

# Motion in Random Potentials

Andreas Knauf

Department Mathematik  
Universität Erlangen-Nürnberg (Germany)

New Perspectives on the  $N$ -body Problem

*Banff International Research Station*

January 13 -18, 2013

# General question

- ▶ Transport properties and ergodic theory of the classical flow generated by Hamiltonian function

$$H(p, q) = \frac{1}{2}\|p\|^2 + V(q),$$

with (random) potential  $V$  on  $\mathbb{R}^d$ .

- ▶ In particular: *asymptotic velocities* for initial conditions  $x_0 = (p_0, q_0)$

$$\bar{v}^\pm(x_0) := \lim_{T \rightarrow \pm\infty} \frac{q(T, x_0) - q_0}{T}.$$

- ▶ Quantum mechanical counterpart has been intensively studied for more than 40 years.
- ▶ A.K. and Christoph Schumacher:  
Classical motion in random potentials.

*Ergodic Theory and Dynamical Systems* **33**, 1–37, 2013

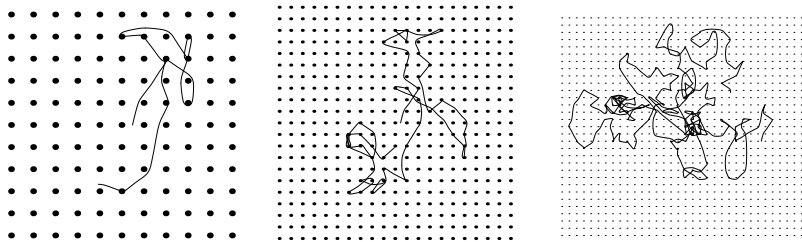
# Periodic potentials

**Known:** Motion in *periodic* 2D coulombic potentials (of finite horizon) is **diffusive**:

For all energies  $E$  above a threshold energy and all probability measures  $\mu$  of initial conditions  $x_0$  on  $H^{-1}(E)$  (of finite second moment and absolutely continuous w.r.t. Liouville measure)

$$\lim_{t \rightarrow \infty} \frac{q(t, x_0)}{\sqrt{t}} \stackrel{\mathcal{D}}{=} N(0, D) \quad (\text{bivariate normal distribution}).$$

A.K.: Ergodic and Topological Properties of Coulombic Periodic Potentials. *Commun. Math. Phys.* **110**, 89-112 ('87)



**Figure:** Diffusion in a periodic coulombic potential. Scale:  $1/\sqrt{t}$   
Left: time  $t = 1$ , mid:  $t = 4$ , right:  $t = 16$

# Periodic vs random scatterers

## Motion in *periodic* 2D **Lorentz gas** (of finite horizon)

- ▶ is diffusive.

L.A. Bunimovich, N.I. Chernov, Ya.G. Sinai: Statistical properties of two-dimensional hyperbolic billiards. *Russ. Math. Surv.* **46**, 47–106 (1991)

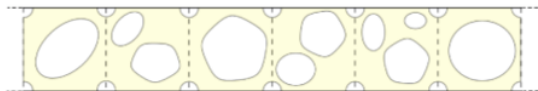
- ▶ is **recurrent** (with probability one it returns infinitely often in any prescribed neighborhood)

J.-P. Conze: Sur un critère de récurrence en dimension 2 pour les marches stationnaires, applications. *Ergodic Theory Dynam. Systems* **19**, 1233–1245 (1999)

K. Schmidt: On joint recurrence. *C. R. Acad. Sci. Paris* **327**, 837–842 (1998)

One expects recurrence for the *random* case, too,  
iff spatial dimension  $d \leq 2$ .

Known for (effective) dimension  $d = 1$ :



Giampaolo Cristadoro, Marcello Seri, Marko Lenci:  
Recurrence for quenched random Lorentz tubes, *Chaos* **20**, (2010)

# Random potentials: The lattice case

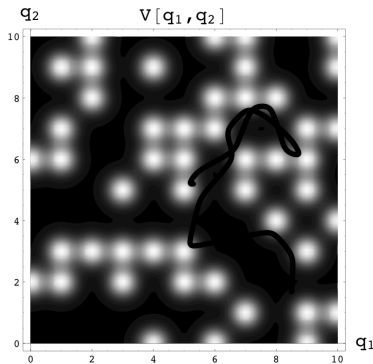
$$H_\omega: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \quad , \quad H_\omega(p, q) = \frac{1}{2} \|p\|^2 + V_\omega(q)$$

with  $\omega \in \Omega := \{1, \dots, N\}^{\mathcal{L}}$  for a lattice  $\mathcal{L} \subseteq \mathbb{R}^d$ ,

- ▶ single site potentials  $W_j: \mathbb{R}^d \rightarrow \mathbb{R}$  ( $j \in \{1, \dots, N\}$ )  
(with  $W_j(q) = \mathcal{O}(\|q\|^{-d-\varepsilon})$  as  $q \rightarrow \infty$ ), and
- ▶ random potential

$$V_\omega : \mathbb{R}^d \rightarrow \mathbb{R},$$
$$V_\omega(q) = \sum_{z \in \mathcal{L}} W_{\omega(z)}(q - z).$$

- ▶  $\mathcal{L}$ -ergodic probability measure  $\beta$  on  $\Omega$ ,
- ▶ Application: crystals with impurities/foreign atoms, alloys



# Random potentials: The Poisson case

- ▶ prescribe intensities  $\rho_j$  for the single site potentials  $W_j$ ,  $j = 1, \dots, N$
- ▶ *marked Poisson process* on  $\mathbb{R}^d$

$$\tilde{\Omega} := \{ \omega \mid \omega \text{ Borel measure on } \mathbb{R}^d \times \{1, \dots, N\} \text{ with} \\ \omega(K \times \{j\}) \in \mathbb{N}_0 \text{ if } K \subseteq \mathbb{R}^d \text{ is compact} \},$$

Lebesgue

- ▶ with measure

$$\beta(\{ \omega \in \tilde{\Omega} \mid \omega(K \times \{j\}) = m \}) = \frac{(\rho_j \lambda^d(K))^m}{m! \exp(\rho_j \lambda^d(K))} \quad (m \in \mathbb{N}_0).$$

- ▶ Poisson potential

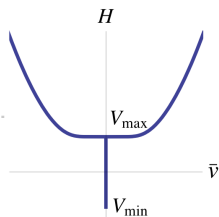
$$V: \tilde{\Omega} \times \mathbb{R}^d \longrightarrow \mathbb{R} \quad , \quad (\omega, q) \longmapsto \int_{\mathbb{R}^d \times J} W_j(q - x) d\omega(x, j).$$

# Dynamics: results

- ▶ Due to ergodic theorem, asymptotic velocities  $\bar{v}_\omega^\pm(x) = \lim_{T \rightarrow \pm\infty} \frac{q_\omega(T, x)}{T}$  exist for  $\beta \otimes \lambda^{2n}$ -a.e.  $(\omega, x)$ , and

$$\bar{v}_\omega^+(x) = \bar{v}_\omega^-(x) =: \bar{v}_\omega(x).$$

- ▶ Joint distribution  $\nu_\omega$  of energy and asymptotic velocity on  $\mathbb{R}^d \times \mathbb{R}$  exists and is  $\beta$ -a.s. independent of  $\omega$
- ▶ mirror symmetry  $(H, \bar{v}) \mapsto (H, -\bar{v})$
- ▶  $d = 1$ : Dichotomy:
  - ▶ Either the energy  $E$  is higher than the supremum of  $V_\omega$ , then the motion is *ballistic* (positive speed), or
  - ▶  $E$  is lower than the supremum of  $V_\omega$ , then the motion is almost surely *bounded*.



# Intermezzo: critical values of the Hamiltonian

- ▶ **Problem:** By conservation of energy, one has to decompose phase space into energy shells in order to do **ergodic theory**. These carry decent measures only for **regular energy values**.
- ▶ critical values of  $H_\omega =$  critical values of  $V_\omega$
- ▶ The closure of the set  $\text{CVal}_\omega \subseteq [V_{\min}, V_{\max}]$  of critical values is  $\beta$ -a.s.  $\omega$ -independent.
- ▶ Example of exponentially decaying ( $W_j(q) = \mathcal{O}(N^{-2|q|})$ ) single-site potentials with  $\overline{\text{CVal}_\omega} = [V_{\min}, V_{\max}]$  !
- ▶ But for faster exponential decay  $\lambda^1(\overline{\text{CVal}_\omega}) = 0$ .



# Two notions of ergodicity of time evolution

- ▶  $H : \Omega \times \mathbb{R}_p^d \times \mathbb{R}_q^d \rightarrow \mathbb{R}$  ,  $H(\omega, p, q) = \frac{1}{2}\|p\|^2 + V_\omega(q)$   
generates motion which is trivial on  $\Omega$
- ▶ Thus never ergodicity on  $H^{-1}(E)$ .
- ▶ Lattice  $\mathcal{L}$  acts on phase space *and* on  $\Omega$ , leaving  $H$  invariant.  
Thus motion on  $(\Omega \times \mathbb{R}^{2d})/\mathcal{L}$ , generated by Hamiltonian  $\hat{H}$ .
- ▶ Motion on compactified energy surface  $\hat{H}^{-1}(E)$  may be ergodic.
- ▶ Motion on energy surfaces  $H_\omega^{-1}(E)$  may be ergodic, too.
- ▶ If motion on  $H_\omega^{-1}(E)$  is ergodic for  $\beta$ -almost all  $\omega$ ,  
then motion on  $\hat{H}^{-1}(E)$  is ergodic, too.
- ▶ but not vice versa.

If the flow on the regular energy surface  $\widehat{H}^{-1}(E)$  is ergodic, then:

- ▶ the asymptotic **velocity** satisfies  $\bar{v}_\omega(x) = 0$  almost surely; but
- ▶ the motion is **unbounded** for almost every initial condition on  $H_\omega^{-1}(E)$  and for  $\beta$ -a.e.  $\omega$ .

# Dynamics: further (negative) results

- ▶  $d \geq 2$ , smooth **bounded potentials**:  
for **no energy**  $E$  (larger nor smaller the supremum of  $V_\omega$ )  
the motion can be **uniformly hyperbolic**.

G. Paternain and M. Paternain: On Anosov Energy Levels of Convex Hamiltonian Systems,  
*Mathematische Zeitschrift* **217**, 367–376 (1994)

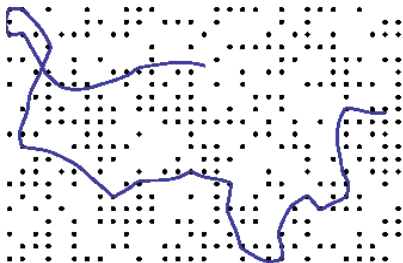
So we do not expect the motion to be ergodic in general.

- ▶ For the **Poisson** potentials, complete dynamics exists for all  $\omega \in \Omega \subseteq \tilde{\Omega}$  with full measure ( $\beta(\Omega) = 1$ ).  
But: for any energy  $E$ , the motion on the energy surface  $H_\omega^{-1}(E)$  is  $\beta$ -a.s. **not ergodic** !

# Dynamics: Coulombic potentials

$d = 2$ , random coulombic potentials (say, with single site potentials  $W_0(q) = 0$  and Yukawa potentials  $W_j(q) = -Z_j \frac{e^{-\mu_j \|q\|}}{\|q\|}$ ):  
For lattice-ergodic probability measures  $\beta$  (with  $\beta(\{\omega = 0\}) = 0$ )

- ▶ the motion is **topologically transitive** for all  $E > E_0$   
(even if it is not uniformly hyperbolic)
- ▶ the periodic orbits are **dense**.
- ▶ the compactified motion is then **ergodic**.



# Motion in a random Coulombic potential

- ▶ In his thesis Christoph Schumacher constructed a *geometric Markov partition* (in the sense of C. Series, with Poincaré surfaces projecting to configuration space trajectories), which is adapted to the lattice action.

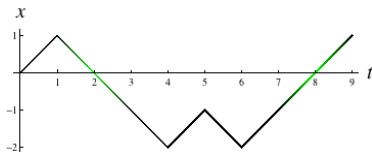
[www.opus.ub.uni-erlangen.de/opus/volltexte/2010](http://www.opus.ub.uni-erlangen.de/opus/volltexte/2010)

- ▶ We try to show a **central limit theorem**, that is, diffusion of the particle in the plane.  
*Difficulty:* Even with uniform hyperbolicity, the **correlations** do not decay exponentially, like in random motion in random environment.

# Slow correlation decay in random media

Herbert Spohn's example

- ▶ random motion on phase space  $\mathbb{R} \times \{-1, 1\}$
- ▶ starting at  $(x_0, v_0) := (0, 1)$
- ▶ zig-zag motion  $x(t) = x([t]) + (t - [t])v([t])$
- ▶ For times  $t \in \mathbb{N}$ : Probability
  - ▶  $\mathbb{P}(\{v(t+1) = v(t)\}) = \frac{1}{2}$  if  $x(t) \neq 0$ ;
  - ▶  $\mathbb{P}(\{v(t+1) = v(t)\}) = 1$  if  $x(t) = 0$  (no scatterer at  $x = 0$ ).



H. van Beijeren, H. Spohn: Transport Properties of the One - Dimensional Stochastic Lorentz Model:  
I. Velocity, Autocorrelation. J. Stat. Phys. **31**, 231–254 (1983)

Velocity autocorrelation  $\mathbb{E}(v(0)v(t))$

- ▶ if scatterer at  $x = 0$ , too:  $\mathbb{E}(v(0)v(t)) = 0$  for  $t \geq 1$
- ▶ else:  $|\mathbb{E}(v(0)v(t))| \sim t^{-3/2}$ .

# Local regularisation

The Hamiltonian flow is incomplete at Coulombic singularities.

Example (Kepler problem:  $V(q) = -\frac{1}{\|q\|}$ )

- ▶ Up to time parametrization geodesics of the **Maupertuis-Jacobi metric**

$$(E - V(q))g_{Euclid} \quad \text{on} \quad \mathbb{R}^2 \setminus \{0\}$$

are the energy  $E$  trajectories of the Kepler problem.

- ▶ At the singularity the metric develops a **cone** with opening angle  $\frac{\pi}{3}$ .
- ▶ **Levi-Civita regularisation**: The Riemann surface

$$\{(q, Q) \in \mathbb{C}^2 \mid q = Q^2\}$$

covers  $\mathbb{C}$  via  $(q, Q) \mapsto q$ , and the lifted Maupertuis-Jacobi metric can be smoothly completed.



# Local regularisation

The Hamiltonian flow is incomplete at Coulombic singularities.

Example (Kepler problem:  $V(q) = -\frac{1}{\|q\|}$ )

- ▶ Up to time parametrization geodesics of the **Maupertuis-Jacobi metric**

$$(E - V(q))g_{Euclid} \quad \text{on} \quad \mathbb{R}^2 \setminus \{0\}$$

are the energy  $E$  trajectories of the Kepler problem.

- ▶ At the singularity the metric develops a **cone** with opening angle  $\frac{\pi}{3}$ .
- ▶ **Levi-Civita regularisation**: The Riemann surface

$$\{(q, Q) \in \mathbb{C}^2 \mid q = Q^2\}$$

covers  $\mathbb{C}$  via  $(q, Q) \mapsto q$ , and the lifted Maupertuis-Jacobi metric can be smoothly completed.





# Local regularisation

The Hamiltonian flow is incomplete at Coulombic singularities.

Example (Kepler problem:  $V(q) = -\frac{1}{\|q\|}$ )

- ▶ Up to time parametrization geodesics of the **Maupertuis-Jacobi metric**

$$(E - V(q))g_{Euclid} \quad \text{on} \quad \mathbb{R}^2 \setminus \{0\}$$

are the energy  $E$  trajectories of the Kepler problem.

- ▶ At the singularity the metric develops a **cone** with opening angle  $\frac{\pi}{3}$ .
- ▶ **Levi-Civita regularisation**: The Riemann surface

$$\{(q, Q) \in \mathbb{C}^2 \mid q = Q^2\}$$

covers  $\mathbb{C}$  via  $(q, Q) \mapsto q$ , and the lifted Maupertuis-Jacobi metric can be smoothly completed.

- ▶ To regularise all singularities of  $V_\omega$  simultaneously we use the natural generalisation:

$$M := \{(q, Q) \in \mathbb{C}^2 \mid f(q) = Q^2\},$$

with  $f: \mathbb{C} \rightarrow \mathbb{C}$  holomorphic,  
 $f(z) = 0, f'(z) \neq 0$  ( $z \in \mathbb{C}$  position of Coulomb singularity).

- ▶  $M$  is an **infinite genus** surface.
- ▶ By direct calculation one sees that for high enough energies the Maupertuis-Jacobi metric exhibits **negative curvature**.

- ▶ To regularise all singularities of  $V_\omega$  simultaneously we use the natural generalisation:

$$M := \{(q, Q) \in \mathbb{C}^2 \mid f(q) = Q^2\},$$

with  $f: \mathbb{C} \rightarrow \mathbb{C}$  holomorphic,  
 $f(z) = 0, f'(z) \neq 0$  ( $z \in \mathbb{C}$  position of Coulomb singularity).

- ▶  $M$  is an **infinite genus** surface.
- ▶ By direct calculation one sees that for high enough energies the Maupertuis-Jacobi metric exhibits **negative curvature**.

# Problems and Strategy

▶ **Problem 1:**

Due to arbitrarily large regions without Coulomb potentials, the negative curvature is not bounded away from zero.

▶ **Strategy:**

But the Riemann surface  $(\mathbf{M}_\omega^*, \mathbf{g}_\omega^*)$  is a *visibility manifold*, that is, for every  $\varepsilon > 0$ , seen from  $p \in \mathbf{M}_\omega^*$  every geodesic of distance  $> r(p, \varepsilon)$  encloses an angle  $< \varepsilon$ .

▶ **Problem 2:**

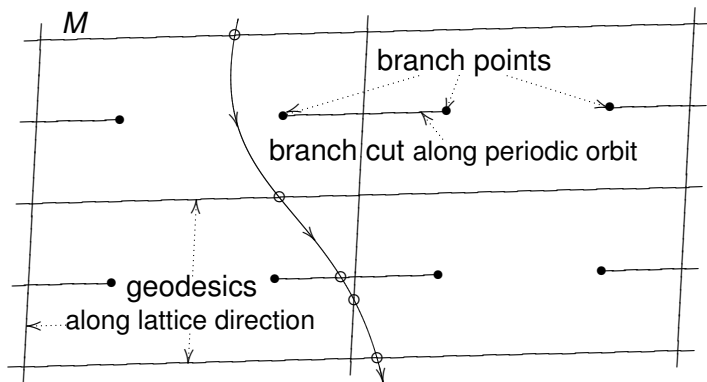
- ▶ The energy surface  $H_\omega^{-1}\{E\}$  has *infinite invariant measure*.
- ▶ Compactification by lattice action leads to finite measure but *nonhyperbolic* system.

▶ **Strategy:**

- ▶ Set up *symbolic dynamics*
- ▶ via *geometric Markov partition*, *i.e.* adapted to the lattice.

# Geometric Poincaré Sections

To encode the winding geodesic we can record the pieces of the web  $N$  of geodesics with piercing points  $\circ$ .



Problem: resulting shift space **not Markov!**

## Theorem (Existence of geometric Markov partition)

*There exists a Markov partition for the geodesic flow on  $M$  whose atoms project to the net  $N$ .*

- ▶ The proof is **constructive** and uses ideas from Bedford, Keane, Series: Ergodic Theory, Symbolic Dynamics and Hyperbolic Spaces

## Theorem (Existence of geometric Markov partition)

*There exists a Markov partition for the geodesic flow on  $M$  whose atoms project to the net  $N$ .*

- ▶ The proof is **constructive** and uses ideas from Bedford, Keane, Series: Ergodic Theory, Symbolic Dynamics and Hyperbolic Spaces

# Thank you!

(Hopefully this presentation was not too chaotic!)

