BÁLINT TÓTH
(University of Bristol and Rényi Institute Budapest)

DIFFUSION IN THE RANDOM LORENTZ GAS

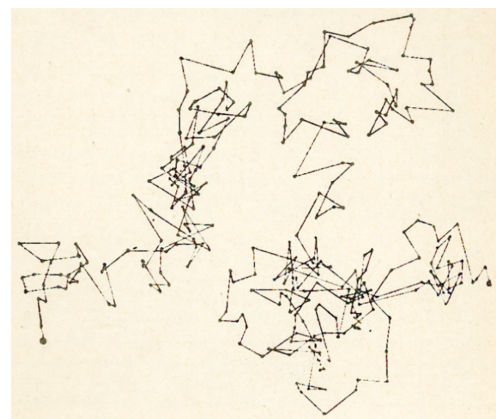
Probability, Analysis and Dynamics
Bristol, 2025-04-09

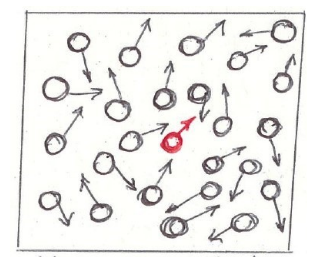
Goal:
Understand mathematically physical diffusion.

Macro: mass/bulk diffusion

[Wikipedia/public]

Micro: tracer/self-diffusion





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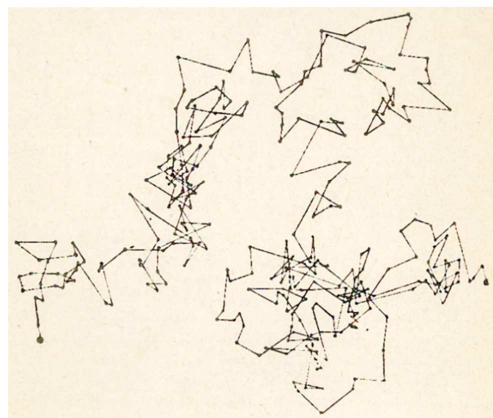
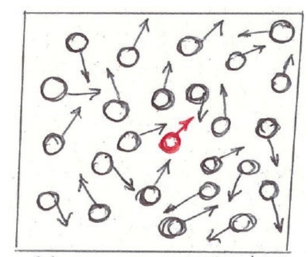




[J Perrin, Les atomes, 1910]

. . . the bottomless well of the past . . .

Empirical:

. . . [Lucretius ($\sim$60 BC)] . . . [J Ingenhousz (1785)] . . .

. . . [R Brown (1827)] . . .

Theoretical:

. . . [A Fick (1855)] . . . [A Einstein (1905)] . . .

. . . [C Pearson & Lord Rayleigh (1905)] . . .

. . . [M Smoluchowski (1906)] . . . [P Langevin (1908)] . . .

. . . [J Perrin (1910)] . . .

Mathematical:

. . . [J Bernoulli (1713)] . . . [A de Moivre (1711-1738)] . . .

. . . [PS Laplace (....-1812)] . . . [A Lyapunov (1901)] . . .

. . . [G Pólya (1922)] . . . [N Wiener (1920-1933)] . . .

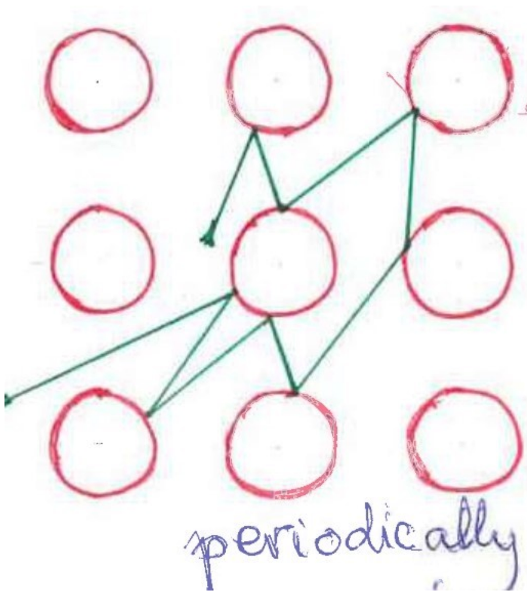
. . . [P Lévy (1920-1940)] . . . [M Kac (1946-....)] . . .

The Lorentz / Ehrenfest Gas - genesis

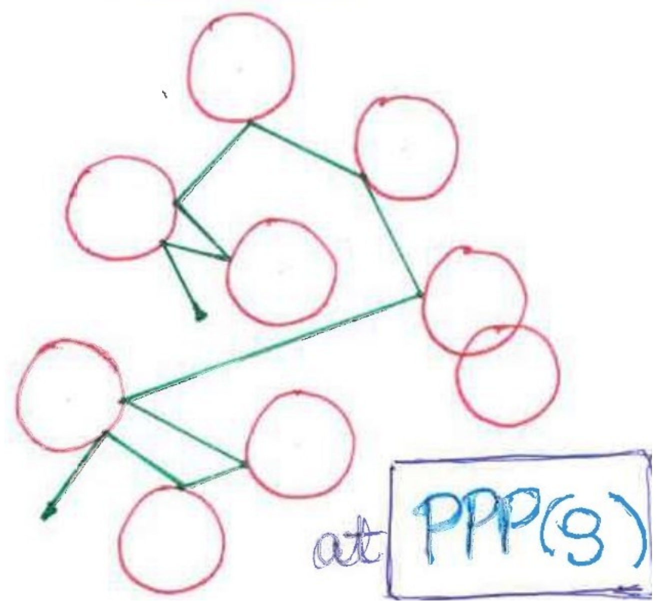
Physics. — "*The motion of electrons in metallic bodies.*" II. By Prof. H. A. LORENTZ.

(Communicated in the meeting of January 28, 1905).

Periodic



Random



Detour:

Tatyana Afanasieva (1876-1964)

Paul Ehrenfest (1880-1933)

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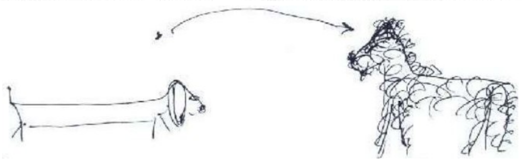
1907:

Über zwei bekannte Einwände gegen das Boltzmannsche H-Theorem.

Von Paul u. Tatiana Ehrenfest.



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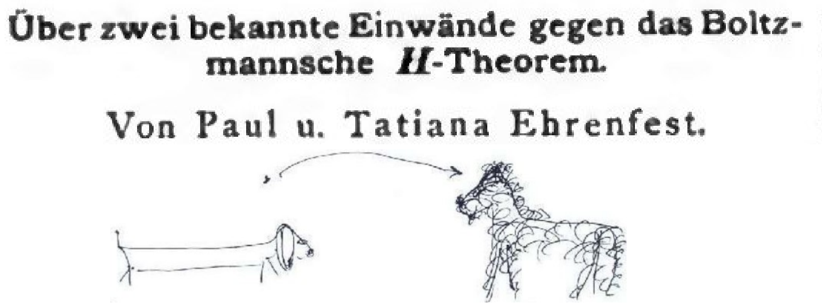

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Von Paul u. Tatiana Ehrenfest.

Genesis of Markov Chains: . . . ,

AA Markov (1906), EH Bruns (1906),

P&T Ehrenfest (1907), O Perron (1907),

G Frobenius (1908), . . .

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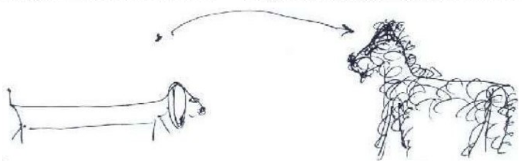

Genesis of Markov Chains: . . . ,

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G Frobenius (1908), . . .

1911:

IV 32. BEGRIFFLICHE GRUNDLAGEN DER STATISTISCHEN AUFFASSUNG IN DER MECHANIK.

Von

P. u. T. EHRENFEST*)

IN ST. PETERSBURG.

In: F Klein (ed): *Encyklopädie der math. Wissenschaften* vol. 4-4

extended book in 1912

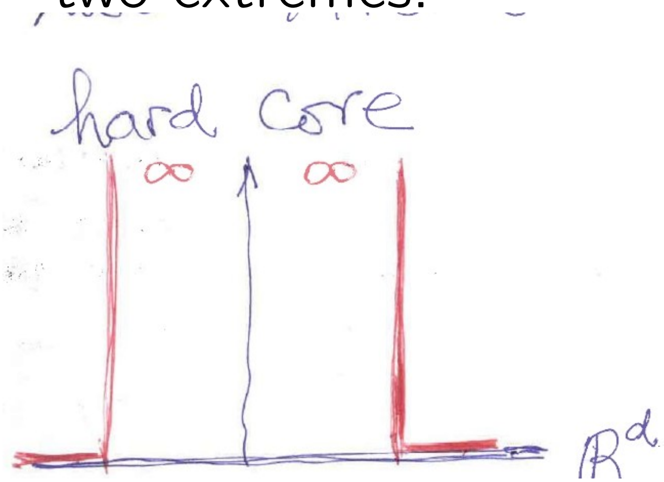
The random Lorentz gas:

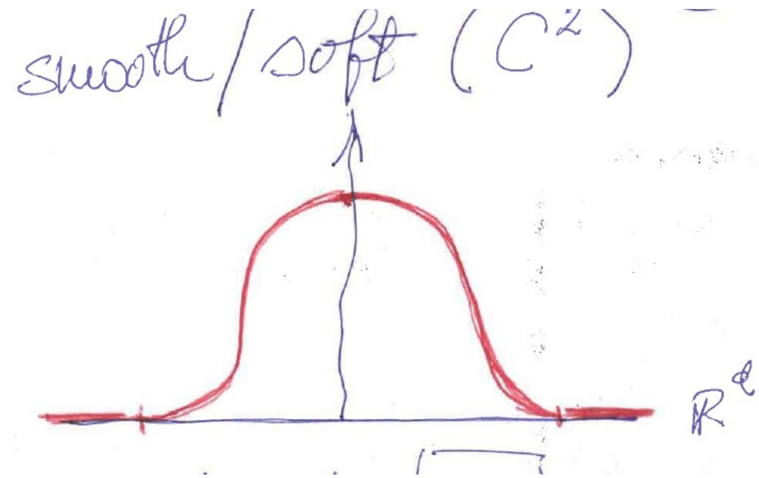
Ingredients:

- A spherically symmetric finite range potential:

$$\varphi : \mathbb{R}^d \mapsto \mathbb{R} \cup \{+\infty\}, \qquad \varphi(x) = \varphi(|x|e) = \varphi(x)\mathbb{1}_{\{|x| \leq r\}}$$

two extremes:





- A PPP ω in $\mathbb{R}^d \setminus \{x : |x| \leq r\}$, of density ϱ.
  Points $q \in \omega$ will be the centres of fixed (∞-mass) scatterers.

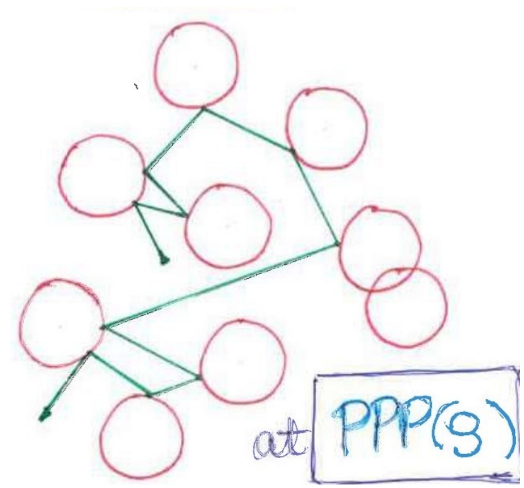
The Lorentz/Ehrenfest trajectory: Particle of mass 1 moves among the fixed scatterers, according to Newtonian dynamics $t \mapsto (V(t)), X(t))$, with i.c. $X(0) = 0 \in \mathbb{R}^d$, $V(0) \in \mathbb{S}^{d-1}$.

In the **soft** case:

$$\Phi(x) := \sum_{q\in\omega} \varphi(x-q), \qquad F(x) = -\nabla\Phi(x) = -\sum_{q\in\omega} \nabla\varphi(x-q)$$

$$\dot{V}(t) = F(X(t)), \qquad \dot{X}(t) = V(t), \qquad + \text{i.c.}$$

In the **hard core** case: the ODE is formal, nevertheless the dynamics is still well defined



Comment on **no trapping**:
h.c.: $r^d\varrho < \theta_c$,
s.c.: $\max|\varphi| < m_c(r^d\varrho)$.

Sources of randomness:

- environment: random placement of scatterers, $\omega \sim \mathsf{PPP}(\varrho)$.
- random direction of initial velocity, e.g., $V(0) \sim \mathtt{UNI}(\mathbb{S}^{\mathrm{d}})$.

and **nothing more**. Dynamics: fully deterministic, Newtonian.

Wanted: $t \gg 1$ scaling behaviour of the trajectory $t \mapsto (V(t), X(t))$

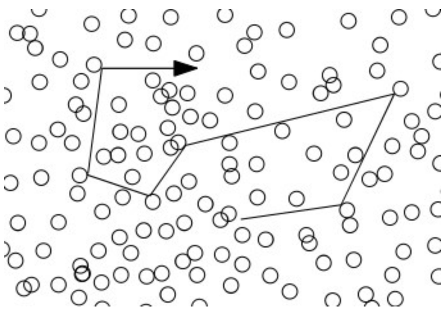
Holy Grail: **?** $T^{-1/2} X(Tt) \Rightarrow W(t)$ **?**
(conditioned on no trapping)

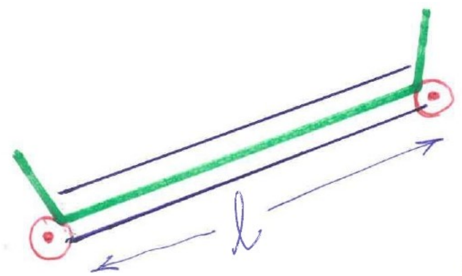
Comment on periodic LG: Factor to cell with periodic b.c.:
Sinai billiard = hyperbolic dynamics on compact state space.
Big Theory, great results since 1980.

[Bunimovich-Sinai (1980)] $d = 2$ ...
[Chernov-Dolgopyat (2009)] $d = 3$ (conditional) ...

Kinetic limits I. Boltzmann-Grad:

$$\varrho = \varepsilon^{-d}, \qquad r = \varepsilon^{d/(d-1)}, \qquad \underbrace{\varrho r^d = \varepsilon^{d/(d-1)}}_{\text{low density}}$$

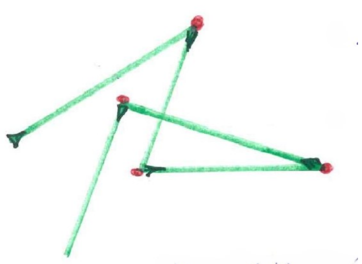




The free flight between successive scatterings

$\ell \sim \texttt{EXP}(1)$

Easy to guess what happens in the BG-limit, as $\varepsilon \to 0$



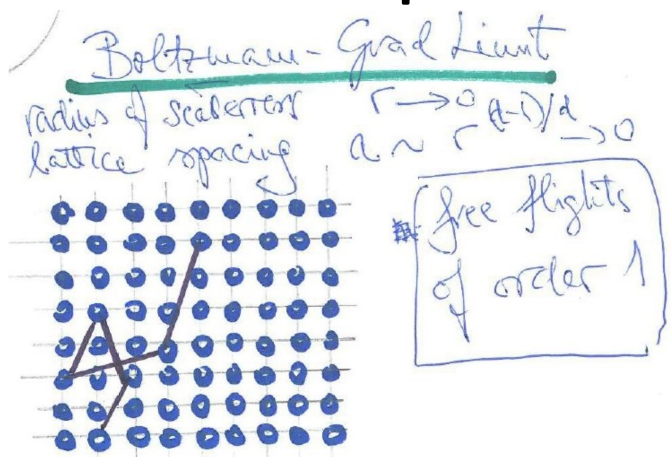
Flight process

- i.i.d $\texttt{EXP}(1)$ flights
- Markovian scatt. with differential cross section $\sigma(v, v') \sim |v - v'|^{3-d}$

Hard to prove.

[G Gallavotti (1970)]
[H Spohn (1978)]
[C Boldrighini, L Bunimovich, YaG Sinai (1982)]

Comment on periodic LG:



[E Caglioti, F Golse (2008)],

. . . ,

[J Marklof, A Strömbergsson (2011)]

The BG-limit: $t \mapsto Y(t)$ a "hidden Markov" flight process with heavy tailed flights.

Kinetic limits II. Weak Coupling:

$$\varrho = \varepsilon^{-d}, \qquad r = \varepsilon, \qquad \underbrace{\text{intensity of potential} \sim \varepsilon^{1/2}}_{\text{weak coupling}}$$

$$\Phi_\varepsilon(x) := \varepsilon^{1/2} \sum_{q \in \varepsilon \cdot \omega} \varphi(\frac{x-q}{\varepsilon}) \qquad \sim \varepsilon^{1/2},$$

$$F_\varepsilon(x) = -\varepsilon^{-1/2} \sum_{q \in \varepsilon \cdot \omega} \nabla\varphi(\frac{x-q}{\varepsilon}) \sim \varepsilon^{-1/2},$$

$$\dot{V}_\varepsilon(t) = F_\varepsilon(X_\varepsilon(t)), \qquad \dot{X}_\varepsilon(t) = V(\varepsilon t), \qquad + \text{i.c.}$$

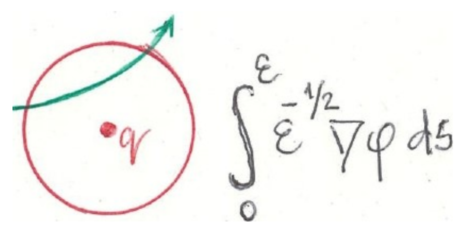
Let's guess the limit together.

- Conservation of energy:

$$\underbrace{|V_\varepsilon(t)|^2}_{E_{\text{kin}}} + \underbrace{\Phi_\varepsilon(X_\varepsilon(t))}_{E_{\text{pot}} \sim \varepsilon^{1/2}} = 1$$

  The particle travels with speed $|V_\varepsilon(t)| = 1 - \mathcal{O}(\varepsilon^{1/2})$.

- In (infinitesimal) time dt it encounters $\sim \varepsilon^{-1} dt$ scatterers.
- Each scatterer has impact $\sim \varepsilon^{1/2}$ on $V_\varepsilon(t)$:



The expected limit: *Spherical Langevin Process*:

$t \mapsto U(t)$: Wiener ("BM") on $\mathbb{S}^{d-1}$, $\quad Y(t) = \int_0^t U(s) ds$.

Not so easy to guess. Even harder to prove.

[H Kesten, G Papanicolaou (1980)]

Two steps limits.

Rnd-BG: [G70],[S78] : $(V_\varepsilon(t), X_\varepsilon(t)) \Rightarrow \underbrace{(U(t), Y(t))}_{\text{Markovian flight proc.}}$

Donsker : $T^{-1/2} Y(Tt) \Rightarrow W(t).$

Rnd-WC: [KP80] : $(V_\varepsilon(t), X_\varepsilon(t)) \Rightarrow \underbrace{(U(t), Y(t))}_{\text{spherical Langevin proc.}}$

Doeblin : $T^{-1/2} Y(Tt) \Rightarrow W(t).$

Per-BG: [MS11] : $(V_\varepsilon(t), X_\varepsilon(t)) \Rightarrow \underbrace{(U(t), Y(t))}_{\text{"hidden Markov" flight proc.}}$

[MT16] : $(T \log T)^{-1/2} Y(Tt) \Rightarrow W(t).$

Can one do better?

Interpolate between the Two Steps Limits and the Holy Grail!

$$? \quad T(\varepsilon)^{-1/2} X_\varepsilon(T(\varepsilon)t) \Rightarrow W(t) \quad ? \qquad (\star)$$

with $T(\varepsilon) \to \infty$ – the faster the better.

Some more recent results

Boltzmann-Grad/Low Density setting.

Theorem. [C Lutsko, BT (2020)] *Let* $d = 3$.
In the Boltzmann-Grad setting, $(\star)$ *holds with* $T(\varepsilon) = \varepsilon^{-3}|\log \varepsilon|^{-2}$

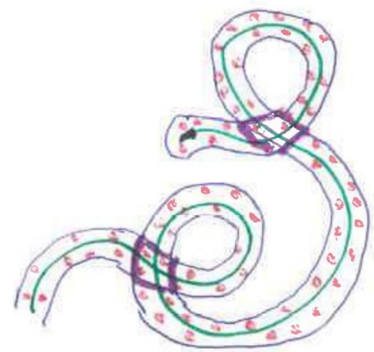
Weak Coupling setting.
Antecedents:
[T Komorowski, L Ryzhyk (2006)]:
In the Weak Coupling setting, $(\star)$ holds in $d \geq 3$ and $T(\varepsilon) = \varepsilon^{-\kappa}$ with some $\kappa > 0$ (but $\kappa \ll 1$).
[L Erdős, M Salmhofer, H-T Yau (2007)]:
Same in quantum setting with $\kappa \approx 1/370$.

Theorem. [BT (2024+)] *Let* $d \geq 3$.
In the Weak Coupling setting, $(\star)$ *holds with* $T(\varepsilon) = \varepsilon^{-(d-2)}$

Explore!

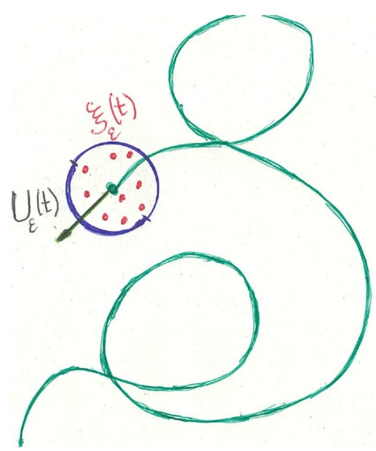
Rather than sample . . .

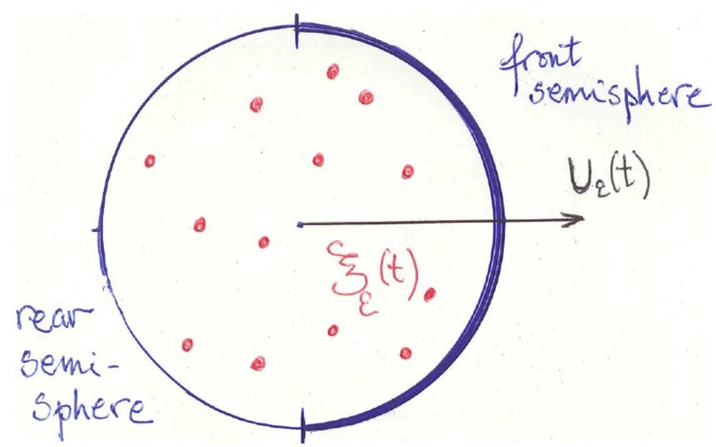
better explore the environment!



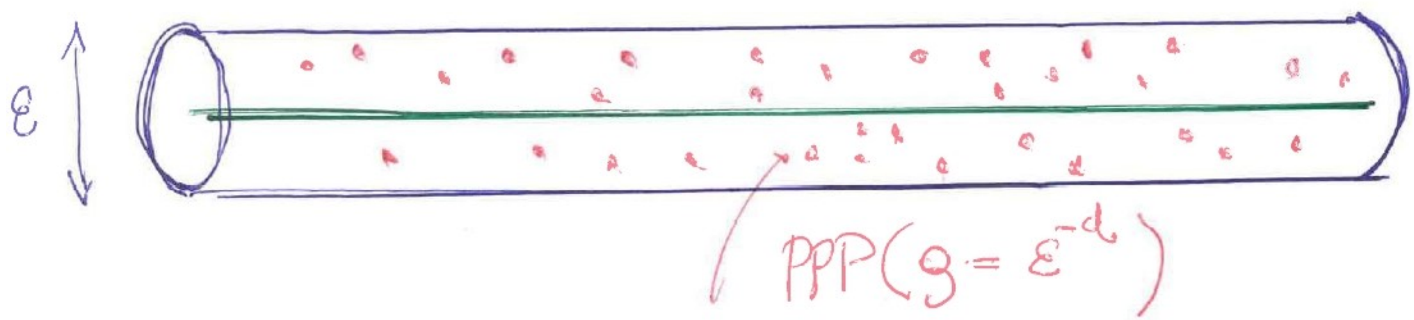
Markovize!

$t \mapsto (U_\varepsilon(t), \xi_\varepsilon(t))$





Probabilistic ingredient for the construction of the Markovized process:



- explicit construction
- the MP $t \mapsto (U_\varepsilon(t), \xi_\varepsilon(t))$ is well-behaved due to
- $\theta_{\varepsilon,n} =$ successive times when $\xi_\varepsilon(t) = \emptyset$.

  $|\theta_{\varepsilon,n+1} - \theta_{\varepsilon,n}| \sim \varepsilon, \quad n \mapsto U_\varepsilon(\theta_{\varepsilon,n})$ is a $O(d)$-invar. RW on $\mathbb{S}^{d-1}$

Limit theorems for the Markovized process.

(i) *Fix* $0 < T < \infty$. *Then, as* $\varepsilon \to 0$,

$$(U_\varepsilon(t), Y_\varepsilon(t)) \Rightarrow \underbrace{(U(t), Y(t))}_{\text{spherical Langevin proc.}}$$

[Key: CLT for RW on $O(d)$.]

(ii) *Let* $T(\varepsilon) \to \infty$ (no matter how fast or slow). *Then, as* $\varepsilon \to 0$,

$$T(\varepsilon)^{-1/2} Y_\varepsilon(T(\varepsilon)t) \Rightarrow W(t)$$

[Key: Martingale approximation + martingale CLT.]

Nothing new or surprising here.

Couple! (the physical and the Markovized processes)

To be proven: Up to $t < T(\varepsilon) = o(\varepsilon^{-d+2})$, with high probability, no ε-neighbourhood of a point left behind is revisited by the Markovized process $t \mapsto Y_\varepsilon(t)$:

$$\Sigma_\varepsilon := \inf\{t : 0 < \exists\, r < \exists\, s < t, \text{such that}$$
$$B_\varepsilon(Y_\varepsilon(r)) \cap B_\varepsilon(Y_\varepsilon(s))^{\mathsf{c}} \cap B_\varepsilon(Y_\varepsilon(t)) \neq \emptyset\}$$

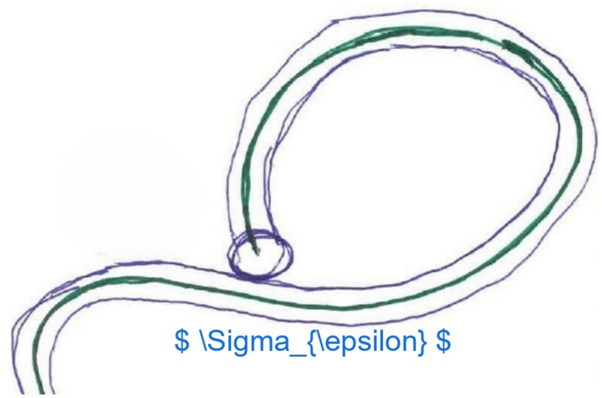
$=$ the first time (t) when a point which was within range ε some time (r) in the past, and left behind (at time $s > r$), is revisited within range ε (at time $t > s$).

By construction (coupling): $\quad \inf\{t : V_\varepsilon(t) \neq U_\varepsilon(t)\} \geq \Sigma_\varepsilon$

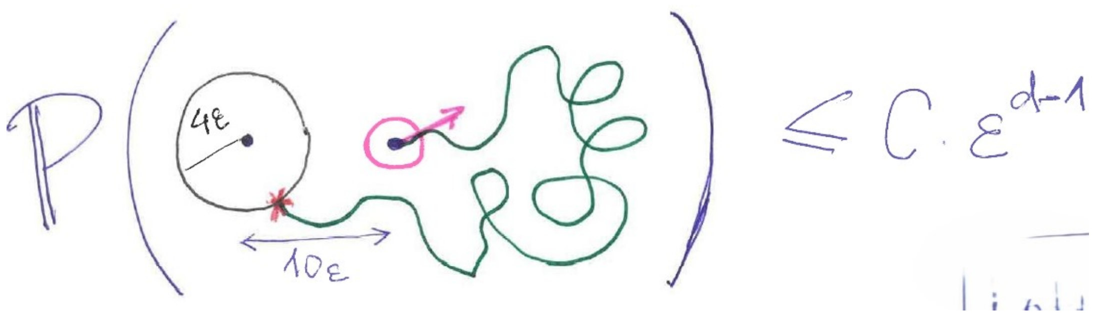
Lower bound on Σ_ε is needed. However, Σ_ε can in principle be very small, if the trajectory $t \mapsto Y_\varepsilon(t)$ is too rough.

Geometry helps:

$$|\ddot{Y}_\varepsilon| = |\dot{U}_\varepsilon| \sim \varepsilon^{-1/2} \ll \varepsilon^{-1}$$



The main probabilistic input



(note the difference from BM)

relies on Green-function (for $t \mapsto Y_{\varepsilon(t)}$) and geometric estimates

Hence (by union bounds and some massaging) the key estimate

$$\mathbf{P}\left(\Sigma_\varepsilon < T\right) < CT\varepsilon^{d-2}. \qquad ☺$$