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Temperature response of heat conducting models

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Chapter 1

Introduction

If we are given a system with an unknown behaviour, how do we approach its study? An intuitive answer is the same that a child with a new, mysterious toy would give: we could "mess" with it and see what happens. More seriously, we can say that to study a system is to study its reaction to external stimuli, which in the context of statistical physics means altering one of the variables of the system.

In general, this could lead to a radically different system that we are no longer able to study in relation to the original one; but if the alteration is small in comparison to its effect, the system maintains a comparable behaviour. In this case, the response of the system can be approximated as linear to the perturbation and we can write the *linear response function* [8]. Integrating the response function over time, we get the *generalized susceptibility* [42]. This means that the linear response function is not only a theoretical tool but it has a clear physical meaning. If we are given a solid, we might be interested in studying how its size is altered if we increase its temperature: in this case, the linear response function is connected to the *thermal expansion coefficient*, how much the system expands when its temperature is increased. At the same time, the *specific heat* of the solid can be retrieved from the response of the internal energy to a thermal perturbation

[15].
The response function is, in turn, determined by the equilibrium fluctuations: this is the *fluctuation-response theorem* [10]; for instance the specific heat, which describes the response of the internal energy to a thermal perturbation, can be expressed from the correlations of the internal energy fluctuations in the unperturbed state. More in general, at equilibrium the linear response of an observable can be written only in terms of the equilibrium correlation between the observable itself and the entropy produced in response to perturbation [24].
Out of equilibrium, however, these results are in general no longer valid.

In general, there are two kinds of systems out of equilibrium [42].
The first one are systems that are in the process of relaxing to equilibrium: for example, when a hot cup of coffee is placed in a room at room temperature, heat will flow from the coffee to the rest of the room; after some time the coffee and the air will have relaxed to a new equilibrium state: the coffee is now at the same temperature of the room. Before that, however, the coffee is not in equilibrium with the room and the process is not reversible: heat will not flow back again from the room to the coffee, warming it up. It is possible to keep changing the external parameters in order to never let the system relax, like in a running combustion engine.
Secondly there are systems that are driven from equilibrium by thermodynamic forces. This kind of systems can be further distinguished into three subgroups: systems under the influence of mechanical nonconservative forces; systems in contact with the environment at different chemical potentials; and systems in contact with parts of the environment at different temperatures.
Out of equilibrium, the linear response can no longer be written just as a correlation between the observable and the entropy produced in response

to perturbation, but another correlation term, called *frenesy*[1], related to the volume of transitions or changes performed in time, will appear. This quantity is time-symmetric, in the sense that trajectories display the same activity if they are spanned in the normal temporal direction or backward in time and it complements entropy production (which is time-antisymmetric) in the description of fluctuating quantities in regimes out of equilibrium [42].

The subject of our study is a conceptually simple one dimensional model of a heat conducting material in contact with two thermostats at adjustable temperatures; if they are set at the same value, we have a system in thermal equilibrium, with all its usual proprieties; the interesting behaviour is when they are not.

The inertial dynamics of the system are modeled as a Fermi-Pasta-Ulam system, a simple toy-model developed in the Fifties; while it was the first computational model in physics [17, 18], it is still in use as a simple model of a conductive body.

A Fermi-Pasta-Ulam chain is composed by a series of masses, with their dynamics determined by a non-linear potential that depends only on the distance between them.

How could we model the effects of the thermostats connected to the chain? We would be tempted to add a thermal white noise term to the dynamics of the extremes of the chain; these oscillators would move as in thermal equilibrium with the thermostat and their thermal fluctuations would propagate along the chain due to the Fermi-Pasta-Ulam interaction. Unfortunately, we would encounter mathematical problems when we apply this method to our model.

In order to obtain an analogue for out of equilibrium systems of the Kubo

[1] It has also been called *traffic* or *dynamical activity*.

formula, a relation between stationary fluctuations of some observable and the response of the system, we need an approach that does not require to explicit the probability density function, which, in contrast with equilibrium, is in general unknown. A suitable one is the *path-integral approach*, a technique that it has proved to be a very powerful tool in various areas of physics, both computationally and conceptually [40].

A realization of a stochastic process is called a trajectory (or path) and, if the dynamics are given, one can in principle compute the probability measure of such paths. The expectation value of observables dependent on the trajectory can be written as a sum (or integral) over all possible trajectories with path weights depending on the dynamics.

The expectation of perturbed observables, to be used in the linear response formula, may be rewritten it term of path weights of the unperturbed dynamics, if its path weights are comparable with those unperturbed. This is always true for mechanical perturbations [15, 16]. The main problem with white noises is that this is not the case when noise prefactors are different, as when we change temperatures. Mathematicians would say that there is no absolute continuity between the two processes. This issue was solved recently for nonequilibrium overdamped systems, for which we now have a thermal response theory [15, 16]. The problem remains open for inertial systems, which is why we are interested in this issue in this thesis.

Instead of relying on an explicit white noise term that has proven to be pathological, the effect of the thermal reservoirs to our Fermi-Pasta-Ulam chain is modeled by applying to the extremes of the chain two *Andersen thermostats*: an algorithm updates the velocity of the oscillator in contact with thermostats with a value extracted from the equilibrium distribution at the given bath temperature [2].

Our goal is to prove that this reformulation is a viable path to the study of out of equilibrium thermal response. In order to do so, we derive a general expression for the linear response function, showing separately the contribution of the entropic and frenetic term, and test it in a simulation with the directly measured linear response of different observables of the system. Hence, for the first time we obtain a fluctuation-response relation for thermal perturbations of a system with full Hamiltonian dynamics and operating out of equilibrium, thus extending previous results available only for systems evolving via overdamped stochastic equations or Markov jump processes [11].

Chapter 2

The thermal response problem

In equilibrium statistical mechanics, all thermodynamics properties are derived from the partition function [33]: once a physicist is given a Hamiltonian, his job is to compute as accurately as possible the partition function, with the appropriate methods for the particular problem (exact analytic calculations, perturbative expansions, numerical calculations and so on). This is not in general possible in non-equilibrium statistical mechanics, but there are many different approaches, whose connections are far from evident, none of them of universal validity.

One of these approaches is the *linear response theory* [10] which allows us to study a system by studying its response to any form of small perturbation (thermal, mechanical, chemical, etc).

2.1 Introduction to stochastic differential equations

For deterministic processes in physics, differential equations are usually written in the form:

$$\frac{dY_t}{dt} = A_t(Y_t) \tag{2.1}$$

where Y_t is some time-dependent physical quantity and $A_t(Y_t)$ a function of this quantity and time. It could also, of course, depend on some other

physical quantities but for the sake of simplicity we will restrict ourselves to the simpler case.

Equation (2.1) can also be written as an update formula [22]:

$$Y_{t+dt} = Y_t + A_t(Y_t)\, dt \tag{2.2}$$

Since, for any t_0, Y_{t_0+dt} is a function of only the value of Y at time t_0, we can say that this process is memoryless. This is a *Markov process.*

It is possible to show that equation (2.2) is the most general form for a deterministic continuous Markov process, since any other form would break consistency [22].

Similarly, the general form for a stochastic continuous Markov process is [22]

$$Y_{t+dt} = Y_t + A_t(Y_t)\, dt + D_t^{1/2}(Y_t)\mathcal{N}_t(dt)^{1/2} \tag{2.3}$$

where $\mathcal{N}_t$ is a function that at every instant extract a value from $N(0,1)$ (a normal distribution with zero mean and unit variance), $A_t(Y_t)$ is the *drift* term and $D_t(Y_t)$ is the *diffusion coefficient.*

To study the stochastic part of the equation (2.3), we write it in the form of a differential equation

$$\frac{dY_t}{dt} = A_t(Y_t) + D_t^{1/2}(Y_t)\frac{\mathcal{N}_t}{(dt)^{1/2}} \tag{2.4}$$

Since, for a Gaussian distribution, $\alpha N(0,1) = N(0,\alpha^2)$:

$$\frac{\mathcal{N}_t}{(dt)^{1/2}} = N\left(0, \frac{1}{dt}\right) \equiv \Gamma_t \tag{2.5}$$

which, in the limit $dt \to 0$, is a Gaussian that keeps widening and lowering. This is called *white noise*, denoted as Γ_t.

What are the characteristics of Γ_t? Its mean is by definition:

$$\langle \Gamma_t \rangle = 0 \tag{2.6}$$

We can write the correlation function as

$$\langle \Gamma_t \Gamma_{t+t'} \rangle = 0 \qquad t' \neq 0 \tag{2.7}$$

and since $\langle \Gamma_t \rangle \sim 1/dt$ goes to infinite in the limit $dt \to 0$:

$$\langle \Gamma_t \Gamma_{t+t'} \rangle = \delta'_t \tag{2.8}$$

It can be shown [21] that the density function of a random variable defined by equations (2.3) and (2.4) satisfies the partial differential equation:

$$\frac{\partial}{\partial t} P_t(y) = -\frac{\partial}{\partial y} \left[A_t(y) P_t(y) \right] + \frac{\partial^2}{2\partial y^2} \left[D_t(y) P_t(y) \right] \tag{2.9}$$

with y a realization of Y_t. This is called the (forward) *Fokker-Planck equation.* We can rewrite it as:

$$\frac{\partial}{\partial t} P_t(y) = L^\dagger P_t(y) \tag{2.10}$$

by introducing the forward generator $L^\dagger$. Its adjoint, the backward generator L, is an operator acting on functions of the process and of the time is defined as:

$$L\ f_t(y) = A_t(y) \nabla f_t(x) + \frac{D_t}{2}(y) \nabla^2 f_t(y) \tag{2.11}$$

with $f_t(y)$ a generic function.

We remark that these are mathematical results, without any particular assumption on the physics of the process.

2.2 Equilibrium linear response theory

Let us take a damped harmonic oscillator [36]

$$\frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + \omega_0^2 x = f(t), \qquad \omega_0^2 = \frac{k}{m} \tag{2.12}$$

how does $f(t)$ affects the system? We expect the solution $x(t)$ to be a linear functional of $f(t)$ in the form

$$x(t) = \int_{-\infty}^{+\infty} dt'\ \mathcal{R}(t - t')\ f(t') \tag{2.13}$$

where $\mathcal{R}(t - t')$ is the *linear response function.*

If we are studying a system at equilibrium, we can easily derive the form of

$\mathcal{R}(t-t')$ since the time-dependent distribution is known and can be written as:

$$\rho(q,p) = \frac{1}{Z(H)} e^{-\beta H(q,p)} \qquad Z(H) = \int dq\ dp\ e^{-\beta H(q,p)} \tag{2.14}$$

where Z(H) is the partition function. We will denote the average value taken with the equilibrium distribution (2.14) as $\langle\ \cdot\ \rangle^{(0)}$. If $A(q,p)$ is a dynamical variable, then its average value when no perturbation is applied is:

$$\langle A\rangle^{(0)} = \int dq\ dp\ A(q,p)\ \rho(q,p) \tag{2.15}$$

If we now perturb the system with a time-dependent potential V, arbitrarily small:

$$H \to H' = H + V \qquad V = -hA(q,p) \tag{2.16}$$

where h is a numerical coefficient and $A(q,p)$ is a dynamic variable. We limit ourselves to effects that are linear in h. The new partition function, in the first order of h, is therefore

$$Z(H+V) \simeq \frac{1}{Z(H)} \int dqdpe^{-\beta H}(1-\beta V) = Z(H)(1-\beta\langle V\rangle) \tag{2.17}$$

We will denote the average value taken with the perturbation h as $\langle\ \cdot\ \rangle^{(h)}$. If we introduce a second dynamic variable $B(q,p)$, we can compute its average $\langle B\rangle^{(h)}$ to first order of f

$$\langle B\rangle^{(h)} \simeq \frac{1}{Z(H)(1-\beta\langle V\rangle)} \int dqdpe^{-\beta H}(1-\beta V)B(q,p)$$

$$\simeq (1+\beta\langle V\rangle)(\langle B\rangle^{(0)} - \beta\langle VB\rangle) \simeq \langle B\rangle^{(0)} + \beta[\langle V\rangle\langle B\rangle - \langle VB\rangle]$$

$$= \langle B\rangle^{(0)} - \beta\langle VB\rangle_c$$

where we have defined $\langle VB\rangle_c$, connected part of $\langle VB\rangle$ as

$$\langle VB\rangle_c \equiv \langle VB\rangle - \langle V\rangle\langle B\rangle \tag{2.18}$$

so that the variation of B is

$$\langle B\rangle^{(h)} - \langle B\rangle^{(0)} = -\beta\langle VB\rangle_c = \beta h\langle BA\rangle_c \tag{2.19}$$

and since the linear response function is defined as

$$\langle B\rangle^{(h)} = \langle B\rangle^{(0)} + h\int_0^t dt'\ R(t-t') + o(h) \tag{2.20}$$

we can write the *static susceptibility* χ_{BA}, which is the derivative of $\langle B\rangle^{(h)}$ with respect of the perturbation h, as

$$\chi_{BA} = \frac{\partial\langle B\rangle^{(h)}}{\partial h}\Big|_{h=0} = \int_0^t dt'\ R_{BA}(t-t') = \beta\langle BA\rangle_c \tag{2.21}$$

This is the *fluctuation-response theorem*: the response of the system to a small perturbation, described by χ_{BA}, is governed by the equilibrium fluctuation $\langle BA\rangle_c$.

But what if the fluctuation is not constant? A very simple form of time-dependent fluctuation is

$$h(t) = \Theta(-t)h \tag{2.22}$$

which can be interpreted as a constant fluctuation applied from $t = -\infty$ to $t = 0$ and then switched off (figure 2.1).

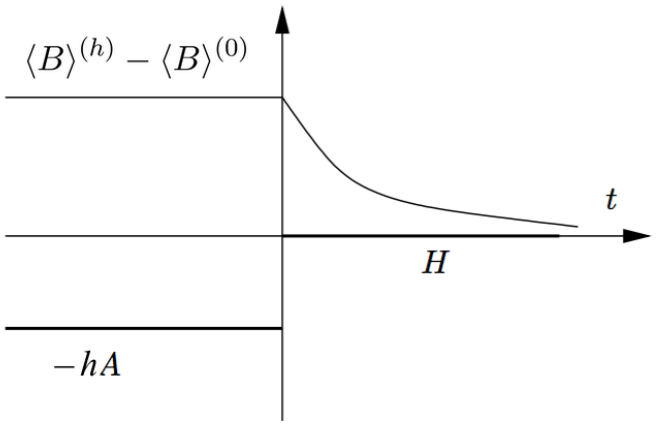


Figure 2.1: Schematic picture of the perturbation $(h(t))$ *and system response* $(\langle B\rangle^{(h)} - \langle B\rangle^{(0)})$

Now $\langle B(t)\rangle^{(h)}$ is a time-dependent variable. For $t < 0$, $\langle B(t)\rangle^{(h)} = \langle B\rangle^{(0)}$ is still constant and consistent with the previous formulation. Working in the analogue of the Heisenberg picture we can derive the form of for positive times

$$\langle B(t)\rangle^{(h)} = \frac{1}{Z(H')}\int dqdp e^{-\beta H'} B(t) \simeq \frac{1+\beta\langle V\rangle}{Z(H)}\int dqdp e^{-\beta H}(1-\beta V)B(t)$$

$$\simeq \langle B\rangle + \beta h\langle B(t)A(0)\rangle_c \tag{2.23}$$

The function $\langle B(t)A(0)\rangle_c$ is the (connected) equilibrium time correlation function of B and A, also called the *Kubo function* $C_{BA}(t)$ [24]. The response function is nothing but the time-derivative of the Kubo function.

We can show that remembering the definition of the response function (2.13)

$$\langle B(t)\rangle^{(h)} - \langle B\rangle^{(0)} = \int_{-\infty}^{t} dt' \mathcal{R}_{BA}(t-t')f(t')$$

$$= f\int_{-\infty}^{0} dt' \mathcal{R}_{BA}(t-t') = f\int_{-\infty}^{0} \mathcal{R}_{BA}(t')dt' \tag{2.24}$$

where the index BA means that we are considering the response of the observable B to a perturbation of A. Since it has to be consisted to (2.23), we can take the derivative of both terms and get

$$\frac{d}{dt}\langle B(t)\rangle^{(h)} = -f\mathcal{R}_{BA}(t) \qquad \frac{d}{dt}\langle B(t)\rangle^{(h)} = \beta f\langle \dot{B}(t)A(0)\rangle_c \tag{2.25}$$

and so we can finally write the response function as

$$\mathcal{R}_{BA}(t) = -\beta\Theta(t)\langle \dot{B}(t)A(0)\rangle_c \equiv -\beta\Theta(t)\dot{C}_{BA} \tag{2.26}$$

where we can see the proportionality between the response function and a time-dependent correlator. This is also called the *Kubo formula*.

Let us write the Fourier-transformat of the linear response function

$$\tilde{\mathcal{R}}_{BA}(\omega) = \int_{-\infty}^{+\infty} dt\, \mathcal{R}_{BA}(t)\, e^{i\omega t} = -\beta\int_{0}^{+\infty} dt\, \dot{C}_{BA}(t)\, e^{i\omega t} \tag{2.27}$$

If we take the imaginary part of the equation we get

$$\tilde{\mathcal{R}}''_{BA}(\omega) = -\beta \int_0^{+\infty} dt\, \dot{C}_{BA}(t)\, sin(\omega t) = -\frac{\beta}{2} \int_{-\infty}^{+\infty} dt\, \dot{C}_{BA}(t)\, sin(\omega t)$$

$$= i\frac{\beta}{2} \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\, \dot{C}_{BA}(t) \tag{2.28}$$

and, integrating by parts, we finally get

$$\tilde{\mathcal{R}}''_{BA}(\omega) = \frac{i\beta}{2}(-i\omega)\tilde{C}_{BA}(t) = \frac{\beta\omega}{2}\tilde{C}_{BA}(t) \tag{2.29}$$

Since it is possible to show that the imaginary part of the Fourier-trasformat of the linear response function ($\tilde{\mathcal{R}}''$) is related to the energy dissipated by a system, this is usually called the *fluctuation–dissipation theorem* [33].

2.3 Non-equilibrium linear response

The previous derivation of the Kubo formula assumes that the system is in equilibrium. We can ask ourself if there is a more general form.
The Fokker-Planck equation (2.10) for a Markov process with probability density $P_t(y)$ (for $t \leq 0$) with the forward generator $L^\dagger$ can be written as:

$$\frac{d}{dt}P_t(y) = L^\dagger P_t(y), \qquad L^\dagger P_{stat}(y) = 0$$

with $P_{stat}(y)$ the stationary probability density. We then turn on the perturbation at $t = 0$ so:

$$L_h^\dagger \equiv L^\dagger + hL_{pert}^\dagger \tag{2.30}$$

where h is a small parameter that let us control the amplitude of the perturbation per unit of time. We want to consider the effect of the perturbation on an observable $\mathcal{O}$. The formal result of a first order Dyson expansion is:

$$\langle \mathcal{O}(t)\rangle^{(h)} - \langle \mathcal{O}(0)\rangle^{(0)} = h \int_0^t \left\langle \frac{L_{pert}^\dagger P_{stat}}{P_{stat}}\, \mathcal{O}(t') \right\rangle^{(0)} dt' \tag{2.31}$$

in terms of time-correlation function for the unperturbed process. This formula, called the *Agarwal-Kubo function*, was first proposed by Agarwal [1], after Kubo's derivation for equilibrium [24], and later rediscovered in different forms [6]; in theory, this could be applied to a non-equilibrium state.

2.3.1 Application to intertial diffusion dynamics

As an example, we try to apply it to a diffusion Langevin dynamics:

$$M\dot{v_t} = -M\gamma v_t + \sqrt{2D}\Gamma_t \tag{2.32}$$

where M is the mass of the particle, γ the viscosity of the fluid, D its diffusion constant and Γ_t the gaussian white noise (2.5). From Einstein relation we know that

$$D = \gamma M k_b T \tag{2.33}$$

with T the temperature and k_b the Boltzmann constant.
We can write a $P_{stat}(x)$ that satisfy the stationary Fokker-Planck equation:

$$0 = \frac{\partial P_{stat}}{\partial t} = L^\dagger P_{stat} = \frac{\partial}{\partial v_t}\gamma v_t P_{stat} + \frac{k_b T}{M}\frac{\partial^2 P_{stat}}{\partial v_t^2} \tag{2.34}$$

If we introduce a thermal perturbation $T \to T + h$, we can write the perturbation in (2.34) as:

$$L_h^\dagger = L^\dagger + hL_{pert}^\dagger \qquad L_{pert}^\dagger = \frac{k_b}{M}\frac{\partial^2}{\partial v^2} \tag{2.35}$$

then Agarwal-Kubo equation gives us a very simple expression for thermal response:

$$\langle \mathcal{O}(t)\rangle_h - \langle \mathcal{O}(0)\rangle_0 = h\int_0^t \left\langle \frac{k_b}{M}\frac{1}{P_{stat}}\frac{\partial^2 P_{stat}}{\partial v^2}\mathcal{O}(t')\right\rangle_0 dt' \tag{2.36}$$

This expression is well-defined and suffers no mathematical problems, if $P_{stat}(x)$ is smooth and the process has only integrable time-correlations.
But, of course, no explicit computations of this formula can be done out of

equilibrium, except for special cases: if we are truly out of equilibrium, we have in general no way of knowing $\frac{\partial^2 P_{stat}}{\partial v^2}/P_{stat}$ or to measure it. While it is generally a well-behaving expression and we have no problem with the hypotheses we had to assume, the expression $\frac{L^\dagger_{pert} P_{stat}}{P_{stat}}$ is just not sufficiently explicit and it is often of little practical use.
We need a different approach that allows us to derive a practically useful expression for linear response formulas.

2.4 The path-integral approach

The notion of path-integral was introduced for the first time in the 1920s by Norbert Wiener as a method to solve problems in the theory of diffusion and Brownian motion. This integral, which is now also called the Wiener integral, has played a central role in the further development of the subject of path integration. It was reinvented in a different form by Richard Feynman in 1942, for the reformulation of quantum mechanics. In the 1950s, path-integrals were studied intensively for solving functional equations in quantum field theory (Schwinger equations). But its results are not limited to the quantum world, the path-integral technique finds newer and newer applications in statistical physics and non-relativistic quantum mechanics, in particular, in solid body physics and the description of critical phenomena (phase transitions), polymer physics and quantum optics, and in many other branches of physics. Most works in theoretical and mathematical physics during the two last decades of the last century contained some elements of the path-integral technique [12].

We can show its application to stochastic processes with a simple example [40]. Let us assume a one-dimensional Markovian process that follows a

Langevin diffusion equation:

$$\dot{x}_t = A_t(x) + D\,\Gamma_t \tag{2.37}$$

where $A_t(x)$ is the drift term and it is the deterministic component of the process, while D is the diffusion coefficient, that we assume constant for simplicity, and Γ_t is the Gaussian white noise. Under these hypotheses we also write the Champman-Kolmogorov equation:

$$P(x_3, t_3|x_1, t_1) = \int_{-\infty}^{+\infty} dx_2 P(x_3, t_3|x_2, t_2) P(x_2, t_2|x_1, t_1) \tag{2.38}$$

with $t_1 < t_2 < t_3$. Such an equation allows us, by partitioning the time interval in $N+1$ steps, $t_0 < t_1 < ... < t_f$, with $t_i = t_0 + i(t_f - t_0)/(N+1)$, to write:

$$P(x_f, t_f|x_0, t_0) = \int_{-\infty}^{+\infty} ... \int_{-\infty}^{+\infty} dx_1 ... dx_N P(x_f, t_f|x_N, t_N) ... P(x_1, t_1|x_0, t_0)$$

This can be interpreted as an integration over all possible paths that the process could follow. We would need the form of $P(x_{i+1}, t_{i+1}|x_i, t_i)$ in order to evaluate this integral, however we will follow an alternative way.
Now, the probability that at a given time t the process takes a value between a and b is:

$$\int_a^b dx P(x, t|x_0, t_0) \tag{2.39}$$

We can iterate this for all the partition, each with its a_i and b_i:

$$\int_{a_1}^{b_1} ... \int_{a_{N-1}}^{b_{N-1}} dx_1 .. dx_{N-1} P(x_f, t_f|x_{N-1}, t_{N-1}) ... P(x_1, t_1|x_0, t_0) \tag{2.40}$$

It is obvious that if we increase the number of time slices and at the same time we take the limit $b_i - a_i \to 0$ the trajectory can be defined with arbitrary precision, if the trajectories are continuous.

For a general Markov process, we can write:

$$P(x, t|x_0, t_0) = \int \mathcal{D}[x(t)] e^{-\int_{t_0}^{t} ds \mathcal{L}[x(s), \dot{x}(s)]} \tag{2.41}$$

where $\mathcal{L}[x(s), \dot{x}(s)]$ is the *stochastic Lagrangian* (also called Onsager-Machlup functional). We can also indentify the *stochastic action* through

$$\mathcal{A}[x(t)] = \int_{t_0}^{t} ds \mathcal{L}[x(s), \dot{x}(s)] \tag{2.42}$$

that allows to write (2.41) as

$$P(x, t|x_0, t_0) = \int \mathcal{D}[x(t)] e^{-\mathcal{A}[x(t)]} \tag{2.43}$$

This formulation allows us to write practically useful expressions for linear response formulas, readily applicable for non equilibrium processes too [5, 7, 9, 14].

As an example, let us apply this to the Wiener process [20, 38]:

$$P(W_2, t_2|W_1, t_1) = \frac{e^{\frac{(W_2 - W_1)^2}{2D(t_2 - t_1)}}}{\sqrt{2\pi(t_2 - t_1)}} \tag{2.44}$$

For $N \to \infty$ we can define a measure of the path-space known as the *Wiener measure* [35, 41]. By substituting (2.44) into (2.40) we get:

$$\prod_{i=1}^{N} \frac{dW_i}{(4\pi h D)^{1/2}} e^{-\frac{1}{4Dh} \sum_i (W_i - W_{i-1})^2} \tag{2.45}$$

which is the desired probability of following a given path.
Taking the limit $h \to 0$ and $N \to \infty$, we can write the exponential in (2.45) in the continues limit as

$$e^{-\frac{1}{4D} \int_{t_0}^{t} d\tau (\frac{dW}{d\tau})^2} \tag{2.46}$$

If we then integrate the expression in (2.40) over all the intermediate points, which is equivalent to a sum over all possible paths, as all the integrands are Gaussians and the convolution of two Gaussians is again a Gaussian, we recover the result of (2.46) for the probability density of the Wiener process. Hence we have expressed the probability density as a path-integral *Wiener integral* [25, 35]

$$P(W, t|W_0, t_0) = \int \mathcal{D}[W(\tau)] e^{-\frac{1}{4D} \int_{t_0}^{t} d\tau (\frac{dW}{d\tau})^2} \tag{2.47}$$

where the expression inside the integral is the continuous version of the integral in (2.40), over all possibile values of the intermediate points.

2.5 Linear response at equilibrium

Let us present a brief description of the path-space approach to the response in equilibrium [29]. A dynamical ensemble gives the weight of a trajectory $[X] = (x_s, 0 \leq s \leq t)$ of the system the expectation value of an observable $\mathcal{O} = \mathcal{O}[X]$ can be written as

$$\langle O \rangle = \int \mathcal{D}[X] P[X] \mathcal{O}[X] = \int \mathcal{D}[X] e^{-\mathcal{A}[X]} P_{eq}[X] \mathcal{O}[X] \tag{2.48}$$

where $\mathcal{D}[X]$ is the formal notation for the volume element on the path-space, P_{eq} is the equilibrium path-probability distribution and we denote with

$$P[X] = e^{-\mathcal{A}[X]} P_{eq}[X] \tag{2.49}$$

the path-probability distribution of the perturbed system, with action $\mathcal{A}$.
At the initial time ($t = 0$), the system is in equilibrium and the two path-probabilities P and P_{eq} differ only because P is in the perturbed ensemble. Since we are at equilibrium, we can assume time-reversibility, which implies the invariance $P_{eq}(\mathcal{T}[X]) = P_{eq}[X]$ under time-reversal $\mathcal{T}$.
We can decompose the action $\mathcal{A}$ into a time-antisymmetric E and a time-symmetric F term

$$\mathcal{A} = \frac{1}{2}(F - E) \tag{2.50}$$

with $\mathcal{T}E = -E$ and $\mathcal{T}F = F$, as they do depend on time because they are defined on paths $[X]$ in the time-interval $[0, t]$.
These are the two components of the action:

- the entropic term (E) given by correlation between the observable and the entropy produced in response to perturbation

- the frenetic term (F) related to the volume of transitions or changes performed in response to perturbation

Expanding (2.48) around equilibrium we get:

$$\langle \mathcal{O} \rangle^{(h)} = \langle \mathcal{O} \rangle^{(0)} - \langle \mathcal{A}[X] \mathcal{O}[X] \rangle^{(0)} \tag{2.51}$$

Remembering that $P_{eq}(\mathcal{T}[X]) = P_{eq}[X]$, the time-reversed observable gives us:

$$\langle \mathcal{O}\mathcal{T} \rangle^{(h)} = \langle \mathcal{O} \rangle^{(0)} - \langle \mathcal{A}\left(\mathcal{T}\left[X\right]\right) \mathcal{O}[X] \rangle^{(0)} \tag{2.52}$$

If we then subtract (2.53) from (2.51) we get

$$\langle \mathcal{O} - \mathcal{O}\mathcal{T} \rangle^{(h)} = -\langle \{\mathcal{A}\left[X\right] \mathcal{A}\left(\mathcal{T}\left[X\right]\right)\} \mathcal{O}[X] \rangle^{(0)} \tag{2.53}$$

to linear order in perturbation.
Now, using that $\mathcal{A}[X] - \mathcal{A}(\mathcal{T}[X]) = -E[X]$ [29] we get

$$\langle \mathcal{O} - \mathcal{O}\mathcal{T} \rangle^{(h)} = \langle E[X] \mathcal{O}[X] \rangle^{(0)} \tag{2.54}$$

If we are studying an observable $\mathcal{O}[X] = \mathcal{O}(x_t)$ that depends on the final time t, we have $\mathcal{O}(\mathcal{T}[X]) = \mathcal{O}(\tilde{x_0})$, where $\tilde{x_0}$ is the initial point of the trajectory with the sign of momentum flipped. And, since we are at equilibrium:

$$\langle \mathcal{O}(\tilde{x}_0) \rangle^{(0)} = \langle \mathcal{O}(x_0) \rangle^{(0)} = \langle \mathcal{O}(x_t) \rangle^{(0)} \tag{2.55}$$

Placing this result in (2.54) we finally get

$$\langle \mathcal{O}(x_t) \rangle^{(h)} - \langle \mathcal{O}(x_t) \rangle^{(0)} = \langle E[X] \mathcal{O}(x_t) \rangle^{(0)} \tag{2.56}$$

In other words, at equilibrium the response is completely given by the correlation with the dissipative part in the action: the entropy flux, E.

2.6 The problem with path-integration

This scheme can be successfully applied to many out of equilibrium processes, where we have a mechanical or even a thermal perturbation [6].
There is, however, a particular case where this approach finds some problem. Let us assume that we have two oscillators with a single degree of freedom [4]:

$$\dot{x}_t = -k_1 x_t + \sqrt{2D_1}\Gamma_t^{(1)}, \qquad \dot{y}_t = -k_2 y_t + \sqrt{2D_2}\Gamma_t^{(2)}$$

where $\Gamma_t^{(1)}$ and $\Gamma_t^{(2)}$ are two independent Gaussian white noises and D_1 and D_2 are the temperature-dependent diffusion constants . If the two diffusion constants are equal, then the two processes have the same support: their typical trajectories look the same and events that have zero probability for one, also have zero probability for the other process. This is not true if $D_1 \neq D_2$, even if $D_1 - D_2 = h$ very small (but still not zero): the two motions remain mutually singular and there is no density of one with respect to the other [32].
We can illustrate this problem in terms of path-integration: let us try to mimic the weight

$$\sim \left[-\int_0^1 ds \frac{\dot{B}^2(s)}{4T} \right] \tag{2.57}$$

of a Brownian path $x_t = \sqrt{2T}B(t)$ at temperature T on a discrete time grid of mesh size $\Delta_t = 1/N$ in the unit time-interval $[t_0 = 0, t_N = 1]$ and let us assign real variables b_i to each time $t_i = 0, 1/N, 2/N, ..., 1$. The Brownian weight resembles the density

$$\mathcal{P}_T[b] = \left(\frac{N}{4\pi T} \right)^{N/2} exp \left[-\frac{N}{4T} \sum_{i=0}^{N-1} (b_i - b_{i+1})^2 \right] \tag{2.58}$$

fixing $b_0 = 0$.
Taking the derivative of the expected value for an observable $\mathcal{O}(b) = O(b_1, ..., b_N)$

with respect to temperature we get the response formula:

$$\frac{1}{2T}\int_{R^N} db \left[\frac{1}{2T}\sum_{i=0}^{N-1}\left(\frac{b_i - b_{i+1}}{1/N}\right)^2 \frac{1}{N} - N\right]\mathcal{O}(b)\mathcal{P}_T[b] \tag{2.59}$$

in between [.], we have the rescaled quadratic variation

$$\mathcal{A}_N(b) \equiv \frac{1}{2T}\sum_{i=0}^{N-1}\frac{(\Delta b_i)^2}{\Delta t}\frac{1}{N} - N \tag{2.60}$$

which has $\mathcal{P}_T$-mean zero, but its variance

$$\int_{R^N} db_1 db_2 ... db_N \mathcal{A}_N^2(b)\mathcal{P}_T[b] \propto N$$

is diverging with $N \to \infty$.

When we try to apply the scheme we have previously presented to processes kept out of equilibrium with different temperatures, problems of incommensurability arise. Mathematically we can say that the two processes are not absolutely continuous with respect to each other [32].
This problem has been overcome in some cases, either introducing an explicit time-discretation to avoid divergence in the response [4, 43] or relaying on a rescaling of the stochastic dynamics in order to derive regular results [16]. More recently, it has been derived a well-defined thermal response formula by standard path-integral techniques [15], but this method is applied only to overdamped dynamics, otherwise the calculations become unfeasible.
We would be interested in obtaining a fluctation-response relation for thermal perturbations of a system with full Hamiltonian dynamics and operating out of equilibrium.

There is, however, a result of the path-integral approach to out of equilibrium linear response that we want to keep in mind. We have shown in the previous section that, in equilibrium, the response is completely given by the correlation with the dissipative part in the action (2.56). This is not

in general true out of equilibrium.

The line of reasoning is essentially unchanged when we are studying linear response out of equilibrium. We can write (2.53) as:

$$\langle \mathcal{O} \rangle^{(h)} = \langle \mathcal{O} \rangle^{(0)} - \langle \mathcal{A}[X]\mathcal{O}[X] \rangle^{(0)} \tag{2.61}$$

where we denoted with $^{(h)}$ some stationary nonequilibrium state where we study the response. We can still decompose $\mathcal{A}$ in E and F, that now refers, respectively, to excess in entropy flux and in dynamical activity with respect to the unperturbed nonequilibrium stationary state. Substituting that into (2.61) we simply get

$$\langle \mathcal{O} \rangle^{(h)} - \langle \mathcal{O} \rangle^{(0)} = \frac{1}{2}\langle S[X]O[X] \rangle^{(0)} - \langle F[X]O[X] \rangle^{(0)} \tag{2.62}$$

Now the frenetic contribution enters as second term in the linear response. It is a non-dissipative term, as it involves time-symmetric changes (remember that $F = F\mathcal{T}$), related, in particular, to dynamical activity and time-symmetric currents. Therefore, we are interested also in studying separately the two terms of linear response.

In the next chapter we will introduce a model for a semi-stochastic system and we will show an algorithmic solution for the thermal response problem for that model.

Chapter 3

Model

In order to achieve a better comprehension of the linear response to temperature changes in systems kept out of equilibrium by heat fluxes, we need a simple model of a conductive solid to study. We will consider a Fermi-Pasta-Ulam chain connected to two thermal reservoirs at two different temperatures as a minimal model of a system conducing heat. We will avoid the pathological white noise term in the dynamics, as discussed in 2.6; the thermalization of the extremes of the chain is, instead, implemented algorithmically.

3.1 The Fermi-Pasta-Ulam model

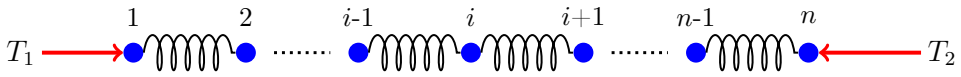


Figure 3.1: Sketch of the model: the oscillators in the chain feel a Fermi-Pasta-Ulam interaction between them, while the first and last are kept at temperatures T_1 and T_2 by Andersen thermostats.

In the early 1950s, considering what numerical investigations could be perormed on a first generation digital computer at Los Alamos National Laboratory, Enrico Fermi suggested to Stanislaw Ulam and John Pasta that

the foundations of statistical mechanics could be explored [26]. The model used in the studies was a discretization of a nonlinear spring which quartic order is given by a potential in form

$$U = \sum_{i}^{N-1} \frac{r_i^2}{2} + \alpha \frac{r_i^3}{3} + \beta \frac{r_i^4}{4} \qquad r_i \equiv x_{i+1} - x_i \tag{3.1}$$

with N unit masses and unit harmonic coupling. The apparent contradiction of the results of the original Fermi-Pasta-Ulam (FPU) experiment conducted in 1953 and 1954 [17] with the hypothesis that essentially any nonlinearity would lead to a system exhibiting ergodic behaviours has become known as the Fermi-Pasta-Ulam Problem[1], that is still an interesting subject of studies in Statistical Mechanics [18]. But the Fermi-Pasta-Ulam model also opened the way to the use of computers to study fundamental questions on the foundations of Statistical Mechanics and is still used as a simple model of a complex system, as in our case.

We have chosen the Fermi-Pasta-Ulam as a minimal model of heat conduction: the thermal fluctuations propagates from the thermalized oscillators along the chain due to the interaction between oscillators. If the temperatures are set to different values, it is an interesting toy-model for a system driven out of equilibrium by a heat flux.

For our purposes, we have settled on $\alpha = -1.5$ and $\beta = 1$. As we can see on figure 3.2, this gives us a potential that is:

- **well-contained**, so that a particularly strong fluctuation do not cause the system to diverge;
- **non-symmetric**, so that an increase on fluctuation leads to a mean increase of the length of the chain (*positive thermal expansion*), as we expect from a real system;
- **with a single minimum**, to simplify the study of the system.

[1] For a review of the current understanding of this paradox, see [19].

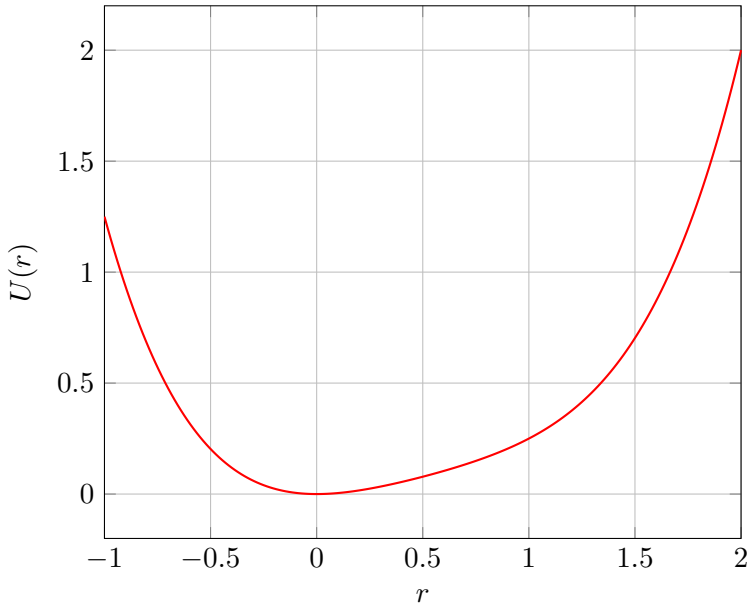


Figure 3.2: FPU potential (U) with $\alpha = -1.5$ and $\beta = 1$

3.2 Thermal reservoirs

This is the core of our solution to the thermal response problem. Both ends of the chain are connected to a thermal reservoir, with a defined temperature. This is modeled with an algorithm that updates the velocity of the extremal oscillators with a value extracted from the equilibrium probability density at the temperature of the reservoir.

$$P_{eq}(v) = \sqrt{\frac{m}{2\pi k_b T}} e^{-\frac{mv^2}{2k_b T}} \tag{3.2}$$

We can therefore set the temperature of the reservoir by changing the parameter T in the distribution, and later change it to model a thermal perturbation of one of the reservoirs. Thermal fluctuations then naturally propagate in the chain due to the Fermi-Pasta-Ulam interaction between the oscillators. Since our goal is to study a non-equilibrium model, the two thermal reservoirs are at two different temperatures T_1 and T_2

The velocity is not updated at fixed time intervals, but the length of every

update interval is stochastic with a simple exponential distribution:

$$P(\Delta t) \propto e^{-\frac{\Delta t}{\tau}} \tag{3.3}$$

with τ a fixed parameter of the simulation, the same for both thermal reservoirs.

This technique is called *Andersen thermostat* [2] and was the first thermostat proposed for molecular dynamics, allowing one to model the dynamics of molecules in a canonical ensemble (where the total number of particles, the volume and the temperature are conserved).

We also note that this technique does not require the extremes of the chain to be in a fixed position, as in physical contact with a thermostat, in order to keep them at the fixed temperature.

3.3 Susceptibility

A thermal perturbation of the system can be written as an increase in temperature of one thermal reservoir:

$$T_2 \to T_2 + h$$

We will denote the probability of a trajectory $[X]$ of a system with thermal reservoirs at temperatures T and T' as $\Pr_{T,T'}[X]$ and the mean value as $\langle\cdot\rangle_{T,T'}$; at the beginning of every trajectory these are fixed at T_1 and T_2.

It is, of course, possible to obtain the susceptivity of the system directly from the definition, computing the mean of an observable $\mathcal{O}$ both in a perturbed and unperturbed simulated system, if we assume h to be small enough

$$\chi_{\mathcal{O}}(t) \simeq \frac{\langle \mathcal{O}(t) \rangle_{T_1,T_2+h} - \langle \mathcal{O}(t) \rangle_{T_1,T_2}}{h} \tag{3.4}$$

Instead, our goal is to write the susceptivity in form of a correlation function between the observable and other quantities, a non-equilibrium analogue of Kubo's formula (2.26). First of all, we write the mean value of an observable

$\mathcal{O}$ in a perturbed system, using the path-integral approach we illustrated in section 2.4

$$\langle \mathcal{O}(t) \rangle_{T_1,T_2+h} = \sum_{[X]} \Pr_{T_1,T_2+h}[X] \cdot \mathcal{O}(x(t)) \tag{3.5}$$

where $\sum_{[X]}$ is the sum over all possible trajectories of the system.
We can multiply and divide this expression for the probability of a trajectory $[X]$ in the unperturbed system $\Pr_{T_1,T_2}[X]$

$$= \sum_{[X]} \Pr_{T_1,T_2}[X] \frac{\Pr_{T_1,T_2+h}}{\Pr_{T_1,T_2}}[X] \cdot \mathcal{O}(x(t))$$

but this is equal to the mean value of a quantity $\frac{\Pr_{T_1,T_2+h}}{\Pr_{T_1,T_2}}[X]$ in the unperturbed system

$$= \left\langle \frac{\Pr_{T_1,T_2+h}}{\Pr_{T_1,T_2}}[X] \cdot \mathcal{O}(x(t)) \right\rangle_{T_1,T_2} \tag{3.6}$$

As we can see, it is possible to compute the mean value of an observable $\mathcal{O}$ in the perturbed system as the mean value of this new observable: $\mathcal{O}$ multiplied by the ratio of the probability of the trajectory in the two systems, in the unperturbed system. The only thing left to do is to compute this ratio.
Our model is semi-deterministic: only the velocity updates are stochastic, the evolution of the system is deterministic. We can therefore write this term as the ratio of the two Maxwell-Boltmann probability of every velocity update and compute $\frac{\Pr_{T_1,T_2+h}}{\Pr_{T_1,T_2}}$ as a product of these ratios:

$$\frac{\Pr_{T_1,T_2+h}}{\Pr_{T_1,T_2}}[X(t)] = \prod_{\alpha}^{n(t)} \frac{\sqrt{\frac{m}{2\pi k_b T_1}} e^{-\frac{m v_{1,\alpha}^2}{2k_b T1}} \sqrt{\frac{m}{2\pi k_b (T_2+h)}} e^{-\frac{m v_{2,\alpha}^2}{2k_b (T_2+h)}}}{\sqrt{\frac{m}{2\pi k_b T_1}} e^{-\frac{m v_{1,\alpha}^2}{2k_b T1}} \sqrt{\frac{m}{2\pi k_b T_2}} e^{-\frac{m v_{2,\alpha}^2}{2k_b T_2}}}$$

$$= \prod_{\alpha}^{n(t)} \sqrt{\frac{T_2}{T_2+h}} e^{\frac{v_{2,\alpha}^2}{2} \frac{h}{T_2(T_2+h)}} \tag{3.7}$$

where we assumed $k_b = 1$ and $m = 1$, α is the index of the velocity update and $n(t)$ is the number of velocity updates before time t; the product is over all the velocity updates until time t.

Therefore, if we are able to simulate a great number of trajectories of the system without perturbation and compute $\frac{\mathrm{Pr}_{T_1,T_2+h}}{\mathrm{Pr}_{T_1,T_2}}[X(t)]$ for each of them, we can obtain the mean value of the perturbed observable without a direct measure on a perturbed system

$$\langle \mathcal{O}(t) \rangle_{T_1,T_2+h} = \frac{\sum_{[X]} \frac{\mathrm{Pr}_{T_1,T_2+h}}{\mathrm{Pr}_{T_1,T_2}}[X(t)] \cdot \mathcal{O}(x(t))}{N} \tag{3.8}$$

where N is the number of trajectories.

If we expand this formula we get, at the first order,

$$\frac{\mathrm{Pr}_{T_1,T_2+h}[X]}{\mathrm{Pr}_{T_1,T_2}[X]}(t) = 1 - \sum_{\alpha}^{n(t)} \left. \frac{\sqrt{\frac{T_2}{T_2+h}} e^{\frac{h v_{2,\alpha}^2}{T_2(T_2+h)}} (T_2 - 2v_{2,\alpha}^2 + h)}{2(T_2+h)^2} \right|_{h=0} h + \mathcal{O}(h^2)$$

$$= 1 - \sum_{\alpha}^{n(t)} \frac{T_2 - v_{2,\alpha}^2}{2T_2^2} h + \mathcal{O}(h^2)$$

where, as before, the sum is over the velocity updates in the trajectory $[X]$ before time t. If we assume h to be very small, we can limit ourselves to the first order and therefore we are able to write the susceptibility

$$\chi_{\mathcal{O}}(t) = \lim_{h\to 0} \frac{\langle \mathcal{O}(t) \rangle_{T_1,T_2+h} - \langle \mathcal{O}(t) \rangle_{T_1,T_2}}{h}$$

$$= \lim_{h\to 0} \frac{\langle \mathcal{O}(t) \rangle_{T_1,T_2} + h \langle \sum_{\alpha}^{n(t)} \frac{T_2 - v_{2,\alpha}^2}{2T_2^2} \mathcal{O}(t) \rangle_{T_1,T_2} - \langle \mathcal{O}(t) \rangle_{T_1,T_2}}{h} =$$

$$= \left\langle \sum_{\alpha}^{n(t)} \frac{v_{2,\alpha}^2 - T_2}{2T_2^2} \mathcal{O}(t) \right\rangle_{T_1,T_2} \tag{3.9}$$

where the sum is over all the velocity updates before time t. As we can see, we have lost an explicit dependency from the size of the perturbation h.

3.4 Entropic and frenetic terms

Since we are dealing with non-equilibrium, we expect that the susceptibility (3.9) can be written as the sum of two terms [4], as we previously discussed in section 2.6:

- an *entropic term* (E), related to the entropy produced in response to perturbation, that is asymmetric under time reversal;
- a *frenetic term* (F), related related to the volume of transitions or changes performed in response to perturbation, that is symmetric under time reversal.

When the perturbation is performed around equilibrium, $T_1 = T_2 = T$ and all the forces are conservative, the entropic and frenetic contributions combine to give back the Kubo formula

$$\chi_{\mathcal{O}}^{eq} = E + F = 2E \tag{3.10}$$

We are therefore interested in writing the susceptibility as a sum of a time-symmetric and time-antisymmetric term, both of them are to be written in form of a correlation between the observable and another quantity.

Let us call $f[X]$ a function of the trajectory $[X]$ and $[X^*]$ the same trajectory run in reverse. It is possibile to write its symmetric and antisymmetric part for time reversal as, respectively, the semisum and semidifference of itself and its time reversed

$$S\{f\} = \frac{1}{2}(f[X] + f[X^*]) \qquad A\{f\} = \frac{1}{2}(f[X] - f[X^*]) \tag{3.11}$$

Likewise we can write the symmetric and antisymmetric part of $\sum_{[X]} f[X]$ as:

$$S\left\{\sum_{[X]} f[X]\right\} = \frac{1}{2}\sum_{[X]}(f[X] + f[X^*])$$

$$A\left\{\sum_{[X]} f[X]\right\} = \frac{1}{2}\sum_{[X]}(f[X] - f[X^*])$$

where, since there is one-to-one correspondence between a trajectory and its reverse, we have wrote it as a sum only over $[X]$. We now have to write in

these forms the susceptibility we recovered in section 3.3:

$$\chi_{\mathcal{O}}(t) = \left\langle \sum_{\alpha}^{n(t)} \frac{v_{2,\alpha}^2 - T_2}{2T_2^2} \mathcal{O}(t) \right\rangle_{T_1,T_2} \tag{3.12}$$

The only time-dependent variable is $v_{2,\alpha}$, the updated velocity of the oscillator connected to the perturbed reservoir. During the forward process, the velocity of that oscillator evolves accordingly to the dynamics of the Fermi-Pasta-Ulam chain until the moment of the update, when it is changed to a new value.

Let us call $v_{2,\alpha}^b$ the velocity of the oscillator the instant before the update with index α. In the time-reversed of the same project the oscillator would have to evolve to a velocity $v_{2,\alpha}$ and then be updated to a velocity $v_{2,\alpha}^b$. Therefore the time-reversed of the updated velocity will be $-v_{2,\alpha}^b$. Remembering (3.9) we can therefore write the frenetic term as

$$F = \frac{1}{2} \left\langle \frac{1}{2T_2^2} \sum_{\alpha} \left[(v_{2,\alpha})^2 - T_2 + (v_{2,\alpha}^b)^2 - T_2 \right] \mathcal{O}(t) \right\rangle_{T_1,T_2} =$$

$$= \frac{1}{4T_2^2} \left\langle \sum_{\alpha} \left[(v_{2,\alpha})^2 + (v_{2,\alpha}^b)^2 - 2T_2 \right] \mathcal{O}(t) \right\rangle_{T_1,T_2} \equiv \langle A(t)\mathcal{O}(t) \rangle_{T_1,T_2} \tag{3.13}$$

and the entropic term as

$$E = \frac{1}{2} \left\langle \frac{1}{2T_2^2} \sum_{\alpha} \left[(v_{2,\alpha})^2 - T_2 - (v_{2,\alpha}^b)^2 + T_2 \right] \mathcal{O}(t) \right\rangle_{T_1,T_2} =$$

$$\frac{1}{4T_2^2} \left\langle \sum_{\alpha} \left[(v_{2,\alpha})^2 - (v_{2,\alpha}^b)^2 \right] \mathcal{O}(t) \right\rangle_{T_1,T_2} \equiv \langle B(t)\mathcal{O}(t) \rangle_{T_1,T_2} \tag{3.14}$$

And of course if we sum these two terms we get the linear response function

$$E + F = \frac{1}{4T_2^2} \left\langle \sum_{\alpha} \left[(v_{2,\alpha})^2 + (v_{2,\alpha}^b)^2 - 2T_2 + (v_{2,\alpha})^2 - (v_{2,\alpha}^b)^2 \right] \mathcal{O}(t) \right\rangle_{T_1,T_2}$$

$$= \frac{1}{4T_2^2} \left\langle \sum_{\alpha} 2 \left[(v_{2,\alpha})^2 - T_2 \right] \mathcal{O}(t) \right\rangle_{T_1,T_2}$$

$$= \left\langle \sum_{\alpha} \frac{(v_{2,\alpha})^2 - T_2}{2T_2^2} \mathcal{O}(t) \right\rangle_{T_1,T_2} = \chi_O(t)$$

We have been able to write a non-equilibrium analogue of the *Kubo formula*: the susceptibility to a thermal perturbation is expressed in form of a correlation between the observable and another quantity. This quantity can be written as a sum of an *entropic* and a *frenetic* term.
We have avoided the problems related to mathematical pathologies of the white noise illustrated in section 2.6 with an algorithmic reformulation of the thermal reservoir.

In the next chapter we will test these results with a computer simulation of our model.

Chapter 4

Simulation

In order to test the results of the previous chapter, we have build a simulation of our model in the programming language C++.
This program will measure different observables and their linear susceptibility in two different ways:

- **direct measure**: the program will simulate both the unperturbed and perturbed system and compute the mean of the observables in the two systems, obtaining the susceptibility as

$$\chi_{\mathcal{O}}(t) \simeq \frac{\langle \mathcal{O}(t) \rangle_{T_1,T_2+h} - \langle \mathcal{O}(t) \rangle_{T_1,T_2}}{h} \tag{4.1}$$

- **sum of the frenetic and entropic terms**: the program will only consider the data from the unperturbed system to compute the frenetic and entropic terms we have derived in section 3.4, obtaining the susceptibility as the sum of these two terms.

4.1 Structure of the simulation

In order to compute the mean of dynamic observables, we need to simulate a great number of trajectories of our system from a stationary state.
It is more reasonable, both for computational cost and the stability of the

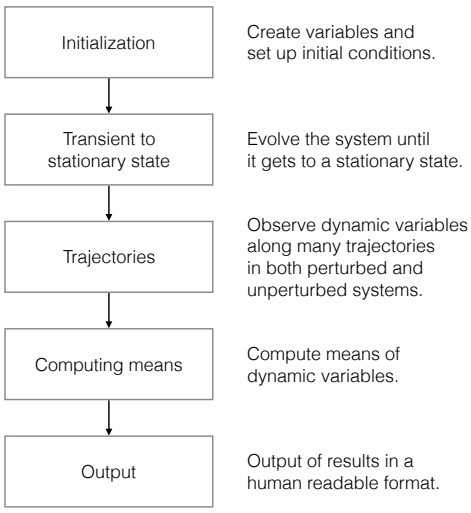


Figure 4.1: Flowchart of the simulation

simulation, to simulate a single long trajectory and split it into smaller fixed-length time intervals, long enough for both a meaningful evolution of the system under the perturbation and to consider each interval independent from the previous one.

But how do we get the system to a stationary state? Since we are not in equilibrium we do not know the stationary probability function, we cannot derive the stationary state from theory. What we can do is let evolve the system for a long time before beginning to measure the observables we are interested in. As we can see in figure 4.2, an observable of the chain (in this case, the length of the chain) gets more stable after $1500 \div 2000$ time-units, but we have chosen to wait 5000 time-units before considering our system to be in a stationary state.

After that, we split the trajectory in time-intervals. As we can see in figure 4.3, at the beginning of every interval the state of the system is copied: this copy will evolve separately and its second thermal reservoir will have a higher temperature $T_2^h = T_2 + h$, in order to simulate the thermal perturbation; this is the *perturbed system*. At every time-step of the interval,

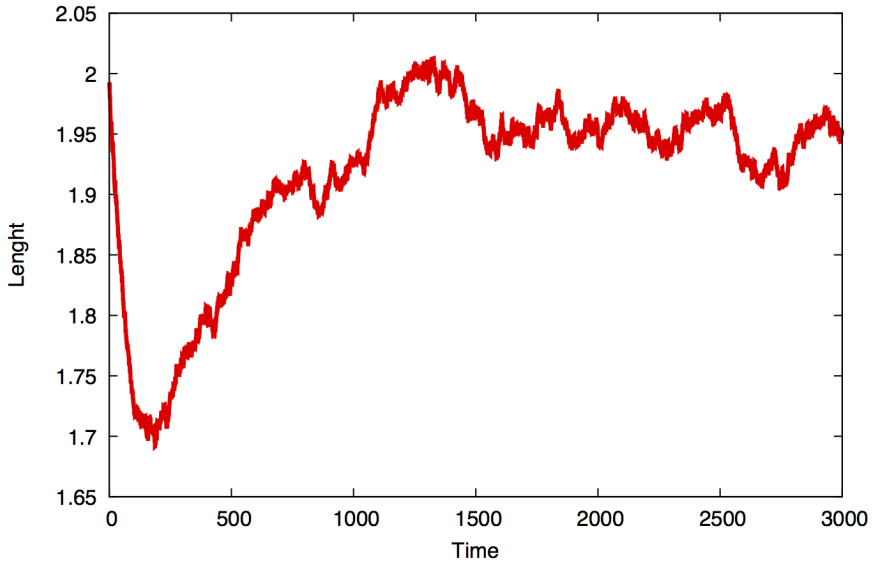


Figure 4.2: Length of the chain after the beginning of the simulation. We can see the system approaching a stationary state after $1500 \div 2000$ *time units.*

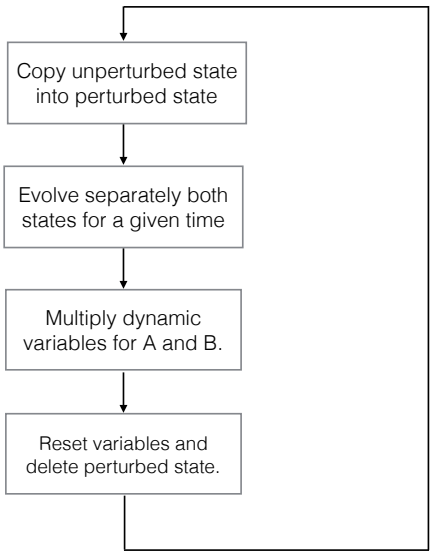


Figure 4.3: Flowchart of the time interval

both the system will evolve as in figure 4.4 and both observables and the quantities $A(t)$ (3.13) and $B(t)$ (3.14) are computed.

The observed values of the dynamic variables in both the perturbed and

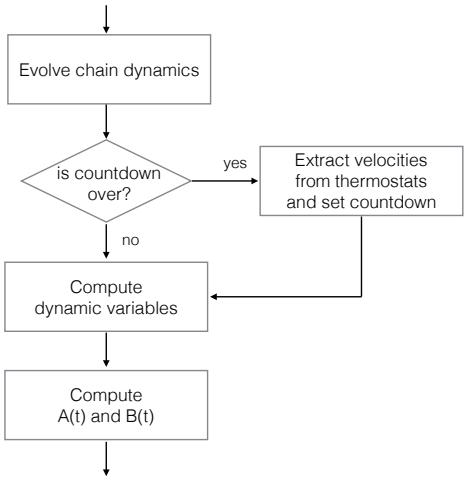


Figure 4.4: Flowchart of a single time-step

unperturbed state are immediately processed in order to compute mean and variance (as discussed in section 4.5) at the end of the simulation. The observed values of dynamic variables in the unperturbed state, $A(t)$, and $B(t)$ are stored until the end of the trajectory when the entropic and frenetic term are computed for all the observables, which are processed to later compute mean and variance. These variables are then deleted before a new trajectory begins.

After a given number of trajectories, the simulation is over. The mean values and variances of the susceptibility for every observable are computed both directly, as in equation (3.4), and as the sum of the frenetic and entropic terms.

The results are outputted in a human readable plain-text format.

4.2 Chain dynamics

Since we already have an expression for the Fermi-Pasta-Ulam potential (3.1), we now need a suitable numerical method to solve the ordinary differential equation (ODE)

$$\ddot{\boldsymbol{x}} = -\nabla U(\boldsymbol{x}) \tag{4.2}$$

Let us consider the Taylor expansion of a function $y(t)$ of t around t_0

$$y(t_0 + \Delta t) = y(t_0) + \Delta t\, y'(t_0) + \frac{1}{2}\Delta t^2\, y''(t_0) + O(\Delta t^3) \tag{4.3}$$

If we limit ourselves to the first order of Δt we get

$$y'(t_0) \approx \frac{y(t_0 + \Delta t) - y(t_0)}{\Delta t} \tag{4.4}$$

this is a first-order method to solve ODEs and it is called the *Eulero method* [34], but it is unsuitable for our model (and to most practical uses) due to two major issues.

First of all the *local error*, given by how we have truncated the Taylor expression, is approximately proportional to Δt^2 and that leads to a *global error* (the error at a fixed time t after how many steps the method needs to take to reach that instant) proportional to Δt.

Secondly, we have to take into account the great instability of the Eulero method: the numerical solution grows very large for equations where the exact solution do not. While this issue does appear in all numerical methods, the Eulero method is particularly susceptible to instability and this cannot practically be limited by reducing the integration interval.

There is an extensive literature of alternative numerical methods [34]. We have chosen for our simulation the *velocity Verlet* method since it allows a sufficient accuracy at a limited computational cost.

Where Eulero method uses the forward difference approximation to the first derivative in differential equations of the first order, *Verlet integration* can be

seen as using the central difference approximation to the second derivative; we can compute the acceleration at the step n as:

$$a_n = \frac{\Delta^2 x_n}{\Delta t^2} = \frac{\frac{x_{n+1}-x_n}{\Delta t} - \frac{x_n - x_{n-1}}{\Delta t}}{\Delta t^2} = \frac{x_{n+1} - 2x_n + x_{n-1}}{\Delta t^2} \tag{4.5}$$

and then we can write the value of x at the $n+1$ step as:

$$x_{n+1} = 2x_n - x_{n-1} + a_n \Delta t^2 \tag{4.6}$$

and the acceleration is known from the Fermi-Pasta-Ulam potential.
There is an alternate formulation of this method, called *velocity Verlet*; this method is mathematically equivalent to the Verlet, but it is not numerically equivalent and is superior on a computer with finite precision [37]

$$x_{n+1} = x_n + v_n \Delta t + \frac{1}{2} a_n \Delta t^2 \tag{4.7}$$

$$v_{n+1} = v_n + \frac{a_n + a_{n+1}}{2} \Delta t \tag{4.8}$$

The local error in position is proportional to Δt^4 and Δt^2 in velocity, while the global error is proportional to Δt^2 in position and Δt in velocity.
We have implemented this method in our simulation with a four step algorithm (figure 4.4), repeated at every time step:

1. Store the previously calculated a_n in another variable;
2. Calculate x_{n+1};
3. Derive a_{n+1} from the Fermi-Pasta-Ulam potential (3.1) using x_{n+1}, since it only depends on position;
4. Calculate v_{n+1}.

The stability of the system is also greatly improved, but we still have to be careful about the length of the integration interval Δt in order to avoid instability in the simulation.

4.3 Thermal reservoirs

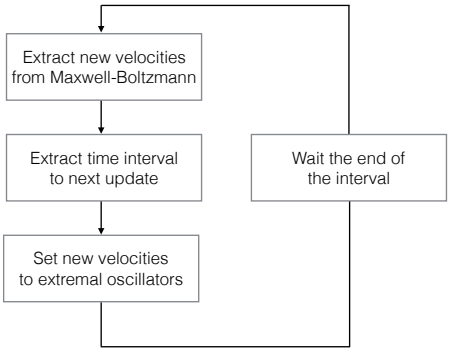


Figure 4.5: Flowchart of the thermal reservoir

As we have discussed in section 3.2, the thermal reservoirs are implemented algorithmically, updating the velocities of the extremal oscillators with values extracted from the Maxwell-Boltzman probability distribution after a stochastically generated time.
We have chosen to use the *BOOST.Random library*, a well-documented open source library of pseudo-random number generators and distributions [31]. The pseudo-random generator we used in our simulation is the `mt19937`, a Mersenell-Twister generator [30]; while 7% slower and requiring 85% more memory than its related `mt11213b`, it gives us a longer cycle: $2^{19937} - 1$ instead of $2^{11213} - 1$. Since our simulation does not use much memory, we consider it a valid trade-off.

The one-dimensional Maxwell-Boltzman distribution

$$\rho_T(v) = \sqrt{\frac{m}{2\pi k_b T}} e^{-\frac{mv^2}{2k_b T}} \tag{4.9}$$

can be seen as a Gaussian distribution with mean $\mu = 0$ and variance $\sigma^2 = k_b T/m$. Since we are not interested in using a particular set of units, we can choose one where $k_b = m = 1$, therefore, remembering the proprieties of the

Gaussian distribution, we can write

$$\rho_T(v) = \sqrt{T}N(0,1) \tag{4.10}$$

where $N(0,1)$ is the Gaussian distribution with zero mean and variance $\sigma^2 = 1$. In this way, we can use `normal_distribution` from the BOOST.Random library, which maps the distribution given by the chosen generator to a normal distribution, to extract a velocity from the Maxwell-Boltzmann distribution of the thermal reservoir; this value is then set as the velocity of the connected oscillators. This is done separately for both thermal reservoirs, each with its temperature.

The algorithm does not update the velocity at a fixed interval but after a time distributed as

$$P(\Delta t) \propto e^{-\frac{\Delta t}{\tau}} \tag{4.11}$$

After every update, the number of time steps before the next update is extracted from this distribution: when the countdown gets to zero, the velocities of both reservoirs are updated again (figure 4.5).
This is implemented using `uniform_real_distribution`, a uniform real distribution from the BOOST.Random library; by applying some algebra to (4.11), we get

$$N_{steps} = -\frac{\tau \log(U(0,1))}{\Delta t} \tag{4.12}$$

where $U(0,1)$ is the uniform real distribution limited between 0 and 1 and Δt is the size of the time step. The result is a real number but the number of steps must obviously be an integer: the value is truncated.
The parameter τ regulates the coupling of the reservoirs with the system; an higher value would reduce their effects on the chain, while a smaller one adds noise to the dynamics of the system. We have set $\tau = 1$ in arbitrary time units.

4.4 Observables

We have chosen and defined within the formalism of this system three different observables we will measure to study their response to a thermal perturbation. Since we are studying their evolution during every interval, they are implemented as an array with a time index.

4.4.1 Chain length

The observable *chain length* ($L(t)$) is the sum of the distances between the oscillators. It is computed at every time step by summing in a cycle over all the oscillators (except the first one) the distance between the position of the oscillator and the previous one:

$$L(t) = \sum_{i=1}^{n} x_i(t) - x_{i-1}(t) \tag{4.13}$$

4.4.2 Fermi-Pasta-Ulam potential energy

The observable *Fermi-Pasta-Ulam potential energy* ($U(t)$) is the value of the sum of the Fermi-Pasta-Ulam potential over all the oscillators. It is, again, computed at every time step with a sum on a cycle over all the oscillators:

$$U(t) = \sum_{i}^{N-1} \left[\frac{r_i^2(t)}{2} + \alpha \frac{r_i^3(t)}{3} + \beta \frac{r_i^4(t)}{4} \right] \qquad r_i(t) \equiv x_{i+1}(t) - x_i(t) \tag{4.14}$$

4.4.3 Kinetic energy of thermalized oscillators

The observable *kinetic energy of thermalized oscillators* ($K(t)$) is the value of the kinetic energy of the oscillators connected to thermal reservoirs (the first and last one in the chain). It is computed at every time step:

$$K(t) = \frac{1}{2} \left(m_1 v_1^2(t) + m_2 v_2^2(t) \right) = \frac{v_1^2(t) + v_2^2(t)}{2} \tag{4.15}$$

since we have set $m_1 = m_2 = 1$.

4.5 Statistical variance

In order to be able to confront different estimates of a physical quantity, in our case the susceptibility, we need to compute its statistical variance.
Since we have a large number of trajectories that we assume independent from each other and identically distributed, we can assume that physical quantities that we measure along these trajectories are realizations from independent and identically distributed variables y_i with $Var(y_i) = \sigma^2 < \infty$. Therefore we can apply the central limit theorem to the estimator mean defined as:

$$\bar{y} = \frac{1}{M} \sum_{i}^{M} y_i \tag{4.16}$$

and, since it is a stochastic variable itself, compute its variance as:

$$\sigma_{\bar{y}}^2 = Var(\bar{y}) = \frac{1}{M^2} Var(\sum_{i}^{M} y_i) \overset{(iid)}{=} \frac{1}{M^2} \sum_{i}^{M} Var(y_i) = \frac{\sigma^2}{M}. \tag{4.17}$$

Since σ^2 is not known, we need to estimate it using its classical sample variance estimator, defined as:

$$\hat{\sigma}^2 = s^2 = \frac{1}{M-1} \sum_{i}^{M} (y_i - \bar{y})^2 \tag{4.18}$$

and thus estimate $\sigma_{\bar{y}}^2$ as

$$\hat{\sigma}_{\bar{y}}^2 = \frac{s^2}{M}. \tag{4.19}$$

An algorithm based on 4.18 would be a *two-pass algorithm* as it would need to cycle two times across the data, first to compute the mean then the variance. For our data size, this is computationally unfeasible: we need a *single-pass algorithm.*

We would be tempted to apply formula of subtraction of squares [28]:

$$s^2 = \frac{1}{M(M-1)} \left(M \sum_{i}^{M} y_i^2 - \left(\sum_{i}^{M} y_i \right)^2 \right) \tag{4.20}$$

Unfortunately, if the dataset we are dealing with is very large and its distribution has a variance significantly smaller than the mean, the terms in

the subtraction in (4.20) will coincide up to a certain significant figure: this would result in a loss of significant figures thus leading to an incorrect result [23, 39]. This is what happens in our case.

There are many algorithms to compute the variance that are more numerically accurate [13, 27]. We have chosen the *Welford method* [23, 39], a simple one-pass algorithm that is arithmetically equivalent to (4.20). It is an iteration formula for deriving the corrected sum of squares for N values from the corrected sum of squares for the first $(N-1)$ of these.

We define recursively two quantities:

$$T_k = T_{k-1} + (y_k - T_{k-1})/k \qquad S_k = S_{k-1} + (y_k - T_{k-1})(y_k - T_k) \quad (4.21)$$

with $S_1 = 0$ and $M_1 = X_1$. After iterating over all the data, we get:

$$\overline{X} = T_N/M \qquad \sigma_X^2 = S_N/M \quad (4.22)$$

This is implemented in our program using the C++ class RunningStat[1].

In order to test our implementation we have generated different sized samples from a Gaussian distribution with known mean and variance using the BOOST libraries, as discussed in section 4.3, and computed s^2 both with our implementation of the Welford algorithm and the subtraction of squares formula. To highlight the problem, we have set a variance five order of magnitude smaller than the mean ($\mu = 10^5$, $\sigma^2 = 1$).

As we can see in figure 4.6, the subtraction of squares formula gives very incorrect results for large samples, while the Welford method gives a better estimate as the sample size increase (figure 4.7), at a very small computational cost ($\sim 5\%$), as shown in figure 4.8.

[1] Which can be found here: `johndcook.com/blog/standard_deviation`

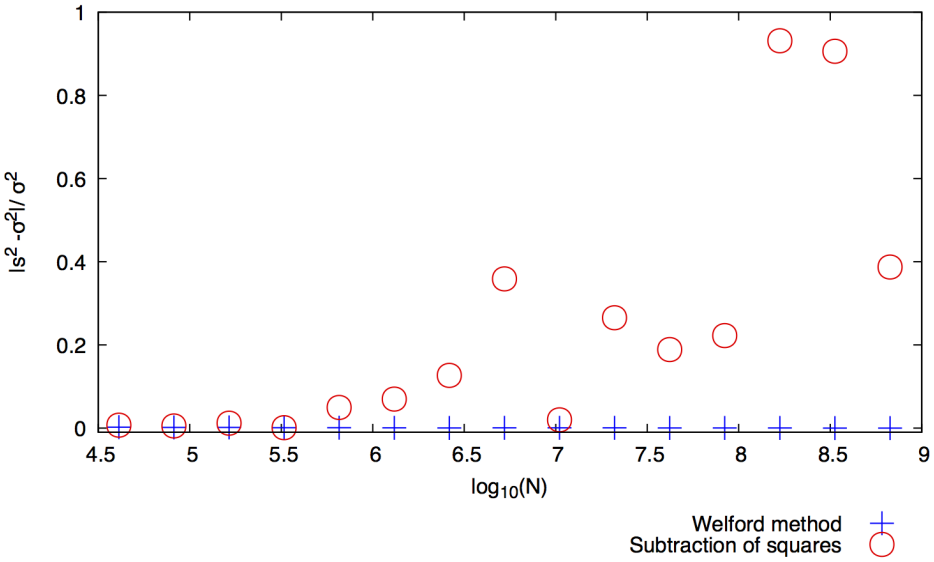


Figure 4.6: Difference between estimated and real variance, both methods.

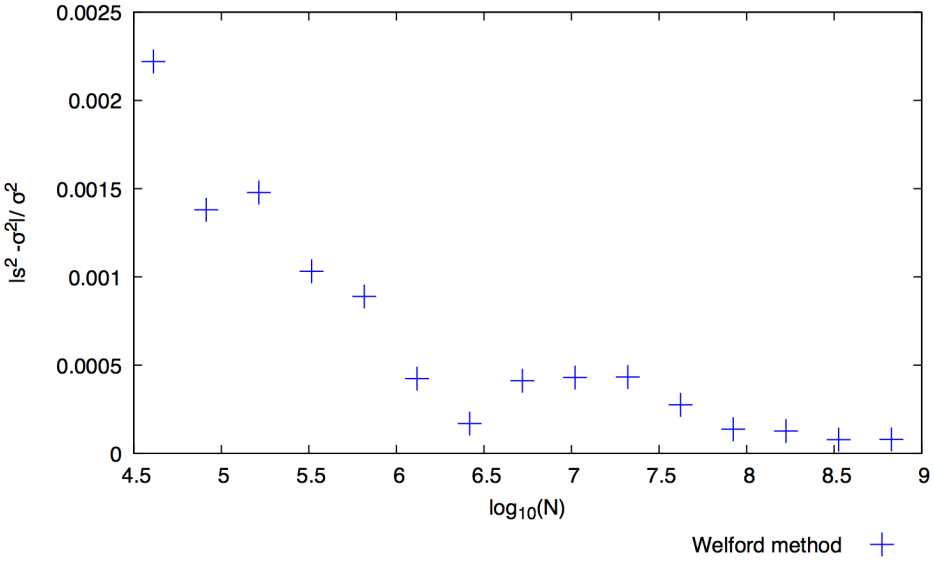


Figure 4.7: Difference between estimated and real variance, Welford method.

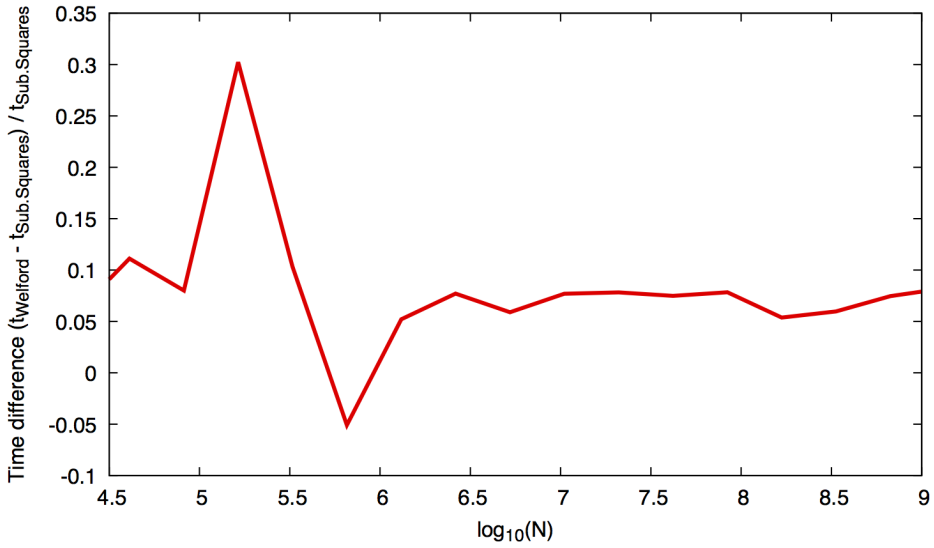


Figure 4.8: Difference in computational time.

Chapter 5

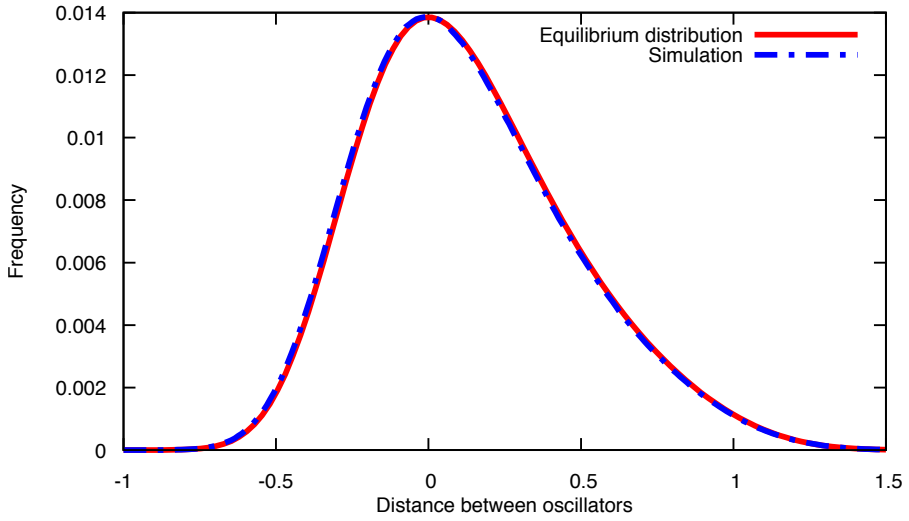
Results

5.1 Equilibrium

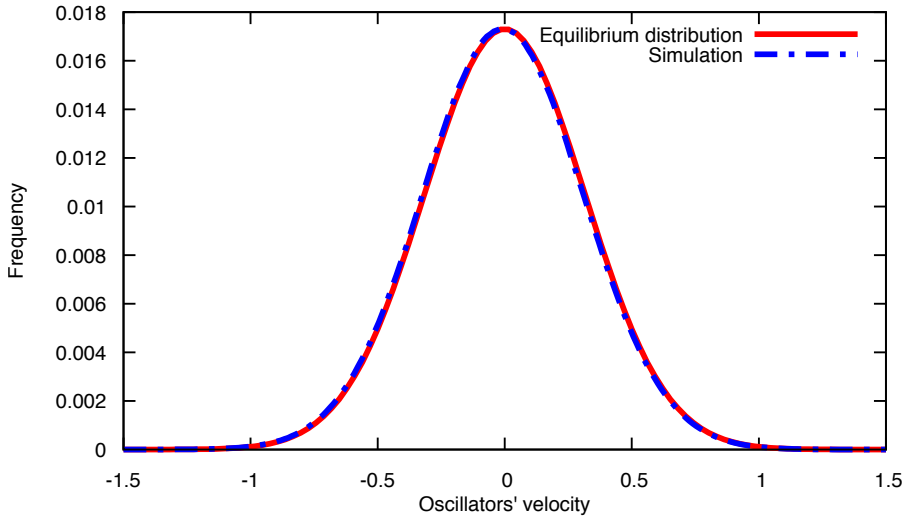
We are interested in testing our simulation by confronting its results with known quantities; in order to do so we place the system in equilibrium by setting the thermal reservoirs to the same temperatures ($T_1 = T_2 = T = 0.1$) and confront the results with those from the known equilibrium probability density function.

The parameters we have set for this simulation are:

Parameter	Variable	Value
Number of oscillators	`N`	10
Number of trajectories	`repeat`	10^5
Length of the time step	`dt`	0.005
Temperature of the first thermostat	`T1`	0.1
Temperature of the second thermostat	`T2`	0.1
Perturbation amplitude	`h`	0.01
Length of the interval	`interval`	70
Length of transient to stationary state	`stable`	5000



(a) Distribution of the distance between oscilators.



(b) Distribution of the velocities.

Figure 5.1: Equilibrium distribution and reconstruction from simulation.

We have recorded, after reaching the stationary (in this case also equilibrium) state, the distance between the oscillators and their velocities the probability density function for these observable is easily obtained as:

$$P_{eq}(r) \propto e^{-\frac{U(r)}{k_b T}} \qquad P_{eq}(v) \propto e^{-\frac{mv^2}{2k_b T}} \tag{5.1}$$

with $U(r)$ the Fermi-Pasta-Ulam potential (3.1) and, as previously discussed, $m = k_b = 1$. As we can see in figures 5.1b and 5.1a, we can be satisfied by the quality of the reconstruction of the probability density from the simulation.

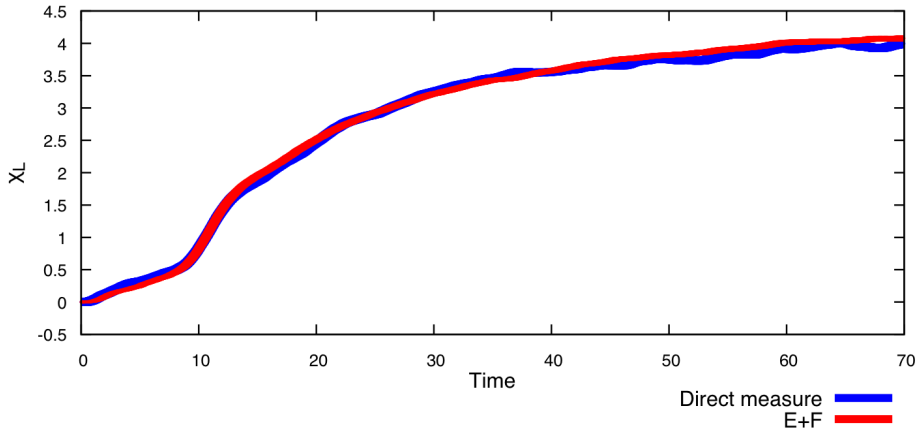
We are also interested in seeing how our simulation reconstructs the form of the susceptibility at equilibrium. If we are around equilibrium and all forces are conservatives, as in our case, we expect the sum of the entropic and frenetic terms to give us the Kubo formula

$$\chi_{\mathcal{O}}^{eq} = E + F = 2E = \frac{1}{2T_2^2} \left\langle \sum_{\alpha} \left[(v_{2,\alpha})^2 - (v_{2,\alpha}^b)^2 \right] \mathcal{O}(t) \right\rangle_{T_1,T_2} \tag{5.2}$$

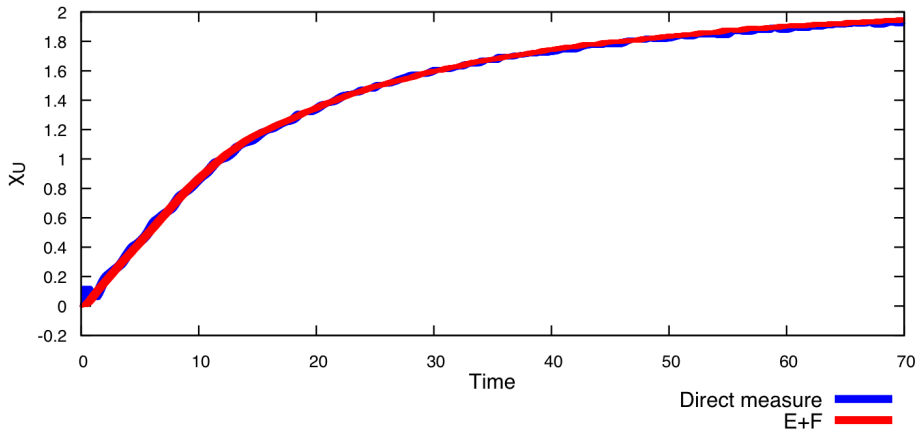
In other words, at equilibrium the response is completely given by the correlation with the dissipative part in the action. This is exactly what happens in our simulation, as we can see in figure 5.2: F coincides with E and their sum $E + E = 2E$ gives us the susceptibility at equilibrium.

5.2 Out of equilibrium

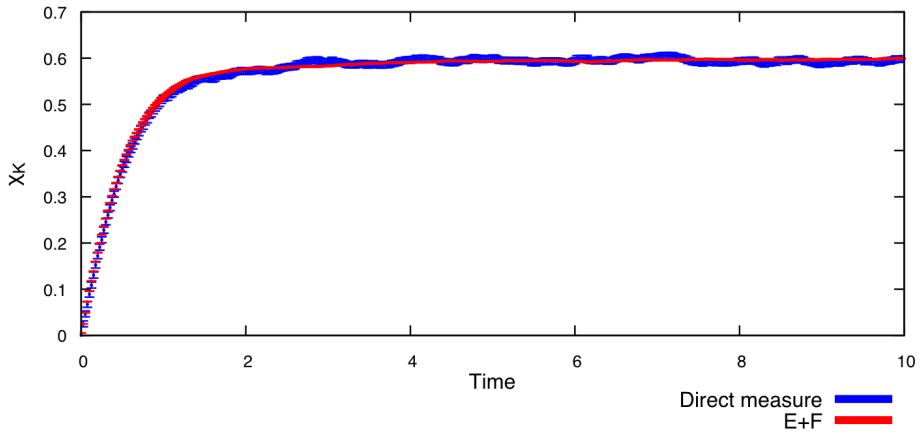
Beside what we already discussed, the final simulation has been set with the following parameters, which have been mostly empirically fine-tuned from the data of many previous simulations:



(a) Susceptibility of the chain length to an increase of T_2 at equilibrium.



(b) Susceptibility of the Fermi-Pasta-Ulam potential energy to an increase of T_2 at equilibrium.



(c) Susceptibility of the kinetic energy of the oscillators connected to thermal reservoir to an increase of T_2 at equilibrium.

Figure 5.2: Estimates of susceptibility at equilibrium to an increase of T_2 with error bars at one sigma: direct measure and sum of the frenetic (F) and entropic (E) terms.

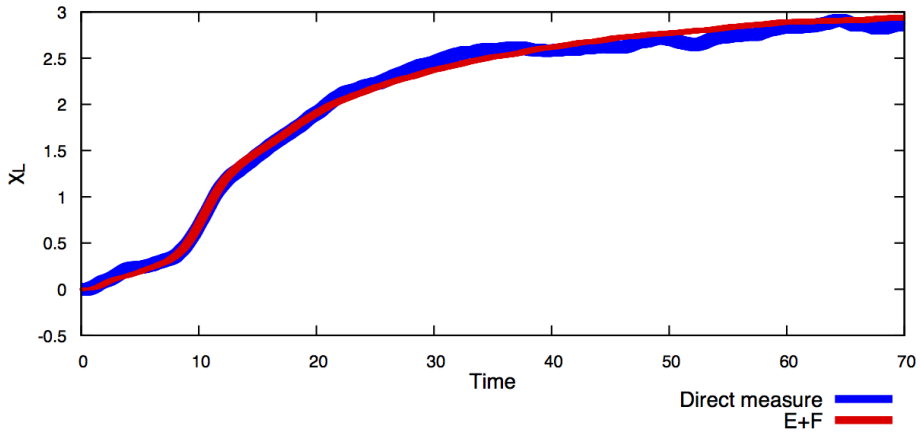
Parameter	Variable	Value
Number of oscillators	`N`	10
Number of trajectories	`repeat`	10^6
Length of the time step	`dt`	0.005
Temperature of the first thermostat	`T1`	0.1
Temperature of the second thermostat	`T2`	0.2
Perturbation amplitude	`h`	0.01
Length of the interval	`interval`	70
Length of transient to stationary state	`stable`	5000

In particular, the length of the interval has been set to allow for the full evolution of the linear response for the observables $L(t)$ and $U(t)$, while $K(t)$ has a very fast evolution and requires a shorter time to get to its final value. With these parameters, a simulation requires over 57 hours on the available machine (~ 0.2 seconds per interval).
The susceptibility of the kinetic energy of the oscillators connected to thermal reservoir is shown in figure 5.5 for a shorter time since it has a faster evolution then the other observables, as we could expect since we are measuring the oscillators directly connected to the thermal reservoir and the perturbation does not have to flow through all the system.

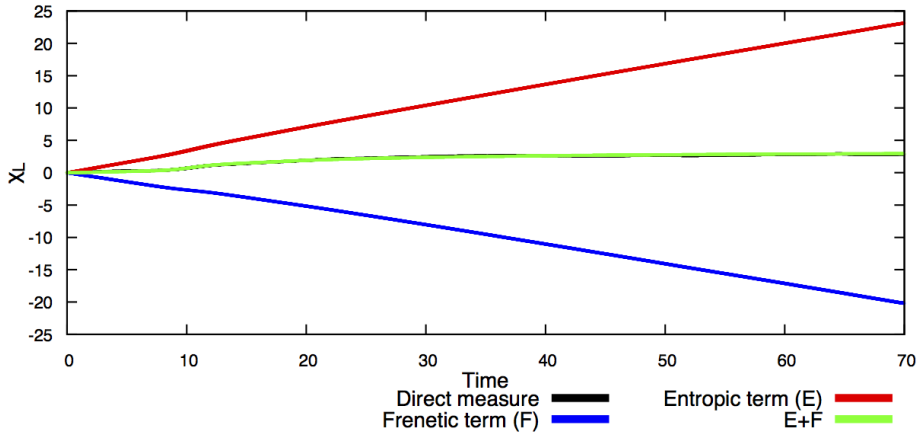
We can see that there is a good agreement between the susceptibility directly measured from the simulation and the form that we derived in sections 3.3 and 3.4, divided in symmetric and antisymmetric part: the frenetic (F) and the entropic part (E); since we are no longer in equilibrium, these contributions are both important to correctly reconstruct the susceptibility as it is clear from the figures in this section.

5.2.1 Susceptibility at different temperatures

The temperature of the thermal reservoirs has an effect on the susceptibility of our model. In order to show it, we have performed different simulations

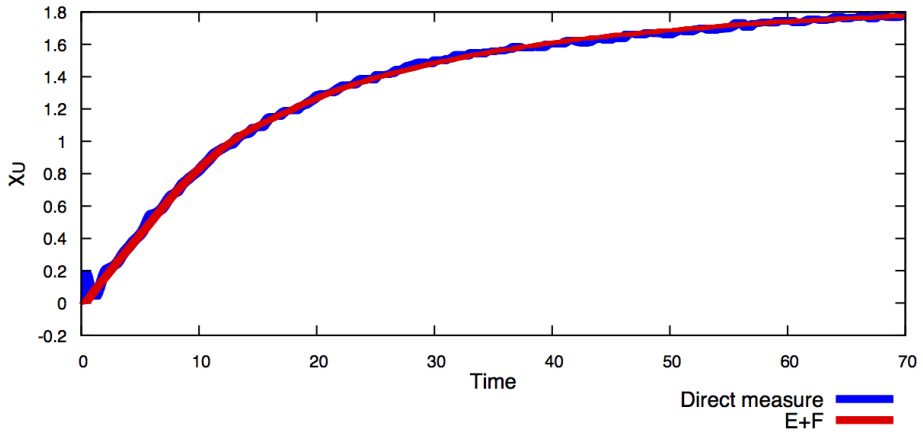


(a) Estimates of χ_L: direct measure and sum of the *frenetic* (F) and *entropic* (E) terms.

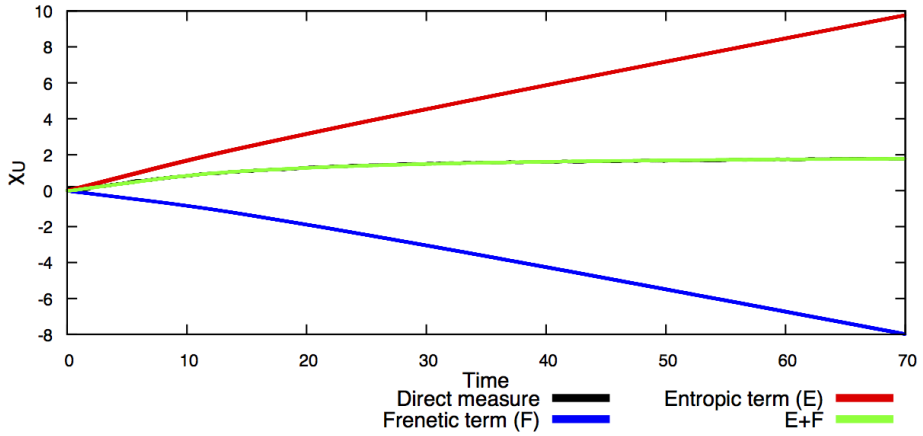


(b) *Frenetic* (F) and *entropic* (E) contributions to χ_L.

Figure 5.3: Susceptibility of the chain length to an increase of T_2 with error bars at one sigma.

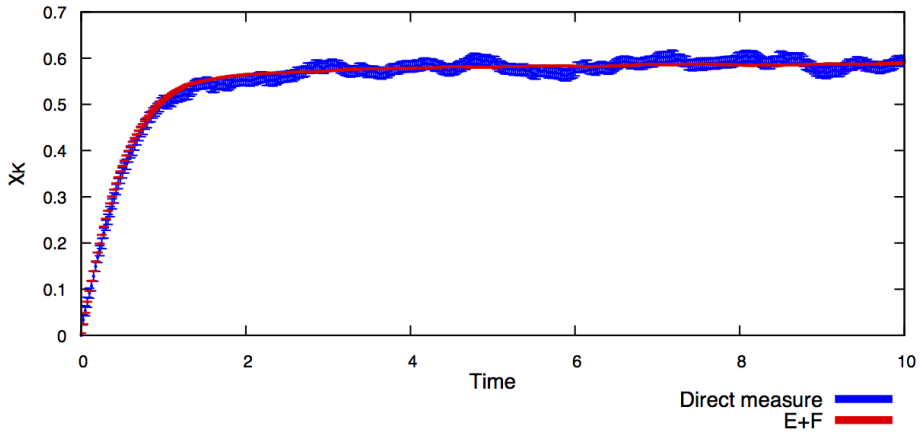


(a) Estimates of χ_U: direct measure and sum of the *frenetic* (F) and *entropic* (E) terms.

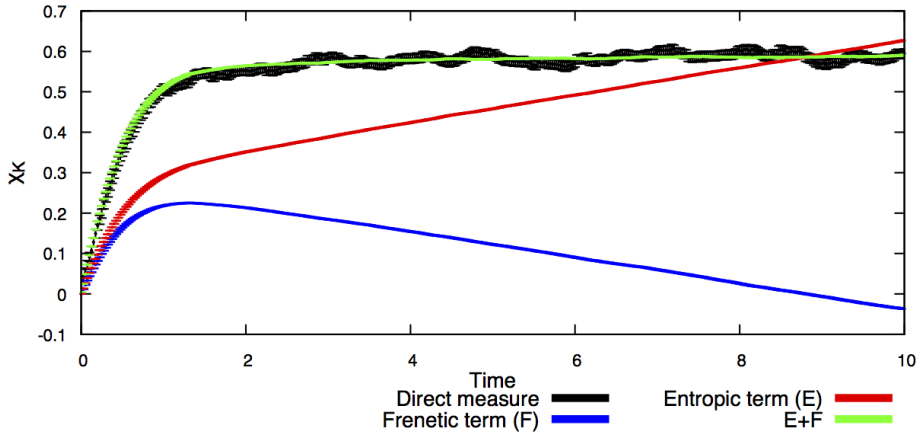


(b) *Frenetic* (F) and *entropic* (E) contributions to χ_U.

Figure 5.4: Susceptibility of the Fermi-Pasta-Ulam potential energy to an increase of T_2 with error bars at one sigma.



(a) Estimates of χ_K: direct measure and sum of the *frenetic* (F) and *entropic* (E) terms.



(b) *Frenetic* (F) and *entropic* (E) contributions to χ_K.

Figure 5.5: Susceptibility of the kinetic energy of the oscillators connected to thermal reservoir to an increase of T_2 with error bars at one sigma.

with the same parameters of table 5.2 and the following temperatures:

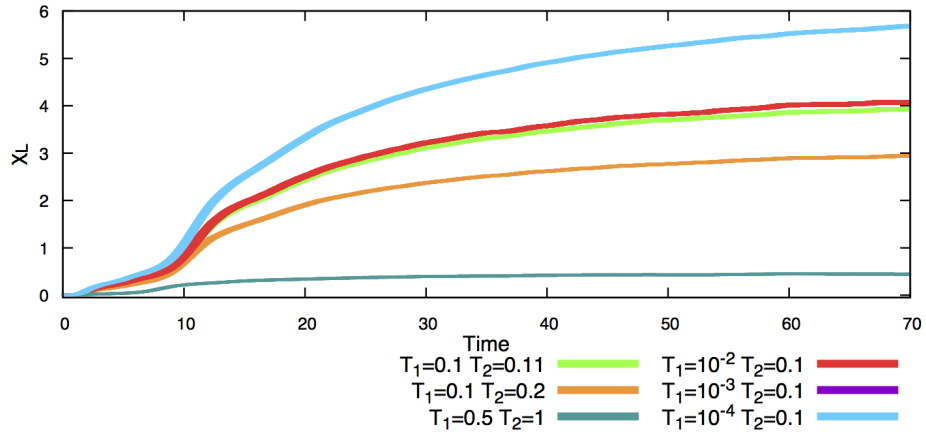
T_1	0.11	0.1	0.2	0.1	0.5	0.1	10^{-2}	0.1	10^{-3}	0.1	10^{-4}
T_2	0.1	0.11	0.1	0.2	1	10^{-2}	0.1	10^{-3}	0.1	10^{-4}	0.1

5.2.2 Moving farther from equilibrium

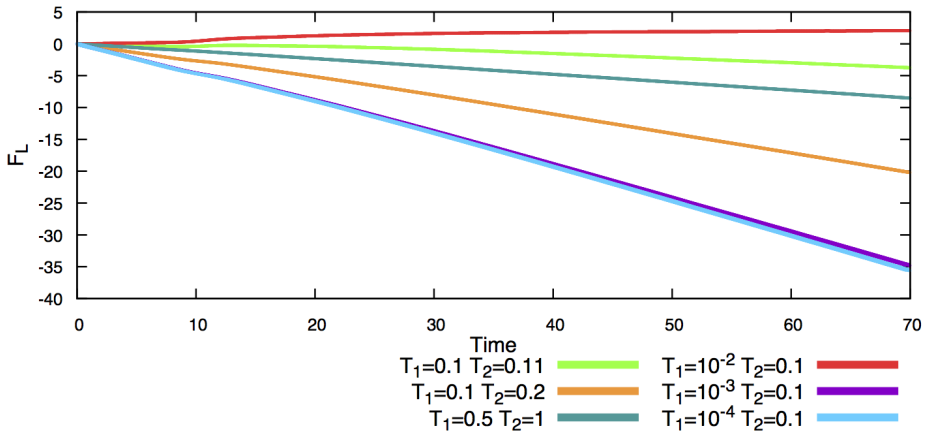
Let us consider how susceptibility is affected by a change of the thermostats' temperatures, while maintaining the perturbed thermostat (T_2) at a higher temperature than the other (T_1). We can see in figure 5.6 that, as we might expect, the farther we move from equilibrium the more susceptibility varies from its value at equilibrium.
We also note the model with $T_1 = 10^{-2}$ $T_2 = 0.1$ presents a positive frenetic and a small entropic term.

5.2.3 Inverting the heat flux

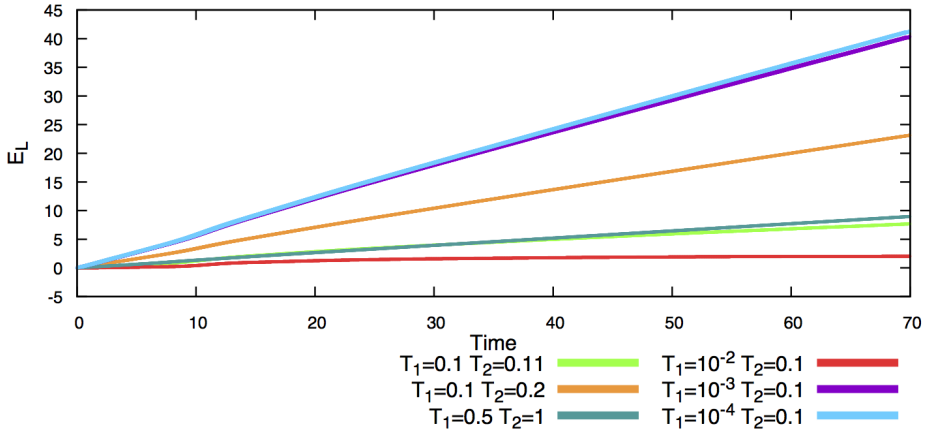
We are also interested in considering how the direction of the heat flux affects susceptibility at different temperatures by exchanging the temperatures in the two thermostats. We note that this has no significant effect in the two first cases, as we can see in figure 5.7, but this does not mean that the dynamics of the system is unaltered: in figure 5.8 we see that the entropic and frenetic terms are dramatically altered by the inversion of the heat flux.



(a) Susceptibility of the chain length to an increase of T_2.

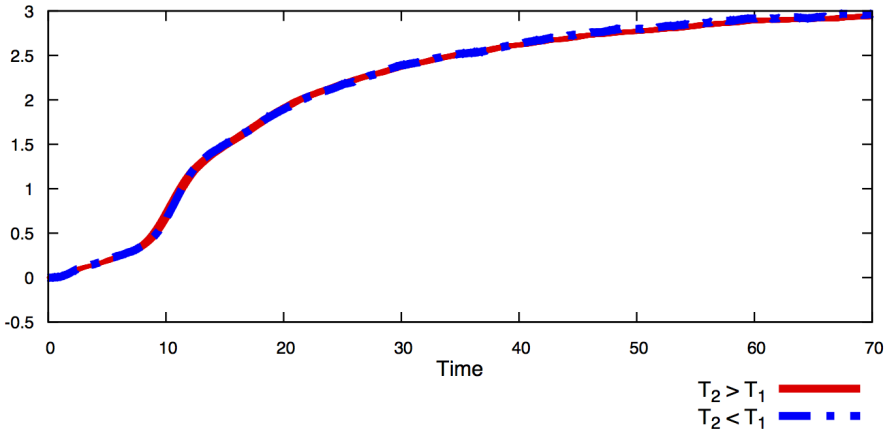


(b) Frenetic term of the susceptibility of the chain length to an increase of T_2.

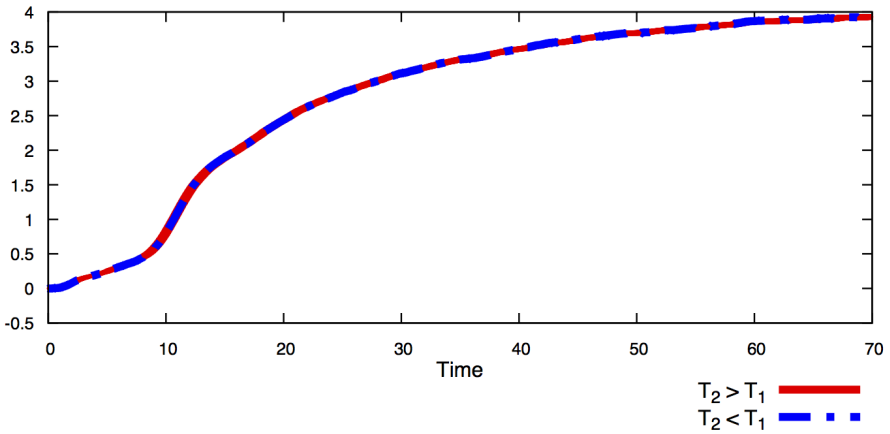


(c) Entropic term of the susceptibility of the chain length to an increase of T_2.

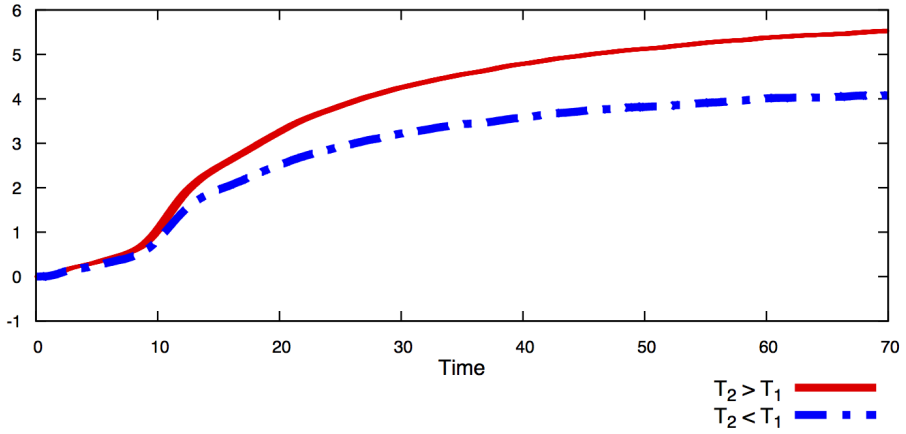
Figure 5.6: Susceptibility of the chain length to an increase of T_2 with error bars at one sigma in models with $T_2 > T_1$.



(a) One thermostat at $T = 0.1$, the other at $T = 0.2$.

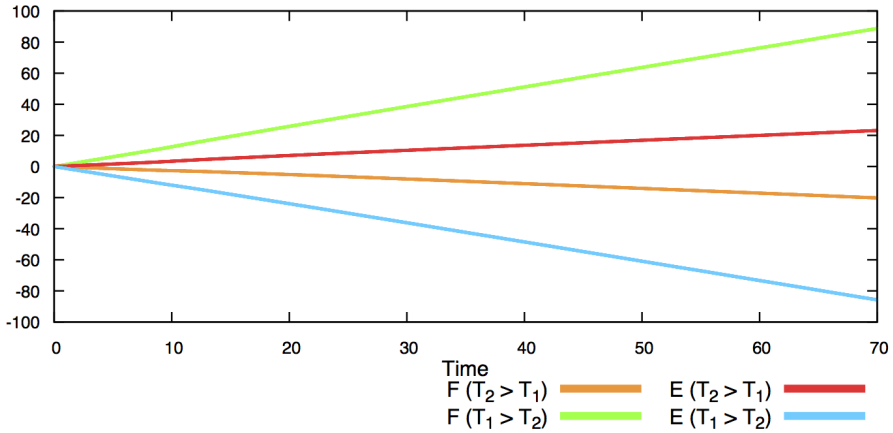


(b) One thermostat at $T = 0.1$, the other at $T = 0.11$.

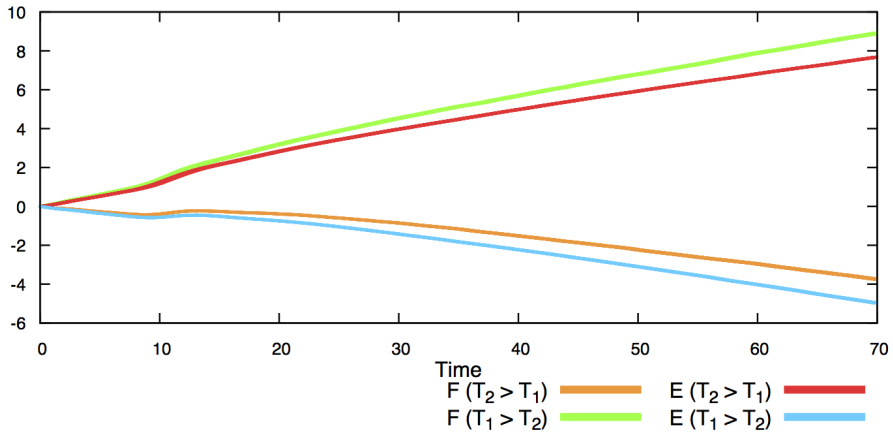


(c) One thermostat at $T = 0.1$, the other at $T = 10^{-3}$.

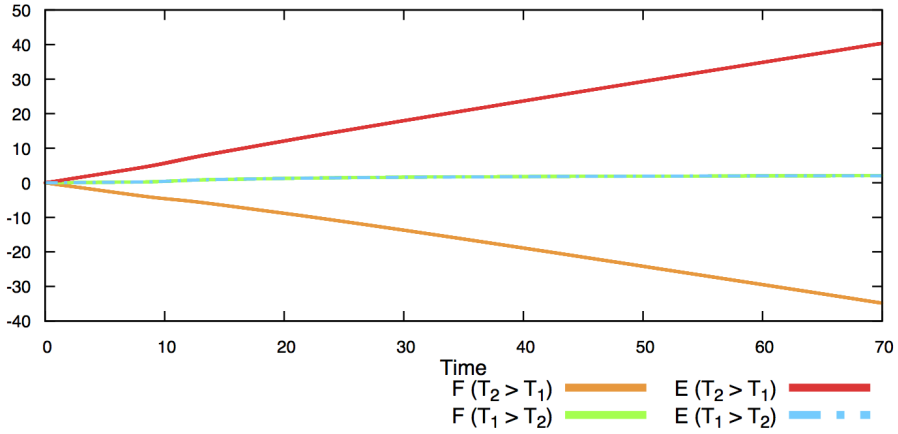
Figure 5.7: Susceptibility of the chain length to an increase of T_2 with error bars at one sigma in models both with $T_2 > T_1$ and $T_1 > T_2$.



(a) One thermostat at $T = 0.1$, the other at $T = 0.2$.



(b) One thermostat at $T = 0.1$, the other at $T = 0.11$.



(c) One thermostat at $T = 0.1$, the other at $T = 10^{-3}$.

Figure 5.8: Frenetic (F) and entropic (E) terms of the susceptibility of the chain length to an increase of T_2 ,with error bars at one sigma, in models both with $T_2 > T_1$ and $T_1 > T_2$.

Chapter 6

Conclusions

We have studied the linear response to a thermal perturbation of a conductive system driven out of equilibrium by an heat flux. By modeling the effects of the thermal reservoir with an algorithm based on Andersen thermostats [2] instead of explicit white noise terms, for the first time we obtain a fluctuation-response relation for thermal perturbations of a system with full Hamiltonian dynamics and operating out of equilibrium, thus extending previous results available only for systems evolving via overdamped stochastic equations or Markov jump processes [11].

Since for $t \to \infty$ the susceptibility of potential energy (χ_U) and length (χ_L) are generalizations of, respectively, the specific heat and the thermal expansion coefficient, we can see that they are not simply connected to a stationary correlation with the heat absorbed from the thermal reservoirs, as it is the case in equilibrium, but we have to also consider a non-dissipative, or frenetic, contribution.

As we remarked in section 3.1, the interaction between the oscillators in our system has a single minimum in order to simplify our study. It would be interesting to further study more complex interactions that have multiple minimum; this could be a road to the study of complex systems that present, out of equilibrium, a negative susceptivity [3, 44].

Resources

The code of the program can be found at `github.com/federicodambrosio/fpu-simulator`. This code is published under the free license BSD 3-Clause License (`opensource.org/licenses/BSD-3-Clause`).
The simulations in chapter 5 have been run on the last version of the code, on September 15th 2016.
The BOOST Libraries can be found at `boost.org`. The BOOST.Random library is currently being integrated into the C++ Standard Library.
Included in the code there is the RunningStats class file from John D. Cook's blog at `johndcook.com/blog/standard_deviation`.

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