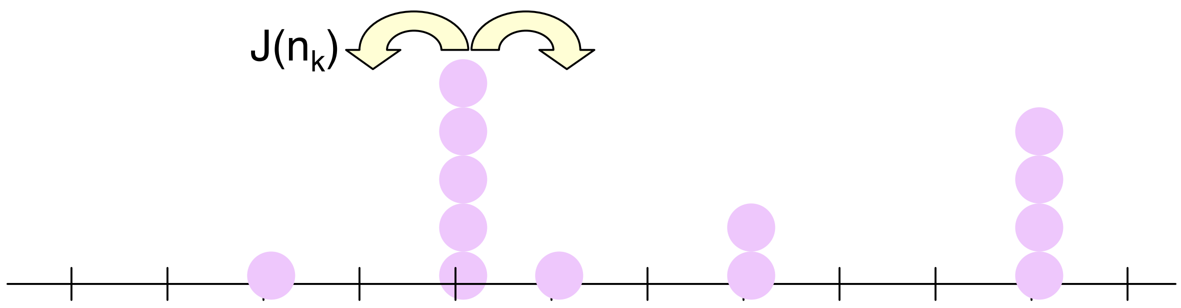


- Zipping rate p_n= w, unzipping rate q_n w

- Detailed balance: $\frac{p_n}{q_{n+1}} = \frac{P^*_{n+1}}{P^*_n}$

- PS free energy at transition a=0: q_n = w (1+ b/n) (random walk in log potential)

Motivations: 2) Dynamics of ZRP on a complete graph (mean field approximation)



Ordered case: $q_n = \exp(-b/n^{\alpha}) \approx 1 - b/n^{\alpha} + \ldots$

$\alpha < 1$ and $b < 0$:

$\alpha = 1$ and $b < -2$:

} Finite density ρ_c at z^* ==> Condensation above ρ_c

$\alpha > 1$ or $b > 0$: $\rho_c = \infty$ (no condensation)

==> $\alpha_c = 1$ (logarithmic potential)

[Evans' 95, Ferrari and Krug '95]

Disordered case: $q_n = \exp(\omega_n - b/n^{\alpha})$ with ω_n mean zero, finite variance, i.i.d.

$\rho_c = \infty$ for $b > 0$, α arbitrary and $b < 0$, $\alpha \geq 1/2$

$\rho_c < \infty$ (Condensation) in the range $b < 0$, $0 < \alpha < 1/2$

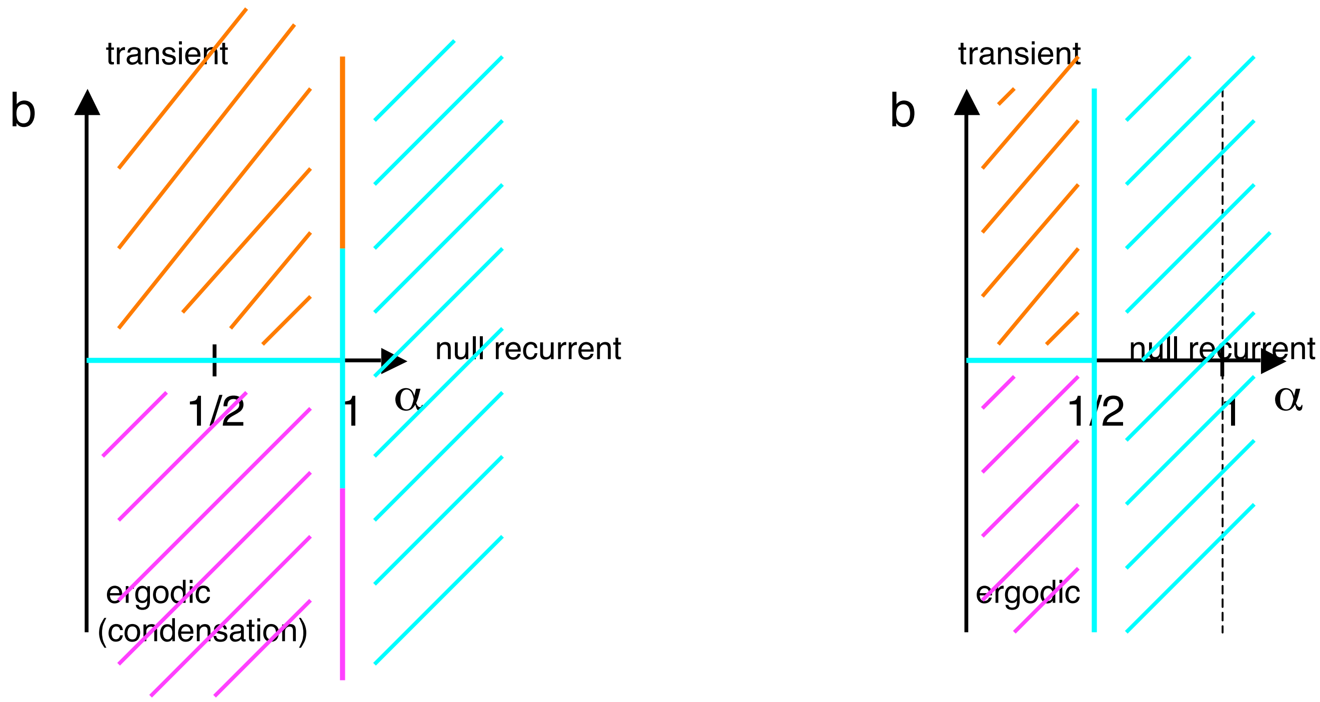
==> $\alpha_c = 1/2$ [Chleboun, Grosskinsky, GMS, 2008]

Other occurrences of the condensation transition:

- Granular shaking
- DNA denaturation
- Network rewiring
- Accumulation of wealth
- Traffic jams

➡ Generic model for condensation in complex systems

Results for similar random walk model in discrete time [Menshikov, Wade, 2006, 2008]



Intriguing results on logarithmic speeds, but poor bounds in transient regime

Theorem: Let b > 0, 0 < α < 1/2 (transient). Then for *a.e.* ω, any ε > 0,

a.s. $(\ln \ln t)^{-(1/\alpha)-\varepsilon} < \eta_t(\omega)/(\ln t)^{1/\alpha} < (\ln \ln t)^{(2/\alpha)+\varepsilon}$

for all but finitely many t.

2. Scaling for diffusion in ordered logarithmic potential

- Redefine b --> -b

- Study large scale relaxation towards equilibrium in terms of function G(x,t) defined by

P(x,t) = P*(x) [1+ G(x,t)]

• Exact solution for arbitrary initial conditions in terms of series of Bessel functions

• Make scaling ansatz with two distinct scaling laws

$$P(x,t) \approx P^*(x) + CP^*(x) \begin{cases} g_\beta\left(\frac{|x|}{t^{1/(b+1)}}\right) t^{-\delta} & \text{for } |x| \leq x_1(t) \\ f_\beta\left(\frac{|x|}{t^{1/2}}\right) t^{-\beta} & \text{for } |x| \geq x_1(t) \end{cases}$$

• Crossover scale

$$t^{1/(b+1)} \ll x_1(t) \ll t^{1/2}$$

Scaling functions:

$$g_\beta(z) = -\frac{4(b+1)}{rZ(2\beta+b-1)} + z^{b+1},$$

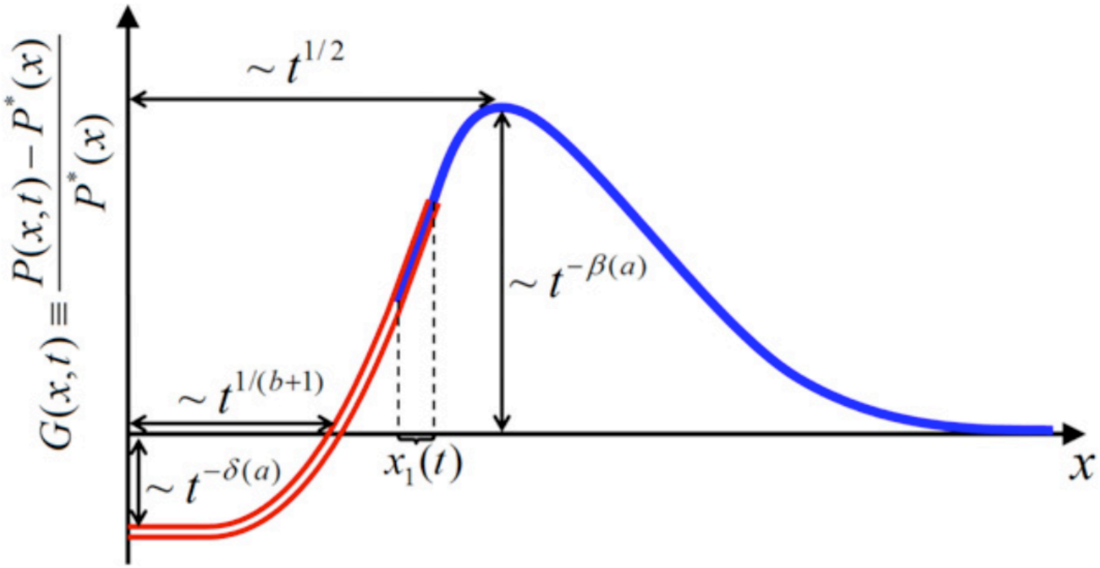
$$f_\beta(u) = u^{b+1}\,{}_1F_1\left(\frac{1+b+2\beta}{2};\frac{b+3}{2};-\frac{u^2}{4}\right)$$

Asymptotically:

$$f_\beta(u) \sim \begin{cases} u^{b+1} & \text{for } u \ll 1 \\ Du^{-2\beta} & \text{for } u \gg 1, \quad \beta < 1 \\ u^{b+1}\mathrm{e}^{-u^2/4} & \text{for } u \gg 1, \quad \beta = 1 \end{cases}$$

Quantities of interest: Scaling exponents β, δ, amplitude C

Plot of G(x,t):



Red: $t^{-\delta}\ g_\beta(x/t^{1/(b+1)})$

Blue: $t^{-\beta}\ f_\beta(x/t^{1/2})$

To leading order in t the two scaling solutions coincide in range of $x_1(t)$

Two distinct dynamical exponents 2, 1+b, with associated relaxation exponents β, δ

Initial value dependence of relaxation exponents of β, δ and of amplitude C:

Consider initial distribution with large-x behaviour

$G_0(x) \sim A\, x^{-a}$ (a > 1-b for normalization)

a =∞ for decay faster than any power

Examples:

$P(x,0)$	$G_0(x)$	a	A
$\delta(x-x_0)$	$\frac{\delta(x-x_0)}{P^*(x)} - 1 \sim -1$	0	-1
$C\mathrm{e}^{-\lvert x\rvert/x_0}$	$\frac{C\mathrm{e}^{-\lvert x\rvert/x_0}}{P^*(x)} - 1 \sim -1$	0	-1
$C\lvert x\rvert^{-(b+1)} + \ell(x)$	$\frac{C\lvert x\rvert^{-(b+1)} + \ell(x)}{P^*(x)} - 1 \sim -1$	0	-1
$C\lvert x\rvert^{-(b-1)} + \ell(x)$	$\frac{C\lvert x\rvert^{-(b-1)} + \ell(x)}{P^*(x)} - 1 \sim CZ\lvert x\rvert^{+1}$	-1	CZ
$P^*(x) + C\lvert x\rvert^{-(b+1)} + \ell(x)$	$\frac{C\lvert x\rvert^{-(b+1)} + \ell(x)}{P^*(x)} \sim CZ\lvert x\rvert^{-1}$	1	CZ
$P^*(\lvert x\rvert + x_0) + \ell(x)$	$\frac{P^*(\lvert x\rvert + x_0) + \ell(x)}{P^*(x)} - 1 \sim -bx_0\lvert x\rvert^{-1}$	1	$-bx_0$
$P^*(x)[1 + \mathrm{e}^{-\lvert x\rvert/x_0}] + \ell(x)$	$\mathrm{e}^{-\lvert x\rvert/x_0} + \frac{\ell(x)}{P^*(x)} \sim \mathrm{e}^{-\lvert x\rvert/x_0}$	∞	
$CP^*(x)[1 + \mathrm{e}^{-\lvert x\rvert/x_0}]$	$C - 1 + C\mathrm{e}^{-\lvert x\rvert/x_0} \sim C - 1$	0	$C-1$

Results for β, δ and amplitude C:

$$\beta = \beta(a) = \begin{cases} \frac{a}{2} & \text{if } a < 2 \\ 1 & \text{if } a > 2 \end{cases}$$

and

$$\delta = \delta(a) = \beta(a) + \frac{b-1}{2}.$$

For $a < 2$, the constant C is

$$C = \frac{\Gamma(1 - a/2)}{2^{b+a+1}\Gamma[(3+b)/2]} \cdot A,$$

- β determines f,g,δ

- β has phase transition at a = 2: depends on a for a < 2

- universality of scaling solution G:
  - (1) independent of small-x details of V(x),
  - (2) independent of small-x details of initial distribution

- a>2: solution does not depend on initial condition, but C is non-universal;
  a ≤ 2: solution depends on initial condition, but C is universal

Selection of solution (large $x \sim \sqrt{t}$):

- Relaxation by propagation of diffusive front from origin towards tails
- Tails of G do not feel this front
- Matching of front solution with asymptotic initial solution ==> $\beta = a/2$
- Normalization (conservation of probability) determines C

- Argument fails for a>2:

- Localized initial G evolve at long times according to

$$G(x,t) \sim t^{-1} f_1\left(\frac{x}{\sqrt{t}}\right)$$

- Heuristics: one expects solution with steepest decay at tails (which is the β=1 solution)

- C is determined by localized perturbation, not by tail

Similar considerations for small x

Mean First Passage Time

Bubbles are rare and hence largely independent because of large initiation energy c_0 ➔ Use random walk model for bubble dynamics

For $p_n = w$, $q_n = w(1+b/n)$:

$$P_n^* = \frac{b-1}{b}\binom{b+n}{b}^{-1}$$

Mean time to create bubble of size N = mean first passage time of random walk from origin to site N

$$T_N = \sum_{n=0}^{N-1}\sum_{k=n}^{N-1} p_k^{-1}\prod_{j=k}^{n-1}\frac{p_j}{q_{j+1}}$$

$\tau = 1/w$ fundamental microscopic time unit

Here:

$$T_N = \tau \sum_{n=0}^{N-1} \sum_{k=n}^{N-1} \frac{\binom{b+k}{b}}{\binom{b+n}{b}}$$

Some algebra

$$T_N = \tau \left[\frac{Nb}{b^2-1} \binom{b+N}{b} - \frac{N(N+1)}{2(b-1)} \right]$$

Large N:

$$T_N = \tau \frac{N^{b+1}}{(b^2-1)\Gamma(b)}$$

==> b-dependence

Comments:

1) Include bubble initiation barrier p_0 = wx:

$$T_N(x) = \tau \frac{b+x-1}{bx} \frac{N^{b+1}}{(b^2-1)\Gamma(b)}$$

==> Only change of time scale (but strong)

2) Equilibrium MBFT (sample up to size M): $T^*_M(x) \equiv \sum_{N=1}^{M} T_N(x) P^*_N$

asymptotically: $$T^*_M(x) = \tau \frac{M^2}{2(b+1)}$$

==> diffusive, NO b-dependence, except in amplitude

3. Logarithmic speed in the presence of disorder

Consider b>0 (b=0 Sinai)

Change definitions slightly (for mathematical convenience):

- $(\omega_x)_{x\geq 1}$ (fixed) sequence of i.i.d.r.v. (random environment)
- $(q_y)_{y\geq 1}$ sequence with $q_0 = 0$ and $q_y = \frac{e^{\omega_y - by^{-\alpha}}}{1+e^{\omega_y - by^{-\alpha}}}$ for $y \geq 1$
- transition probabilities

$$\mathrm{P}_\omega[X_{t+h} = y+1 \mid X_t = y] = (1-q_y)h + o(h),$$
$$\mathrm{P}_\omega[X_{t+h} = y-1 \mid X_t = y] = q_y h + o(h), \qquad \text{if } y \geq 1$$

Conditions:

- Condition S: $\mathbb{E}[\omega_1] = 0, \quad \sigma^2 := \mathbb{E}[\omega_1^2] \in (0, +\infty)$

- Condition K: There exists a $\theta_0 > 0$ such that $\mathbb{E}[e^{\theta\omega_1}] < \infty$ for all $|\theta| < \theta_0$

Main result:

Theorem 1.1 *Under Conditions S and K, we have for $\mathbb{P}$-almost all realizations of ω,*

$$\lim_{t\to\infty} \frac{X_t}{(C^*(\ln\ln t)^{-1}\ln t)^{\frac{1}{\alpha}}} = 1, \qquad \mathrm{P}_\omega\text{-}a.s.,$$

with $C^* = \frac{2\alpha b}{\sigma^2(1-2\alpha)}$.

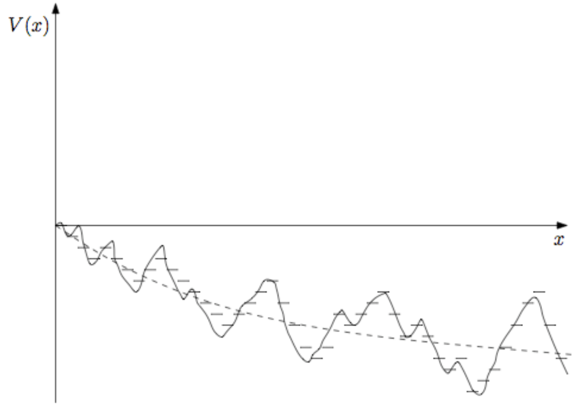
Heuristics: X_t gets trapped in deep potential wells and performs random walk between wells.

- Define potential: $$U(x) := \sum_{y=1}^{\lfloor x \rfloor} \ln \frac{q_y}{1-q_y} = \sum_{y=1}^{\lfloor x \rfloor} (\omega_y - b y^{-\alpha})$$

  (random walk in random potential)

- Couple potential to drifted Brownian motion, using Conditions S and K

$$V(x) := \sigma W(x) - \tfrac{b}{1-\alpha} x^{1-\alpha}$$



- Consider without loss of generality

  "good" environments

$$\Gamma(t) := \left\{ \omega : \left| \sum_{i=1}^{\lfloor x \rfloor} \omega_i - \sigma W(x) \right| \leq K \ln \ln t \ , \ x \in [0, \ln^M t] \right\}$$

$M > 1/\alpha$ and $t > e$

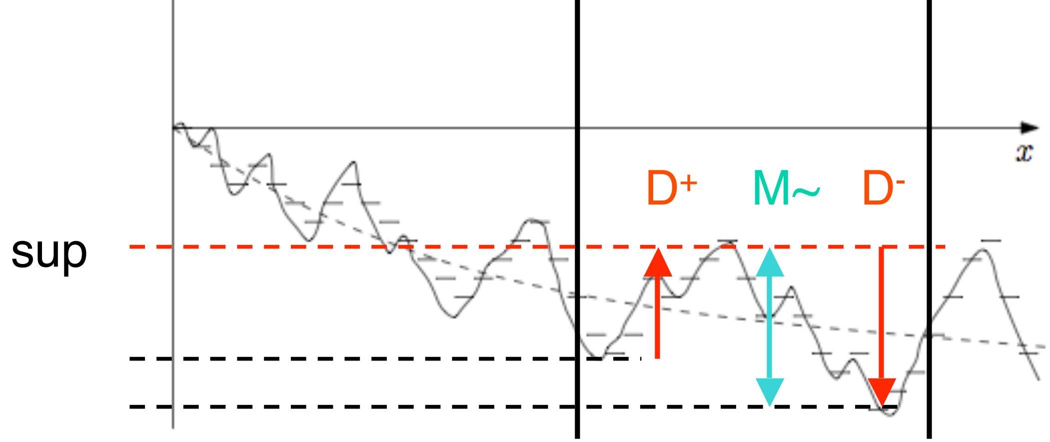
➢ Search for deep potential wells where the particle gets trapped for a long time

➢ Define for an interval [x,y]:

- maximal Drawup $D^{+}_{[x,y]}(f) := \sup_{u\in[x,y]}(f(u) - \inf_{v\in[x,u]} f(v))$

- maximal Drawdown $D^{-}_{[x,y]}(f) := \sup_{u\in[x,y]}(f(u) - \inf_{v\in[u,y]} f(v))$

- maximal Excursion $\tilde{M} := \max_{y\in I} U(y) - \min_{y\in I} U(y)$



➢ Results from Fribergh, Gantert, Popov (2010)

- A) Confinement probability: particle gets trapped for exponential times ~ $e^{H(I)}$

Proposition 2.2 *Let $I = [a, b]$ with $0 \le a < b < \infty$ be an interval of $\mathbb{Z}^+$. Let $H(I) := D_I^+(U) \wedge D_I^-(U)$ and $\tilde{M} := \max_{y \in I} U(y) - \min_{y \in I} U(y)$. For $a < x < b$ we have*

$$\mathrm{P}_\omega^x[\tau_{\{a,b\}} \ge t] \le \exp\left\{ - \frac{t}{K_2 (b-a)^3 (b - a + \tilde{M}) e^{H(I)}} \right\}$$

with K_2 a positive constant.

==> To find P of order one: Look for potential wells of depths H(I) ~ ln(t)

- B) Escape probability from a --> b

Proposition 2.3 *Let $I = [a, b]$ with $0 \leq a < b < \infty$ be an interval of $\mathbb{Z}^+$ and $h := \arg\max_{x \in [a,b]} U(x)$. For any $t > 1$,*

$$\mathrm{P}_\omega^a[\tau_b < t] \leq K_3 t \frac{\pi(h)}{\pi(a)}$$

with K_3 a positive constant.

where $\pi(x)$ is reversible measure defined by $\pi(0)=1$ and detailed balance

$\pi(x)\ (1-q_x) = \pi(x+1)\ q_{x+1}$

==> $\pi(x) = e^{-U(x)} + e^{-U(x+1)}$

==> $$\frac{\pi(h)}{\pi(a)} \leq e^{-V(h)+V(a)}(2K_1+1) \quad \ln t$$

for $h < \ln^M(t)$ with $M > 1/\alpha$ and for good environments

- Analyse V(x): Distribution of D^+ for Brownian motion W with power law drift not known

- Approximate power law drift by linear drift ν

- Take interval of exponential random length T with mean μ:

$$P\left[D^+_{[0,T]}(W^{(\nu)}) > a\right] = \frac{e^{\nu a}}{\cosh(a\sqrt{2\mu^{-1}+\nu^2}) + \frac{\nu}{\sqrt{2\mu^{-1}+\nu^2}}\sinh(a\sqrt{2\mu^{-1}+\nu^2})}$$

Easy to show:

Corollary 2.1 *Suppose that* $\nu < 0$ *and that* a, ν *and* μ *are functions the real variable* $t > 0$. *If* $a|\nu| \to \infty$, $\nu^2\mu \to \infty$ *and* $a(\mu|\nu|)^{-1} \to 0$ *as* $t \to \infty$, *then*

$$P\left[D^+_{[0,T]}(W^{(\nu)}) > a\right] = \frac{1}{1 + \frac{1}{2\nu^2\mu}e^{2|\nu|a}}(1 + o(1))$$

as $t \to \infty$.

➢ Rough argument: Look for first trap (max drawup) s' of order ln(t); Observe:

(i) Corollary 2.1 gives for $s' = [C \ln(t) / \ln(\ln(t)]^{1/\alpha}$

$$P(s') = \begin{cases} 0 & \text{for } C < C^* \\ 1 & \text{for } C > C^* \end{cases} \qquad \text{with } C^* = 2\alpha b/(\sigma^2(1-2\alpha))$$

(ii) Deviation of linear potential from power law potential such that s' is good lower bound, jump in P suggests that it is also good upper bound

==> position $s(t) = [C^* \ln(t) / \ln(\ln(t)]^{1/\alpha}$ (heuristically) as claimed in Theorem

(Precise argument: Make sure that

(i) around position s(t) and drawup length ln(t) probability P behaves in the "right" way to yields a.s. convergence

(ii) randomness of interval length in Corollary 2.1 does not matter)

4. Conclusions

1. Unusual scaling behaviour of diffusion in a log potential:

- Two distinct scaling forms of relaxation
- Initial-distribution dependence of dynamical exponents
- Phase transition to regime with no dependence

2. Sensitivity of mean bubble formation time on entropic amplitude in PS model and hence to order of transition

3. Detailed almost sure result for logarithmic speed in the presence of disorder

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