# Chaos and transport in nonequilibrium systems

*Summary of Ph.D. dissertation*

**Dolowschiák Márk**

MTA-ELTE Theoretical Physics Research Group
Supervisor: Dr. Kovács Zoltán

Statistical physics, biological physics és physics of quantum systems PhD Program
Director: Prof. Kürti Jenő

PhD School in Physics
Director: Prof. Horváth Zalán

Eötvös Loránd University, 2009

# 1. Introduction

In the Ph.D. dissertation I have investigated numerically the transport properties of nonequilibrium systems with chaotic dynamics. I have performed the numerical experiments on the dynamically thermostated Lorentz gas subjected to external fields. The dissertation consists of two parts: the investigation of the *conjugate pairing rule* describing the symmetry of the Liapunov exponents, and the investigation of the *fluctuation formula* related to the distribution of fluctuations characterizing the dynamics. In these two subjects I have performed the following numerical experiments:

1. investigation of the conjugate pairing rule in the periodic Lorentz gas thermostated by Gaussian Isokinetic thermostat and subjected to external magnetic field;
2. investigation of the fluctuation formula in the the periodic Lorentz gas thermostated by Gaussian Isokinetic thermostat and subjected to external magnetic field;
3. investigation of the fluctuation formula in the Nosé-Hoover thermostated Lorentz gas;
4. investigation of the fluctuation formula in the Lorentz gas thermostated by deterministic scatterings.

# 2. Numerical investigation of the conjugate pairing rule

## 2.1. Introduction

According to the observations based on numerical experiments, some thermostated systems fulfill the conjugate pairing rule: from the $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_N$ Liapunov exponents the non-zero ones obey the

$$\lambda_i + \lambda_{N+1-i} = C$$

formula independently from the index $i$, where $C \leq 0$.

This behavior is very similar to the symmetry can be proven for Hamiltonian systems, which corresponds to the $C = 0$ choice. There has been two conjectures born for the possible explanation of the conjugate pairing rule: the time reversal symmetry of the system's dynamics, and some kind of nontrivial Hamiltonian property of the system's dynamics.

## 2.2. Objectives

The objective of the numerical experiment is investigating the conjugate pairing rule in a system, where the two conjectures supposed to play a role in the appearance of the conjugate Liapunov pairs (i.e., reversibility and Hamiltonian property) can be affected separately.

## 2.3. Methodology

The 3-dimensional periodic Lorentz gas thermostated by the Gaussian Isokinetic thermostat has been subjected to external magnetic field, therefore the reversibility and the Hamiltonian property of the system's dynamics can be affected by the direction of the magnetic field.

We have shown that the dynamics of the 3-dimensional periodic Lorentz gas thermostated by Gaussian Isokinetic thermostat with $|\mathbf{B}| \neq 0$ magnetic and $|\mathbf{E}| \neq 0$ electric fields is reversible if and only if the plane defined by $\mathbf{E}$ and $\mathbf{B}$ coincides with a symmetry plane of the lattice.

It can be shown that the system's equations of motion can be derived from a Hamiltonian if $\mathbf{B} = \mathbf{0}$. This Hamiltonian has been generalized by us to cases, where the system is subjected to $\mathbf{B} \neq \mathbf{0}$ magnetic field and the $\mathbf{E}\mathbf{B} = 0$ condition is met.

In the numerical experiment we have calculated the $\lambda_i(t)$ Liapunov exponents during several $t = 10^7$ long trajectories with the Gramm-Schmidt reortogonalization algorithm. The time evolution of the trajectory has been performed by an event driven algorithm, which ensures that not a single collision with the scatterers has been missed during the computed trajectory of the particle. Furthermore, this algorithm is far more efficient numerically than the generally used one, which steps the equations of motion with equal time intervals. In the numerical experiment I have investigated the following configurations:

- *reversible, but not Hamiltonian configurations:* the plane defined by $\mathbf{E} \neq \mathbf{0}$ and $\mathbf{B} \neq \mathbf{0}$ coincides with a symmetry plane of the lattice, however $\mathbf{EB} \neq 0$;
- *Hamiltonian, but not reversible configurations:* $\mathbf{EB} = 0$ condition holds, however the plane defined by $\mathbf{E} \neq \mathbf{0}$ and $\mathbf{B} \neq \mathbf{0}$ does not coincide with any of the symmetry planes of the lattice;
- *not reversible and not Hamiltonian configurations:* the plane defined by $\mathbf{E} \neq \mathbf{0}$ and $\mathbf{B} \neq \mathbf{0}$ does not coincide with any of the symmetry planes of the lattice and the $\mathbf{EB} = 0$ condition does not hold.

## 2.4. Results

**T1/1** *I have shown that the 3-dimensional Lorentz gas thermostated by the Gaussian Isokinetic thermostat and subjected to external magnetic field obeys the conjugate pairing rule (if* $\mathbf{E} \neq \mathbf{0}$, $\mathbf{B} \neq \mathbf{0}$*) only if the* $\mathbf{EB} = \mathbf{0}$ *condition holds. This condition coincides with the case, where* $\mathbf{B} \neq \mathbf{0}$ *and generalized Hamiltonian has been found.*

## 2.5. Conclusions

The numerical result described in **T1/1** thesis shows that the reversibility plays no role in obeying the conjugate pairing rule. Contrarily, the Hamiltonian formulation of the dynamics can play the key role in the appearance of the symmetry described by the rule. This numerical result has been confirmed by theoretical results found after its publication.

# 3. Numerical investigation of the fluctuation formula

## 3.1. Introduction

The fluctuation formula was found by D.J. Evans, E.G.D. Cohen and G. Morris in a numerical experiment, where the motion of particles interacting with Lennard-Jones potential and subjected to dissipation was investigated. They found that the probability of states with negative $\xi_\tau$ entropy production rate (i.e., violating the second law of thermodynamics) is exponentially smaller that the probability of states with positive entropy production rate:

$$\Pi_\tau(-\xi) = e^{-\tau\xi_\tau}\,\Pi_\tau(\xi)\,. \tag{1}$$

In this formula $\xi_\tau$ denotes the entropy production averaged over the $\tau$ interval, and $\Pi_\tau(\xi)$ is the probability density function of this quantity.

After publishing this numerical result several research groups started to investigate the symmetry described by the formula with the use of theoretical methods. Two significant results have been found: the *Evans-Searles fluctuation theorem* and the *Gallavotti-Cohen fluctuation theorem*, which one describes the fluctuations of the $\sigma_\tau$ phase space contraction rate instead of the $\xi_\tau$ entropy production rate.

G. Gallavotti has gone beyond the Gallavotti-Cohen fluctuation formula with his conceptual proposal, called the *chaotic hypothesis*. According to this hypothesis if we want to calculate the average of an observable of a nonequilibrium system, we can consider it as an Anosov system, and therefore we can use the results derived for Anosov systems.

## 3.2. Investigating the role of time reversibility

### 3.2.1. Objectives

The time reversal symmetry plays an important role in the derivation of both the Gallavotti-Cohen and the Evans-Searles fluctuation theorems. Accordingly, it would be interesting to investigate the affects of breaking the time reversal symmetry when the fluctuation formula is fulfilled.

### 3.2.2. Methodology

In the case of the periodic Lorentz gas thermostated by the Gaussian Isokinetic thermostat and subjected to magnetic field the reversibility of the dynamics can be affected by the direction of the magnetic field according to section 2.3. In the numerical experiment I have computed the $\Pi_\tau(\xi)$ probability density function during several $t = 10^8$ long trajectories with various $\tau$ parameters. In the numerical experiment I have investigated the following configurations:

1. *time reversible configurations:* with the $\mathbf{B} = \mathbf{0}$ choice the equations of motion of the system are invariant under time reversal;
2. *reversible configurations:* the plane defined by $\mathbf{E} \neq \mathbf{0}$ and $\mathbf{B} \neq \mathbf{0}$ coincides with a symmetry plane of the lattice;
3. *nonreversible configurations:* any configuration different from the ones above.

### 3.2.3. Results

**T2/1** *I have shown that in the 2- and 3-dimensional periodic Lorentz gas thermostated by the Gaussian Isokinetic thermostat and subjected to external magnetic field the entropy production rate fluctuations obey the Gallavotti-Cohen and the Evans-Searles fluctuation formula independently of the strengths and direction of the* $\mathbf{E}$ *and* $\mathbf{B}$ *fields.*

### 3.2.4. Conclusions

The numerical result formulated in the **T2/1** thesis shows that reversibility is not a necessary condition for obeying the fluctuation formulas, therefore fluctuation theorems could be formulated in more general terms.

## 3.3. Investigating the Nosé-Hoover thermostated Lorentz gas

### 3.3.1. Objectives

In the Lorentz gas thermostated by Gaussian Isokinetic thermostat the values of the phase space contraction rate and the entropy production rate are equal at each point of time, however this identity does not hold in general. It could be interesting to investigate the Gallavotti-Cohen and the Evans-Searles fluctuation formulas in a system, where the fluctuations of the above two quantities follow different distributions, therefore obeying the these two formulas can be investigated independently. The Lorentz gas thermostated by the Nosé-Hoover thermostat meets these requirements. There is one more reason supporting the numerical investigation of this system: namely, Anosov systems have compact phase space, therefore the fluctuations of the $\sigma$ quantity are bounded, however this property is not fulfilled by the Nosé-Hoover thermostated Lorentz gas.

### 3.3.2. Methodology

In the numerical experiment I have investigated the Gallavotti-Cohen and the Evans-Searles fluctuation formulas in the Nosé-Hoover thermostated Lorentz gas. In the simulation I have computed the $\Pi_\tau(\sigma)$ and $\Pi_\tau(\xi)$ probability density functions of the $\sigma_\tau$ and $\xi_\tau$ quantities along several $t = 10^8$ long trajectories with various $\tau$ and $\mathbf{E}$ parameters.

### 3.3.3. Results

**T3/1** *I have shown that the entropy production rate fluctuations always obey the Evans-Searles fluctuation formula in the 2- and 3-dimensional Nosé-Hoover thermostated Lorentz gas.*

**T3/2** *I have shown that in case of larger fluctuations the phase space contraction rate fluctuations deviate significantly from the Gallavotti-Cohen fluctuation formula in the 2- and 3-dimensional Nosé-Hoover thermos-*

*tated Lorentz gas. It can be observed that smaller phase space contraction rate fluctuations obey the Gallavotti-Cohen fluctuation formula far from equilibrium, however closer to equilibrium the proportion of fluctuations obeying the Gallavotti-Cohen fluctuation formula decreases significantly.*

### 3.3.4. Conclusions

The numerical result formulated in the **T3/1** thesis is in tune with the expected behavior and serves further numerical evidences on that the Evans-Searles fluctuation formula is valid in the broad range of systems.

The observation formulated in the **T3/2** thesis affects the chaotic hypothesis in its grounds, since I have shown that the Nosé-Hoover thermostated Lorentz gas cannot be treated as an Anosov system when calculating the averages of certain dynamical quantities.

## 3.4. Investigating the Lorentz gas thermostated by deterministic scatterings

### 3.4.1. Objectives

As a response to the negative results regarding the Gallavotti-Cohen fluctuation formula formulated in the **T3/2** thesis, such theoretical considerations have been born, which account the singularities caused by the collisions for the deviations from the formula. Accordingly, it would be interesting to investigate such a thermostating mechanism, which is incorporated into the collisions, therefore solely singularities are in the averaged phase space contraction rate.

### 3.4.2. Methodology

In the numerical experiment I have investigated the Gallavotti-Cohen and the Evans-Searles fluctuation formulas in the Lorentz gas thermostated by deterministic scatterings. In the simulation I have computed the $\Pi_\tau(\sigma)$ and

$\Pi_\tau(\xi)$ probability density functions of the $\sigma_\tau$ and $\xi_\tau$ quantities along several $t = 10^8$ long trajectories with various $\tau$ and $\mathbf{E}$ parameters.

### 3.4.3. Results

**T4/1** *I have shown that the entropy production rate fluctuations always obey the Evans-Searles fluctuation formula in the 2-dimensional Lorentz gas thermostated by deterministic scatterings*

**T4/2** *I have shown that – similarly to the Nosé-Hoover thermostated Lorentz gas – in case of larger fluctuations the phase space contraction rate fluctuations deviate significantly from the Gallavotti-Cohen fluctuation formula in the 2-dimensional Lorentz gas thermostated by deterministic scatterings. It can be observed that smaller phase space contraction rate fluctuations obey the Gallavotti-Cohen fluctuation formula far from equilibrium, however closer to equilibrium the proportion of fluctuations obeying the Gallavotti-Cohen fluctuation formula decreases significantly.*

**T4/3** *I have shown that the phase space contraction rate fluctuations of the Lorentz gas thermostated by deterministic scatterings are in good agreement with the modified fluctuation formula can be derived for a particle described by the Langevin equation and placed into moving harmonic potential:*

$$\lim_{\tau\to\infty} \frac{1}{\tau} \ln \frac{\Pi_\tau(\sigma)}{\Pi_\tau(-\sigma)} = f\left(\sigma/\sigma_+\right)\sigma_+ \,, \tag{2}$$

*where*

$$f\left(\sigma/\sigma_+\right)\sigma_+ = \begin{cases} \sigma & 0 \le \sigma < \sigma_+ \\ \sigma - \frac{\sigma_+}{4}\left(\frac{\sigma}{\sigma_+} - 1\right)^2 & \sigma_+ \le p < 3\sigma_+ \\ 2\sigma_+ & p \ge 3\sigma_+ \,. \end{cases}$$

### 3.4.4. Conclusions

The numerical result formulated in the **T4/1** thesis is in tune with the expected behavior and serves further numerical evidences on that the Evans-Searles fluctuation formula is valid in the broad range of systems.

The observation formulated in the **T3/2** thesis affects the chaotic hypothesis in its grounds, since I have shown that – beyond the Nosé-Hoover thermostated Lorentz gas – the Lorentz gas thermostated by deterministic scatterings cannot be treated as an Anosov system when calculating the averages of certain dynamical quantities.

The result formulated in the **T4/3** thesis shows – similarly to the case of Nosé-Hoover Lorentz gas – that in thermostated billiards the phase space contraction rate fluctuations do not obey the Gallavotti-Cohen fluctuation formula in its original form, however a modified form shown in 2 seems to be valid.

# Publications supporting the thesis


[1] M. Dolowschiák and Z. Kovács, *Breaking conjugate pairing in thermostatted billiards by magnetic field*, Phys. Rev. E **62**, 7894 (2000)

[2] M. Dolowschiák and Z. Kovács, *Fluctuation formula for nonreversible dynamics in the thermostated Lorentz gas*, Phys. Rev. E **66**, 066217 (2002)

[3] M. Dolowschiák and Z. Kovács, *Fluctuation Formula in the Nose-Hoover thermostated Lorentz gas*, Phys. Rev. E **71**, 025202(R) (2005)