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Thermodynamic uncertainty relation

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1 Introduction

In the last two decades a great effort has been made to describe microscopic system's dynamics through the use of stochastic mechanics for the reason that such kind of systems are mainly characterized by the presence of a non-negligible fluctuating component. Moreover, recent experimental achievement along with numerical computations give us the access to a plethora of data to be compared with theoretical results and this in turn of course stimulates the search for more results. In this sense stochastic mechanics has proved to be a comprehensive framework for the description of many systems that exhibit some sort of randomness. One of the most important areas in which this kind of approach finds a lot of applications is the one concerning biomolecular systems where one studies, for example, the dynamics of complicated objects such as proteins or DNA or alternatively active systems such as molecular motors. This is possible thanks to a coarse-graining process that involves the many degrees of freedom of the system (that is often too difficult to describe in every detail) thus obtaining a limited number of important parameters that are then used in the model. It was in this framework that the thermodynamic uncertainty principle made its first appearance, precisely in [1]. In fact, one of the main objectives of stochastic thermodynamics, as we will call stochastic mechanics when applied to biomolecules or systems in contact with a heat bath, is to find relations between meaningful observables such as entropy, diffusion coefficients or the production rate of a molecule in a chemical reaction. In the above mentioned article the uncertainty relation is found for continuous time Markov chains used to model biomolecular processes on an arbitrary discrete network. In this case it involves a generic observable and entropy production, namely

$$\left\langle \Delta R^2 \right\rangle_t \geq \frac{2k_B \left\langle R \right\rangle_t^2}{t\sigma} \tag{1.1}$$

where $\left\langle R \right\rangle_t$ and $\left\langle \Delta R^2 \right\rangle_t$ are respectively the average and the variance of the selected observable (in [1] only the number of consumed or produced molecules, or counting processes that count the number of jumps between two or more links of the network are considered as observables) and σ_t is the entropy production per unit time. Moreover, this result is valid for stationary states and near to equilibrium states. The physical significance of the thermodynamic uncertainty relation is more evident if we define

$$\epsilon_t^2 \equiv \frac{\left\langle \Delta R^2 \right\rangle_t}{\left\langle R \right\rangle_t^2} \tag{1.2}$$

that is a quantity that measures the precision associated to the observable X. In fact thanks to this it is possible to rewrite (1.1) as follows

$$\epsilon_t^2 \Sigma_t \geq 2k_B \tag{1.3}$$

where $\Sigma_t = t\sigma$ is the entropy produced up to time t. It is evident that if we want to obtain a higher precision (namely a smaller ϵ_t^2) we might have to rise up the entropy production (in a way that (1.3) is satisfied). In other words (1.3) gives us informations about the cost of the precision of the system's dynamics.

Another similar result has been obtained in [2] where, differently from the previous article, the thermodynamic uncertainty relation has been obtained thanks to large deviations theory.

The main limit of this kind of relation is that it is valid only for stationary states and hence the subsequent works have mainly focused on extending this result to transient times and pure nonequilibrium states. A first approach to this more general setting can be found in [3] and [4] but this time the thermodynamic uncertainty relation is discussed also for general Langevin systems. More specifically, the authors consider systems with an arbitrary number of degrees of freedom for which it is possible to write the following set of coupled stochastic differential equations

$$\dot{\mathbf{x}}(t) = \frac{d\mathbf{x}(t)}{dt} = \mathbf{A}(x(t), t) + \sqrt{2}\mathbf{G}(x(t), t) \cdot \xi(\mathbf{t}) \tag{1.4}$$

where $\mathbf{A}(x(t), t)$ is the drift vector and $\mathbf{G}(x(t), t)$ is the diffusion matrix. As for $\xi(\mathbf{t})$, it is the Gaussian white noise vector which is the source of randomness. In this case the issue is faced tanks to a path integral approach and linear response theory. In fact, the crucial point of the paper is where the system is perturbed by modifying the drift vector in the following way

$$\widetilde{\mathbf{A}}\left(x\left(t\right),t\right)=\mathbf{A}\left(x\left(t\right),t\right)+\alpha\mathbf{y}\left(x\left(t\right),t\right) \tag{1.5}$$

where α is a small perturbation parameter and $\mathbf{y}\left(x\left(t\right),t\right)$ is an arbitrary vector. This leads to a modified probability density function for the considered degrees of freedom

$$P\left(\mathbf{x}\left(t\right),t\right)\qquad\Longrightarrow\qquad P^{\alpha}\left(\mathbf{x}\left(t\right),t\right) \tag{1.6}$$

from which, as we will see in the next section, it is possible to show that, for sufficiently small α, the following inequality holds

$$2\big\langle\Delta R^2\big\rangle_t\geq\frac{\Big(\big\langle R\big\rangle_t^{\alpha}-\big\langle R\big\rangle_t\Big)^2}{C\left(t\right)} \tag{1.7}$$

where the $\langle\cdot\rangle^{\alpha}$ stands for the average taken with respect to the modified probability density function and $C\left(t\right)$ is the cost function defined as follows (using $\mathbf{B}\left(x\left(t\right),t\right)=\mathbf{G}\left(x\left(t\right),t\right)\cdot\mathbf{G}\left(x\left(t\right),t\right)$)

$$C_y\left(t\right)=\frac{\alpha^2}{4}\int_0^t ds\big\langle\mathbf{y}\mathbf{B}^{-1}\mathbf{y}\big\rangle_s \tag{1.8}$$

In (1.7), $R\left(x,t\right)$ is an observable, for example an integrated current (this last condition is not necessary but useful as we will see soon). Moreover we know that it is possible to associate to the set of Langevin equations (1.4) a set of Fokker-Planck equations, namely

$$\begin{aligned}\partial_t P\left(\mathbf{x}\left(t\right),t\right)&=-\nabla\mathbf{J}\left(\mathbf{x}\left(t\right),t\right)\\ \mathbf{J}\left(\mathbf{x}\left(t\right),t\right)&=\big(\mathbf{A}\left(\mathbf{x}\left(t\right),t\right)-\nabla\mathbf{B}\left(\mathbf{x}\left(t\right),t\right)\big)P\left(\mathbf{x}\left(t\right),t\right)\end{aligned} \tag{1.9}$$

hence identifying $\mathbf{J}\left(\mathbf{x}\left(t\right),t\right)$ with a probability current. At this point if we chose

$$\bar{\mathbf{y}}\left(\mathbf{x}\left(t\right),t\right)=\frac{\mathbf{J}\left(\mathbf{x}\left(t\right),t\right)}{P\left(\mathbf{x}\left(t\right),t\right)} \tag{1.10}$$

that is a velocity in probability space we get that

$$C_{\bar{y}}\left(t\right)=\frac{\alpha^2}{4}\int_0^t ds\big\langle\bar{\mathbf{y}}\mathbf{B}^{-1}\bar{\mathbf{y}}\big\rangle_s=\frac{\alpha^2}{4}\int_0^t ds\Big\langle\frac{\mathbf{J}\mathbf{B}^{-1}\mathbf{J}}{P^2}\Big\rangle_s=\frac{\alpha^2}{4}\big\langle\Sigma\big\rangle_t \tag{1.11}$$

namely the cost function (for this particular perturbation) can be intrpreted as an object proportional to the entropy production $\big\langle\Sigma\big\rangle_t$. It is moreover possible to show that (1.7) can be rewritten as

$$\big\langle\Delta R^2\big\rangle_t\geq\frac{2\left(t\big\langle\dot{R}\big\rangle_t\right)^2}{\big\langle\Sigma\big\rangle_t} \tag{1.12}$$

where $\big\langle\dot{R}\big\rangle_t=\frac{\partial}{\partial t}\big\langle R\big\rangle_t$, and if $R\left(x,t\right)$ is an integrated current then $\big\langle\dot{R}\big\rangle_t$ is the averaged current. However, it must be pointed out that this result is only valid for systems whose Langevin equations have coefficients that havo no explicit time dependence.

We see that (1.12) can be compared to (1.1), in fact in [1] they considered only observables for which, at steady states, it is possible to write

$$\big\langle R\big\rangle_t=t\big\langle j\big\rangle \tag{1.13}$$

whith $\big\langle j\big\rangle$ a current independent of time. Remembering that we defined $t\sigma=\Sigma_t$ equation (1.1) can be rewritten as

$$\big\langle\Delta R^2\big\rangle_t\geq\frac{2k_B\left(t\langle j\rangle\right)^2}{\Sigma_t} \tag{1.14}$$

In conclusion if we make the following matches

$$\big\langle\dot{R}\big\rangle_t\Leftrightarrow t\big\langle j\big\rangle\qquad\qquad\big\langle\Sigma\big\rangle_t\Leftrightarrow\frac{\Sigma_t}{k_B} \tag{1.15}$$

we recognize the same analytical structure between (1.12) and (1.14). But we must remember that the last derivation shown here was applied to Langevin systems that can be in a purely non-equilibrium state while the first approach we discussed is plausible for jump processes in a steady state. Nevertheless these similarities have suggested that the thermodynamic uncertainty relation can be obtained with a more general approach independent of the particular process that is being considered: again Dechant and Sasa in the latest version of [4] came up with a solution, that is just to characterise the processes by their probability density function. Indeed, in total generality we can define a probability measure on a probability space $\omega \in \Omega$ that is

$$\int d\mathbb{P} = \int_{\Omega} d\omega P(\omega, t) = 1 \qquad\qquad \langle R \rangle_t = \int_{\Omega} d\omega P(\omega, t) R(\omega) \tag{1.16}$$

where $R(\omega)$ is again a generic observable. At this point, as already done before and in the spirit of linear response theory we imagine to slightly perturb the system and the perturbation to be dependent of a small perturbation parameter α so to obtain a new probability density function $P^{\alpha}(\omega, t)$. We stress that the perturbation can either be a physically one or a virtual one. By doing so we can define the Kullback-Leibler divergence, an object that has a crucial importance in this thesis

$$\mathbb{H}_t(P^{\alpha}|P) = \int_{\omega} d\omega P^{\alpha}(\omega, t) \ln\left[\frac{P^{\alpha}(\omega, t)}{P(\omega, t)}\right] \tag{1.17}$$

The latter is usually handled in information theory and indeed it encodes the information on how different $P^{\alpha}(\omega, t)$ and $P(\omega, t)$ are. Moreover we stress that this quantity can be canclulated for two arbitrary probability measures under very weak assumptions. With this it is possible to obtain the following result

$$2\langle \Delta R^2 \rangle_t \geq \frac{\left(\langle R \rangle_t^{\alpha} - \langle R \rangle_t\right)^2}{\mathbb{H}_t(P^{\alpha}|P)} \tag{1.18}$$

that has again an identical form as (1.7). We can hence say that for a Langevin system with a Gaussian white noise the Kullback-Leibler divergence is nothing else than the cost function $C(t)$. We have also seen that by chosing a particular perturbation (see equation (1.10)) the cost becomes proportional to the perturbation parameter α squared and the average entropy production $\langle \Sigma \rangle_t$, hence suggesting that for a given system one must calculate the Kullback-Leibler divergence and then choose a suitable perturbation to obtain the entropy production. This is what was done in [4] for both Langevin systems with Gaussian white noise (showing that it is the same as (1.7)) and jump processes.
Instead, in this thesis, we calculate some explicit inequalities coming from (1.18), not necessarily aiming to obtain an entropic interpretation of the Kullback-Leibler divergence but eventually relating it to some others observables. We will also re-derive equation (1.18) in a different way with respect to Dechant and Sasa in [4]. Moreover the non-equilibrium inequalities that we obtain in this thesis, compared to thermodynamic relations involving entropy production, involve cost functions that are more rooted in the time-symmetric activations of the system. These functions care of how agitated the system is rather than of how it is dissipating. For example, a measure of agitation for discrete systems is the mean number of jumps per unit time. This is clearly not a measure of dissipation, it is more a quantification of the mean level of activity in the system. Concerning Langevin systems instead, a connection to other observables is more difficult. What we have done in this case was to provide an explicit formula for the Kullback-Leibler divergence for Markov and non-Markov Brownian systems with dissipation, external force and Gaussian noise (white and coloured) in one dimension. Moreover, choosing as observable $R = x$, namely position, we obtain some interesting plots that give us information about the system's dynamics. It should be underlined that all the results obtained in this thesis are valid also for pure non-equilibrium.

2 Preliminaries

In this section we show two possible derivations of the thermodynamic uncertainty relation valid from equilibrium to pure non-equilibrium. The first one which can be found in [3] is valid, as already said in the introduction, only for Langevin systems whith Gaussian white noise while the second one is appliable to every system for which it is possible to define a probability measure. The reason why we show the first one is that some strategies used in the proof whill be systematically used throughout the wole thesis. Actually as for the second derivation we will only obtain a non-equilibrium inequality that with further work can eventually lead to the thermodynamic uncertainty relation. Neverthless this last approach is the basis from which all the results of this thesis will be obtained.

2.1 First proof

As already said, we consider a system obeying the following set of coupled stochastic differential equations

$$\dot{\mathbf{x}}(t) = \frac{d\mathbf{x}(t)}{dt} = \mathbf{A}(x(t), t) + \sqrt{2}\mathbf{G}(x(t), t) \cdot \xi(\mathbf{t}) \tag{2.1}$$

Here $A(x(t), t)$ stands for the drift vector, $G(x(t), t,)$ is the diffusion matrix (of dimension $d \times d$) and ξ is the Gaussian white noise vector, which is the source of randomness. The vector components have the following features

$$\langle \xi_\alpha(t) \rangle = 0 \qquad\qquad \langle \xi_\alpha(t)\, \xi_\beta(s) \rangle = \delta_{\alpha,\beta}\delta(t-s) \tag{2.2}$$

with all higher order expected values equal to 0. The characteristic of ξ of being delta correlated makes the dynamic Markovian, in this specific case having an uncountable state space.
The notation "$\dot{x}(t)$" in equation (2.1) is a formal writing which is easy to remember and pleasant to see but sometimes, as in this case, it is more convenient to write it in incremental form

$$d\mathbf{x}(t) = x_{\alpha,i+1} - x_{\alpha,i} = A_{\alpha,i}(x_i)\, h + \sqrt{2}G(x_i)_{\alpha,\beta,i}\, \xi_{\beta,i}\sqrt{h} \tag{2.3}$$

where the time interval in which we are interested $[0, T]$ has been divided into N small intervals such that $dt = h = \frac{T}{N}$, $t = ih$ and greek letters stand for vector and matrix components (the number of dimension is set to d). Same indices are, as always, meant in Einstein notation. The components $\xi_{\alpha,i}$ again obey $\langle \xi_{\alpha,i} \rangle = 0$ and $\langle \xi_{\alpha,i}\xi_{\beta,j} \rangle = \delta_{\alpha,\beta}\delta_{i,j}$.
We now follow [5], performing the same reasoning but in an arbitrary number of dimensions. We consider the joint probability density functional for the vector $\mathbf{x}(t)$ which can be written as

$$P(\mathbf{x}|\xi, \mathbf{x_0}) = \prod_{i,\alpha}^{N} \delta\left(x_{\alpha,i+1} - x_{\alpha,i} - A_{\alpha,i}(x_i)\, h - \sqrt{2}G(x_i)_{\alpha,\beta,i}\, \xi_{\beta,i}\sqrt{h} - x_{\alpha,0}\delta_{i,0}\right) \tag{2.4}$$

Instead, we are more interested in

$$P(\mathbf{x}|\mathbf{x}_0) = \int d\xi \rho(\xi)\, P(\mathbf{x}|\xi, \mathbf{x_0}) \tag{2.5}$$

which is the joint probability functional where we have integrated out the noise. In other words, we are considering the mean value with respect all possible realizations of ξ. To compute $P(\mathbf{x}|\mathbf{x}_0)$ we recall the Fourier representation of the Dirac delta

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx} dk \tag{2.6}$$

and hence we can rewrite equation (2.4) in the following way

$$P(\mathbf{x}|\xi, \mathbf{x}_0) = \prod_{i,\alpha}^{N,d} \int \frac{dk_{\alpha,i}}{2\pi} \exp\Big[-ik_{\alpha,i}\Big(x_{\alpha,i+1} - x_{\alpha,i} - A_{\alpha,i}(x_i)\, h - \sqrt{2}G(x_i)_{\alpha,\beta,i}\, \xi_{\beta,i}\sqrt{h} - x_{\alpha,0}\delta_{i,0}\Big)\Big] \tag{2.7}$$

To integrate over all possible realizations of $\xi(t)$ we must also consider the probability density function $p(\xi_i)$, which we know must be Gaussian

$$p(\xi_{\alpha,i}) = \frac{1}{\sqrt{2\pi}} \exp\left[-\xi_{\alpha,i}^2/2\right] \tag{2.8}$$

Hence, we finally obtain

$$\begin{gathered} P(\mathbf{x}|\mathbf{x}_0) = \int P(\mathbf{x}|\xi, \mathbf{x_0}) \prod_{i,\alpha}^{N,d} p(\xi_{\alpha,i})\, d\xi_{\alpha,i} = \\ \prod_{i,\alpha}^{N,d} \int \frac{d\xi_{\alpha,i}}{\sqrt{2\pi}} \int \frac{dk_{\alpha,i}}{2\pi} \exp\Big[-ik_{\alpha,i}\Big(x_{\alpha,i+1} - x_{\alpha,i} - A_{\alpha,i}(x_i)\, h + \\ -\sqrt{2} G(x_i)_{\alpha,\beta,i}\, \xi_{\beta,i} \sqrt{h} - x_{\alpha,0}\delta_{i,0}\Big) - \frac{1}{2}\sum_{\beta} \xi_{\alpha,i}\xi_{\beta,i}\delta_{\alpha,\beta}\Big] \end{gathered} \tag{2.9}$$

By using the well known rules of Gaussian integration we get rid of the ξ dependence

$$\begin{gathered} P(\mathbf{x}|\mathbf{x}_0) = \prod_{i,\alpha}^{N,d} \int \frac{dk_{\alpha,i}}{2\pi} \exp\Big[-ihk_{\alpha,i}\Big(\frac{x_{\alpha,i+1} - x_{\alpha,i}}{h} - A_{\alpha,i}(x_i) - \frac{x_{\alpha,0}\delta_{i,0}}{h}\Big) + \\ - h\sum_{\beta,\gamma} k_{\alpha,i} G(x_i)_{\alpha,\beta,i}\, G(x_i)_{\beta,\gamma,i}\, k_{\gamma,i}\Big] \end{gathered} \tag{2.10}$$

We now set

$$\begin{gathered} \Delta_{\alpha,i} = \frac{x_{\alpha,i+1} - x_{\alpha,i}}{h} - A_{\alpha,i}(x_i) - \frac{x_{\alpha,0}\delta_{i,0}}{h} \\ B_{\alpha,\gamma,i} = \sum_{\beta} G(x_i)_{\alpha,\beta,i}\, G(x_i)_{\beta,\gamma,i} \end{gathered}$$

By completing the square in equation (2.10) and using the notation above

$$\begin{gathered} P(\mathbf{x}|\mathbf{x}_0) = \prod_{i,\alpha}^{N,d} \int \frac{dk_{\alpha,i}}{2\pi} \exp\Big[-ihk_{\alpha,i}\Delta_{\alpha,i} - h\sum_{\gamma} k_{\alpha,i}B_{\alpha,\gamma,i}k_{\gamma,i}\Big] = \\ \mathbf{Z}^{-1} \prod_{i} \exp\left[-\frac{h}{4}\sum_{\alpha,\beta} \Delta_{\alpha,i}\left(B^{-1}\right)_{\alpha,\beta,i} \Delta_{\beta,i}\right] \end{gathered} \tag{2.11}$$

where again we used Gaussian integration. Moreover we note that

$$\mathbf{Z} \propto \prod_i \left(\det B_{\alpha,\beta,i}\right)^{-\frac{1}{2}}$$

is independent of $A_{\alpha,i}(x_i)$.

We now return to the continuum notation by changing sums into integrals and noting that $\dot{\mathbf{x}}(t) = \lim_{h\to 0} \frac{x_{\alpha,i+1} - x_{\alpha,i}}{h}$ and $\delta(t - t_0) = \lim_{h\to 0} \frac{\delta_{i,0}}{h}$. The probability density function thus becomes (using matrix notation)

$$\begin{gathered} P(\mathbf{x}|\mathbf{x}_0) = \exp\Big[-\frac{1}{4}\int_0^T \Big[\Big(\dot{\mathbf{x}}(t) - \mathbf{A}(x(t), t) - \mathbf{x}(0)\,\delta(t - t_0)\Big)\left(\mathbf{B}^{-1}\right)(x(t), t)\, \cdot \\ \cdot\Big(\dot{\mathbf{x}}(t) - \mathbf{A}(x(t), t) - \mathbf{x}(0)\,\delta(t - t_0)\Big)\Big] dt\Big] \cdot \mathbf{Z}^{-1}\Big(\mathbf{B}(x(t), t), x(t), t\Big) \end{gathered} \tag{2.12}$$

Using a notation borrowed from field theory we have

$$\int \mathcal{D}[\mathbf{x}(t)]\, P(\mathbf{x}|\mathbf{x}_0) = 1 \qquad\qquad \langle R(\mathbf{x}(t), t)\rangle \int \mathcal{D}[\mathbf{x}(t)]\, R(\mathbf{x}(t), t)\, P(\mathbf{x}|\mathbf{x}_0) \tag{2.13}$$

where $R(\mathbf{x}(t), t)$ is a generic observable, this notation will be useful in short.
From now on we follow [3] and set $\mathbf{x}(0) = 0$ for simplicity. Let us consider the scaled cumulant generating function which is well known to be

$$\mathcal{K}_Q(h,T) = \frac{1}{T} \ln \left\langle \exp\left[h \int_0^T \dot{Q}(t)\, dt \right] \right\rangle \tag{2.14}$$

where $\dot{Q}(t)$ is a generalized current defined via the Stratonovich product

$$\dot{Q}(t) = \Omega(\mathbf{x}(t), t) \circ \dot{\mathbf{x}}(t) \tag{2.15}$$

where $\Omega(\mathbf{x}(t), t)$ is a function of coordinates and time and $\dot{\mathbf{x}}(t)$ is the same of equation (2.1). Writing equation (2.14) more explicitly

$$\begin{aligned} \mathcal{K}_Q(h,T) = \frac{1}{T} \ln \int \mathcal{D}[\mathbf{x}(t)] \exp\Bigg[h \int_0^T \dot{Q}(t)\, dt - \frac{1}{4} \int_0^T \bigg[\Big(\dot{\mathbf{x}}(t) - \mathbf{A}(x(t), t) \Big) \cdot \\ \cdot \mathbf{B}^{-1}(x(t), t) \Big(\dot{\mathbf{x}}(t) - \mathbf{A}(x(t), t) \Big) \bigg] dt \Bigg] \cdot \mathbf{Z}^{-1}\Big(\mathbf{B}(x(t), t), x(t), t \Big) \end{aligned} \tag{2.16}$$

that can be equivalently written as

$$\begin{aligned} \mathcal{K}_Q(h,T) = \frac{1}{T} \ln \int \mathcal{D}[\mathbf{x}(t)] \exp\Bigg[h \int_0^T \dot{Q}(t)\, dt + \\ + \int_0^T \bigg[-\frac{1}{4} \Big(\dot{\mathbf{x}}(t) - \mathbf{A}(x(t), t) - \mathbf{Y}(x(t), t) \Big) \mathbf{B}^{-1}(x(t), t) \cdot \\ \cdot \Big(\dot{\mathbf{x}}(t) - \mathbf{A}\big((x(t), t) - \mathbf{Y}(x(t), t) \Big) - \frac{1}{4} \mathbf{Y}(x(t), t) \mathbf{B}^{-1}(x(t), t) \mathbf{Y}(x(t), t) + \\ + \frac{1}{2} \mathbf{Y}\big(x(t), t\big) \mathbf{B}^{-1}\Big(x(t), t \Big(\dot{\mathbf{x}}(t) - \mathbf{A}(x(t), t) - \mathbf{Y}(x(t), t) \Big) \bigg] dt \Bigg] \\ \cdot \mathbf{Z}^{-1}\Big(\mathbf{B}(x(t), t), x(t), t \Big) \end{aligned} \tag{2.17}$$

where $\mathbf{Y}(x(t), t)$ is a vector function throught which we imagine to perturb the drift vector $\mathbf{A}(x(t), t)$ and that will be discussed better later. We note that

$$\begin{aligned} P^Y(\mathbf{x}|\mathbf{x}_0) = \exp\Bigg[-\frac{1}{4} \int_0^T \big[(\dot{\mathbf{x}}(t) - \mathbf{A}(x(t), t) - \mathbf{Y}(x(t), t)) \left(\mathbf{B}^{-1} \right)(x(t), t) \cdot \\ \cdot (\dot{\mathbf{x}}(t) - \mathbf{A}(x(t), t) - \mathbf{Y}(x(t), t)) \big] dt \Bigg] \cdot \mathbf{Z}^{-1}(\mathbf{B}(x(t), t), x(t), t) \end{aligned} \tag{2.18}$$

corresponds to the probability density function obtained from the perturbed Langevin equation

$$\dot{\mathbf{x}}(t) = \widetilde{\mathbf{A}}(x(t), t) + \sqrt{2}\mathbf{G}(x(t), t) \cdot \xi(t) \tag{2.19}$$

with $\widetilde{\mathbf{A}}(x(t), t) = \mathbf{A}(x(t), t) + \mathbf{Y}(x(t), t)$. Furthermore we stress that being Z independent of $\mathbf{A}(x(t), t)$ the perturbation does not change this term. The scaled cumulant generating function thus becomes

$$\begin{aligned} \mathcal{K}_Q(h,T) = \frac{1}{T} \ln \int \mathcal{D}[\mathbf{x}(t)] P^Y(\mathbf{x}|\mathbf{x}_0) \exp\Bigg[h \int_0^T \dot{Q}(t)\, dt + \\ + \int_0^T \bigg[-\frac{1}{4} \mathbf{Y}(x(t), t) \mathbf{B}^{-1}(x(t), t) \mathbf{Y}(x(t), t) + \\ + \frac{1}{2} \mathbf{Y}\big(x(t), t\big) \mathbf{B}^{-1}(x(t), t) \Big(\dot{\mathbf{x}}(t) - \mathbf{A}(x(t), t) - \mathbf{Y}(x(t), t) \Big) \bigg] dt \Bigg] \end{aligned} \tag{2.20}$$

The following term

$$\frac{1}{2}\mathbf{Y}\left(x\left(t\right),t\right)\mathbf{B}^{-1}\left(x\left(t\right),t\right)\Big(\dot{\mathbf{x}}\left(t\right)-\mathbf{A}\left(x\left(t\right),t\right)-\mathbf{Y}\left(x\left(t\right),t\right)\Big)=\frac{1}{\sqrt{2}}\mathbf{Y}\left(x\left(t\right),t\right)\mathbf{G}^{-1}\left(x\left(t\right),t\right)\cdot\xi\left(t\right) \tag{2.21}$$

averages to zero because of its is proportionality to $\xi\left(t\right)$. We now use Jensen inequality which states that $\langle e^{x}\rangle\geq e^{\langle x\rangle}$ so that we can get a lower bound for the scaled cumulant generating function

$$\begin{gathered}\mathcal{K}_{Q}\left(h,T\right)=\frac{1}{T}\ln\int\mathcal{D}\left[\mathbf{x}\left(t\right)\right]P^{Y}\left(\mathbf{x}|\mathbf{x}_{0}\right)\exp\Bigg[h\int_{0}^{T}\dot{Q}\left(t\right)dt+\\ +\int_{0}^{T}\left[-\frac{1}{4}\mathbf{Y}\left(x\left(t\right),t\right)\mathbf{B}^{-1}\left(x\left(t\right),t\right)\mathbf{Y}\left(x\left(t\right),t\right)\right]\Bigg]\geq\\ \frac{1}{T}\int\mathcal{D}\left[\mathbf{x}\left(t\right)\right]P^{Y}\left(\mathbf{x}|\mathbf{x}_{0}\right)\left[\int_{0}^{T}\left[h\dot{Q}\left(t\right)t-\frac{1}{4}\mathbf{Y}\left(x\left(t\right),t\right)\mathbf{B}^{-1}\left(x\left(t\right),t\right)\mathbf{Y}\left(x\left(t\right),t\right)\right]dt\right]=\\ \frac{1}{T}\left[h\int_{0}^{T}\langle\dot{Q}\left(t\right)\rangle^{Y}dt-\frac{1}{4}\int_{0}^{T}\langle\mathbf{Y}\left(x\left(t\right),t\right)\mathbf{B}^{-1}\left(x\left(t\right),t\right)\mathbf{Y}\left(x\left(t\right),t\right)\rangle^{Y}dt\right]\end{gathered} \tag{2.22}$$

Let us open a brief parenthesis about equation (2.1). It is known that we can equivalently solve the problem using the Fokker-Plank equations

$$\begin{gathered}\partial_{t}P\left(\mathbf{x}\left(t\right),t\right)=-\nabla\mathbf{J}\left(\mathbf{x}\left(t\right),t\right)\\ \mathbf{J}\left(\mathbf{x}\left(t\right),t\right)=\big(\mathbf{A}\left(\mathbf{x}\left(t\right),t\right)-\nabla\mathbf{B}\left(\mathbf{x}\left(t\right),t\right)\big)P\left(\mathbf{x}\left(t\right),t\right)\end{gathered} \tag{2.23}$$

In the modified dynamics they become

$$\begin{gathered}\partial_{t}P^{Y}\left(\mathbf{x}\left(t\right),t\right)=-\nabla\mathbf{J}^{Y}\left(\mathbf{x}\left(t\right),t\right)\\ \mathbf{J}^{Y}\left(\mathbf{x}\left(t\right),t\right)=\big(\mathbf{A}\left(\mathbf{x}\left(t\right),t\right)+\mathbf{Y}\left(\mathbf{x}\left(t\right),t\right)-\nabla\mathbf{B}\left(\mathbf{x}\left(t\right),t\right)\big)P\left(\mathbf{x}\left(t\right),t\right)\end{gathered} \tag{2.24}$$

We hence identify $\mathbf{J}\left(x\left(t\right),t\right)$ as a probability current that obeys a continuity equation. Moreover, from now on we assume that $\mathbf{A}\left(\mathbf{x}\left(t\right),t\right)$ and $\mathbf{B}\left(\mathbf{x}\left(t\right),t\right)$ have no explicit time dependence. In this case, by choosing

$$\mathbf{Y}\left(\mathbf{x}\left(t\right),t\right)=\alpha\frac{\mathbf{J}\left(\mathbf{x}\left(t\right),\left(1+\alpha\right)t\right)}{P\left(\mathbf{x}\left(t\right),\left(1+\alpha\right)t\right)} \tag{2.25}$$

we have that

$$P^{Y}\left(\mathbf{x}\left(t\right),t\right)=P\left(\mathbf{x}\left(t\right),\left(1+\alpha\right)t\right)\qquad\qquad\mathbf{J}^{Y}\left(\mathbf{x}\left(t\right),t\right)=\mathbf{J}\left(\mathbf{x}\left(t\right),\left(1+\alpha\right)t\right) \tag{2.26}$$

obey equations (2.24) as one can easily check by using the hypothesis of non-explicit time dependence of $\mathbf{A}\left(\mathbf{x}\left(t\right),t\right)$ and $\mathbf{B}\left(\mathbf{x}\left(t\right),t\right)$. Now we evaluate the expected values of equation (2.22) (we will now call $P\left(\mathbf{x}|\mathbf{x}_{0}\right)=P\left(\mathbf{x}\left(t\right),t\right)$ implying the initial conditions), for the first one we have

$$\begin{gathered}h\int_{0}^{T}\langle\dot{Q}\left(t\right)\rangle^{Y}dt=h\int_{0}^{T}dt\int\mathcal{D}\left[\mathbf{x}\left(t\right)\right]P^{Y}\left(\mathbf{x}\left(t\right),t\right)\dot{Q}\left(t\right)=\\ h\int_{0}^{T}dt\int\mathcal{D}\left[\mathbf{x}\left(t\right)\right]P\left(\mathbf{x}\left(t\right),\left(1+\alpha\right)t\right)\frac{dQ}{dt}\left(t\right)=\\ h\int_{0}^{\left(1+\alpha\right)T}\frac{dt}{\left(1+\alpha\right)}\int\mathcal{D}\left[\mathbf{x}\left(t\right)\right]P\left(\mathbf{x}\left(t\right),t\right)\frac{\left(1+\alpha\right)dQ}{dt}\left(t\right)=\\ h\langle Q\rangle\left(\left(1+\alpha\right)T\right).\end{gathered} \tag{2.27}$$

where in the third line we made a change of variable $t'=\left(1+\alpha\right)t$ and then we relabelled the new variable $t'=t$. As for the second piece we recognise the cost function $C\left(t\right)$ (see equation (1.8)) for which it holds that

$$\begin{gathered}C\left(t\right)=\frac{1}{4}\int_{0}^{T}\langle\mathbf{Y}\left(x\left(t\right),t\right)\mathbf{B}^{-1}\left(x\left(t\right)\right)\mathbf{Y}\left(x\left(t\right),t\right)\rangle^{Y}dt=\\ \frac{1}{4}\int_{0}^{T}dt\int\mathcal{D}\left[\mathbf{x}\left(t\right)\right]P^{Y}\left(\mathbf{x}\left(t\right),t\right)\mathbf{Y}\left(x\left(t\right),t\right)\mathbf{B}^{-1}\left(x\left(t\right)\right)\mathbf{Y}\left(x\left(t\right),t\right)dt=\\ \frac{1}{4}\int_{0}^{T}dt\int\mathcal{D}\left[\mathbf{x}\left(t\right)\right]P\left(\mathbf{x}\left(t\right),\left(1+\alpha\right)t\right)\mathbf{Y}\left(x\left(t\right),t\right)\mathbf{B}^{-1}\left(x\left(t\right)\right)\mathbf{Y}\left(x\left(t\right),t\right)\end{gathered} \tag{2.28}$$

We substitute (2.25) into (2.28) so that, as already said in the introduction, the cost function becomes proportional to the entropy production (actually this is true if $\mathbf{J}(t) = \mathbf{J}^{irr}(t)$, namely if th probability current is only related to irreversible processes), in fact

$$\begin{gathered}\frac{\alpha^2}{4}\int_0^T dt \int \mathcal{D}[\mathbf{x}(t)]\, P(\mathbf{x}(t), (1+\alpha)t)\, \frac{[\mathbf{J}(\mathbf{x}(t), (1+\alpha)t)]^2\, \mathbf{B}^{-1}(x(t))}{[P(\mathbf{x}(t), (1+\alpha)t)]^2} = \\ \frac{\alpha^2}{4}\int_0^{(1+\alpha)T} \frac{dt}{(1+\alpha)} \int \mathcal{D}[\mathbf{x}(t)]\, P(\mathbf{x}(t), t)\, \frac{[\mathbf{J}(\mathbf{x}(t), t)]^2\, \mathbf{B}^{-1}(x(t))}{[P(\mathbf{x}(t), t)]^2} = \\ \frac{\alpha^2}{4(1+\alpha)}\int_0^{(1+\alpha)T} \left\langle \frac{\mathbf{J}\mathbf{B}^{-1}\mathbf{J}}{P^2}\right\rangle(t)\, dt = \frac{\alpha^2}{4(1+\alpha)}\langle\Sigma\rangle((1+\alpha)T)\end{gathered} \tag{2.29}$$

where we have set $\int_0^{(1+\alpha)T} \langle \frac{\mathbf{J}\mathbf{B}^{-1}\mathbf{J}}{P^2}\rangle(t)\, dt = \langle\Sigma\rangle((1+\alpha)T)$ that is the entropy production. Moreover, in the secon line of (2.29) we again made a change of the time variable. Finally we obtain

$$\mathcal{K}_Q(h, T) \geq \frac{1}{T}\left[h\langle Q\rangle((1+\alpha)T) - \frac{\alpha^2}{4(1+\alpha)}\langle\Sigma\rangle((1+\alpha)T)\right] \tag{2.30}$$

Let us now consider the first part of equation (2.30). We have (considering h as a small parameter)

$$\begin{gathered}\mathcal{K}_Q(h, T) = \frac{1}{T}\ln\left\langle \exp\left[h\int_0^T \dot{Q}(t)\, dt\right]\right\rangle \approx \\ \frac{1}{T}\ln\left[h\langle Q\rangle(T) + \frac{h^2}{2}\langle Q^2\rangle(T)\right] \approx \frac{1}{T}\left[h\langle Q\rangle(T) + \frac{h^2}{2}\langle \Delta Q^2\rangle(T)\right]\end{gathered} \tag{2.31}$$

and hence (2.30) becomes

$$\begin{gathered}\frac{1}{T}\left[h\langle Q\rangle(T) + \frac{h^2}{2}\langle \Delta Q^2\rangle(T)\right] \geq \frac{1}{T}\Big[h\langle Q\rangle((1+\alpha)T) + \\ - \frac{\alpha^2}{4(1+\alpha)}\langle\Sigma\rangle((1+\alpha)T)\Big]\end{gathered} \tag{2.32}$$

We then note that if α is small we can taylor expand the averaged integrated current

$$\begin{gathered}\langle Q\rangle((1+\alpha)T) \approx \langle Q\rangle(T) + \frac{\partial}{\partial(\alpha T)}\left[\langle Q\rangle((1+\alpha)T)\right]\Big|_{\alpha=0}\cdot \alpha T = \\ \langle Q\rangle(T) + \alpha T\langle \dot{Q}\rangle(T)\end{gathered} \tag{2.33}$$

and inserting (2.33) in (2.32) we obtain

$$\frac{h^2}{2}\langle \Delta Q^2\rangle(T) \geq h\alpha T\langle \dot{Q}\rangle(T) - \frac{\alpha^2}{4}\langle\Sigma\rangle(T) + \mathcal{O}\left(\alpha^3\right) \tag{2.34}$$

The last step consists in making a clever choice for the expansion parameter α in a way that the two pieces on the right of (2.34) become proportional, we hence pose

$$\alpha = \frac{2hT\langle \dot{Q}\rangle(T)}{\langle\Sigma\rangle(T)} \tag{2.35}$$

in a way that α and h are of the same order. Equation (2.34) hence becomes

$$\frac{\langle \Delta Q^2\rangle(T)}{2} \geq \frac{\left(T\langle \dot{Q}\rangle(T)\right)^2}{\langle\Sigma\rangle(T)} \tag{2.36}$$

This is the thermodynamic uncertainty relation we were looking for. By putting $\mathcal{D}^Q(T) = \dfrac{\langle \Delta Q^2\rangle(T)}{2T}$ and $\overline{\sigma}_T = \dfrac{\langle\Sigma\rangle(T)}{T}$, where the first is the generalized time-dependent diffusivity and the latter is the time-averaged entropy production rate, we get an alternative version of equation (2.36)

$$\mathcal{D}^Q(T)\,\overline{\sigma}_T \geq \langle \dot{Q}\rangle^2(T) \tag{2.37}$$

2.2 General derivation

There is an alternative way to derive the previous result, in some ways easier to obtain and also more general. This approach is also used in another article written by Dechant and Sasa, see [4].
The starting point is again the scaled cumulant generating function

$$\mathcal{K}_Q(h,T) = \frac{1}{T}\ln\left\langle \exp\left[h\int_0^T \dot{Q}(t)\,dt\right]\right\rangle^{\mathbb{P}} = \frac{1}{T}\ln\int d\mathbb{P}\exp\left[h\int_0^T \dot{Q}(t)\,dt\right] \tag{2.38}$$

where we used that

$$\big\langle O(\mathbf{x}(t),t)\big\rangle^{\mathbb{P}} = \mathbb{E}_{\mathbb{P}}[O(\mathbf{x}(t),t)] = \int d\mathbb{P}\,[O(\mathbf{x}(t),t)] \tag{2.39}$$

We now switch to a new probability measure $\mathbb{Q}$ which must be absolutely continuous with respect to $\mathbb{P}$. This can be done thanks to the formal relation

$$\frac{1}{T}\ln\int d\mathbb{P}\exp\left[h\int_0^T \dot{Q}(t)\,dt\right] = \frac{1}{T}\ln\int d\mathbb{Q}\frac{d\mathbb{P}}{d\mathbb{Q}}\exp\left[h\int_0^T \dot{Q}(t)\,dt\right] \tag{2.40}$$

where $\dfrac{d\mathbb{P}}{d\mathbb{Q}}$ is the Radon-Nikodym derivative [6], which is widely used in Girsanov's work [7]. In the latter it is explained, for exemple for a process $X(t)$ adapted to the natural filtration $\{\mathcal{F}^{\mathcal{W}}(t)\}$ of a simple Wiener process $\{\mathcal{W}(t)\}$, that the Radon-Nikodym derivative is equivalent to the Doléans-Dade exponential [8]

$$\mathcal{E}[X(t)] = \exp\Big[X(t) - \frac{\Delta X^2(t)}{2}\Big] = \frac{d\mathbb{P}}{d\mathbb{Q}}\Big|_{\mathcal{F}^{\mathcal{W}}(t)} \tag{2.41}$$

We will abandon the the $\cdot\big|_{\mathcal{F}^{\mathcal{W}}(t)}$ notation in favour of a more agile t subscript. Using Jensen's inequality on equation (2.40) we get that

$$\begin{gathered}\mathcal{K}_Q(h,T) = \frac{1}{T}\ln\int d\mathbb{Q}\frac{d\mathbb{P}}{d\mathbb{Q}}\exp\left[h\int_0^T \dot{Q}(t)\,dt\right] \geq \\ \frac{1}{T}\left[h\int d\mathbb{Q}[\int_0^T \dot{Q}(t)\,dt] + \int d\mathbb{Q}\ln\left[\frac{d\mathbb{P}}{d\mathbb{Q}}\right]_T\right] = \\ \frac{1}{T}\left[h\langle Q\rangle^{\mathbb{Q}}(T) - \mathbb{H}(\mathbb{Q}|\mathbb{P})(T)\right]\end{gathered} \tag{2.42}$$

Here

$$\mathbb{H}(\mathbb{Q}|\mathbb{P})(T) = \int d\mathbb{Q}\ln\left[\frac{d\mathbb{Q}}{d\mathbb{P}}\right]_T = \left\langle\ \ln\left(\frac{d\mathbb{Q}}{d\mathbb{P}}\right)_T\right\rangle^{\mathbb{Q}}$$

stands for the relative entropy between the two probability measures $\mathbb{P}$ and $\mathbb{Q}$, also known as Kullback-Leibler divergence [9].
By doing the same reasoning we made in the previous subsection (see equation (2.31)) we expand the scaled cumulant generating function in powers of h, which is an arbitrarly small parameter. We obtain

$$T\mathcal{K}_Q(h,T) \approx h\langle Q\rangle^{\mathbb{P}}(T) + \frac{h^2}{2}\langle \Delta Q^2\rangle^{\mathbb{P}}(T) \geq h\langle Q\rangle^{\mathbb{Q}}(T) - \mathbb{H}(\mathbb{Q}|\mathbb{P})(T) \tag{2.43}$$

As we will see in the next sections, if we take the probability measure $\mathbb{Q}$ "close" to $\mathbb{P}$ in a sense that $d\mathbb{Q} = d\mathbb{P}^{\alpha}$, where α is a small perturbation parameter such that $\alpha = 0 \implies d\mathbb{Q} = d\mathbb{P}^{\alpha}$, it is possible to suppose that it will be always possible to make a taylor expansion of the Kullback-Leibler and that at leading order in α we get

$$\mathbb{H}(\mathbb{P}|\mathbb{Q}) = \mathbb{H}(\mathbb{P}|\mathbb{P}^{\alpha}) \equiv \frac{\alpha^2}{4}\langle\Sigma\rangle(T) \tag{2.44}$$

where $\langle\Sigma\rangle(T)$ is a function independent of α and, at this level of generality, can not be identified as entropy production. Instead, concerning the currents, we get

$$\langle Q\rangle^{\mathbb{Q}}(T) - \langle Q\rangle^{\mathbb{P}}(T) = \langle Q\rangle^{\mathbb{P}^{\alpha}}(T) - \langle Q\rangle^{\mathbb{P}}(T) \equiv \alpha\delta\langle Q\rangle(T) \tag{2.45}$$

Here $\delta\langle Q\rangle(T)$ can be interpreted as the susceptibility of $Q(t)$ to the α-dependent perturbation (we again stress that the latter must not necessarily be a phisically realisable perturbation, what matters is that it generates a probability measure $\mathbb{P}^{\alpha}$ slightly different from $\mathbb{P}$). Formally we can define it as follows

$$\delta\langle Q\rangle(T) = \frac{\delta}{\delta\alpha}\langle Q\rangle^{\mathbb{P}^{\alpha}}(T) \tag{2.46}$$

where $\frac{\delta}{\delta\alpha}\cdot$ stands for functional derivation. Equation (2.43) can hence be rewritten as follows

$$\frac{h^2}{2}\langle\Delta Q^2\rangle(T) \geq h\alpha\delta\langle Q\rangle(T) - \frac{\alpha^2}{4}\langle\Sigma\rangle(t) \tag{2.47}$$

where we have abandoned the $\mathbb{P}$ superscript over $\frac{h^2}{2}\langle\Delta Q^2\rangle^{\mathbb{P}}(T)$. At this point the trick consists in making again a clever choice for α. Since h is an arbitrarily small parameter (used to make a series expansion of the scaled cumulant generating function) and so must be α, we set them proportional in such a way that also the two pieces of the right hand side of (2.47) become proportional, namely

$$\alpha = \frac{2h\delta\langle Q\rangle(T)}{\langle\Sigma\rangle(T)} \tag{2.48}$$

so that finally (2.47) becomes

$$\langle\Delta Q^2\rangle(T) \geq \frac{2\left(\delta\langle Q\rangle(T)\right)^2}{\langle\Sigma\rangle(T)} \tag{2.49}$$

that is a non-equilibrium inequality independent both from h and α. For future convenience we also define the function $I(T)$ which will have an important role in this thesis in the following way

$$I(T) = \frac{2\left(\delta\langle Q\rangle(T)\right)^2}{\langle\Sigma\rangle(T)\cdot\langle\Delta Q^2\rangle(T)} \leq 1 \tag{2.50}$$

Given the generality of the α-dependent perturbation, $\mathbb{H}(\mathbb{P}|\mathbb{Q})(T)$ (and hence $\langle\Sigma\rangle(T)$) can take very diferent forms. For instance, as already said, Dechant and Sasa have discussed how to recover the thermodynamic uncertainty relation using a peculiar perturbation and in that case they have shown that $\langle\Sigma\rangle(T)$ is the entropy production of the system. We will show that complementary choices can give interestin non-equilibrium inequalities where $\langle\Sigma\rangle(T)$ becomes a time symmetric object estimating how "active" the system is. For instance, for jump processes this is quantified by the average number of jumps per unit time.
In the following sections we will hence analyse different systems, namely jump and diffusion processes, calculaiting the Kullback-Leibler divergence for different kinds of perturbations, trying to relate the result to physical observables and analysing the non-equilibrium inequalities that arise from those calculations. We again stess that this is possible thanks to the generality of this approach and to the weak conditions under which the Kullback-Leibler divergence exists.

3 Jump processes

Before starting the actual calculations we make a short introduction about Markov processes. It is known such kind of processes is a random variable X that is characterised by a state space $\mathcal{S}$ and a time parameter, namely we have $X_t \in \mathcal{S}$. Time can either be a discrete index or a continuous parameter while the state space $\mathcal{S}$ can be either discrete and finite, discrete and countable or continuous. The simplest case is of course the one relative to discrete time and discrete state space and for which we have the most theorems and results. If the state space becomes countable we lose some results but the biggest part of them still work. Moreover, it can be shown that also if time becomes continuous (but keeping the state space discrete) the situation does not change much and hence the mathematical approach remains the same. Instead, things change a lot if the state space becomes continuous and this situation will be faced in the next section. Hence for now we will focus on discrete state space with elements $i_n \in \mathcal{S}$ showing some results that are valid for this case. First of all, in total generality we define a conditional probability for a process $(X_n)_{0\leq n\leq N+M}$, where the time index n is for now discrete, as follows

$$\mathbb{P}(X_{N+1} = i_{N+1}, \dots, X_{N+M} = i_{N+M} | X_0 = i_0, \dots, X_N = i_N) = \frac{\mathbb{P}(X_0 = i_0, \dots, X_{N+M} = i_{N+M})}{\mathbb{P}(X_0 = i_0, \dots, X_N = i_N)} \tag{3.1}$$

that is valid for all stochastic processes with discrete time. Here i_n is the state at time n. The main feature of Markov processes is the Markov propriety that states that for such kind of processes it holds that

$$\begin{gathered}\mathbb{P}\big(X_{N+1} = i_{N+1}, \dots, X_{N+M} = i_{N+M} | X_0 = i_0, \dots, X_N = i_N\big) = \\ \mathbb{P}(X_{N+1} = i_{N+1}, \dots, X_{N+M} = i_{N+M} | X_N = i_N)\end{gathered} \tag{3.2}$$

that is the system has no memory on what happened before time N. Moreover we define the transition matrix

$$p_{ij} = \mathbb{P}(X_{n+1} = j | X_n = i) \tag{3.3}$$

that is a $d \times d$ matrix (d is the dimension of the state space) whose elements are the probabilities of jumping from state i to state j. It hence has the propriety that the sum of the row's elements is 1, namely

$$\sum_{j=1}^{d} p_{ij} = 1 \tag{3.4}$$

With these we can write the joint probability of N successive events as

$$\mathbb{P}\big(X_1 = i_1, X_2 = i_2, \dots, X_N = i_N\big) = \mathbb{P}\left(X_1 = i_1\right) p_{i_1,i_2} p_{i_2,i_3} \dots p_{i_{N-1},i_N} \tag{3.5}$$

that is again a consequence of the Markov propriety. Moreover the probability of reaching state j from state i after n jumps is the (i, j)th element of the nth power of the transition matrix.
As for continuous time Markov chains the fundamental object is the K-matrix for with it holds that $i \neq j \implies K_{i,j} \geq 0$ and $K_{i,i} \leq 0$ and moreover

$$\sum_{j}^{d} K_{i,j} = 0 \qquad\qquad \sum_{j\neq i}^{d} K_{i,j} = -K_{i,i} \tag{3.6}$$

All the proprieties of this kind of matrices are well illustrated in [11], with the only difference that in this text they are called Q-matrices (we will use the letter Q for other purposes so we use K instead to avoid confusion). From now on we will focus on some of them that will be useful soon. First of all we have that it is possible to define a transition matrix $(P_{i,j}(t) : t \geq 0)$ also for continuous time Markov chains (note that we now have a continuous time variable) that obeys the following differential equations

$$\frac{d}{dt} P_{i,j}(t) = \sum_{l}^{d} P_{i,l}(t) K_{l,j} \qquad\qquad \frac{d}{dt} P_{i,j}(t) = \sum_{l}^{d} K_{i,l} P_{l,j}(t) \tag{3.7}$$

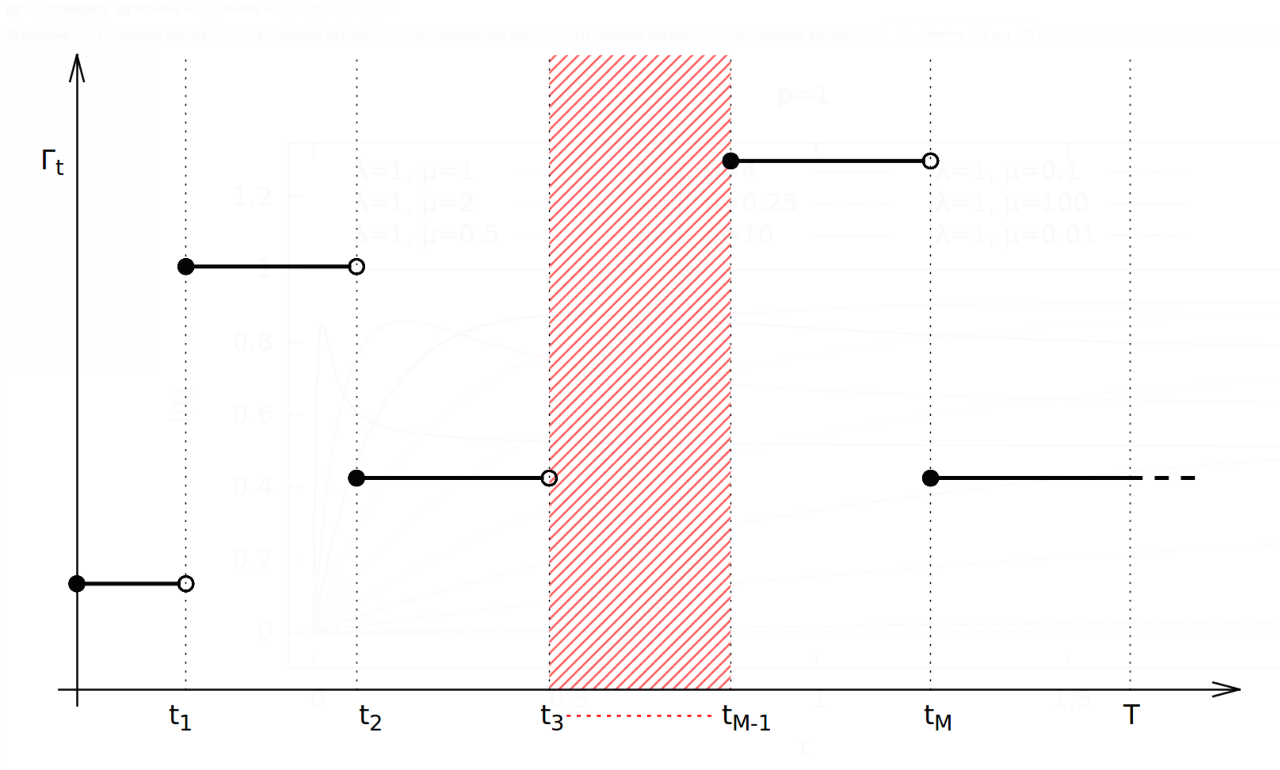
that are respectively the forward and the backward equation. Its formal solution is

$$P_{i,j}\left(t\right)=\exp\left[t\cdot K_{i,j}\right] \tag{3.8}$$

that is a matrix exponential. It can be shown that the so defined transition matrix has the propriety given in (3.4). The problem of this definition is that a matrix exponential is often too complicated to calculate and hence this approach is not often used to solve problems. In fact, as we will see in the next subsection, to describe systems with the aid of continuous time Markov chains we will build up a probability density function for a given path in state space using two fundamental building blocks

$$\mathbb{P}\left(X_{t+dt}=j|X_t=i\right)=K_{i,j}dt \qquad\qquad \mathbb{P}\left(X_{t+s}=i|X_t=i\right)=\exp\left[K_{i,i}t\right] \tag{3.9}$$

that are respectively the probability that a jump occurs from i to j in an infinitesimal time interval dt and the probability that after a time t the system remains in i. From now on we will refer to a given path in state space up to time T as Γ_T. To write a probability density function for the latter we imagine a total of N states with M jumps occurred at times t_m from state i_m^- to i_m^+ (see figure below).



Scheme of a continuous time Markov jump process

For such a situation and using (3.9) we obtain

$$P\left(\Gamma_T|\Gamma_0\right)=P\left(\Gamma_0\right)\cdot\exp\left[K_{i_M^+,i_M^+}\left(T-t_M\right)\right]\prod_{m=1}^{M}\left[\exp\left[K_{i_m^-,i_m^-}\left(t_m-t_{m-1}\right)\right]K_{i_m^-,i_m^+}dt\right] \tag{3.10}$$

where Γ_0 is the starting point of Γ_T. This result will be immediately used in the following subsection.

3.1 General case

We will now focus on calculating $\mathbb{H}\left(\mathbb{P}^\alpha|\mathbb{P}\right)(T)$ (we will use $\mathbb{P}^\alpha$ instead of $\mathbb{Q}$) for two simple jump processes using continuous time Markov chains: Poisson process (the most simple example) and a two state Markov chain. The step immediately following this calculation will be of course to plug the result in equation (2.43) in order to obtain a nonequilibrium inequality. We will keep this treatment

general as long as possible, specializing to the matter in hand when needed.
To calculate the Kullback-Leibler divergence it is convenient to rewrite (3.10) as a function of the modified coefficients of the K-matrix $K^{\alpha}_{i,j} = (1+\alpha) K_{i,j}$. We see indeed that this modification does not affect the validity of the constraints (3.6), so that $K^{\alpha}_{i,j}$ is still a K-matrix. We can hence equivalently rewrite equation (3.10) as

$$\begin{aligned} P\big(\Gamma_T|\Gamma_0\big) = P(\Gamma_0) \prod_{m=1}^{M+1} \exp\left[\tau_m K^{\alpha}_{i^-_m, i^-_m} - \alpha \tau_m K_{i^-_m, i^-_m}\right] \prod_{m=1}^{M} \left[\left(K^{\alpha}_{i^-_m, i^+_m} - \alpha K_{i^-_m, i^+_m}\right) dt\right] = \\ P(\Gamma_0) \exp\left[\sum_{m}^{M+1} \left(\tau_m K^{\alpha}_{i^-_m, i^-_m} - \alpha \tau_m K_{i^-_m, i^-_m}\right)\right] \prod_{i \neq j}^{N} \left[K^{\alpha}_{i,j} - \alpha K_{i,j}\right]^{n_{ij}} (dt)^n \end{aligned} \tag{3.11}$$

where $\tau_m = t_m - t_{m-1}$, $\tau_{M+1} = T - t_M$, $i^+_M = i^-_{M+1}$ (these choices where made to make the future calculation more agile), n_{ij} is the number of times the system jumps from state i to state j up to time T and n is the total number of jumps again up to time T. Moreover remembering that, as in the previous section, we take α as a small parameter it follows that

$$\prod_{i \neq j}^{N} \left[K^{\alpha}_{i,j} - \alpha K_{i,j}\right]^{n_{ij}} = \prod_{i \neq j}^{N} K^{\alpha\, n_{ij}}_{i,j} \left[1 - \frac{\alpha}{1+\alpha}\right]^{n_{ij}} = \prod_{i \neq j}^{N} K^{\alpha\, n_{ij}}_{i,j} \left[\frac{1}{1+\alpha}\right]^{n_{ij}} \tag{3.12}$$

so that

$$P(\Gamma_T|\Gamma_0) = P^{\alpha}(\Gamma_T|\Gamma_0) \exp\left[-\alpha \sum_{m}^{M+1} \tau_m K_{i^-_m, i^-_m} - \sum_{i \neq j}^{N} n_{ij} \ln(1+\alpha)\right] \tag{3.13}$$

We note that the $(dt)^n$ term was absorbed by the definition of $P^{\alpha}(\Gamma_T|\Gamma_0)$. At this point we note that $d\mathbb{P} = P(\Gamma_T|\Gamma_0)\, d\Gamma$ and similarly $d\mathbb{P}^{\alpha} = P^{\alpha}(\Gamma_T|\Gamma_0)\, d\Gamma$, using this result it is obvious that

$$\frac{d\mathbb{P}^{\alpha}}{d\mathbb{P}}(T) = \frac{P^{\alpha}(\Gamma_T|\Gamma_0)\, d\Gamma}{P(\Gamma_T|\Gamma_0)\, d\Gamma} = \exp\left[\alpha \sum_{m}^{M+1} \tau_m K_{i^-_m, i^-_m} + \sum_{i \neq j}^{N} n_{ij} \ln(1+\alpha)\right] \tag{3.14}$$

From the definition of the Kullback-Leibler divergence it is easy to see that

$$\begin{aligned} \mathbb{H}(\mathbb{P}^{\alpha}|\mathbb{P})(T) = \int d\mathbb{P}^{\alpha} \ln\left[\frac{d\mathbb{P}^{\alpha}}{d\mathbb{P}}(T)\right] = \\ \int_{[0,T]} d\mathbb{P}^{\alpha} \left[\alpha \sum_{m}^{M+1} \tau_m K_{i^-_m, i^-_m} + \sum_{i \neq j}^{N} n_{ij} \ln(1+\alpha)\right] = \\ \alpha \langle \sum_{m}^{M+1} \tau_m K_{i^-_m, i^-_m} \rangle^{\alpha} + \sum_{i \neq j}^{N} \langle n_{ij}(T) \rangle^{\alpha} \ln(1+\alpha) \end{aligned} \tag{3.15}$$

where $\langle \cdot \rangle^{\alpha}$ is intended as an average with respect to the modified probability measure $\mathbb{P}^{\alpha}$. Moreover we note that the first term of the last line is nothing else than the averaged sum over all states of the escape rate (relabelling the indices) $K_{j,j}$ times the averaged number of visits in state j again times the permanence time in state j. The whole sum can thus been rewritten as the double sum over all states i and j of the average number of times that the system jumps from i to j times $K_{j,j}$ again times the average permanence time in the state j. In formulae

$$\langle \sum_{m}^{M+1} \tau_m K_{i^-_m, i^-_m} \rangle^{\alpha} = \sum_{j}^{N} K_{j,j} \langle n_j(T) \rangle^{\alpha} \langle \tau_j \rangle^{\alpha} = \sum_{i}^{N} \sum_{j}^{N} K_{j,j} \langle n_{ij}(T) \rangle^{\alpha} \langle \tau_j \rangle^{\alpha} \tag{3.16}$$

where $\langle n_j(T)\rangle$ is the averaged number of visits to state j up to time T and it clearly holds that $\langle n_j(T)\rangle = \sum_i^N \langle n_{ij}(T)$, hence

$$
\begin{aligned}
&\mathbb{H}(\mathbb{P}^\alpha|\mathbb{P})(T) = \alpha \sum_i^N \sum_j^N K_{j,j} \langle n_{ij}(T)\rangle^\alpha \langle \tau_j \rangle^\alpha + \sum_{i\neq j}^N \langle n_{ij}(T)\rangle^\alpha \ln(1+\alpha) = \\
&\sum_{i\neq j}^N \langle n_{ij}(T)\rangle^\alpha \Big[\alpha K_{j,j}\langle \tau_j\rangle^\alpha + \ln(1+\alpha)\Big] = \sum_{i\neq j}^N \langle n_{ij}(T)\rangle^\alpha \Big[-\frac{\alpha}{1+\alpha} + \ln(1+\alpha)\Big]
\end{aligned}
\tag{3.17}
$$

where in the last line we used the fact that

$$
\langle \tau_m \rangle^\alpha = -\frac{1}{K_{j,j}^\alpha} = -\frac{1}{(1+\alpha)K_{j,j}}
$$

In the end, by expanding the α-dependent part of the last term of equation (3.17) we obtain our final result

$$
\mathbb{H}(\mathbb{P}^\alpha|\mathbb{P})(T) = \frac{\alpha^2}{2}\sum_{i\neq j}^N \langle n_{ij}(T)\rangle^\alpha + \mathcal{O}\left(\alpha^3\right) \tag{3.18}
$$

At this point we note that $\langle n_{ij}(T)\rangle^\alpha$ is a quantity that depends on the perturbation parameter α so that we can formally write

$$
\langle n_{ij}(T)\rangle^\alpha = \langle n_{ij}(T)\rangle + \alpha \left(\frac{\partial}{\partial\alpha}\langle n_{ij}(T)\rangle^\alpha\Big|_{\alpha=0}\right) \tag{3.19}
$$

hence by putting back in equation back into (3.18) and neglecting higher order terms in α we obtain

$$
\mathbb{H}(\mathbb{P}^\alpha|\mathbb{P})(T) = \frac{\alpha^2}{2}\sum_{i\neq j}^N \langle n_{ij}(T)\rangle + \mathcal{O}\left(\alpha^3\right) \tag{3.20}
$$

Although this formula could seem very simple at first sight, it is usually very difficult to calculate the $\langle n_{ij}(T)\rangle$ term, even in the two states case.
Instead, in case of a simple Poisson process with escape rate λ it is very easy to calculate. In fact we have $\langle n_{ij}(T)\rangle = \langle n(T)\rangle = \lambda T$, and hence

$$
\mathbb{H}(\mathbb{P}^\alpha|\mathbb{P})(T) = \frac{\alpha^2}{2}\lambda T + \mathcal{O}\left(\alpha^3\right) \tag{3.21}
$$

In the next section we will obtain the same result in a slightly different and more direct way to demonstrate that the this formula is indeed correct.
Turning back to equation (3.20) we note that $n_{ij}(T)$ can be rewritten as follows

$$
n_{ij}(T) = \frac{1}{2}\left(n_{ij}(T) + n_{ji}(T)\right) + \frac{1}{2}\left(n_{ij}(T) - n_{ji}(T)\right) \tag{3.22}
$$

Concerning the second term we have that by relabelling indices

$$
\frac{1}{2}\sum_{i\neq j}^N \left(n_{ij}(T) - n_{ji}(T)\right) = \frac{1}{2}\sum_{i\neq j}^N \left(n_{ij}(T) - n_{ij}(T)\right) = 0 \tag{3.23}
$$

and hence (3.20) becomes

$$
\mathbb{H}(\mathbb{P}^\alpha|\mathbb{P})(T) = \frac{\alpha^2}{4}\sum_{i\neq j}^N \langle n_{ij}(T) + n_{ji}(T)\rangle = \frac{\alpha^2 T}{4}\sum_{i\neq j}^N \langle \Psi_{ij}(T)\rangle \tag{3.24}
$$

where we have used the definition of the "frenesy"

$$
\Psi_{ij}(T) = \frac{1}{T}\left(n_{ij}(T) + n_{ji}(T)\right) \tag{3.25}
$$

With equation (3.24) we immediately recognize

$$\langle \Sigma \rangle (T) = T \sum_{i \neq j}^{N} \langle \Psi_{ij} (T) \rangle \qquad \bar{\sigma} (T) = \frac{\langle \Sigma \rangle (T)}{T} = \sum_{i \neq j}^{N} \langle \Psi_{ij} (T) \rangle \tag{3.26}$$

We stress that this treatment is also valid for irreversible processes (such as the following ones treated in next subsections) and hence $\langle \Sigma \rangle (T)$ can not always be considered as the entropy production as for those kind of systems entropy in not defined.
Having these informations we would like to use equation (2.49). We only need to know what kind of form $\delta \langle Q \rangle (T)$ takes, from its definition we have that

$$\alpha \delta \langle Q \rangle = \langle Q \rangle^{\alpha} (T) - \langle Q \rangle (T) \tag{3.27}$$

We note that the perturbation we have made $K_{i,j}^{\alpha} = (1 + \alpha) K_{i,j}$ is such that, using equation (3.10), the perturbed probability measure is equivalent to the old one with dilated time by a factor $(1 + \alpha)$, namely

$$P^{\alpha} (\Gamma_T | \Gamma_0) = P \left(\Gamma_{(1+\alpha)T} | \Gamma_0 \right) \implies \langle Q \rangle^{\alpha} (T) = \langle Q \rangle ((1 + \alpha) T) \tag{3.28}$$

As the perturbation parameter is small we have that (3.27) becomes

$$\alpha \delta \langle Q \rangle = \langle Q \rangle ((1 + \alpha) T) - \langle Q \rangle (T) \approx \langle Q \rangle (T) + \alpha T \left(\frac{\partial}{\partial \alpha T} \langle Q \rangle (T) \Big|_{\alpha = 0} \right) - \langle Q \rangle (T) = \alpha T \langle \dot{Q} \rangle (T) \tag{3.29}$$

hence indentifying

$$\delta \langle Q \rangle (T) = T \langle \dot{Q} \rangle (T) \tag{3.30}$$

Consequently equation (2.49) becomes

$$\langle \Delta Q^2 \rangle (T) \geq \frac{2 \left(T \langle \dot{Q} \rangle (T) \right)^2}{\langle \Sigma \rangle (T)} \tag{3.31}$$

that is the same as (2.36). This form is peculiar for systems where the perturbation has the same effect of a time scaling of the probability measure, as we will see for a generic diffusion processes it will not hold. Finally, putting (3.26) in (3.31) we obtain

$$\langle \Delta Q^2 \rangle (T) \geq \frac{2T \left(\langle \dot{Q} \rangle (T) \right)^2}{\sum_{i \neq j}^{N} \langle \Psi_{ij} (T) \rangle} \tag{3.32}$$

3.2 Example I: Poisson Process

We now consider a simple Poisson process for which the $K_{i,j}$ matrix has the following form

$$K_{i,j} = \begin{bmatrix} -\lambda & \lambda & 0 & 0 & \dots \\ 0 & -\lambda & \lambda & 0 & \dots \\ 0 & 0 & -\lambda & \lambda & \dots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix} \tag{3.33}$$

so that (3.10) becomes

$$P (\Gamma_T | \Gamma_0) = P (\Gamma_0) \exp [-\lambda T] (\lambda)^n \tag{3.34}$$

with n the number of jumps up to time T. We now consider the ratio between this path probability (which we will call from now on $P^{\lambda} (\Gamma_T | \Gamma_0)$) and the one obtained with a different parameter μ ($P^{\mu} (\Gamma_T | \Gamma_0)$)

$$\frac{P^{\lambda} (\Gamma_T | \Gamma_0)}{P^{\mu} (\Gamma_T | \Gamma_0)} = \exp [- (\lambda - \mu) T] \left(\frac{\lambda}{\mu} \right)^n \tag{3.35}$$

because $P(\Gamma_0)$ is not affected by the driving parameter change. Moreover we again have that $P^\lambda(\Gamma_T|\Gamma_0)\, d\Gamma = d\mathbb{P}^\lambda$, so that

$$\frac{d\mathbb{P}^\lambda}{d\mathbb{P}^\mu} = \frac{P^\lambda(\Gamma_T|\Gamma_0)\, d\Gamma}{P^\mu(\Gamma_T|\Gamma_0)\, d\Gamma} = \exp\left[-(\lambda-\mu)\, T\right]\left(\frac{\lambda}{\mu}\right)^n \tag{3.36}$$

We can now easily calculate the relative entropy

$$\mathbb{H}\left(\mathbb{P}^\mu|\mathbb{P}^\lambda\right)(T) = \int d\mathbb{P}^\mu \ln\left[\left.\frac{d\mathbb{P}^\mu}{d\mathbb{P}^\lambda}\right|_{\mathcal{F}^{\mathcal{Y}}(T)}\right] = -\int_{[0,T]} d\mathbb{P}^\mu\left[(\mu-\lambda)\, T + n\ln\left(\frac{\lambda}{\mu}\right)\right] \tag{3.37}$$

Let us now set $\mu = (1+\alpha)\,\lambda$ with α an arbitrarily small parameter. In this way what we have obtained is a small perturbation of the original dynamics with driving parameter λ. Thus

$$\begin{aligned}\mathbb{H}\left(\mathbb{P}^\mu|\mathbb{P}^\lambda\right)(T) = -\int_{[0,T]} d\mathbb{P}^\mu\left[\alpha\lambda T + n\ln\left(\frac{1}{1+\alpha}\right)\right] = \\ -\alpha\lambda T - (1+\alpha)\,\lambda T\ln\left(\frac{1}{1+\alpha}\right)\end{aligned} \tag{3.38}$$

where we used the fact that $\int_{[0,T]} d\mathbb{P}^\mu n = \mu T$ and that there are no other random variables. Expanding up to second order in α the term with the logarithm, $(1+\alpha)\ln\left(\frac{1}{1+\alpha}\right) = -\alpha - \frac{1}{2}\alpha^2 + \mathcal{O}\left(\alpha^3\right)$, we get

$$\mathbb{H}\left(\mathbb{P}^\mu|\mathbb{P}^\lambda\right)(T) = \frac{\alpha^2}{2}\lambda T \tag{3.39}$$

We notice that this result coincides with what we have obtained in the last section, namely equation (3.21). At this point we finally make use of this result putting it in equation (3.31) and noting that $\langle\Sigma\rangle(T) = 2\lambda T$ we obtain (abandoning the λ superscript)

$$\left\langle\Delta Q^2\right\rangle(T) \geq \frac{T\left(\langle\dot{Q}\rangle(T)\right)^2}{\lambda} \tag{3.40}$$

or equivalently

$$\mathcal{D}^Q(T)\,\overline{\sigma}_T \geq \langle\dot{Q}\rangle^2(T) \tag{3.41}$$

With $\mathcal{D}^Q(T) = \frac{\left\langle\Delta Q^2\right\rangle(T)}{2T}$ and $\overline{\sigma}_T = \frac{\langle\Sigma\rangle(T)}{T} = 2\lambda$.
The treatment of the current terms will be performed in detail in the next subsection.

3.3 Example II: Two states process

Let us now examine a different situation: a two states continuous Markov chain. This is a simple system that is often treated during undergraduate curses but its dynamics, differently from the simple Poisson process, is no longer time homogeneous, and this will lead to non trivial results. First of all we analyse its K matrix that is

$$K_{i,j} = \begin{bmatrix}-\lambda & \lambda \\ \mu & -\mu\end{bmatrix} \tag{3.42}$$

Moreover we note that through a relabelling of the states the dynamic is the same of a system with the following K matrix

$$\widetilde{K}_{i,j} = \begin{bmatrix}-\lambda & \lambda & 0 & 0 & 0 & \dots \\ 0 & -\mu & \mu & 0 & 0 & \dots \\ 0 & 0 & -\lambda & \lambda & 0 & \dots \\ 0 & 0 & 0 & -\mu & \mu & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots\end{bmatrix} \tag{3.43}$$

This means that if $\lambda = \mu$ we should obtain the same results of the previous subsection and, furthermore, it will give us some computational advantages.
The starting point is again (2.43). From now on, as at the beginning of this section, averages taken with respect to the perturbed probability measure $\mathbb{P}^\alpha$ will be indicated by $\langle\cdot\rangle^\alpha$. We should now calculate $\mathbb{H}_i\left(\mathbb{P}^\alpha|\mathbb{P}\right)(T)$, where the i subscript stands for state in which the sistem is at time 0, but this is a complicated task and thus we will rely on a result contained in [12]. For this purpose we set a new notation

$$\gamma_i^{\mathbb{P}} \implies \begin{cases} \gamma_1^{\mathbb{P}} = \lambda \\ \gamma_2^{\mathbb{P}} = \mu \end{cases} \qquad \gamma_i^{\mathbb{P}^\alpha} \implies \begin{cases} \gamma_1^{\mathbb{P}^\alpha} = \lambda^\alpha = (1+\alpha)\,\lambda \\ \gamma_2^{\mathbb{P}^\alpha} = \mu^\alpha = (1+\alpha)\,\mu \end{cases} \tag{3.44}$$

We have that

$$\mathbb{E}_{\mathbb{P}^\alpha}\left[\ln\left(\frac{d\mathbb{P}^\alpha}{d\mathbb{P}}(T)\right)\Big|X(0)=i\right] = \mathbb{H}_i\left(\mathbb{P}^\alpha|\mathbb{P}\right)(T) = BT + A_i\left[1-\exp\left[-\left(\lambda^\alpha+\mu^\alpha\right)T\right]\right] \tag{3.45}$$

with

$$A_1 = \frac{\lambda^\alpha\left(b_1-b_2\right)}{\left(\lambda^\alpha+\mu^\alpha\right)^2} \qquad A_2 = \frac{\mu^\alpha\left(b_2-b_1\right)}{\left(\lambda^\alpha+\mu^\alpha\right)^2} \qquad B = \frac{\mu^\alpha b_1 + \lambda^\alpha b_2}{\lambda^\alpha+\mu^\alpha} \tag{3.46}$$

and

$$b_i = \gamma_i^{\mathbb{P}} - \gamma_i^{\mathbb{P}^\alpha} + \gamma_i \ln\left[\frac{\gamma_i^{\mathbb{P}^\alpha}}{\gamma_i^{\mathbb{P}}}\right] = -\alpha\gamma_i^{\mathbb{P}} + (1+\alpha)\,\gamma_i^{\mathbb{P}}\ln\left[1+\alpha\right] \tag{3.47}$$

As usual, we take α small so that we can expand (3.47) in Taylor series

$$b_i = \frac{1}{2}\alpha^2\gamma_i^{\mathbb{P}} + \mathcal{O}\left(\alpha^3\right) \tag{3.48}$$

We now proceed with the calculation of the relative entropy

$$\begin{gathered} \mathbb{H}\left(\mathbb{P}^\alpha|\mathbb{P}\right)(T) = \mathbb{E}_{\mathbb{P}^\alpha}\left[\ln\left(\frac{d\mathbb{P}^\alpha}{d\mathbb{P}}(T)\right)\right] = \\ \sum_i \mathbb{E}_{\mathbb{P}^\alpha}\left[\ln\left(\frac{d\mathbb{P}^\alpha}{d\mathbb{P}}(T)\right)\Big|X(0)=i\right]P\left[X(0)=i\right] = \\ P\big[X(0)=1\big]\mathbb{H}_1\left(\mathbb{P}^\alpha|\mathbb{P}\right)(T) + P\left[X(0)=2\right]\mathbb{H}_2\left(\mathbb{P}^\alpha|\mathbb{P}\right)(T) = \\ \Big[BT + \big[A_1P\big[X(0)=1\big] + A_2P\big[X(0)=2\big]\big]\left[1-\exp\left[-\left(\lambda+\mu\right)T\right]\right]\Big]\alpha^2 + \mathcal{O}\left(\alpha^3\right) \end{gathered} \tag{3.49}$$

with

$$A_1 = \frac{\lambda\left(\lambda-\mu\right)}{2\left(\lambda+\mu\right)^2}\alpha^2 \qquad A_2 = \frac{\mu\left(\mu-\lambda\right)}{2\left(\lambda+\mu\right)^2}\alpha^2 \qquad B = \frac{\mu\lambda}{\mu+\lambda}\alpha^2 \tag{3.50}$$

Moreover we pose $P_i = P\big[X(0)=i\big]$ so that

$$\begin{gathered} \mathbb{H}\left(\mathbb{P}^\alpha|\mathbb{P}\right)(T) = \\ \left[\frac{\mu\lambda}{\mu+\lambda}T + \left[P_1\frac{\lambda\left(\lambda-\mu\right)}{2\left(\lambda+\mu\right)^2} + P_2\frac{\mu\left(\mu-\lambda\right)}{2\left(\lambda+\mu\right)^2}\right]\left[1-\exp\left[-\left(\lambda+\mu\right)T\right]\right]\right]\alpha^2 + \mathcal{O}\left(\alpha^3\right) \end{gathered} \tag{3.51}$$

By posing $\mu = \lambda$ we see that $A_i = 0$ and (3.51) reduces to (3.39). Furthermore we note that

$$\lim_{T\to\infty}\mathbb{H}\left(\mathbb{P}^\alpha|\mathbb{P}\right)(T) \approx \left[\frac{\mu\lambda}{\mu+\lambda}T\right]\alpha^2 \tag{3.52}$$

and this is the same result we would obtain by choosing $P_1 = \dfrac{\mu}{\mu+\lambda}$ and $P_2 = \dfrac{\lambda}{\mu+\lambda}$ in (3.51), namely starting from the stationary distribution (the probability distribution to which the system tends as time goes to infinity).
Instead, we would like to start from a situation that is not stationary and for this reason we will analyse the situation in total generality by putting $P_1 = p$ and $P_2 = 1-p$ so that (3.51) becomes

$$\mathbb{H}\left(\mathbb{P}^\alpha|\mathbb{P}\right)(T) = \left[\frac{\mu\lambda}{\mu+\lambda}T + \frac{(\lambda-\mu)\left[p\left(\lambda+\mu\right)-\mu\right]}{2\left(\lambda+\mu\right)^2}\left[1-\exp\left[-\left(\lambda+\mu\right)T\right]\right]\right]\alpha^2 \tag{3.53}$$

Again, by setting

$$\left\langle\Sigma\right\rangle(T) = 4\left[\frac{\mu\lambda}{\mu+\lambda}T + \frac{(\lambda-\mu)\left[p\left(\lambda+\mu\right)-\mu\right]}{2\left(\lambda+\mu\right)^2}\left[1-\exp\left[-\left(\lambda+\mu\right)T\right]\right]\right] \tag{3.54}$$

and, as before, by noting

$$\left\langle Q\right\rangle^\alpha(T) = \left\langle Q\right\rangle\left(\left(1+\alpha\right)T\right) \approx \left\langle Q\right\rangle(T) + \alpha T\left\langle \dot{Q}\right\rangle(T) \tag{3.55}$$

(because changing simultaneously λ e μ by a factor $1+\alpha$ is the same as performing a time scaling of the same factor) we are able to use equation (2.34)

$$\frac{h^2}{2}\left\langle\Delta Q^2\right\rangle(T) \geq h\alpha T\left\langle\dot{Q}\right\rangle(T) - \frac{\alpha^2}{4}\left\langle\Sigma\right\rangle(T)$$

where, once more, by posing

$$\alpha = \frac{2hT\left\langle\dot{Q}\right\rangle(T)}{\left\langle\Sigma\right\rangle(T)} \tag{3.56}$$

we get

$$\left\langle\Delta Q^2\right\rangle(T) \geq \frac{\left(T\left\langle\dot{Q}\right\rangle(T)\right)^2}{2\left[\frac{\mu\lambda}{\mu+\lambda}T + \frac{(\lambda-\mu)\left[p\left(\lambda+\mu\right)-\mu\right]}{2\left(\lambda+\mu\right)^2}\left[1-\exp\left[-\left(\lambda+\mu\right)T\right]\right]\right]} \tag{3.57}$$

that is clearly the same as equation (3.31).
It is time now to treat the current terms. For this purpose we will use a counting process that counts the times the system returns to state 1 after being at 2. In other words, if we decide to start from state 1 at time 0 and T_m is the time at which the mth jump occurs $i \to j$, $i \neq j$ and we define

$$\tau_n = \inf\{t \in [0,T]\,|t > T_{2m-1} \wedge X(t) = 1\} \tag{3.58}$$

we have that

$$Q(t) = N(t) = n \qquad \text{when} \qquad t \in [\tau_n, \tau_{n+1}) \tag{3.59}$$

We are thus interested in $m(t) = \left\langle N\right\rangle(t)$ and subsequently in $\left\langle\dot{N}\right\rangle(t)$ and $\left\langle\Delta N^2\right\rangle(t)$ (from now on we will abandon the $\mathbb{P}$ superscript in the $\left\langle\,\cdot\,\right\rangle$ notation). A well known result of renewal theory states that, for a counting process, it holds that

$$\left\langle N\right\rangle(T) = m(T) = F(T) + \int_0^T m(T{-}s)\,F'(s)\,ds \tag{3.60}$$

where $F(t)$ is the survival function, $F_i(t) = 1{-}e^{-\gamma_i t}$ and $F_i'(t) = f_i(t)$ is the probability density function of jumping from i to the other state. In fact

$$\begin{gathered} m(t) = \mathbb{E}\left[N(t)\right] = \int_0^\infty \mathbb{E}\left[N(t)\,|\tau_1 = s\right]f(s)\,ds = \\ \int_0^t \mathbb{E}\left[N(t)\,|\tau_1 = s\right]f(s)\,ds + \int_t^\infty 0ds = \int_0^t \mathbb{E}\left[\left(1+N(t-s)\right)\right]f(s)\,ds = \\ \int_0^t \left[1+\mathbb{E}\left[N(t-s)\right]\right]f(s)\,ds = F(t) + \int_0^t m(t-s)\,f(s)\,ds \end{gathered} \tag{3.61}$$

The fact that $\mathbb{E}\left[N\left(t\right)|\tau_1 = s\right] = \mathbb{E}\left[\left(1 + N\left(t - s\right)\right)\right]$ justifies the name of "renewal process". Moreover, for this particular system, it holds

$$F\left(T\right) = \int_0^T F_1\left(T - s\right) F_2'\left(s\right) ds = \left[F_1 \star F_2\right]\left(T\right) \tag{3.62}$$

where $\star$ stands for convolution.
To solve (3.60) we make use of Laplace-Stieltjes transform, for which it holds that

$$\mathcal{L}^*\left[h\left(t\right)\right] = \hat{h}\left(s\right) \qquad\qquad \mathcal{L}^*\left[\left[h_1 \star h_2\right]\left(t\right)\right] = \hat{h}_1\left(s\right) \cdot \hat{h}_2\left(s\right) \tag{3.63}$$

so that we can make (3.60) an algebraic equation

$$\hat{m}\left(s\right) = \hat{F}\left(s\right) + \hat{m}\left(s\right) \cdot \hat{F}\left(s\right) \implies \hat{m}\left(s\right) = \frac{\hat{F}\left(s\right)}{1 - \hat{F}\left(s\right)} = \frac{\hat{F}_1\left(s\right) \cdot \hat{F}_2\left(s\right)}{1 - \hat{F}_1\left(s\right) \cdot \hat{F}_2\left(s\right)} \tag{3.64}$$

Moreover we have that

$$\mathcal{L}^*\left[F_i\left(t\right)\right] = \mathcal{L}^*\left[1 - e^{-\gamma_i t}\right] = 1 - \frac{s}{s + \gamma_i} \tag{3.65}$$

so that (3.64) becomes

$$\hat{m}\left(s\right) = \frac{\left(1 - \frac{s}{s+\lambda}\right)\left(1 - \frac{s}{s+\mu}\right)}{1 - \left(1 - \frac{s}{s+\lambda}\right)\left(1 - \frac{s}{s+\mu}\right)} = \frac{\lambda\mu}{s\left(s + \lambda + \mu\right)} \tag{3.66}$$

Another well known rule of Laplace-Stieltjes transform is that

$$\hat{h}\left(s\right) = \mathcal{L}^*\left[h\left(t\right)\right] = \mathcal{L}\left[h'\left(t\right)\right] \tag{3.67}$$

where $\mathcal{L}\left[\cdot\right]$ stands for standard Laplace transform. Hence

$$\left\langle \dot{N} \right\rangle\left(t\right) = m'\left(t\right) = \mathcal{L}^{-1}\left[\hat{m}\left(s\right)\right] = \mathcal{L}^{-1}\left[\frac{\lambda\mu}{s\left(s + \lambda + \mu\right)}\right] = \frac{\mu\lambda}{\mu + \lambda}\left(1 - e^{-t\left(\mu+\lambda\right)}\right) \tag{3.68}$$

and

$$\left\langle N \right\rangle\left(t\right) = m\left(t\right) = \int_0^t m'\left(s\right) ds = \frac{\mu\lambda}{\mu + \lambda} t + \frac{\mu\lambda}{\left(\mu + \lambda\right)^2}\left(e^{-t\left(\mu+\lambda\right)} - 1\right) \tag{3.69}$$

We will later put these results in equation (3.57), but first we calculate

$$\left\langle \Delta N^2 \right\rangle\left(t\right) = \mathrm{Var}\left[N\left(t\right)\right] = \mathbb{E}\left[N^2\left(t\right)\right] - \left[\mathbb{E}\left[N\left(t\right)\right]\right]^2 = g\left(t\right) - m^2\left(t\right) \tag{3.70}$$

We now focus on $g\left(t\right)$. We have that, similarly to (3.61)

$$\begin{gathered} g\left(t\right) = \mathbb{E}\left[N^2\left(t\right)\right] = \int_0^\infty \mathbb{E}\left[N^2\left(t\right)|\tau_1 = s\right] f\left(s\right) ds = \\ \int_0^t \mathbb{E}\left[N^2\left(t\right)|\tau_1 = s\right] f\left(s\right) ds + \int_t^\infty 0 ds = \int_0^t \mathbb{E}\left[\left(1 + N\left(t - s\right)\right)^2\right] f\left(s\right) ds = \\ \int_0^t \left[1 + 2\mathbb{E}\left[N\left(t - s\right)\right] + \mathbb{E}\left[N^2\left(t - s\right)\right]\right] f\left(s\right) ds = \\ F\left(t\right) + 2\int_0^t m\left(t - s\right) f\left(s\right) ds + \int_0^t g\left(t - s\right) f\left(s\right) ds \end{gathered} \tag{3.71}$$

or

$$g\left(t\right) = F\left(t\right) + 2\left[m \star F\right]\left(t\right) + \left[g \star F\right]\left(t\right)$$

As before, we use Laplace-Stieltjes to get an algebraic equation

$$\begin{aligned}\hat{g}(s) &= \hat{F}(s) + 2\hat{m}(s)\hat{F}(s) + \hat{g}(s)\hat{F}(s) \\ \hat{g}(s) &= \frac{\hat{F}(s)}{1-\hat{F}(s)}\left(1+2\hat{m}(s)\right) = \hat{m}(s) + 2\hat{m}^2(s)\end{aligned} \tag{3.72}$$

Again

$$\hat{g}(s) = \mathcal{L}^*\left[g(t)\right] = \mathcal{L}\left[g'(t)\right] \qquad g'(t) = \mathcal{L}^{-1}\left[\hat{g}(s)\right] = m'(t) + \mathcal{L}^{-1}\left[\hat{m}^2(s)\right] \tag{3.73}$$

thus

$$\begin{aligned}g'(t) =& m'(t) + \mathcal{L}^{-1}\left[\left[\frac{\lambda\mu}{s(s+\lambda+\mu)}\right]^2\right] = \frac{\mu\lambda}{\mu+\lambda}\left(1 - e^{-t(\mu+\lambda)}\right) + \\ &+ 2\left[\frac{\mu\lambda}{\mu+\lambda}\right]\left[te^{-t(\mu+\lambda)} + 2\frac{e^{-t(\mu+\lambda)}}{\mu+\lambda} - \frac{2}{\mu+\lambda}\right]\end{aligned} \tag{3.74}$$

Finally we have

$$\begin{aligned}\left\langle \Delta N^2\right\rangle(t) = \int_0^t g'(s)\,ds - m^2(t) = \frac{\mu\lambda t}{(\mu+\lambda)^3}\left[\lambda^2+\mu^2 - 4\mu\lambda e^{-t(\mu+\lambda)}\right] + \\ + \frac{\mu\lambda}{(\mu+\lambda)^4}\left[\left(\lambda^2+\mu^2\right)\left(e^{-t(\mu+\lambda)}-1\right) + \mu\lambda\left(3 - 2e^{-t(\mu+\lambda)} - e^{-2t(\mu+\lambda)}\right)\right]\end{aligned} \tag{3.75}$$

We now put all together by substituting (3.68) and (3.75) into (3.57)

$$\begin{aligned}&\frac{2}{(\mu+\lambda)^2}\left[\lambda^2+\mu^2-4\mu\lambda e^{-T(\mu+\lambda)}\right] + \\ &+\frac{2}{T(\mu+\lambda)^3}\left[\left(\lambda^2+\mu^2\right)\left(e^{-T(\mu+\lambda)}-1\right) + \mu\lambda\left(3-2e^{-T(\mu+\lambda)} - e^{-2T(\mu+\lambda)}\right)\right] \geq \\ &\frac{\left[1-e^{-T(\mu+\lambda)}\right]^2}{1+\frac{(\lambda-\mu)\left[p(\lambda+\mu)-\mu\right]}{2\lambda\mu T(\lambda+\mu)}\left[1-e^{-(\lambda+\mu)T}\right]}\end{aligned} \tag{3.76}$$

We now have to see if this inequality holds or not and we start considering stationary states, namely as $T\to\infty$, thus we shall first verify (3.76) in this case. We obtain

$$\frac{2}{(\mu+\lambda)^2}\left[\lambda^2+\mu^2\right] \geq 1 \implies (\mu-\lambda)^2 \geq 0 \tag{3.77}$$

which means that the inequality holds and that it becomes an equality for a standard Poisson process. Let us return to the general case. We set

$$\begin{aligned}h(t,\lambda,\mu) = &\left[\frac{2}{(\mu+\lambda)^2}\left[\lambda^2+\mu^2-4\mu\lambda e^{-T(\mu+\lambda)}\right] + \frac{2}{T(\mu+\lambda)^3}\cdot\right. \\ &\left.\cdot\left[\left(\lambda^2+\mu^2\right)\left(e^{-T(\mu+\lambda)}-1\right) + \mu\lambda\left(3-2e^{-T(\mu+\lambda)}-e^{-2T(\mu+\lambda)}\right)\right]\right].\end{aligned} \tag{3.78}$$

so that (3.76) becomes

$$I(T) = \frac{\left[1-e^{-(\lambda+\mu)T}\right]^2}{h(T,\lambda,\mu)\left[1+\frac{(\lambda-\mu)\left[p(\lambda+\mu)-\mu\right]}{2\lambda\mu T(\lambda+\mu)}\left[1-e^{-(\lambda+\mu)T}\right]\right]} \leq 1 \tag{3.79}$$

We now want to verify whether this inequality holds or not and, being the above expression too complicated to do it analytically, we will do it by plotting $I(T)$ for different values of the available parameters. First of all we notice that the dynamics of the system is determined only by the ratio of the two driving parameters λ and μ up to a time rescaling and consequently, as a matter of convenience, we will plot $I(T)$ setting $\lambda = 1$. In the following plots the p parameter is fixed for each figure (the considered values of p are $\{0,\ 1/4,\ 1/2,\ 3/4,\ 1\}$) to see whether the inequality holds for every initial condition (for example $p = 1$ means that we are considering the dynamics to start from state 1). That is what we have obtained

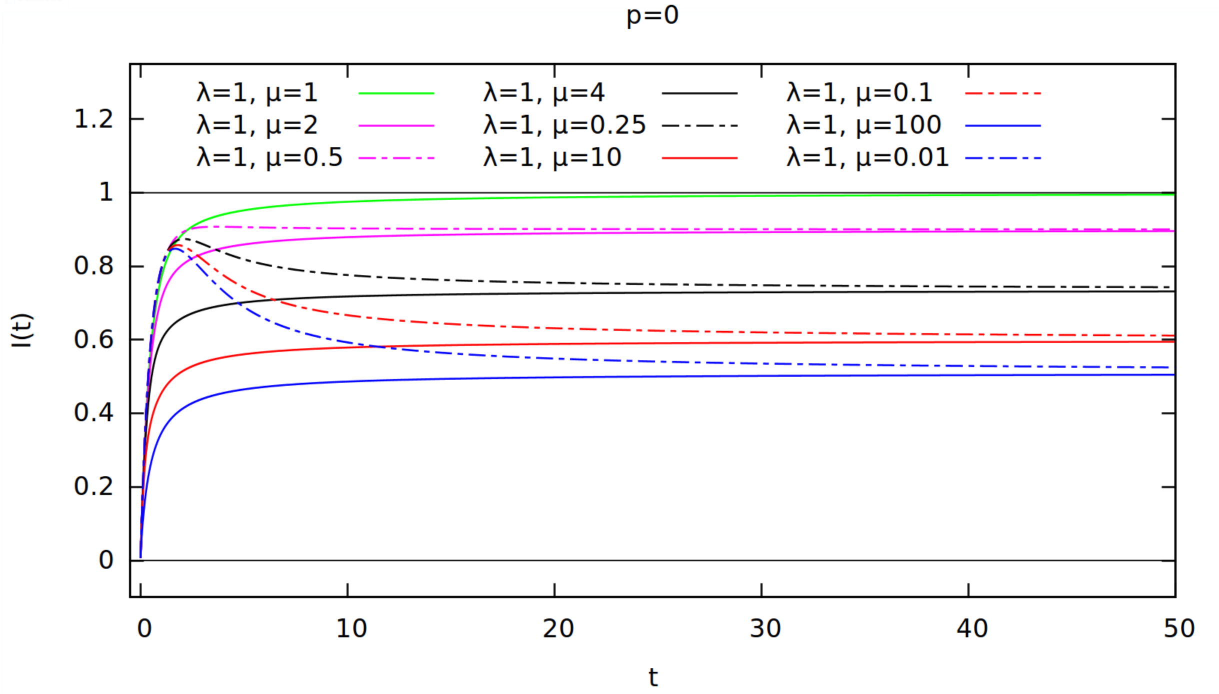


Figure 1: Plot of $I(T)$ with fixed $p = 0$

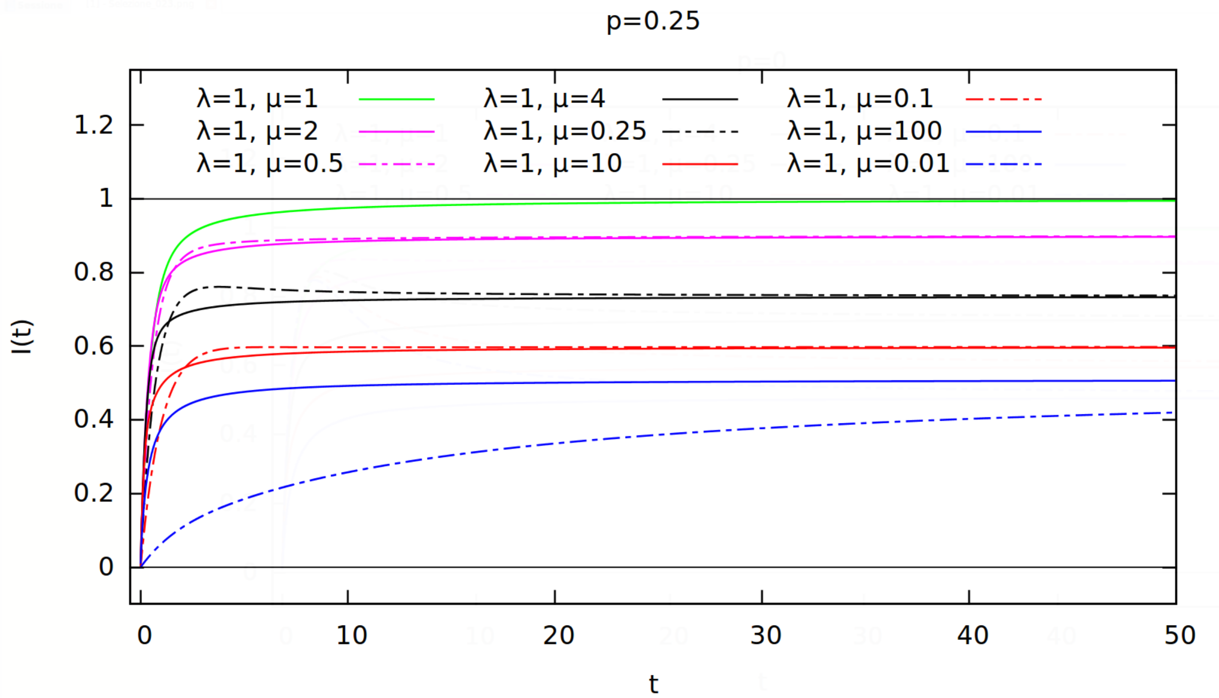


Figure 2: Plot of $I(T)$ with fixed $p = 0.25$

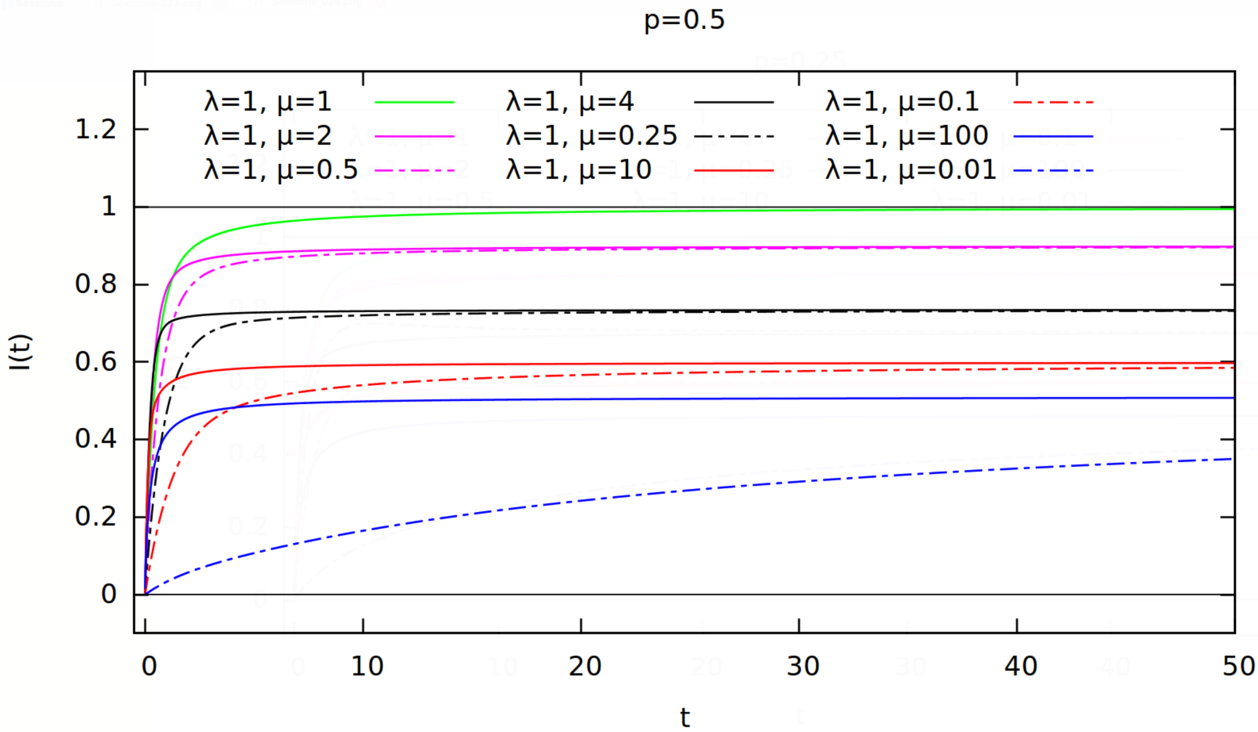


Figure 3: Plot of $I(T)$ with fixed $p = 0.5$

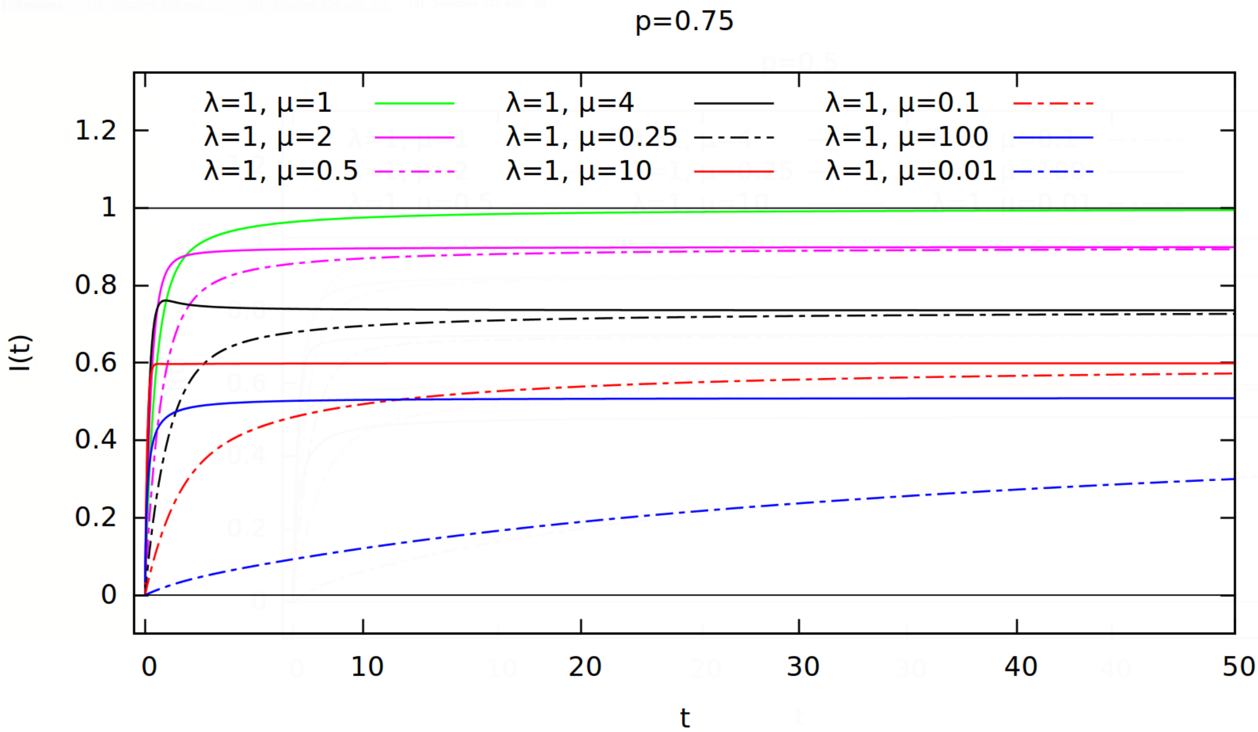


Figure 4: Plot of $I(T)$ with fixed $p = 0.75$

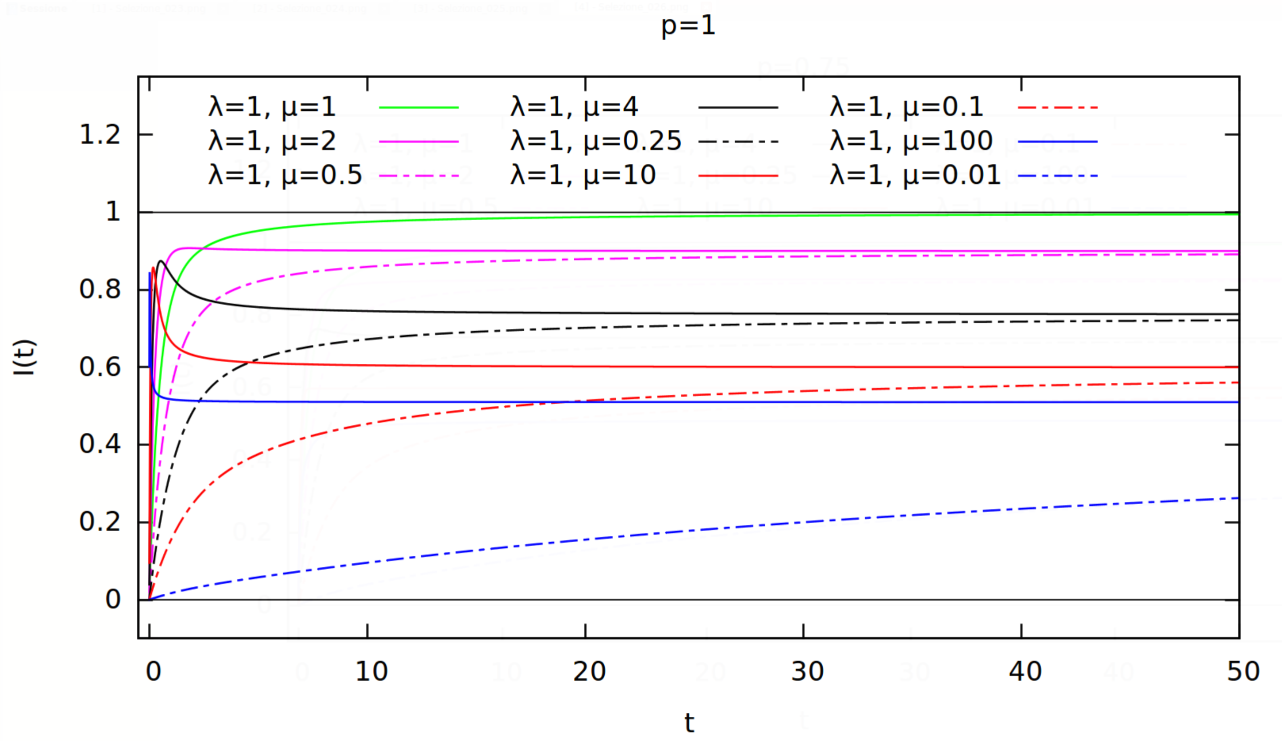


Figure 5: Plot of $I(T)$ with fixed $p = 1$

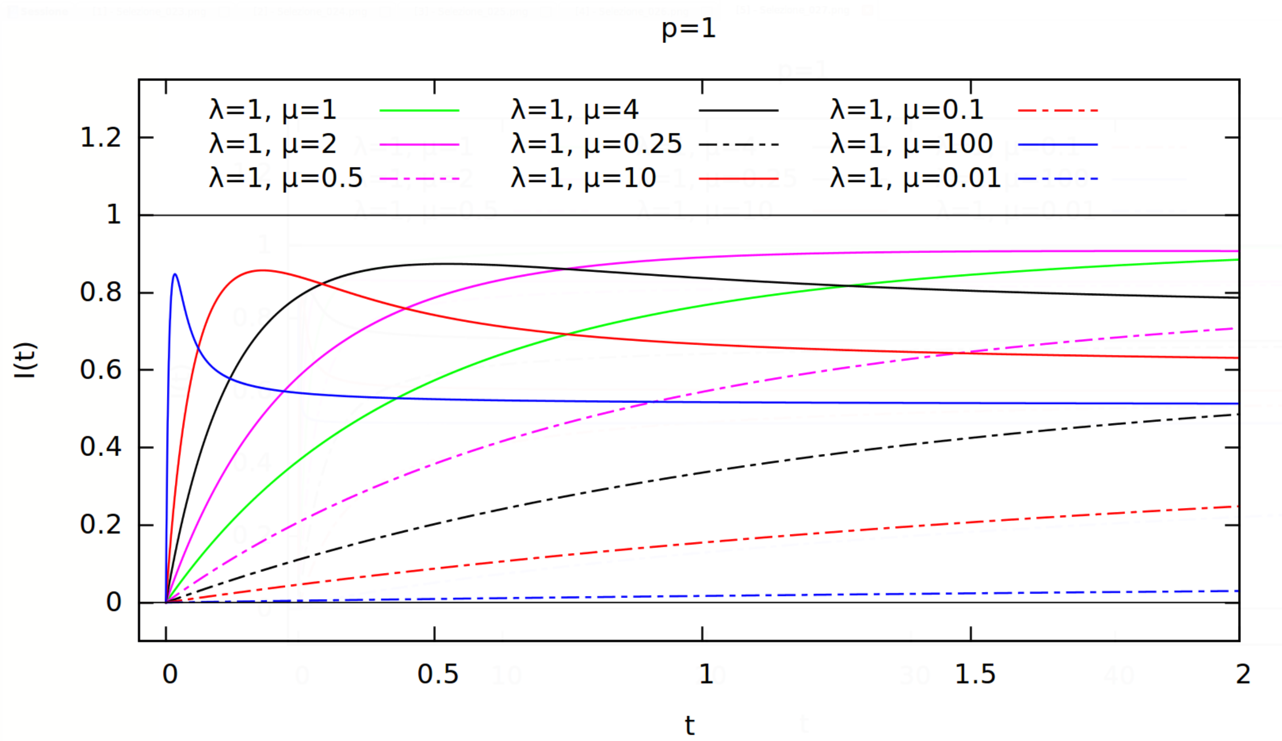


Figure 6: Zoomed plot of $I(T)$ with fixed $p = 1$

Figure 6 is a zoom of figure 5 in order to better show the short time behaviour of the dynamics with $p = 1$. We see that all the curves plotted above lie in the region $\{(x, y)\,|0 \leq y \leq 1\, x \geq 0$ of the plane and this means that the inequality is verified. Moreover, if we have μ_1 and μ_2 such that $\mu_1 = \dfrac{1}{\mu_2}$ we observe, as expected, the same large time behaviour.

4 Markov diffusion processes

From an historical point of view, the Langevin equation was initially formulated to describe Brownian motion, in which we can imagine a mesoscopic particle bathed in a fluid at thermal equilibrium and subject to a random force due to the many random collisions with the fluids molecules and to a friction caused by the fluid's viscosity. Mathematically speaking this can be translated in a first order stochastic differential equation, which is precisely the first version of Langevin equation

$$m\frac{d\vec{v}}{dt}(t) = -\gamma\vec{v}(t) + \vec{f}(t) \tag{4.1}$$

where $\vec{f}(t)$ is the aforementioned random force and γ is the friction coefficient (in first approximation one could use Stoke's law for which $\gamma = 6\pi R\mu$, assuming that the Brownian particle is a sphere with radius R and that the fluid has viscosity μ). We should now focus on the source of randomness of the process that is, as mentioned above, the chaotic thermal motion of the fluid's molecules. We also considered as hypothesis a mesoscopic particle, which means that the Brownian particle is little enough to be hit by a small number of molecules so that there happen to be temporary imbalances of the force exerted on the particle, and big in such a manner to be hit by a number of molecules large enough to make this fluctuating force Gaussian. For this reason, from now on we use the same notation of (2.1) and (2.10) putting $\vec{f}(t) = f_i(t) = G_0\xi_i(t)$ with

$$\langle \xi_i(t)\rangle = 0 \qquad\qquad \langle \xi_i(t)\,\xi_j(s)\rangle = \delta_{i,j}\delta(t-s) \tag{4.2}$$

and all higher moments are either zero or a function of $\langle \xi_i(t)\,\xi_i(s)\rangle$.
Equation (4.1) is well known from the early decades of the XX century, and since then it has been widely studied. Instead, we will focus on a generalized version of this equation that includes an external force which can be constant, such as in the case of gravitational force or a constant electric field (assuming that the Brownian particle is charged, of course), time dependent (oscillating electric field), position dependent (for example an harmonic potential) or both time and position dependent. We thus obtain an equation of the form

$$\frac{d\vec{x}}{dt}(t) = \vec{v}(t)$$

$$m\frac{d\vec{v}}{dt}(t) = -\gamma\vec{v}(t) + \vec{F}(x,t) + G_0\vec{\xi}(t) \tag{4.3}$$

Our purpose will be, as might be expected, to derive new nonequilibrium inequalities by explicitly calculating the Kullback-Leibler divergence and the excess current and variance of a given current. Of course, apart from the case of constant force which is trivial, the simplest case is the one with no position dependence, this means that for a given t the force is constant in space. We will start from this simpler case.

4.1 Time dependent force

As previously said, we now consider the particular case of time dependent external force, so that equation (4.3) becomes

$$m\frac{d\vec{v}}{dt}(t) = -\gamma\vec{v}(t) + \vec{F}(t) + G_0\vec{\xi}(t) \tag{4.4}$$

For simplicity we will consider the unidimensional case knowing that, being the components of the random force independent stochastic variables with correlation equal to 0, the results that will be obtained in this section will be valid for each component of $\vec{x}(t)$ and $\vec{v}(t)$. The most efficient way to formally solve the unidimensional version of equation (4.4) is through the use of Laplace transforms. In fact, remembering that $\mathcal{L}\left[\frac{df}{dt}(t)\right](k) = k\mathcal{L}[f(t)](k) - f(0^+)$ we obtain the following algebraic equation

$$\begin{aligned}\hat{v}(k)\left[k+\frac{\gamma}{m}\right] &= v_0 + \frac{\hat{F}(k)}{m} + \frac{G_0}{m}\hat{\xi}(k) \\ \hat{v}(k) &= \frac{1}{\left[k+\frac{\gamma}{m}\right]}\left[v_0 + \frac{\hat{F}(k)}{m} + \frac{G_0}{m}\hat{\xi}(k)\right]\end{aligned} \tag{4.5}$$

where it is clear that $v_0 = v(0)$. From now on we set

$$\hat{\chi}_v(k) = \frac{1}{\left[k+\frac{\gamma}{m}\right]} \qquad\qquad \chi_v(t) = \exp\left[-\frac{\gamma}{m}t\right] \tag{4.6}$$

that is the velocity response function, namely, as we will see, it is the function that embodies the informations of how the velocity behaves as an external force is applied to the system.
By transforming back to real time we get

$$v(t) = v_0\chi_v(t) + \frac{1}{m}\int_0^t \chi_v(t-s)F(s) + \frac{G_0}{m}\int_0^t \chi_v(t-s)\xi(s) \tag{4.7}$$

Thus equation (4.7) becomes

$$v(t) = v_0 e^{\left[-\frac{\gamma}{m}t\right]} + \frac{1}{m}\int_0^t e^{\left[-\frac{\gamma}{m}(t-s)\right]}\cdot\left[F(s) + G_0\xi(s)\right] \tag{4.8}$$

We now calculate the velocity correlation, which will be useful later. By definition we have

$$\begin{aligned} C(t_2,t_1) = \langle v(t_2)v(t_1)\rangle = \Big\langle v_0^2 e^{\left[-\frac{\gamma}{m}(t_1+t_2)\right]} + \\ +\frac{v_0}{m}e^{\left[-\frac{\gamma}{m}t_1\right]}\int_0^{t_2} ds_2 e^{\left[-\frac{\gamma}{m}(t_2-s_2)\right]}\cdot\left[F(s_2)+G_0\xi(s_2)\right] + \\ +\frac{v_0}{m}e^{\left[-\frac{\gamma}{m}t_2\right]}\int_0^{t_1} ds_1 e^{\left[-\frac{\gamma}{m}(t_1-s_1)\right]}\cdot\left[F(s_1)+G_0\xi(s_1)\right] + \\ +\int_0^{t_1}\frac{ds_1}{m}\int_0^{t_2}\frac{ds_2}{m}e^{\left[-\frac{\gamma}{m}(t_1+t_2-s_1-s_2)\right]}\left[F(s_1)+G_0\xi(s_1)\right]\left[F(s_2)+G_0\xi(s_2)\right]\Big\rangle = \\ \phi_v(t_1)\phi_v(t_2) + v_0^2 e^{\left[-\frac{\gamma}{m}(t_1+t_2)\right]} + \frac{v_0}{m}\left[e^{\left[-\frac{\gamma}{m}t_1\right]}\phi_v(t_2) + e^{\left[-\frac{\gamma}{m}t_2\right]}\phi_v(t_1)\right] + \\ +\frac{G_0^2}{m^2}\int_0^{t_1} ds_1\int_0^{t_2} ds_2 e^{\left[-\frac{\gamma}{m}(t_1-s_1)\right]}e^{\left[-\frac{\gamma}{m}(t_2-s_2)\right]}\delta(s_2-s_1)\end{aligned} \tag{4.9}$$

where we defined the velocity susceptibility to an external force $F(t)$. As we previously said, the response function $\chi_v(t)$ plays a fundamental role in expressing how the velocity behaves after an external force is applied.

$$\phi_v(t) = \int_0^t ds e^{\left[-\frac{\gamma}{m}(t-s)\right]}F(s) \tag{4.10}$$

Let us now focus on the last term of equation (4.9), which can be simplified as follows

$$\begin{aligned} \frac{G_0^2}{m^2}e^{\left[-\frac{\gamma}{m}(t_2+t_1)\right]}\int_0^{t_1} ds_1\int_0^{t_2} ds_2 e^{\left[\frac{\gamma}{m}(s_2+s_1)\right]}\delta(s_2-s_1) = \\ \frac{G_0^2}{m^2}e^{\left[-\frac{\gamma}{m}(t_2+t_1)\right]}\int_0^{\infty} ds_1\int_0^{\infty} ds_2 e^{\left[\frac{\gamma}{m}(s_2+s_1)\right]}\theta(t_1-s_1)\theta(t_2-s_2)\delta(t_1-s_1) = \\ \frac{G_0^2}{m^2}e^{\left[-\frac{\gamma}{m}(t_2+t_1)\right]}\int_0^{\infty} ds_1 e^{\left[\frac{2\gamma}{m}s_1\right]}\theta(t_1-s_1)\theta(t_2-s_1) = \\ \frac{G_0^2}{m^2}e^{\left[-\frac{\gamma}{m}(t_2+t_1)\right]}\int_0^{\min(t_1,t_2)} ds_1 e^{\left[\frac{2\gamma}{m}s_1\right]} = \frac{G_0^2}{2\gamma m}e^{\left[-\frac{\gamma}{m}(t_2+t_1)\right]}\left[e^{\left[\frac{2\gamma}{m}\min(t_1,t_2)\right]} - 1\right]\end{aligned} \tag{4.11}$$

where in the last row we used the fact that

$$\theta\left(t_1-s_1\right)\theta\left(t_2-s_1\right)=\theta\left(\min\left(t_1,t_2\right)-s_1\right)$$

Furthermore it is known that $2\min\left(t_1,t_2\right)=\left(t_1+t_2\right)-\left|t_1-t_2\right|$ so that (4.11) becomes

$$\frac{G_0^2}{2\gamma m}e^{\left[-\frac{\gamma}{m}\left(t_2+t_1\right)\right]}\left[e^{\left[\frac{2\gamma}{m}\min\left(t_1,t_2\right)\right]}-1\right]=\frac{G_0^2}{2\gamma m}\left[e^{\left[-\frac{\gamma}{m}\left|t_1-t_2\right|\right]}-e^{\left[-\frac{\gamma}{m}\left(t_1+t_2\right)\right]}\right] \tag{4.12}$$

and hence the two point velocity correlation $C\left(t_1,t_2\right)$ finally becomes

$$\begin{aligned}\left\langle v\left(t_2\right)v\left(t_1\right)\right\rangle=\frac{G_0^2}{2\gamma m}\left[e^{\left[-\frac{\gamma}{m}\left|t_1-t_2\right|\right]}-e^{\left[-\frac{\gamma}{m}\left(t_1+t_2\right)\right]}\right]+\\+\phi_v\left(t_1\right)\phi_v\left(t_2\right)+v_0^2e^{\left[-\frac{\gamma}{m}\left(t_1+t_2\right)\right]}+\frac{v_0}{m}\left[e^{\left[-\frac{\gamma}{m}t_1\right]}\phi_v\left(t_2\right)+e^{\left[-\frac{\gamma}{m}t_2\right]}\phi_v\left(t_1\right)\right]\end{aligned} \tag{4.13}$$

From this expression we can finally infer the value of G_0. First we consider the correlation function at equal times, which stands for the mean square velocity. We have

$$\left\langle v^2\left(t\right)\right\rangle=\frac{G_0^2}{2\gamma m}\left[1-e^{\left[-\frac{2\gamma t}{m}\right]}\right]+\phi_v^2\left(t\right)+v_0^2e^{\left[-\frac{2\gamma t}{m}\right]}+\frac{2v_0}{m}e^{\left[-\frac{2\gamma t}{m}\right]}\phi_v\left(t\right) \tag{4.14}$$

If we take the limit $t\to\infty$ and set $F\left(t\right)=0$, we know from equipartition theorem that

$$\frac{m}{2}\left\langle v^2\left(\infty\right)\right\rangle_{F=0}=\frac{G_0^2}{4\gamma}=\frac{1}{2}k_BT\qquad\Longrightarrow\qquad G_0=\sqrt{2\gamma k_BT} \tag{4.15}$$

At this point it is interesting to calculate the variance of the velocity, which by definition is

$$\mathrm{Var}\left[v\left(t\right)\right]=\left\langle\left(v\left(t\right)-\left\langle v\left(t\right)\right\rangle\right)^2\right\rangle=\left\langle v^2\left(t\right)\right\rangle-\left\langle v\left(t\right)\right\rangle^2 \tag{4.16}$$

In fact, the knowledge of this quantity will be useful later on. For this purpose, it is necessary to calculate

$$\left\langle v\left(t\right)\right\rangle^2=\left[v_0e^{\left[-\frac{\gamma}{m}t\right]}+\phi_v\left(t\right)\right]^2=\phi_v^2\left(t\right)+v_0^2e^{\left[-\frac{2\gamma}{m}t\right]}+\frac{2v_0}{m}e^{\left[-\frac{2\gamma}{m}t\right]}\phi_v\left(t\right) \tag{4.17}$$

Hence we get

$$\mathrm{Var}\left[v\left(t\right)\right]=\left\langle\Delta v^2\left(t\right)\right\rangle=\frac{k_BT}{m}\left[1-e^{\left[-\frac{2\gamma t}{m}\right]}\right] \tag{4.18}$$

We note that $\Delta v^2\left(t\right)$ does not depend on the external force. This is reasonable because the variance is a measure of the indetermination of the process, which is of course due to the fluctuating force coming from the thermal bath. On the other hand the external force is a deterministic component of the process and hence does not contribute to the variance, instead it is obviously present in the mean velocity expression becoming the only contribution at large times.
We now focus on the position instead of velocity, calculating the mean displacement, variance and probability distribution which will be useful to calculate the Kullback-Leibler divergence of the process. Of course we have

$$\begin{aligned}x\left(t\right)=x_0+\int_0^t v\left(s\right)ds=x_0+\int_0^t ds\left[v_0e^{\left[-\frac{\gamma}{m}s\right]}+\int_0^s\frac{e}{m}^{\left[-\frac{\gamma}{m}\left(s-q\right)\right]}\left[F\left(q\right)+\right.\right.\\\left.\left.+\sqrt{2\gamma k_BT}\xi\left(q\right)\right]\right]=x_0+\frac{v_0m}{\gamma}\left[1-e^{\left[-\frac{\gamma}{m}t\right]}\right]+\phi_x\left(t\right)+\sqrt{2\gamma k_BT}\psi_x\left(t\right)\end{aligned} \tag{4.19}$$

with

$$\phi_x\left(t\right)=\int_0^t ds\phi_v\left(s\right)\qquad\qquad\psi_x\left(t\right)=\int_0^t ds\psi_v\left(s\right)=\frac{1}{m}\int_0^t ds\int_0^s dqe^{\left[-\frac{\gamma}{m}\left(s-q\right)\right]}\xi\left(q\right) \tag{4.20}$$

that are respectively the position's susceptibilities to the external force $F(t)$ and to the random force $\xi(t)$. It is also possible to express these relations through

$$\phi_x(t) = \frac{1}{m}\int_0^t ds\chi_x(t{-}s)\,F(s) \qquad\qquad \psi_x(t) = \frac{1}{m}\int_0^t ds\chi_x(t{-}s)\,\xi(q) \tag{4.21}$$

where

$$\chi_x(t) = \int_0^t ds\chi_v(t) \tag{4.22}$$

is the position response function that has an analogous meaning of $\chi_v(t)$. Moreover it clearly holds that $\langle\psi_x(t)\rangle = \langle\psi_v(t)\rangle = 0$. It is obvious that, being the other terms of (4.19) not aleatory and thus equal to their mean, it holds that

$$\langle x(t)\rangle = x_0 + \frac{v_0 m}{\gamma}\left[1 - e^{\left[-\frac{\gamma}{m}t\right]}\right] + \phi_x(t) \tag{4.23}$$

Moreover, the position's variance can be found starting from its definition

$$\mathrm{Var}[x(t)] = \langle\Delta x^2(t)\rangle = \langle(x(t) - \langle x(t)\rangle)^2\rangle \tag{4.24}$$

To calculate this quantity we use, as one would expect, equation (4.19) and (4.23)

$$\begin{gathered}\langle(x(t) - \langle x(t)\rangle)^2\rangle = 2\gamma k_B T\langle\psi_x^2(t)\rangle = 2\gamma k_B T\int_0^t ds_1\int_0^t ds_2\langle\psi_v(s_1)\,\psi_v(s_2)\rangle = \\ \frac{2\gamma k_B T}{m^2}\int_0^t ds_1\int_0^t ds_2\left[\int_0^{s_1} dq_1\int_0^{s_2} dq_2 e^{\left[-\frac{\gamma}{m}(s_1-q_1)\right]}e^{\left[-\frac{\gamma}{m}(s_2-q_2)\right]}\langle\xi(q_1)\,\xi(q_2)\rangle\right]\end{gathered} \tag{4.25}$$

The term between square brackets in the last line has already been calculated in (4.12), thus (4.25) becomes

$$\begin{gathered}\langle\Delta x^2(t)\rangle = \frac{k_B T}{m}\int_0^t ds_1\int_0^t ds_2\left[e^{\left[-\frac{\gamma}{m}|s_1-s_2|\right]} - e^{\left[-\frac{\gamma}{m}(s_1+s_2)\right]}\right] = \\ \frac{k_B T}{m}\left[\int_0^t ds_1\int_0^{s_1} ds_2 e^{\left[-\frac{\gamma}{m}(t_1-t_2)\right]} - \left(\int_0^t ds_1 e^{\left[-\frac{\gamma}{m}s_1\right]}\right)^2\right] = \\ \frac{k_B T}{\gamma}\left[2\left[t - \frac{m}{\gamma}\left[1 - e^{\left[-\frac{\gamma}{m}t\right]}\right]\right] - \frac{m}{\gamma}\left[1 - e^{\left[-\frac{\gamma}{m}t\right]}\right]^2\right] = \\ \frac{k_B T}{\gamma}\left[2t + \frac{m}{\gamma}\left[4e^{\left[-\frac{\gamma}{m}t\right]} - e^{\left[-\frac{2\gamma}{m}t\right]} - 3\right]\right]\end{gathered} \tag{4.26}$$

Again this result does not depend on the external force, the reason is the same as before the external force is a deterministic component of the process and does not contribute to the random part of it, thus it does not appear in the variance's expression. We have thus obtained both the mean value and the variance of the position, these two objects would be enough to characterize the probability density function of the random variable $x(t)$ if this was a Gaussian variable. Fortunately, it was nicely shown in [13] that $x(t)$ has a Gaussian distribution with mean and variance given respectively by (4.23) and (4.26). We thus obtain

$$\begin{gathered}P(x,t|x_0,v_0) = \left[\frac{\gamma}{2\pi k_B T\left[2t + \frac{m}{\gamma}\left[4e^{\left[-\frac{\gamma}{m}t\right]} - e^{\left[-\frac{2\gamma}{m}t\right]} - 3\right]\right]}\right]^{\frac{1}{2}}\cdot \\ \cdot\exp\left[-\frac{\gamma\left(x(t) - x_0 - \frac{v_0 m}{\gamma}\left[1 - e^{\left[-\frac{\gamma}{m}t\right]}\right] - \phi_x(t)\right)^2}{2k_B T\left[2t + \frac{m}{\gamma}\left[4e^{\left[-\frac{\gamma}{m}t\right]} - e^{\left[-\frac{2\gamma}{m}t\right]} - 3\right]\right]}\right]\end{gathered} \tag{4.27}$$

But we are not done yet, in fact the v_0 dependence of the probability density function is somewhat troublesome and we want to get rid of it. To do so, we must average with respect to all possible initial velocities, using the probability density function relative to v_0. Mathematically

$$P(x,t|x_0) = \int_{-\infty}^{\infty} dv_0 P(v_0)\, P(x,t|x_0,v_0) \tag{4.28}$$

with of course $\int_{-\infty}^{\infty} dv_0 P(v_0) = 1$. In order to obtain an analytical expression for $P(v_0)$ we must remember the physical situation from which we started, namely a Brownian particle in a thermal bath at a certain temperature T and hence the initial velocity v_0 follows the Boltzman statistics. In fact, if $F(t) = 0$ for $t \leq 0$ (which we will assume hereafter) the initial velocity probability density function takes the following form

$$P(v_0) = \sqrt{\frac{m}{2\pi k_B T}} \exp\left[-\frac{mv_0^2}{2k_B T}\right] \tag{4.29}$$

Before plugging this result in equation (4.28) we rewrite (4.27) in a slightly different notation, in fact remembering equation (4.22) we put

$$\langle x(t)\rangle_{v_0} = x_0 + \phi_x(t) \qquad\qquad \chi_x(t) = \int_0^t ds\chi_v(s) = \frac{m}{\gamma}\left[1 - e^{\left[-\frac{\gamma}{m}t\right]}\right] \tag{4.30}$$

so that

$$P(x,t|x_0,v_0) = \left[\frac{1}{2\pi\langle\Delta x^2(t)\rangle}\right]^{\frac{1}{2}} \exp\left[\frac{(x - \langle x(t)\rangle_{v_0} - v_0\chi_x(t))^2}{2\langle\Delta x^2(t)\rangle}\right] \tag{4.31}$$

We can now proceed with the calculation of (4.28) using this new notation

$$P(x,t|x_0) = \int_{-\infty}^{\infty} dv_0 \sqrt{\Delta} \exp\left[-\frac{(x - \langle x(t)\rangle_{v_0} - v_0\chi_x(t))^2}{2\langle\Delta x^2(t)\rangle} - \frac{mv_0^2}{2k_B T}\right] \tag{4.32}$$

with

$$\Delta = \frac{m}{(2\pi)^2 k_B T\langle\Delta x^2(t)\rangle} \tag{4.33}$$

Let us focus on the argument of the exponential of equation (4.32). We have that

$$\begin{aligned} &\frac{-\left(x - \langle x(t)\rangle_{v_0}\right)^2 - v_0^2\chi_x^2(t) + 2v_0\chi_x(t)\left(x - \langle x(t)\rangle_{v_0}\right)}{2\langle\Delta x^2(t)\rangle} - \frac{mv_0^2}{2k_B T} = \\ &-\frac{\left(x - \langle x(t)\rangle_{v_0}\right)^2}{2\langle\Delta x^2(t)\rangle} + \frac{v_0\chi_x(t)\left(x - \langle x(t)\rangle_{v_0}\right)}{\langle\Delta x^2(t)\rangle} - v_0^2\left(\frac{m}{2k_B T} + \frac{\chi_x^2(t)}{2\langle\Delta x^2(t)\rangle}\right) \end{aligned} \tag{4.34}$$

The first term does not depend on v_0 and can be brought out from the integral of equation (4.32), on the other hand the other two terms depend on v_0 and in order to perform the integration it is useful to complete the square so that equation (4.32) becomes

$$\begin{aligned} P(x,t|x_0) = \sqrt{\Delta}\exp&\left[-\frac{\left(x - \langle x(t)\rangle_{v_0}\right)^2}{2\langle\Delta x^2(t)\rangle} + \frac{1}{4}\left(\frac{\left(x - \langle x(t)\rangle_{v_0}\right)\chi_x(t)}{\langle\Delta x^2(t)\rangle}\right)^2 \cdot\right. \\ &\left.\cdot\left(\frac{m}{2k_B T} + \frac{\chi_x^2(t)}{2\langle\Delta x^2(t)\rangle}\right)^{-1}\right] \int_{-\infty}^{\infty} dv_0 \exp\left[-\left(v_0\left(\frac{m}{2k_B T} + \frac{\chi_x^2(t)}{2\langle\Delta x^2(t)\rangle}\right)^{\frac{1}{2}} + \right.\right. \\ &\left.\left. - \frac{1}{2}\left(\frac{\left(x - \langle x(t)\rangle_{v_0}\right)\chi_x(t)}{\langle\Delta x^2(t)\rangle}\right)\left(\frac{m}{2k_B T} + \frac{\chi_x^2(t)}{2\langle\Delta x^2(t)\rangle}\right)^{-\frac{1}{2}}\right)^2\right] \end{aligned} \tag{4.35}$$

Changing variable with the following substitution

$$\xi = v_0\left(\frac{m}{2k_B T} + \frac{\chi_x^2(t)}{2\langle\Delta x^2(t)\rangle}\right)^{\frac{1}{2}} \implies dv_0 = d\xi\left(\frac{m}{2k_B T} + \frac{\chi_x^2(t)}{2\langle\Delta x^2(t)\rangle}\right)^{-\frac{1}{2}} \tag{4.36}$$

and performing the Gaussian integration (4.35) becomes

$$\begin{gathered}P\left(x,t|x_0\right)=\frac{1}{\sqrt{\frac{2\pi k_BT\langle\Delta x^2(t)\rangle}{m}\left(\frac{m}{k_BT}+\frac{\chi_x^2(t)}{\langle\Delta x^2(t)\rangle}\right)}}\exp\left[-\frac{\left(x-\langle x\left(t\right)\rangle_{v_0}\right)^2}{2\langle\Delta x^2\left(t\right)\rangle}+\right.\\ \left.\frac{1}{2}\left(\frac{\left(x-\langle x\left(t\right)\rangle_{v_0}\right)\chi_x\left(t\right)}{\langle\Delta x^2\left(t\right)\rangle}\right)^2\left(\frac{m}{k_BT}+\frac{\chi_x^2\left(t\right)}{\langle\Delta x^2\left(t\right)\rangle}\right)^{-1}\right]=\\ \frac{1}{\sqrt{2\pi\Big(\langle\Delta x^2\left(t\right)\rangle+\frac{k_BT}{m}\chi_x^2\left(t\right)\Big)}}\exp\left[-\frac{\left(x-\langle x\left(t\right)\rangle_{v_0}\right)^2}{2\Big(\langle\Delta x^2\left(t\right)\rangle+\frac{k_BT}{m}\chi_x^2\left(t\right)\Big)}\right]\end{gathered}\tag{4.37}$$

From this expression we see that we have again a Gaussian distribution whith mean and variance respectively equal to

$$\begin{gathered}\mu\left(t\right)=\langle x\left(t\right)\rangle_{v_0}=x_0+\phi_x\left(t\right)\\ \sigma^2\left(t\right)=\langle\Delta x^2\left(t\right)\rangle+\frac{k_BT}{m}\chi_x^2\left(t\right)=\frac{2k_BT}{\gamma}\left[t-\frac{m}{\gamma}\left(1-e^{\left[-\frac{\gamma}{m}t\right]}\right)\right]\end{gathered}\tag{4.38}$$

so that finally we get

$$P\left(x,t|x_0\right)=\frac{1}{\sqrt{2\pi\sigma^2\left(t\right)}}\exp\left[-\frac{\left(x-\mu\left(t\right)\right)^2}{2\sigma^2\left(t\right)}\right]\tag{4.39}$$

At this point we want to use what we have just obtained to deduce new nonequilibrium inequalities , i.e. we want to plug in our results into equation (2.43). Here, the only piece that is missing is the Kullback-Leibler divergence $\mathbb{H}\left(\mathbb{Q}|\mathbb{P}\right)(t)$ which we are now going to calculate. To do this, we have to chose a particular perturbation and see what kind of form the Kullback-Leibler divergence takes. We will take two different paths and see which one leads to a better result.
First of all we want to properly calculate the relative entropy for a general perturbation of the system, whose probability density function is still a Gaussian but with different parameters

$$P^{\alpha}\left(x,t|x_0\right)=\frac{1}{\sqrt{2\pi\sigma_{\alpha}^2\left(t\right)}}\exp\left[-\frac{\left(x-\mu_{\alpha}\left(t\right)\right)^2}{2\sigma_{\alpha}^2\left(t\right)}\right]\tag{4.40}$$

From the definition of relative entropy we have that

$$\begin{gathered}\mathbb{H}\left(P^{\alpha}|P\right)(t)=\int_{-\infty}^{\infty}dxP^{\alpha}\left(x,t\right)\ln\left(\frac{P^{\alpha}\left(x,t\right)}{P\left(x,t\right)}\right)=\\ \int_{-\infty}^{\infty}dxP^{\alpha}\left(x,t\right)\ln\left(P^{\alpha}\left(x,t\right)\right)-\int_{-\infty}^{\infty}dxP^{\alpha}\left(x,t\right)\ln\Big(P\left(x,t\right)\Big)\end{gathered}\tag{4.41}$$

Let us focus on the first piece of this expression. It is easy to see that

$$\begin{gathered}\int_{-\infty}^{\infty}dxP^{\alpha}\left(x,t\right)\ln\left(P^{\alpha}\left(x,t\right)\right)=-\frac{1}{2}\ln\left(2\pi\sigma_{\alpha}^2\left(t\right)\right)-\int_{-\infty}^{\infty}dxP^{\alpha}\left(x,t\right)\frac{\left(x-\mu_{\alpha}\left(t\right)\right)^2}{2\sigma_{\alpha}^2\left(t\right)}=\\ -\frac{1}{2}\left(1+\ln\left(2\pi\sigma_{\alpha}^2\left(t\right)\right)\right)\end{gathered}\tag{4.42}$$

Turning to the second part of equation (4.41) we see that

$$\begin{gathered}\int_{-\infty}^{\infty}dxP^{\alpha}\left(x,t\right)\ln\left(P\left(x,t\right)\right)=-\frac{1}{2}\ln\left(2\pi\sigma^2\left(t\right)\right)-\int_{-\infty}^{\infty}dxP^{\alpha}\left(x,t\right)\frac{\left(x-\mu\left(t\right)\right)^2}{2\sigma^2\left(t\right)}=\\ -\frac{1}{2}\ln\left(2\pi\sigma^2\left(t\right)\right)-\int_{-\infty}^{\infty}dxP^{\alpha}\left(x,t\right)\frac{\left(x^2-2x\left(t\right)\mu\left(t\right)+\mu^2\left(t\right)\right)}{2\sigma^2\left(t\right)}=\\ -\frac{1}{2}\ln\left(2\pi\sigma^2\left(t\right)\right)-\frac{\langle\widetilde{x}^2\left(t\right)\rangle-2\mu_{\alpha}\left(t\right)\mu\left(t\right)+\mu^2\left(t\right)}{2\sigma^2\left(t\right)}\end{gathered}\tag{4.43}$$

Remembering that $\langle \widetilde{x}^2(t)\rangle = \sigma_\alpha^2(t) + \mu_\alpha^2(t)$, equation (4.43) becomes

$$\begin{aligned} &-\frac{1}{2}\ln\left(2\pi\sigma^2(t)\right) - \frac{\sigma_\alpha^2(t) + \mu_\alpha^2(t) - 2\mu_\alpha(t)\mu(t) + \mu^2(t)}{2\sigma^2(t)} = \\ &-\frac{1}{2}\ln\left(2\pi\sigma^2(t)\right) - \frac{\sigma_\alpha^2(t) + \left(\mu_\alpha(t) - \mu(t)\right)^2}{2\sigma^2(t)} \end{aligned} \tag{4.44}$$

Putting (4.44) and (4.42) in (4.41) we finally obtain our result

$$\mathbb{H}(P^\alpha|P)(t) = \frac{1}{2}\ln\left(\frac{\sigma^2(t)}{\sigma_\alpha^2(t)}\right) + \frac{\sigma_\alpha^2(t) + \left(\mu_\alpha(t) - \mu(t)\right)^2}{2\sigma^2(t)} - \frac{1}{2} \tag{4.45}$$

We now consider our first kind of perturbation, recalling that the starting point of this treatment is the Langevin equation (4.3), we thus modify its dynamic by adding a small additional external force

$$m\frac{v}{dt}(t) = -\gamma v(t) + F(t) + \beta(t) + \sqrt{2\gamma k_B T}\xi(t) \tag{4.46}$$

hence obtaining a new probability density that has of corse the form of (4.40) whit variance $\sigma_\alpha^2 = \sigma^2$ (the variance, as we have seen, does not depend on the external forces and is thus unchanged) and mean

$$\mu_\alpha(t) = \mu(t) + \frac{1}{m}\int_0^t ds \int_0^s dq e^{\left[-\frac{\gamma}{m}(s-q)\right]}\beta(q) \tag{4.47}$$

Using this result along with equation (4.38) and putting them into (4.45) we get

$$\mathbb{H}(P^\alpha|P)(t) = \frac{\gamma\left(\int_0^t ds \int_0^s dq e^{\left[-\frac{\gamma}{m}(s-q)\right]}\beta(q)\right)^2}{4k_B T m^2\left[t - \frac{m}{\gamma}\left(1 - e^{\left[-\frac{\gamma}{m}t\right]}\right)\right]} \tag{4.48}$$

In the spirit of the previous sections we imagine the modification of the dynamics made through the additional force $\beta(t)$ to be small, and hence proportional to a small perturbation parameter α so that $\beta(t) = \alpha\widetilde{\beta}(t)$. In this way equation (4.48) can be rewritten as follows

$$\mathbb{H}(P^\alpha|P)(t) = \frac{\alpha^2}{4}\langle\Sigma\rangle(t) \tag{4.49}$$

of course with

$$\langle\Sigma\rangle(t) = \frac{\gamma\left(\int_0^t ds \int_0^s dq e^{\left[-\frac{\gamma}{m}(s-q)\right]}\widetilde{\beta}(q)\right)^2}{k_B T m^2\left[t - \frac{m}{\gamma}\left(1 - e^{\left[-\frac{\gamma}{m}t\right]}\right)\right]} \tag{4.50}$$

We now have to use this result to obtain a nonequilibrium inequality, which is the main purpose of this thesis. As it was already done, to this end we use (2.43) so that

$$\frac{h^2}{2}\left\langle \Delta Q^2\right\rangle(t) \geq h\left\langle Q\right\rangle^\beta(t) - h\left\langle Q\right\rangle(t) - \frac{\alpha^2}{4}\langle\Sigma\rangle(t) \tag{4.51}$$

where $Q(t)$ is a generic current and $\langle\cdot\rangle^\beta$ is an average taken with respect to the modified dynamic. It is convenient at this point to consider $Q(t) = x(t)$ because $\left\langle \Delta x^2\right\rangle(t)$ is proportional to the diffusion constant (which is a measurable quantity) and moreover we have already calculated the important quantities. In fact we have that

$$\left\langle x\right\rangle_{v_0}(t) = \mu(t) \qquad \left\langle x\right\rangle_{v_0}^\beta(t) = \mu_\alpha(t) \qquad \left\langle \Delta x^2\right\rangle_{v_0}(t) = \sigma(t) \tag{4.52}$$

where $\left\langle\ \cdot\ \right\rangle_{v_0}$ is intended as the average after having performed the integration with respect to the initial velocity probability density function $P(v_0)$. With these informations (4.51) becomes

$$\begin{aligned} &\frac{h^2}{2}\sigma(t) \geq h\Big[\mu_\alpha(t) - \mu(t)\Big] - \frac{\alpha^2}{4}\langle\Sigma\rangle(t) = \\ &\frac{h\alpha}{m}\left[\int_0^t ds \int_0^s dq e^{\left[-\frac{\gamma}{m}(s-q)\right]}\widetilde{\beta}(q)\right] - \frac{\alpha^2}{4}\langle\Sigma\rangle(t) \end{aligned} \tag{4.53}$$

As usual we pose

$$\alpha = \frac{2h\Big[\int_0^t ds \int_0^s dq e^{\left[-\frac{\gamma}{m}(s-q)\right]} \widetilde{\beta}(q)\Big]}{m\langle\Sigma\rangle(t)} \tag{4.54}$$

thus (4.53) becomes

$$\sigma(t) \geq \frac{2\Big[\int_0^t ds \int_0^s dq e^{\left[-\frac{\gamma}{m}(s-q)\right]} \widetilde{\beta}(q)\Big]^2}{m^2\langle\Sigma\rangle(t)} = \frac{2k_BT}{\gamma}\left[t - \frac{m}{\gamma}\Big(1 - e^{\left[-\frac{\gamma}{m}t\right]}\Big)\right] \tag{4.55}$$

Remembering the definition of $\sigma^2(t)$ (equation (4.38)) we see that (4.55) takes the form of the trivial inequality $1 \geq 1$. Of course we are not satisfied with this result, although it is clear that the relation is manifestly always verified. In fact we would like to obtain an expression that explicitly depends on the external force of equation (4.4) and that exhibits some more interesting behaviour. For this purpose what we do is to perturb the dynamics of the system in a different way, namely by modifying the friction coefficient γ in such a way that $\widetilde{\gamma} = (1+\alpha)\gamma$. This modification obviously induces a change in the average value of the position and in the variance. As for the average value μ_α we obtain that

$$\begin{gathered}\langle x(t)\rangle^\alpha = \mu_\alpha(t) = x_0 + \frac{1}{m}\int_0^t ds \int_0^s dq e^{\left[-\frac{\widetilde{\gamma}}{m}(s-q)\right]} F(q) = \\ x_0 + \frac{1}{m}\int_0^t ds \int_0^s dq e^{\left[-\frac{\gamma}{m}(s-q)\right]} F(q) - \frac{\alpha\gamma}{m^2}\int_0^t ds \int_0^s dq\,(s-q)\, e^{\left[-\frac{\gamma}{m}(s-q)\right]} F(q)\end{gathered} \tag{4.56}$$

where we performed a Taylor expansion of the perturbed velocity response function

$$\widetilde{\chi}_v(t) = e^{\left[-\frac{\widetilde{\gamma}}{m}(s-q)\right]} = e^{\left[-\frac{\gamma}{m}(s-q)\right]} - \frac{\alpha\gamma}{m}(s-q)\, e^{\left[-\frac{\gamma}{m}(s-q)\right]} \tag{4.57}$$

Therefore using equation (4.56) we get

$$\mu_\alpha(t) - \mu(t) = -\frac{\alpha\gamma}{m^2}\int_0^t ds \int_0^s dq\,(s-q)\, e^{\left[-\frac{\gamma}{m}(s-q)\right]} F(q) \tag{4.58}$$

With regard to the variance, starting from equation (4.38) we see that putting $\rho = \frac{\gamma}{m} \implies \rho_\alpha = (1+\alpha)\rho$

$$\sigma_\alpha^2(t) = \frac{2k_BT}{m}\frac{1}{\rho_\alpha}\left[t - \frac{1}{\rho_\alpha}\Big(1 - e^{-\rho_\alpha t}\Big)\right] \tag{4.59}$$

We temporarily put aside the $\frac{2k_BT}{m}$ term and, as usual, we expand the remaining part in powers of α up to second order. Thus

$$\begin{gathered}\frac{1}{\rho_\alpha}\left[t - \frac{1}{\rho_\alpha}\Big(1 - e^{-\rho_\alpha t}\Big)\right] = \frac{1}{\rho_\alpha}\left[t - \frac{1}{\rho_\alpha}\left[1 - e^{-\rho t}\Big(1 - \alpha\rho t + \frac{(\alpha\rho t)^2}{2}\Big)\right]\right] = \\ \frac{1}{\rho_\alpha}\left[t - \frac{1}{\rho}\Big(1 - e^{-\rho t}\Big) + \frac{\alpha}{\rho}\left(1 - e^{-\rho t}(1+\rho t)\right) + \frac{\alpha^2}{\rho}\Big(e^{-\rho t}\Big(1 + \rho t + \frac{(\rho t)^2}{2}\Big) - 1\Big)\right] = \\ \frac{1}{\rho}\Big[t - \frac{1}{\rho}\Big(1 - e^{-\rho t}\Big) - \frac{\alpha}{\rho}\Big(\rho t\left(1 + e^{-\rho t}\right) + 2e^{-\rho t} - 2\Big) + \\ + \frac{\alpha^2}{\rho}\Big(e^{-\rho t}\Big(1 + 2\rho t + \frac{(\rho t)^2}{2}\Big) + 3e^{-\rho t} - 3\Big)\Big]\end{gathered} \tag{4.60}$$

The variance can hence be written as

$$\sigma_\alpha^2(t) = \frac{2k_BT}{m}\frac{1}{\rho_\alpha}\left[t - \frac{1}{\rho_\alpha}\Big(1 - e^{-\rho_\alpha t}\Big)\right] = \sigma^2(t) - \alpha\Gamma(t) + \alpha^2\Omega(t) \tag{4.61}$$

with

$$\begin{gathered}\Gamma(t) = \frac{1}{\rho^2}\Big(\rho t\left(1 + e^{-\rho t}\right) + 2e^{-\rho t} - 2\Big) \\ \Omega(t) = \frac{1}{\rho^2}\Big(e^{-\rho t}\Big(1 + 2\rho t + \frac{(\rho t)^2}{2}\Big) + 3e^{-\rho t} - 3\Big)\end{gathered} \tag{4.62}$$

At this point we put (4.61) in (4.45), so that the Kullback-Leibler divergence becomes

$$\begin{aligned}
&\mathbb{H}\left(P^{\alpha}|P\right)(t)=\frac{1}{2}\ln\left(\frac{\sigma^{2}(t)}{\sigma^{2}(t)-\alpha\Gamma(t)+\alpha^{2}\Omega(t)}\right)+\\
&+\frac{\sigma^{2}(t)-\alpha\Gamma(t)+\alpha^{2}\Omega(t)}{2\sigma^{2}(t)}+\frac{\left(\mu_{\alpha}(t)-\mu(t)\right)^{2}}{2\sigma^{2}(t)}-\frac{1}{2}=\\
&-\frac{1}{2}\ln\left(1-\frac{\alpha\Gamma(t)}{\sigma^{2}(t)}+\frac{\alpha^{2}\Omega(t)}{\sigma^{2}(t)}\right)-\frac{\alpha\Gamma(t)}{2\sigma^{2}(t)}+\frac{\alpha^{2}\Omega(t)}{2\sigma^{2}(t)}+\frac{\left(\mu_{\alpha}(t)-\mu(t)\right)^{2}}{2\sigma^{2}(t)}=\\
&\left[\frac{\alpha\Gamma(t)}{2\sigma^{2}(t)}\right]^{2}+\frac{\left(\mu_{\alpha}(t)-\mu(t)\right)^{2}}{2\sigma^{2}(t)}
\end{aligned} \tag{4.63}$$

Note that the second order term $\Omega(t)$ does not appear in this expression. Now, using equation (4.58) and the definition of $\Gamma(t)$ and $\sigma^2(t)$ we obtain

$$\begin{aligned}
&\mathbb{H}\left(P^{\alpha}|P\right)(t)=\frac{\alpha^{2}}{4}\langle\Sigma\rangle(t)=\\
&\frac{\alpha^{2}}{4}\left[\left[\frac{\rho t\left(1+e^{-\rho t}\right)+2\left(e^{-\rho t}-1\right)}{\rho t-\left(1-e^{-\rho t}\right)}\right]^{2}+\frac{\left[\rho^{3}\int_{0}^{t}ds\int_{0}^{s}dq\,(s-q)\,e^{-\rho(s-q)}f(q)\right]^{2}}{\rho t-\left(1-e^{-\rho t}\right)}\right]
\end{aligned} \tag{4.64}$$

where

$$f(q)=\left[\frac{m}{k_{B}T\gamma^{2}}\right]^{\frac{1}{2}}F(q) \tag{4.65}$$

in such a way that $f(q)$ is an dimensionless quantity. We thus note that this expression of the Kullback-Leibler divergence is more interesting than (4.48) indeed for the explicit dependence of the external force.

By doing the exact same calculation as in the first section, i.e. starting from equation (2.43) and as usual setting

$$\alpha=\frac{2h\left[\delta\langle Q\rangle(T)\right]}{\langle\Sigma\rangle(t)} \tag{4.66}$$

we obtain the familiar expression

$$\left\langle\Delta Q^{2}\right\rangle(t)\geq\frac{2\left(\delta\langle Q\rangle(t)\right)^{2}}{\langle\Sigma\rangle(t)} \tag{4.67}$$

where the value of $\langle\Sigma\rangle(t)$ can be easily deduced from equation (4.64) and moreover we assumed that we could write the excess current (the difference between the perturbed average of the current and its unperturbed average) in the following way

$$\langle Q\rangle^{\alpha}(T)-\langle Q\rangle(T)=\alpha\delta\langle Q\rangle(T) \tag{4.68}$$

We will discuss this point more deeply in a moment.

Remembering the definition of the function $I(t)$ which was given in the first section (equation (2.50)) we can write

$$I(t)=\frac{2\left(\delta\langle Q\rangle(t)\right)^{2}}{\left\langle\Delta Q^{2}\right\rangle(t)\cdot\langle\Sigma\rangle(t)}=\frac{2\left(\delta\langle Q\rangle(t)\right)^{2}}{\left\langle\Delta Q^{2}\right\rangle(t)\left[\left[\frac{\rho t(1+e^{-\rho t})+2(e^{-\rho t}-1)}{\rho t-(1-e^{-\rho t})}\right]^{2}+\frac{\left[\rho^{3}\int_{0}^{t}ds\int_{0}^{s}dq(s-q)e^{-\rho(s-q)}f(q)\right]^{2}}{\rho t-(1-e^{-\rho t})}\right]}\leq 1 \tag{4.69}$$

and it is valid for a generic current $Q(x,t)$.

If we choose to take $Q(x,t)=x$ than it holds that

$$\langle x\rangle^{\alpha}(T)-\langle x\rangle(T)=\alpha\delta\langle x\rangle(T)=\mu_{\alpha}(t)-\mu(t)=-\frac{\alpha\gamma}{m^{2}}\int_{0}^{t}ds\int_{0}^{s}dq\,(s-q)\,e^{\left[-\frac{\gamma}{m}(s-q)\right]}F(q) \tag{4.70}$$

where we have used equation (4.58). We thus deduce that

$$\delta\langle x\rangle(T) = -\frac{\gamma}{m^2}\int_0^t ds\int_0^s dq\,(s-q)\,e^{\left[-\frac{\gamma}{m}(s-q)\right]}F(q) \tag{4.71}$$

First of all we see that the hypothesis made in (4.68) is legitimate and moreover it is clear that this relation is very different with respect to (3.30) where we obtained

$$\delta\langle Q\rangle(t) = t\langle\dot{Q}\rangle(t) \tag{4.72}$$

This is a consequence of the fact that the perturbation used in this section does not correspond to a time rescaling for the perturbed probability density function.
At this point, using x as our current and thus putting equations (4.38) and (4.71) into (4.67) we obtain the following nonequilibrium inequality

$$\begin{aligned}\Big[\rho t - \left(1-e^{-\rho t}\right)\Big] \geq \left[\rho^3\int_0^t ds\int_0^s dq\,(s-q)\,e^{-\rho(s-q)}f(q)\right]^2 \cdot \\ \cdot\left[\left[\frac{\rho t\left(1+e^{-\rho t}\right)+2\left(e^{-\rho t}-1\right)}{\rho t-(1-e^{-\rho t})}\right]^2 + \frac{\left[\rho^3\int_0^t ds\int_0^s dq\,(s-q)\,e^{-\rho(s-q)}f(q)\right]^2}{\rho t-(1-e^{-\rho t})}\right]^{-1}\end{aligned} \tag{4.73}$$

where we got rid of the constant terms involving k_B, m and T to make $F(q)$ dimensionless. Instead, equation (4.69) can be written as follows

$$I(t) = \frac{\left[\rho^3\int_0^t ds\int_0^s dq\,(s-q)\,e^{-\rho(s-q)}f(q)\right]^2}{\frac{\left[\rho t\left(1+e^{-\rho t}\right)+2\left(e^{-\rho t}-1\right)\right]^2}{\rho t-(1-e^{-\rho t})} + \left[\rho^3\int_0^t ds\int_0^s dq\,(s-q)\,e^{-\rho(s-q)}f(q)\right]^2} \leq 1 \tag{4.74}$$

From the last expression it is obvious that the considered nonequilibrium inequality is always verified. In the next section we explore the behaviour of this inequality for some particular external forces.

4.1.1 Constant force

As previously said in the introduction to this section, a constant force can be obtained if we imagine the Brownian particle to be charged and to be subject to a constant Electric field. We consider the Brownian particle to be initially in an equilibrium state and to turn on the external constant force at $t = 0$. The first thing to do is to calculate

$$\rho^3 f\int_0^t ds\int_0^s dq\,(s-q)\,e^{-\rho(s-q)} = f\Big[\rho t\left(1+e^{-\rho t}\right)+2\left(e^{-\rho t}-1\right)\Big] \tag{4.75}$$

Inserting this expression in (4.74) we obtain

$$I(t) = \frac{f^2}{f^2+\frac{1}{\rho t-(1-e^{-\rho t})}} \leq 1 \tag{4.76}$$

In the following we show its behaviour for some values of ρ and f. Here, it is interesting to see that as time goes to infinity (as the system reaches the stationary state) we obtain an equivalence independently from the value of the parameters, differently from the two states jump process where the inequality becomes an equality (at infinite times) only in the case of same jump rates (namely for the Poisson process). This happens because at large times the dynamic of the system in determined by the constant force, which is the deterministic component of the system, and hence the relation becomes an equality.

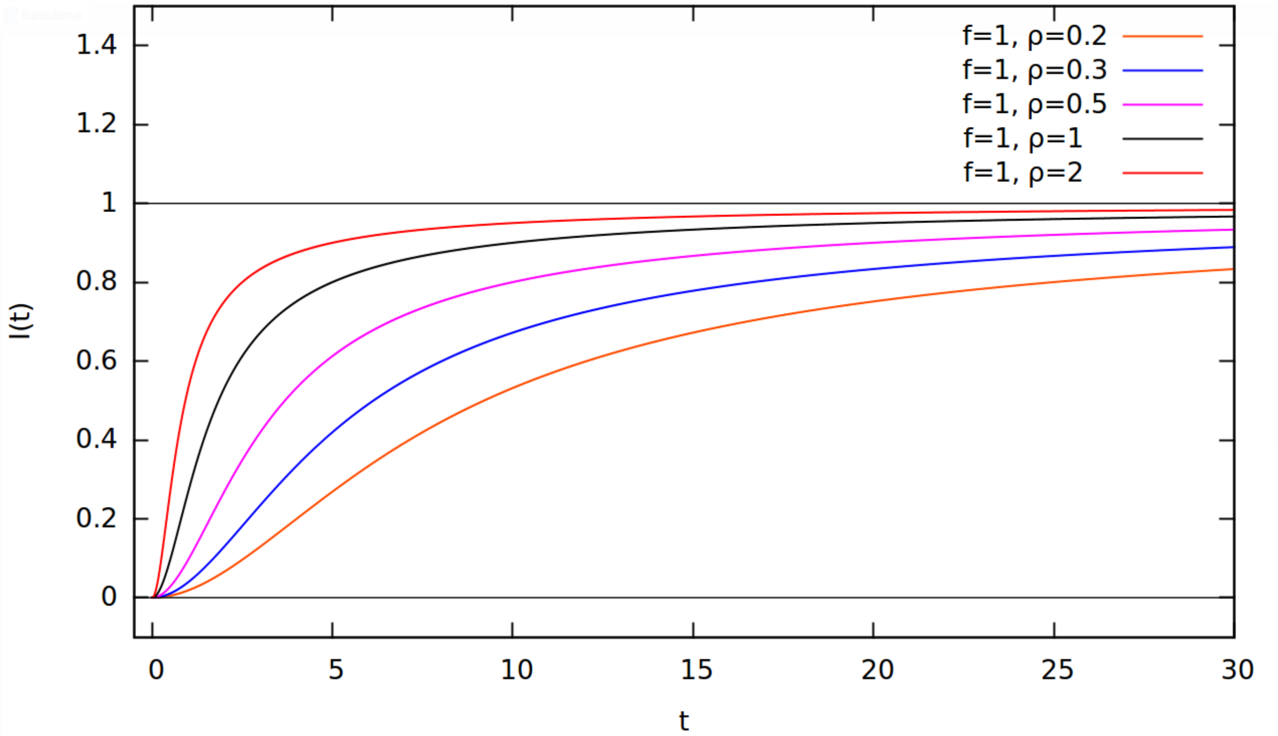


Figure 7: Plot of $I(t)$ with constant external force and fixed $f = 1$

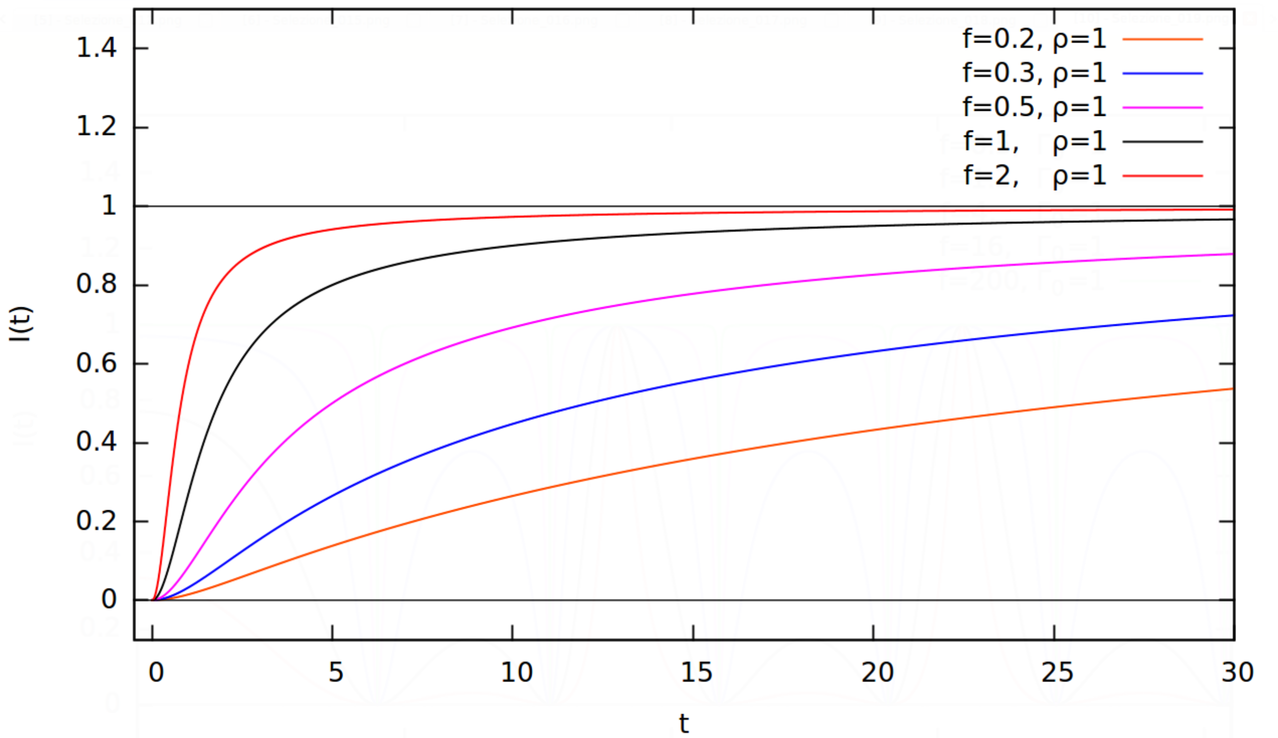


Figure 8: Plot of $I(t)$ with constant external force and fixed $\rho = 1$

4.1.2 Impulsive force

We now consider a peculiar kind of force that is useful to describe some kind of forces that are exerted for a very short time. These kind of forces are called impulsive and can be modelled through the use of a Dirac delta, namely

$$F(t) = F\frac{\delta(t)}{\rho} \tag{4.77}$$

where ρ has been introduced in such a way that $\frac{\delta(t)}{\rho}$ is dimensionless. Such a force could be obtained for example again imagining our Brownian particle to be charged and turning an electric field for a very short time compared to the characteristic time of the system.
Of course, in order to visualise the behaviour of the nonequilibrium inequality, we again want to use (4.74). To do so we must calculate

$$\begin{gathered}\rho^3\int_0^t ds\int_0^s dq\,(s-q)\,e^{-\rho(s-q)}f(q) = \rho^2 f\int_0^t ds\int_0^s dq\,(s-q)\,e^{-\rho(s-q)}\delta(q) = \\ \frac{\rho^2 f}{2}\int_0^t ds\,(s)\,e^{-\rho s} = \frac{f}{2}\Big[1-e^{-\rho s}(\rho t+1)\Big]\end{gathered} \tag{4.78}$$

where we used the fact that

$$\int_0^t dsg(s)\,\delta(s) = \frac{g(0)}{2} \tag{4.79}$$

Finally we put equation (4.78) in (4.74) so that we obtain

$$I(t) = \frac{f^2\Big[1-e^{-\rho s}(\rho t+1)\Big]^2}{\dfrac{4\Big[\rho t\left(1+e^{-\rho t}\right)+2\left(e^{-\rho t}-1\right)\Big]^2}{\rho t-(1-e^{-\rho t})}+f^2\Big[1-e^{-\rho s}(\rho t+1)\Big]^2} \leq 1 \tag{4.80}$$

Plotting this inequality for different values of the impulsive force amplitude f and the damping constant ρ (for every value of the force we plotted 3 curves for $\rho = 0.5, 1, 2$) we observe a very different behaviour with respect to the constant force case. In fact, for large times, we do not obtain an equality any more; this happens because for large times, after a certain time needed for the relaxation of the system, the random component dominates and hence the relation remains an inequality. On the other hand, for small times, we note that the more the magnitude of the impulse is big, the more the relation becomes an equality: this is explained with the same argument of before, namely that the deterministic component dominates on the random one.

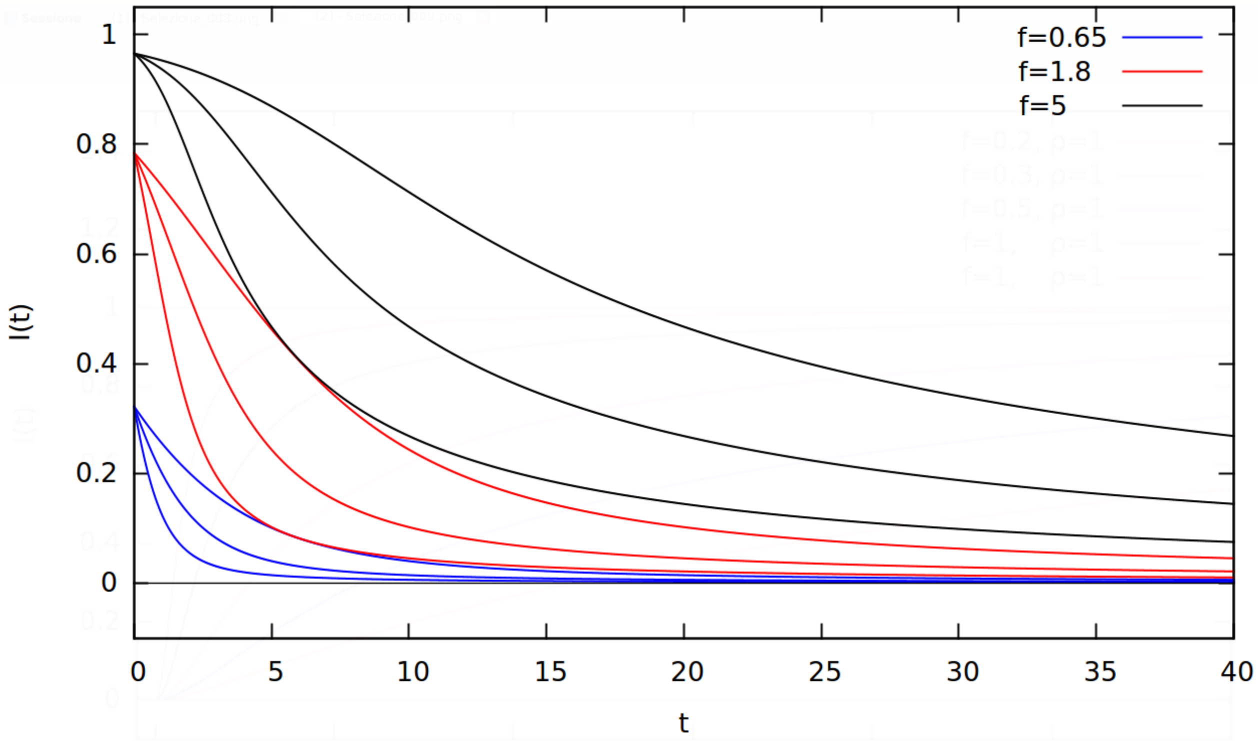


Figure 9: Plot of $I(t)$ with impulsive external force, for every value of f three curves were plotted with $\rho = 0.5, 1, 2$ (the curves that decrease more rapidly are those related to a bigger damping constant ρ)

5 Non-Markov diffusion processes with time dependent force

In recent years an ever-growing interest was addressed towards non-Markovianity of diffusive processes. In fact, considering for example the situation taken into account in the previous subsection, if the characteristic time of the dynamics of the Brownian particle τ_B is not much greater than the typical time scales of the fluid components (τ_F), then we can not any more consider the Gaussian random force as a white noise, namely it exhibits a correlation at different times that is not a delta function. In this case, we call it coloured noise.

The first step towards non-Markovianity can be made if we take the time correlation function of the Gaussian noise to be exponentially decreasing, in fact this will be our first example in the next subsection and it will be shown that the differences with the Markov case are very small. Instead, in a more general case, the memory kernel (as we will call the noise correlation function from now on) can have an arbitrary form and many efforts have been made to correctly describe through the use of this object the stochastic motion of, for example, ions in a charged or neutral plasma [14] or of a tracer in a visco-elastic fluid where some features of the Navier-Stokes equation must be implemented [15]. For all these reasons, we consider a generalized version of Langevin equation that exhibits some memory effects, it can be written in the following form

$$\frac{dv}{dt}(t) = -\int_0^t \Gamma\left(t-t'\right) v\left(t'\right) dt' + \frac{F(t)}{M} + \frac{\eta(t)}{M} \tag{5.1}$$

where we used a different notation for the random force precisely because it is not a white noise any more (but still Gaussian). Moreover we use M instead of m for future usefulness. The function $\Gamma(t-t')$ is the memory kernel, the reason why we referred to it as the time correlation function of the noise is explained by a famous work made by R. Kubo [16] where it is shown that, for a particle of mass M immersed in a thermal bath at equilibrium and at a temperature T, the following equality holds

$$\langle \eta(t)\, \eta(s) \rangle = k_B T M \Gamma\left(|t-s|\right) \tag{5.2}$$

This relation is also known in scientific literature as the second fluctuation dissipation theorem, and it will be of great help in the following calculations. It is, of course, still true that $\langle \eta(t) \rangle = 0$.

Turning back to equation (5.1), in order to formally solve it, we proceed in the same way as the previous subsection, i.e. with the aid of Laplace transforms. We obtain

$$\begin{aligned} \hat{v}(k)\left[k + \hat{\Gamma}(k)\right] &= v_0 + \frac{\hat{F}(k)}{M} + \frac{\hat{\eta}(k)}{M} \\ \hat{v}(k) &= \hat{\chi}_v(k)\left[v_0 + \frac{\hat{F}(k)}{M} + \frac{\hat{\eta}(k)}{M}\right] \end{aligned} \tag{5.3}$$

where

$$\hat{\chi}_v(k) = \frac{1}{\left[k + \hat{\Gamma}(k)\right]} \tag{5.4}$$

We note that we recover Markov dynamics by setting $\Gamma(t) = 2\frac{\gamma}{M}\delta(t)$. In fact, in this case, we have

$$\int_0^t \Gamma\left(t–t'\right) v\left(t'\right) dt' = 2\frac{\gamma}{M}\int_0^t \delta\left(t–t'\right) v\left(t'\right) dt' = 2\frac{\gamma}{M}\int_0^t \delta\left(t'\right) v\left(t-t'\right) = \frac{\gamma}{M} v(t) \tag{5.5}$$

so that (5.1) becomes (4.4) and moreover

$$\mathcal{L}\big[\Gamma(t)\big](k) = \hat{\Gamma}(k) = \int_0^{+\infty} e^{-kt}\Gamma(t)\, dt = 2\frac{\gamma}{M}\int_0^{+\infty} e^{-kt}\delta(t)\, dt = \frac{\gamma}{M} \tag{5.6}$$

so that from equation (5.4) we recover (4.6). In both (5.5) and (5.6) we used the fact that

$$\int_0^t dsg(s)\,\delta(s) = \frac{g(0)}{2} \tag{5.7}$$

Transforming (5.3) back

$$\begin{gathered}v(t) = v_0\chi_v(t) + \frac{1}{M}\int_0^t \chi_v(t-s)\,F(s) + \frac{1}{M}\int_0^t \chi_v(t-s)\,\eta(s) = \\ v_0\chi_v(t) + \phi_v(t) + \psi_v(t)\end{gathered} \tag{5.8}$$

where the meaning of $\phi_v(t)$ and $\psi_v(t)$ is obvious. Moreover by setting

$$\chi_x(t) = \int_0^t ds\chi_v(s) \tag{5.9}$$

it is easily verified that

$$\begin{gathered}x(t) = x_0 + \int_0^t v(s) = \\ x_0 + v_0\chi_x(t) + \frac{1}{M}\int_0^t \chi_x(t-s)\,F(s) + \frac{1}{M}\int_0^t \chi_x(t-s)\,\eta(s) = \\ x_0 + v_0\chi_x(t) + \phi_x(t) + \psi_x(t)\end{gathered} \tag{5.10}$$

Noting that $\langle\psi_v(t)\rangle = \langle\psi_x(t)\rangle = 0$, we obtain that

$$\begin{gathered}\langle v(t)\rangle = v_0\chi_v(t) + \phi_v(t) \\ \langle x(t)\rangle = x_0 + v_0\chi_x(t) + \phi_x(t)\end{gathered} \tag{5.11}$$

In order to obtain the probability density function $P(x,t|x_0,v_0)$, the only thing we still need is the variance $\langle\Delta x^2(t)\rangle$ (being the pdf Gaussian). From its definition

$$\begin{gathered}\langle\Delta x^2(t)\rangle = \left\langle\left(x(t) - \langle x(t)\rangle\right)^2\right\rangle = \langle\psi_x(t)\,\psi_x(t)\rangle = \\ \frac{1}{M^2}\int_0^t ds_1\int_0^t ds_2\int_0^{s_1} dq_1\int_0^{s_2} dq_2\chi_v(s_1-q_1)\,\chi_v(s_2-q_2)\,\langle\eta(q_1)\,\eta(q_2)\rangle = \\ \frac{k_BT}{M}\int_0^t ds_1\int_0^t ds_2\int_0^{s_1} dq_1\int_0^{s_2} dq_2\chi_v(s_1-q_1)\,\chi_v(s_2-q_2)\,\Gamma(|q_1-q_2|)\end{gathered} \tag{5.12}$$

We now follow the the derivation of [17], initially focusing on

$$\int_0^{s_1} dq_1\int_0^{s_2} dq_2\chi_v(s_1-q_1)\,\chi_v(s_2-q_2)\,\Gamma(|q_1-q_2|) \tag{5.13}$$

Let us take the double Laplace transform of (5.13)

$$\begin{gathered}\int_0^\infty ds_1e^{-ks_1}\int_0^\infty ds_2e^{-k's_2}\int_0^{s_1} dq_1\int_0^{s_2} dq_2\chi_v(s_1-q_1)\,\chi_v(s_2-q_2)\,\Gamma(|q_1-q_2|) = \\ \int_0^\infty dq_1\int_{q_1}^\infty ds_1\int_0^\infty dq_2\int_{q_2}^\infty ds_2e^{-k(s_1-q_1)}\chi_v(s_1-q_1)\,e^{-k'(s_2-q_2)}\chi_v(s_2-q_2)\cdot \\ \cdot e^{-kq_1}e^{-k'q_2}\Gamma(|q_1-q_2|) = \\ \int_0^\infty dq_1\int_0^\infty d\tau_1\int_0^\infty dq_2\int_0^\infty d\tau_2e^{-k\tau_1}\chi_v(\tau_1)\,e^{-k'\tau_2}\chi_v(\tau_2)\cdot \\ \cdot e^{-kq_1}e^{-k'q_2}\Gamma(|q_1-q_2|) = \\ \hat{\chi}_v(k)\,\hat{\chi}_v(k')\int_0^\infty dq_1\int_0^\infty dq_2e^{-kq_1}e^{-k'q_2}\Gamma(|q_1-q_2|)\end{gathered} \tag{5.14}$$

where in second line we noted that $\int_0^\infty ds_i \int_0^{s_i} dq_1 = \int_0^\infty dq_i \int_{q_i}^\infty ds_i$ and after that we set $\tau_i = s_i - q_i$. Focusing on the last double integral of equation (5.14)

$$\begin{gathered}\int_0^\infty dq_1 \int_0^\infty dq_2 e^{-kq_1} e^{-k'q_2} \Gamma\left(|q_1 - q_2|\right) = \\ \int_0^\infty dq_1 \int_0^\infty dq_2 e^{-k(q_1-q_2)} e^{-q_2(k+k')} \Gamma\left(|q_1 - q_2|\right) = \\ \int_0^\infty dq_2 \int_{-q_2}^\infty d\sigma e^{-k\sigma} e^{-q_2(k+k')} \Gamma\left(|\sigma|\right) = \\ \int_0^\infty dq_2 \left(\hat{\Gamma}(k) + \int_{-q_2}^0 d\sigma e^{-k\sigma} \Gamma\left(|\sigma|\right)\right) e^{-q_2(k+k')} = \\ \frac{\hat{\Gamma}(k)}{k+k'} + \int_0^\infty dq_2 \frac{e^{-q_2(k+k')}}{k+k'} e^{kq_2} \Gamma(q_2) = \frac{\hat{\Gamma}(k) + \hat{\Gamma}(k')}{k+k'}\end{gathered} \tag{5.15}$$

where to obtain the last line from the second-last one we used integration by parts. Putting this result back into (5.14) and remembering (5.1) we obtain

$$\hat{\chi}_v(k)\hat{\chi}_v(k') \frac{\hat{\Gamma}(k) + \hat{\Gamma}(k')}{k+k'} = \frac{\hat{\chi}_v(k) + \hat{\chi}_v(k')}{k+k'} - \hat{\chi}_v(k)\hat{\chi}_v(k') \tag{5.16}$$

The last piece is clearly the double Laplace transform of $\chi_v(s_1)\chi_v(s_2)$, instead as for the first piece we note that in equation (5.15) we showed that the double Laplace transform of $\Gamma(|q_1 - q_2|)$ is

$$\mathcal{L}\Big[\mathcal{L}\Big[\Gamma\left(|q_1 - q_2|\right)\Big](k')\Big](k) = \frac{\hat{\Gamma}(k) + \hat{\Gamma}(k')}{k+k'} \tag{5.17}$$

Using this parallelism we see that

$$\mathcal{L}\Big[\mathcal{L}\Big[\chi_v\left(|q_1 - q_2|\right)\Big](k')\Big](k) = \frac{\hat{\chi}_v(k) + \hat{\chi}_v(k')}{k+k'} \tag{5.18}$$

Finally we remember that we started taking the double Laplace transform of equation (5.13) obtaining (5.16), hence we conclude that

$$\int_0^{s_1} dq_1 \int_0^{s_2} dq_2 \chi_v(s_1 - q_1)\chi_v(s_2 - q_2)\Gamma\left(|q_1 - q_2|\right) = \chi_v\left(|s_1 - s_2|\right) - \chi_v(s_1)\chi_v(s_2) \tag{5.19}$$

Now, turning back to equation (5.12), we have to calculate the following

$$\begin{gathered}\langle \Delta x^2(t) \rangle = \frac{k_B T}{M} \int_0^t ds_1 \int_0^t ds_2 \Big[\chi_v\left(|s_1 - s_2|\right) - \chi_v(s_1)\chi_v(s_2)\Big] = \\ \frac{k_B T}{M}\left[\int_0^t ds_1 \int_0^t ds_2 \chi_v\left(|s_1 - s_2|\right) - \int_0^t ds_1 \chi_v(s_1) \int_0^t ds_2 \chi_v(s_2)\right] = \\ \frac{k_B T}{M}\left[2\int_0^t ds_1 \int_0^{s_1} ds_2 \chi_v(s_1 - s_2) - \chi_x(t)\chi_x(t)\right] = \\ \frac{k_B T}{M}\left[2\int_0^t ds_1 \int_0^{s_1} dq \chi_v(q) - \chi_x(t)\chi_x(t)\right] = \\ \frac{k_B T}{M}\Big[2\chi(t) - \chi_x(t)\chi_x(t)\Big]\end{gathered} \tag{5.20}$$

where we defined

$$\chi(t) = \int_0^t ds \chi_x(s) \tag{5.21}$$

We now have all the pieces to build the probability density function which is, as already said, Gaussian. Hence

$$P(x,t|v_0,x_0) = \frac{1}{\sqrt{2\pi\langle\Delta x^2(t)\rangle}}\exp\left[-\frac{(x-\langle x(t)\rangle)^2}{2\langle\Delta x^2(t)\rangle}\right] = \tag{5.22}$$

$$\frac{1}{\sqrt{\frac{2\pi k_B T}{M}\left[2\chi(t)-\chi_x^2(t)\right]}}\exp\left[-\frac{M\left(x-x_0-v_0\chi_x(t)-\phi_x(t)\right)^2}{2k_BT\left[2\chi(t)-\chi_x^2(t)\right]}\right]$$

As already done in the previous subsection, we want to get rid of the v_0 dependence which is somewhat problematic. To do so we again use the Boltzman statistics for the v_0 probability density function (equation (4.29)) so that

$$P(x,t|x_0) = \int_{-\infty}^{-\infty} dv_0 P(v_o)\, P(x,t|v_0,x_0) \tag{5.23}$$

To simplify the notation we set

$$\langle x(t)\rangle_{v_0} = x_0 + \phi_x(t) \qquad\qquad \Delta = \frac{M}{(2\pi)^2 k_B T\langle\Delta x^2(t)\rangle} \tag{5.24}$$

so that equation (5.23) becomes

$$P(x,t|x_0) = \int_{-\infty}^{\infty} dv_0\sqrt{\Delta}\exp\left[-\frac{\left(x-\langle x(t)\rangle_{v_0}-v_0\chi_x(t)\right)^2}{2\langle\Delta x^2(t)\rangle} - \frac{Mv_0^2}{2k_BT}\right] \tag{5.25}$$

We note that this expression is identical to equation (4.32), and hence we already know the result, namely

$$P(x,t|x_0) = \frac{1}{\sqrt{2\pi\sigma^2(t)}}\exp\left[-\frac{\left(x-\mu(t)\right)^2}{2\sigma^2(t)}\right] \tag{5.26}$$

with

$$\sigma^2(t) = \langle\Delta x^2(t)\rangle + \frac{k_BT}{M}\chi_x^2(t) = \frac{2k_BT}{M}\chi(t) \qquad\qquad \mu(t) = x_0 + \phi_x(t) \tag{5.27}$$

The fact that the above calculations are the same for Markov and non-Markov was to be expected as the whole derivation done in this section follows the same steps of the previous section with the only difference that here the response functions $\chi_v(t)$ and $\chi_x(t)$ are not determined yet while for the Markov case they were known (because we knew the the memory kernel was). In fact we see that substituting Markov response functions into (5.27) we obtain the previous results.
Now that we have the probability density function we can proceed with the calculation of the Kullback-Leibler divergence. To do so, as usual, we have to perturb the dynamics and we imagine this perturbation to be dependent on a small parameter α such that if this parameter is equal to zero we recover the original dynamics. In the last subsection we saw that adding a small new force doesn't lead to interesting results whereas perturbing the friction coefficient does. In the non-Markov case the corresponding term to the friction coefficient is the memory kernel, hence perturbing the latter determines a variation in the response function $\chi_v(t)$. In total generality we can write

$$\chi_*^\alpha(t) \approx \chi_*(t) + \alpha\left(\frac{\partial\chi_*^\alpha(t)}{\partial\alpha}\bigg|_{\alpha=0}\right) \tag{5.28}$$

where the $*$ subscript means that this relation holds for all $\chi_v(t)$, $\chi_x(t)$ and $\chi(t)$. Moreover we note that in equation (5.28) we performed a Taylor expansion only at first order because, as we see in equation (4.63), no higher orders are involved in the calculation of the Kullback-Leibler divergence.

Hence we find for the relative entropy

$$
\begin{gathered}
\mathbb{H}\Big(P^{\alpha}|P\Big)\left(t\right)=\frac{1}{2}\ln\left(\frac{\sigma^{2}\left(t\right)}{\sigma_{\alpha}^{2}\left(t\right)}\right)+\frac{\sigma_{\alpha}^{2}\left(t\right)+\left(\mu_{\alpha}\left(t\right)-\mu\left(t\right)\right)^{2}}{2\sigma^{2}\left(t\right)}-\frac{1}{2}= \\
-\frac{1}{2}\ln\left(\frac{\chi^{\alpha}\left(t\right)}{\chi\left(t\right)}\right)+\frac{\chi^{\alpha}\left(t\right)}{2\chi\left(t\right)}+\frac{M\Big(\phi_{x}^{\alpha}\left(t\right)-\phi_{x}\left(t\right)\Big)^{2}}{4k_{B}T\chi\left(t\right)}-\frac{1}{2}= \\
-\frac{1}{2}\ln\left[1+\frac{\alpha\left(\frac{\partial\chi^{\alpha}(t)}{\partial\alpha}\Big|_{\alpha=0}\right)}{\chi\left(t\right)}+\alpha^{2}\Omega\left(t\right)\right]+\frac{1}{2}\left[1+\frac{\alpha\left(\frac{\partial\chi^{\alpha}(t)}{\partial\alpha}\Big|_{\alpha=0}\right)}{\chi\left(t\right)}+\alpha^{2}\Omega\left(t\right)\right]+ \\
+\frac{M\Big(\phi_{x}^{\alpha}\left(t\right)-\phi_{x}\left(t\right)\Big)^{2}}{4k_{B}T\chi\left(t\right)}-\frac{1}{2}= \\
\frac{\alpha^{2}}{4}\left[\left(\frac{\left(\frac{\partial\chi^{\alpha}(t)}{\partial\alpha}\Big|_{\alpha=0}\right)}{\chi\left(t\right)}\right)^{2}+\frac{\left(\int_{0}^{t}ds\left(\frac{\partial\chi_{x}^{\alpha}(t-s)}{\partial\alpha}\Big|_{\alpha=0}\right)F\left(s\right)\right)^{2}}{k_{B}TM\chi\left(t\right)}\right]=\frac{\alpha^{2}}{4}\langle\Sigma\rangle\left(t\right)
\end{gathered}
\tag{5.29}
$$

Where we have used the fact that

$$
\begin{gathered}
\phi_{x}^{\alpha}\left(t\right)-\phi_{x}\left(t\right)=\frac{1}{M}\int_{0}^{t}ds\chi_{x}^{\alpha}\left(t\text{–}s\right)F\left(s\right)-\frac{1}{M}\int_{0}^{t}ds\chi_{x}\left(t\text{–}s\right)F\left(s\right)= \\
\frac{1}{M}\int_{0}^{t}ds\chi_{x}\left(t\text{–}s\right)F\left(s\right)+\frac{\alpha}{M}\int_{0}^{t}ds\left(\frac{\partial\chi_{x}^{\alpha}\left(t-s\right)}{\partial\alpha}\Big|_{\alpha=0}\right)F\left(s\right)-\frac{1}{M}\int_{0}^{t}ds\chi_{x}\left(t\text{–}s\right)F\left(s\right)= \\
\frac{\alpha}{M}\int_{0}^{t}ds\left(\frac{\partial\chi_{x}^{\alpha}\left(t-s\right)}{\partial\alpha}\Big|_{\alpha=0}\right)F\left(s\right)
\end{gathered}
\tag{5.30}
$$

Moreover, the $\alpha^2\Omega\left(t\right)$ term in (5.29) corresponds to the second order term of the Taylor expansion and, as previously said, it cancels out. Moreover, it is easily verified that if we take $\Gamma\left(t\right)=\frac{\gamma}{M}\delta\left(t\right)$ we recover the result obtained in equation (4.63). Now the last step consists in using (2.43) (as we have already often done), namely

$$
\frac{h^{2}}{2}\left\langle\Delta Q^{2}\right\rangle\left(t\right)\geq h\left\langle Q\right\rangle^{\alpha}\left(t\right)-h\left\langle Q\right\rangle\left(t\right)-\mathbb{H}\left(P^{\alpha}|P\right)\left(t\right)
\tag{5.31}
$$

where $Q\left(t\right)$ is a generic current. By setting

$$
\left\langle Q\right\rangle^{\alpha}\left(t\right)-\left\langle Q\right\rangle\left(t\right)=\alpha\delta\left\langle Q\right\rangle\left(t\right)
\tag{5.32}
$$

so that (5.31) becomes

$$
\frac{h^{2}}{2}\left\langle\Delta Q^{2}\right\rangle\left(t\right)\geq h\alpha\delta\left\langle Q\right\rangle-\frac{\alpha^{2}}{4}\langle\Sigma\rangle\left(t\right)
\tag{5.33}
$$

we can make the already well known substitution

$$
\alpha=\frac{2h\delta\left\langle Q\right\rangle\left(t\right)}{\langle\Sigma\rangle\left(t\right)}
\tag{5.34}
$$

so that equation (5.31) becomes

$$
\left\langle\Delta Q^{2}\right\rangle\left(t\right)\geq\frac{2\left(\delta\left\langle Q\right\rangle\left(t\right)\right)^{2}}{\langle\Sigma\rangle\left(t\right)}
\tag{5.35}
$$

Again, to make some explicit calculations that are analytically not too difficult to handle we take the generic current $Q\left(t\right)$ to be the position x of which we know mean and variance (equation (5.27)). We just have to calculate

$$
\left\langle x\right\rangle^{*}\left(t\right)-\left\langle x\right\rangle\left(t\right)=\alpha\delta\left\langle x\right\rangle\left(t\right)=\phi_{x}^{\alpha}\left(t\right)-\phi_{x}\left(t\right)=\frac{\alpha}{M}\int_{0}^{t}ds\left(\frac{\partial\chi_{x}^{\alpha}\left(t-s\right)}{\partial\alpha}\Big|_{\alpha=0}\right)F\left(s\right)
\tag{5.36}
$$

where we have used (5.30). We hence identify

$$\delta\langle x\rangle(t)=\frac{1}{M}\int_0^t ds\left(\frac{\partial\chi_x^\alpha(t-s)}{\partial\alpha}\Big|_{\alpha=0}\right)F(s) \tag{5.37}$$

again showing that relation (5.32) is valid.
With these informations (5.35) becomes

$$\frac{2k_BT}{M}\chi(t)\geq\frac{2\left(\int_0^t ds\left(\frac{\partial\chi_x^\alpha(t-s)}{\partial\alpha}\Big|_{\alpha=0}\right)F(s)\right)^2}{M^2\left[\left(\frac{\left(\frac{\partial\chi^\alpha(t)}{\partial\alpha}\Big|_{\alpha=0}\right)}{\chi(t)}\right)^2+\frac{\left(\int_0^t ds\left(\frac{\partial\chi_x^\alpha(t-s)}{\partial\alpha}\Big|_{\alpha=0}\right)F(s)\right)^2}{k_BTM\chi(t)}\right]} \tag{5.38}$$

or equivalently

$$I(t)=\frac{2\left(\delta\langle x\rangle(t)\right)^2}{\langle\Sigma\rangle(t)\cdot\langle\Delta x^2\rangle(t)}=\frac{\left(\int_0^t ds\left(\frac{\partial\chi_x^\alpha(t-s)}{\partial\alpha}\Big|_{\alpha=0}\right)F(s)\right)^2}{\left[K_BTM\frac{\left(\left(\frac{\partial\chi^\alpha(t)}{\partial\alpha}\Big|_{\alpha=0}\right)\right)^2}{\chi(t)}+\left(\int_0^t ds\left(\frac{\partial\chi_x^\alpha(t-s)}{\partial\alpha}\Big|_{\alpha=0}\right)F(s)\right)^2\right]}\leq 1 \tag{5.39}$$

which is a generalized version of (4.74). Note that this non-equilibrium inequality is aslo always verified as we have the ratio of a squared quantity $\left(\int_0^t ds\left(\frac{\partial\chi_x^\alpha(t-s)}{\partial\alpha}\Big|_{\alpha=0}\right)F(s)\right)^2$ and the same quantity plus another positive quantity. In fact, being $\chi(t)$ proportional to $\sigma^2(t)$ (see equation (5.27)), it is in turn positive. We are now going to analyse this inequality for some particular memory kernels.

5.1 Exponential memory kernel

As mentioned above in the previous subsection the first step towards non-Markovianity can be made by using an exponentially decaying memory kernel which we can imagine being dependend on two parameters, namely

$$\Gamma(t)=\beta\lambda e^{-\lambda t}\qquad\Longrightarrow\qquad\hat{\Gamma}(k)=\frac{\beta\lambda}{k+\lambda} \tag{5.40}$$

from this we obtain the response function which we know its Laplace transform to be equal to

$$\hat{\chi}_v(k)=\frac{1}{\left[k+\hat{\Gamma}(k)\right]}=\frac{k+\lambda}{k^2+k\lambda+\beta\lambda} \tag{5.41}$$

From tables we obtain the inverse Laplace transform of (5.41) that is

$$\chi_v(t)=e^{-\frac{\lambda}{2}t}\left[\cosh(\omega t)+\frac{\lambda}{2\omega}\sinh(\omega t)\right] \tag{5.42}$$

with $2\omega=\sqrt{\lambda(\lambda-4\beta)}$. As for $\chi_x(t)$ and $\chi(t)$ we have that

$$\chi_x(t)=\frac{1}{\beta}\left[1-e^{-\frac{\lambda}{2}t}\left[\left(\frac{\lambda-2\beta}{2\omega}\right)\sinh(\omega t)+\cosh(\omega t)\right]\right] \tag{5.43}$$

$$\chi(t)=\frac{1}{\beta}\left[t+\left(\frac{\lambda-\beta}{\lambda\beta}\right)\left[e^{-\frac{\lambda}{2}t}\cosh(\omega t)-1\right]+\left(\frac{\lambda-3\beta}{2\beta\omega}\right)e^{-\frac{\lambda}{2}t}\sinh(\omega t)\right] \tag{5.44}$$

Before proceeding with the verification of the thermodynamic uncertainty principle we make some considerations on the parameters appearing in the memory kernel. We remember that at the beginning of this section we made the consideration that a familiar situation in which non-markovianity can arise is the case of a Brownian particle whose characteristic time (τ_B) is not much greater than the characteristic time scale of the fluid components(τ_F), hence we could make a reasonable guess and put

$$\beta = \frac{\gamma}{M} = \frac{1}{\tau_B} \qquad\qquad \lambda = \frac{\gamma}{m} = \frac{1}{\tau_F} \tag{5.45}$$

where m is the mass of the fluid molecules. In fact we see that if λ tends to infinity we obtain

$$\lim_{\lambda\to+\infty} \beta\lambda e^{-\lambda t} = \frac{\gamma}{M}\delta\left(t\right) \tag{5.46}$$

so that if the characteristic time of the microscopic particles is small we recover the delta-correlated white noise of the previous section. Moreover if we suppose

$$\frac{\beta}{\lambda} = \frac{m}{M} \ll 1 \implies \omega = \frac{\lambda}{2}\sqrt{1 - \frac{4\beta}{\lambda}} \approx \frac{\lambda}{2}\left(1 - \frac{2\beta}{\lambda}\right) = \frac{\lambda}{2} - \beta \tag{5.47}$$

we see that under this hypotesis, in addition to the condition of $\lambda \gg 1$, equation (5.42) becomes

$$\begin{aligned} \lim_{\lambda\to+\infty} \chi_v\left(t\right) \approx \lim_{\lambda\to+\infty} e^{-\frac{\lambda}{2}t}\left[\frac{e^{\frac{\lambda}{2}-\beta} + e^{-\frac{\lambda}{2}+\beta}}{2} + \frac{\lambda}{2\left(\frac{\lambda}{2}-\beta\right)}\left(\frac{e^{\frac{\lambda}{2}-\beta} - e^{-\frac{\lambda}{2}+\beta}}{2}\right)\right] = \\ \lim_{\lambda\to+\infty}\left[\frac{e^{-\beta} + e^{-\lambda+\beta}}{2} + \frac{\lambda}{2\left(\frac{\lambda}{2}-\beta\right)}\left(\frac{e^{-\beta} - e^{-\lambda+\beta}}{2}\right)\right] = e^{-\beta t} = e^{-\frac{\gamma}{M}t} \end{aligned} \tag{5.48}$$

which is exactly equal to (4.6). We conclude that if $\frac{\gamma}{m} \gg 1$ along with th condition that the mass of the Brownian particle to be much bigger the fluid's particle mass we recover the Markov dynamics of the previous section. After this preamble we can proceed with the study of the behaviour of (5.39). We shall consider constant force for two reasons first of all is is of course the simplest case (very simple as we will see) and secondly we will have the opportunity to compare the results with those obtained in the previous subsections. Before all we note that for a constant force

$$\int_0^t ds\left(\frac{\partial\widetilde{\chi}_x\left(t-s\right)}{\partial\alpha}\Big|_{\alpha=0}\right)F = F\left(\frac{\partial\widetilde{\chi}\left(t\right)}{\partial\alpha}\Big|_{\alpha=0}\right) \tag{5.49}$$

thus (5.39) becomes

$$I\left(t\right) = \frac{\frac{F^2}{K_BTM}}{\left[\frac{1}{\chi(t)} + \frac{F^2}{K_BTM}\right]} \leq 1 \tag{5.50}$$

Noting that $\chi\left(t\right)$ can be made dimensionless by multiplying it by β^2 we rewrite equation (5.50) as

$$I\left(t\right) = \frac{f^2}{\frac{1}{\beta^2\chi(t)} + f^2} \leq 1 \tag{5.51}$$

where, as we have already seen, we have set

$$f\left(q\right) = \left[\frac{1}{k_BTM\beta^2}\right]^{\frac{1}{2}} F\left(q\right) = \left[\frac{M}{k_BT\gamma^2}\right]^{\frac{1}{2}} F\left(q\right) \tag{5.52}$$

which is also a dimensionless quantity.
In Figure number 10 we can observe the behaviour of equation (5.51) compared to Markov case with same β (the curves with the same colour as the ones in the legend are the one relative to the non-Markov case while the ones near to them correspond to the Markov case). Let us remember that

$$\omega = \frac{\lambda}{2}\sqrt{1 - \frac{4\beta}{\lambda}} \tag{5.53}$$

and hence if $\lambda \leq 4\beta$ (or $M \leq 4m$) we obtain an imaginary quantity and the dynamics corresponds to damped oscillations of the particle. Thus, in figure 10 we decided to consider λ slightly grater than 4β so that the dynamics is still the one we are familiar with and moreover it was seen that even for λ not so big with respect to 4β the difference between Markov and non-Markov is impossible to see (so we took λ as little as possible without changing the dynamics). Nevertheless, even if the chosen λ is the smallest possible, the differences are still very little and for this reason we show an enlarged particular of figure 10 in figure 11. In these figures (where we have set $f = 0.5$) the coloured curves correspond to the weak non-Markov dynamics while the grey curves near to them are the Markov ones with same $\beta = \frac{\gamma}{M}$ obtained in the previous section with a constant external force. The little differences that we have just found between the two dynamics justifies the word weak non-Markovianity (it had to be expected being the exponential a rapidly decreasing function).
For the sake of completeness we analyse the opposite situation where λ is much smaller than β in order to observe aforementioned damped oscillations of the particle. The two parameters where chosen so that the oscillations are maximized with respect to the damping given by the exponential nature of the memory kernel so that we focus on what happens as we vary the dimensionless force f. Figure 12 shows that at (very) large times the same behaviour as before is restored, it had to be expected as after a transient time the system reaches a steady state where the deterministic component of the dynamics (the constant force) dominates making the non equilibrium inequality (5.51) an equality. Instead we see that at short times a certain periodicity is visible in figure 13 the damping effect of the exponential is still evident whereas at very short times the damping is very difficult to see (figure 14). This situation will be better analysed in the next subsection.

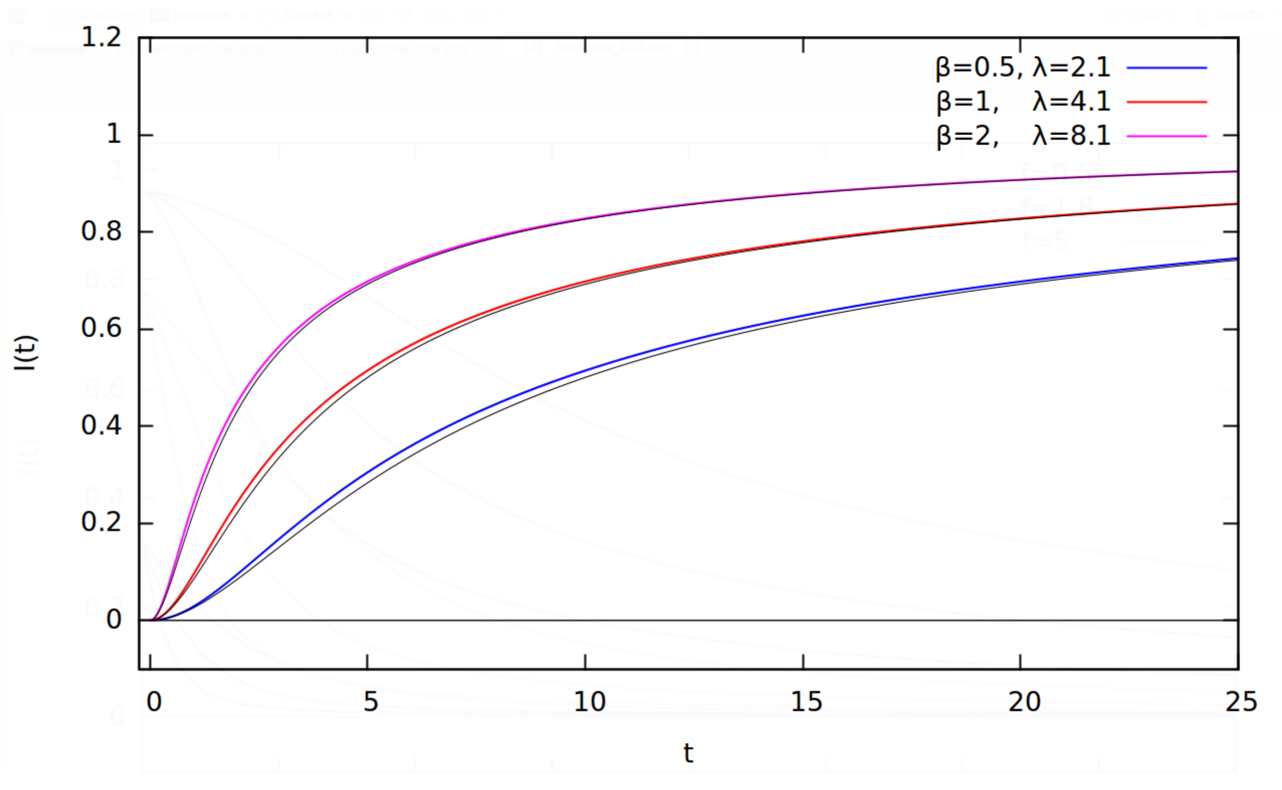


Figure 10: Plot of $I(t)$ for exponential memory kernel, coloured curves are related to non-Markov dynamics whereas grey curves are related to the corresponding Markov dynamics such that $\beta = \frac{\gamma}{M}$

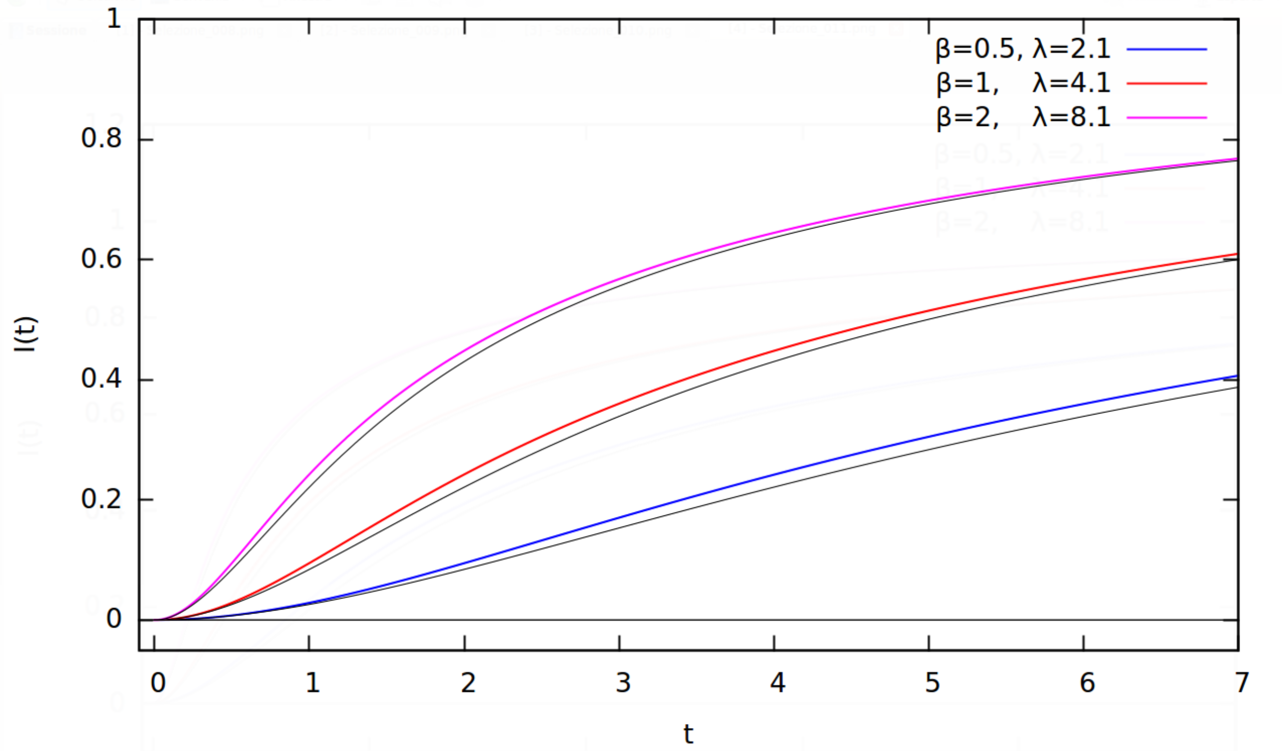


Figure 11: Zoom of figure 10 to better see the differences between non- Markov and Markov dynamics

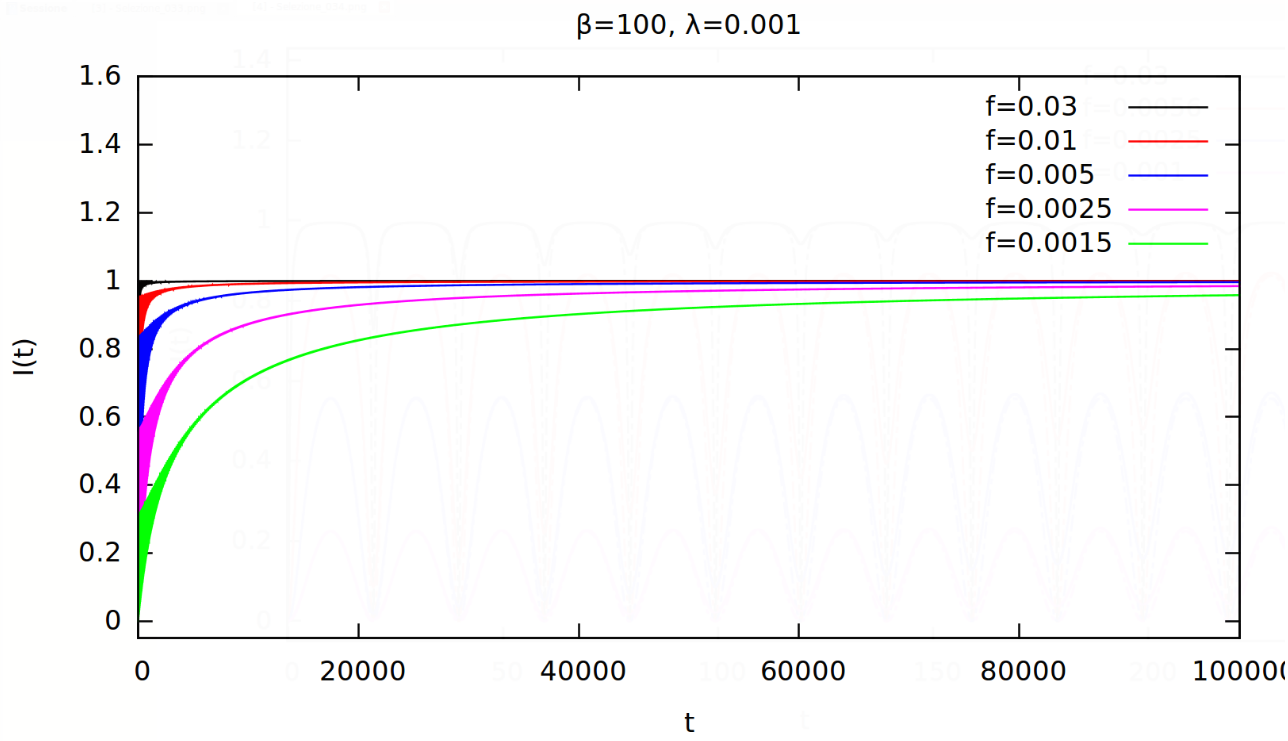


Figure 12: Plot of $I(t)$ for exponential memory kernel with $\lambda \ll \beta$, for large times we recover the previous dynamics

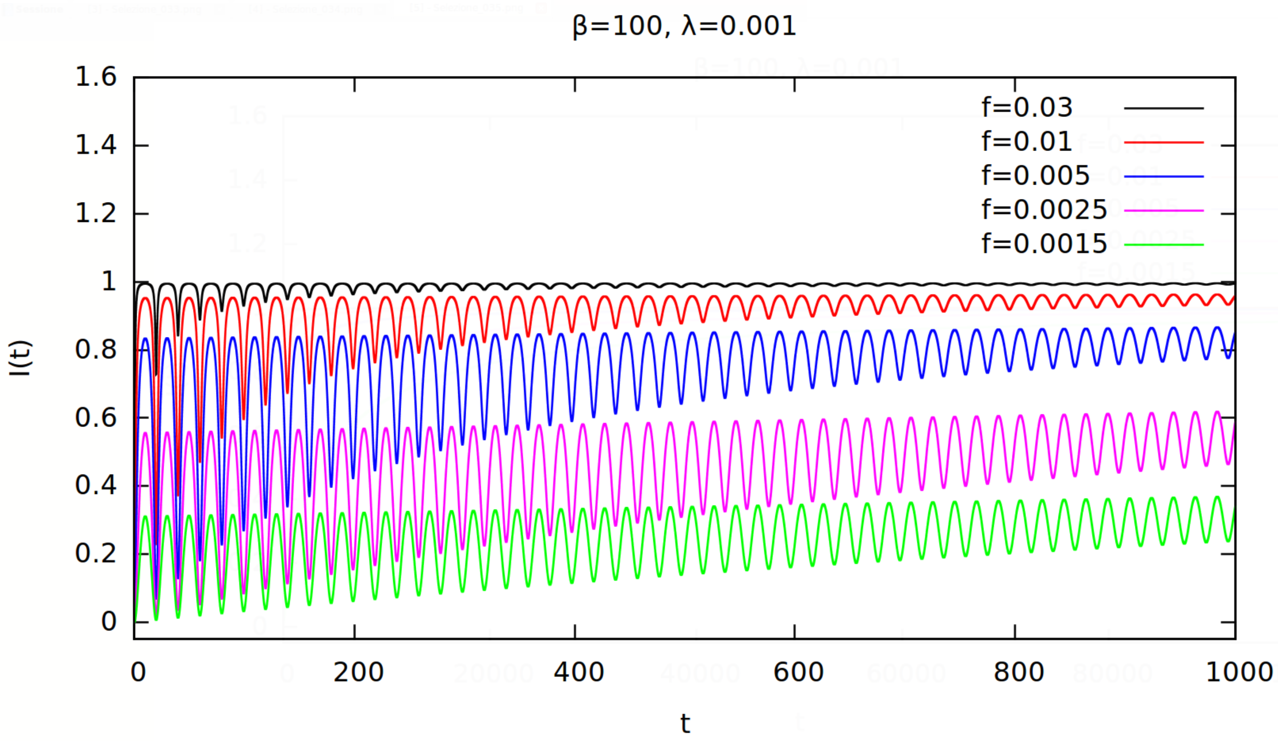


Figure 13: Plot of $I(t)$ for exponential memory kernel with $\lambda \ll \beta$, damped oscillations of the Brownian particle are evident

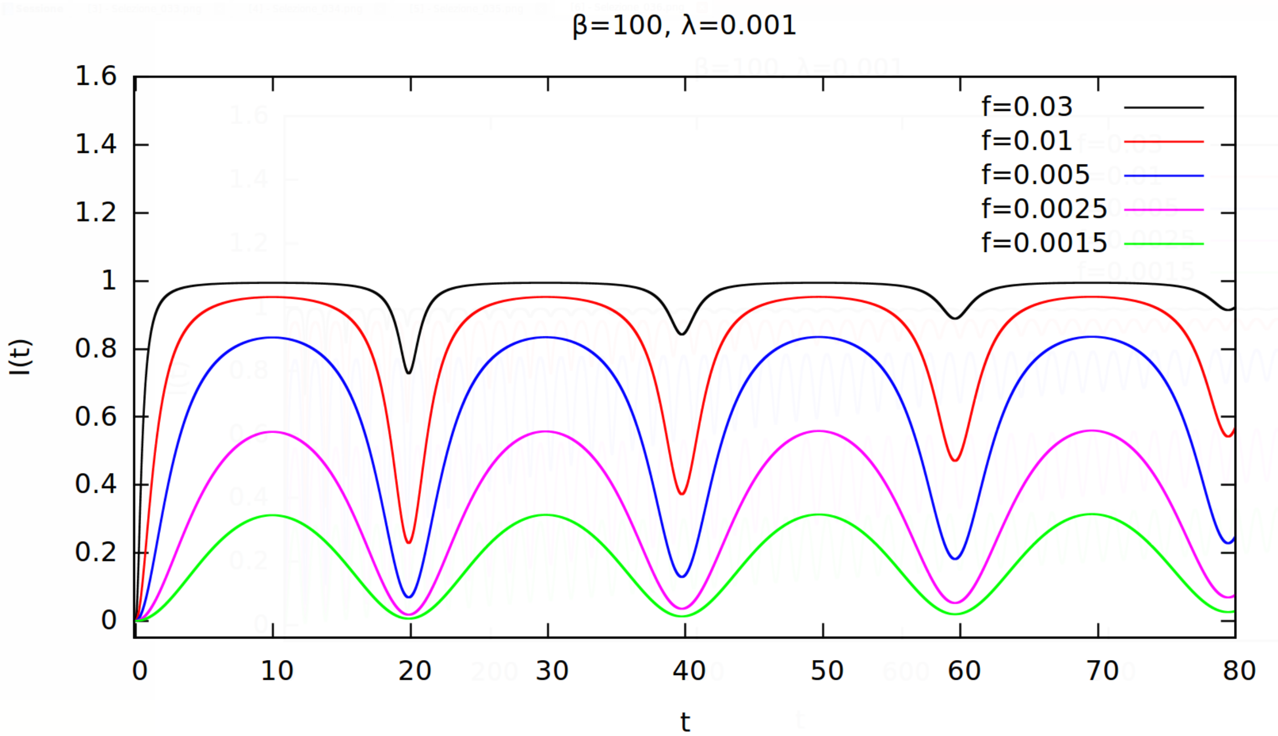


Figure 14: Plot of $I(t)$ for exponential memory kernel with $\lambda \ll \beta$, for very short times the damping is really difficult to see

5.2 Constant memory kernel

In the previous subsection we considered an exponential memory kernel which corresponds to the week non-Markovianity condition because of it rapidly decaying behaviour. Physically this means that the system keeps memory of the past only for a very rapidly and that the present is not affected by what happened in the infinite past. In more general situation it is of course not always like this but it is usually expected that the the memory kernel decays to zero after a certain characteristic time with some kind of power law or function with an initial rapid decay followed by a slow final decay. The reason why this is true is due to the fact that the thermal bath needs a finite time to respond to the fluctuations of the system. The case of a thermal bath responding infinitely quickly to those fluctuations corresponds to the memory kernel being a delta function, hence recovering Markov dynamics.
On the other hand, the opposite situation could be a very sluggish bath responding extremely slowly to the motion of the Brownian particle whose memory kernel could be in first approximation taken as a constant, namely $\Gamma(t) = \Gamma_0$. Although this is a strongly idealised situation, there are cases where for short times compared to the response time of the bath this approximation is reasonable. Before making some more considerations, let us note that using the generalised Langevin equation we obtain:

$$\begin{gathered}\frac{dv}{dt}(t) = -\int_0^t \Gamma\left(t-t'\right) v\left(t'\right) dt' + \frac{F(t)}{M} + \frac{\eta(t)}{M} = \\ -\int_0^t \Gamma_0 v\left(t'\right) dt' + \frac{F(t)}{M} + \frac{\eta(t)}{M} = -\Gamma_0\Big(x(t) - x(0)\Big) + \frac{F(t)}{M} + \frac{\eta(t)}{M}\end{gathered} \tag{5.54}$$

The $-\Gamma_0\Big(x(t) - x(0)\Big)$ term is a restoring force corresponding to an harmonic potential of the form:

$$\phi(x, x_0) = \frac{1}{2}\Gamma_0 (x - x_0)^2 \implies F(x) = -\frac{\partial}{\partial x}\phi(x, x_0) = -\Gamma_0 (x - x_0) \tag{5.55}$$

This effect is called dynamic caging and can be observed for example if a small light particle is immersed in a bath of bigger and heavier particles. It can happen that the little test particle gets trapped in a sort of spatial cage made by the heavy particles of the bath and only with the aid of the rare fluctuations of the bath that open some holes in the cage the test particle is able to escape. After that it is very likely that the latter get caught again in a new cage. We thus expect that some sort of periodicity to arise also in the thermodynamic uncertainty relation. For this purpose we calculate as usual the response function using Laplace transform of the memory kernel:

$$\hat{\Gamma}(k) = \frac{\Gamma_0}{k} \implies \hat{\chi}_v(k) = \frac{1}{k + \hat{\Gamma}(k)} = \frac{k}{k^2 + \Gamma_0} \tag{5.56}$$

so that:

$$\begin{gathered}\chi_v(t) = \cos\left(\sqrt{\Gamma_0} t\right) \qquad \chi_x(t) = \int_0^t ds \chi_v(s) = \frac{\sin\left(\sqrt{\Gamma_0} t\right)}{\sqrt{\Gamma_0}} \\ \chi(t) = \int_0^t ds \chi_x(s) = \frac{1 - \cos\left(\sqrt{\Gamma_0} t\right)}{\Gamma_0}\end{gathered} \tag{5.57}$$

With the aid of these relations we explore the behaviour of equation (5.39), as usual starting from a constant external force. We have the same situation of equations (5.49) and (5.50), hence we obtain:

$$I(t) = \frac{\frac{F^2}{K_B T M}}{\left[\frac{1}{\chi(t)} + \frac{F^2}{K_B T M}\right]} \leq 1 \tag{5.58}$$

In order to make the force dimensionless we multiply numerator and denominator by $\frac{1}{\Gamma_0}$ so that becomes:

$$I(t) = \frac{\frac{F^2}{K_B T M \Gamma_0}}{\left[\frac{1}{\Gamma_0 \chi(t)} + \frac{F^2}{K_B T M \Gamma_0}\right]} = \frac{f^2}{\left[\frac{1}{1 - \cos\left(\sqrt{\Gamma_0} t\right)} + f^2\right]} \leq 1 \tag{5.59}$$

with $f = F \cdot (k_B T M \Gamma_0)^{-\frac{1}{2}}$ dimensionless.
In figure 15 this relation is plotted for a fixed force and variable Γ_0 and we note that the effect is just a change of the periodicity of the curves. Instead, in figure 16, Γ_0 is fixed while we let the force variable. As in the previous cases, as the external force rises the inequality tends to saturate to an equality (except for the case where $1 - \cos\left(\sqrt{\Gamma_0} t\right) = 0$), this happens because as the deterministic part of the dynamic becomes dominant with respect to the fluctuations of the system the Jensen inequality becomes an equality and so does (5.59).

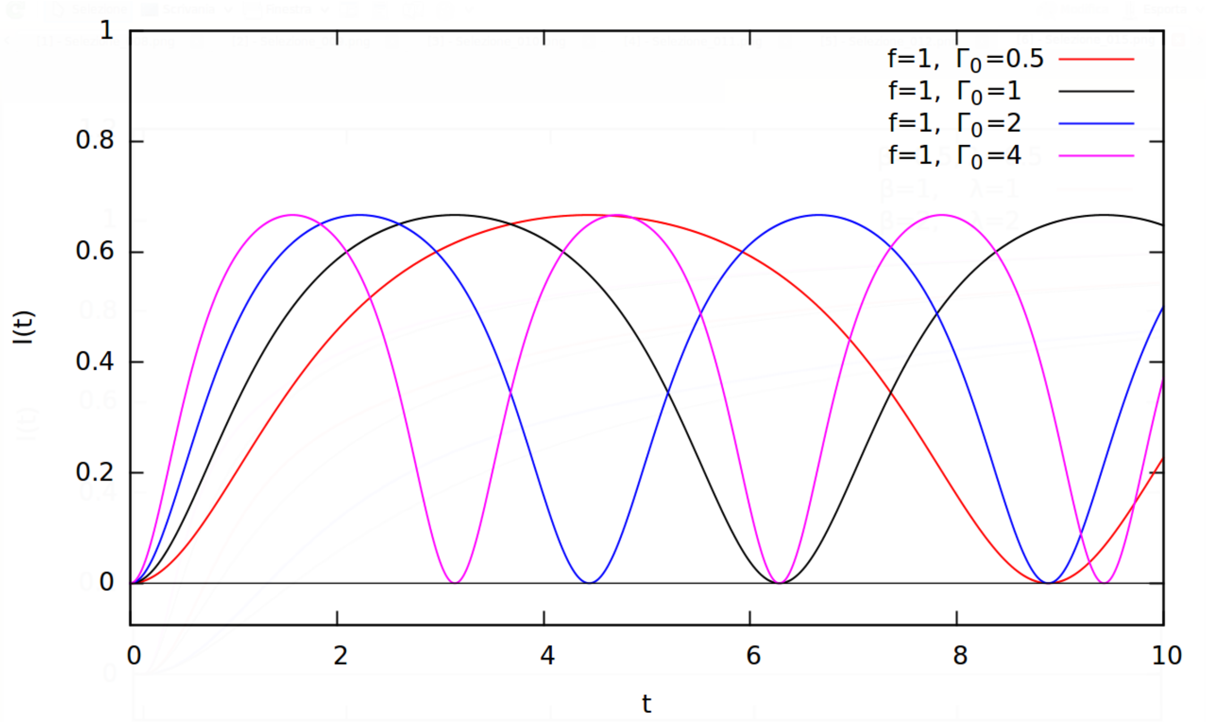


Figure 15: Plot of $I(t)$ for constant memory kernel and constant force with $f = 1$

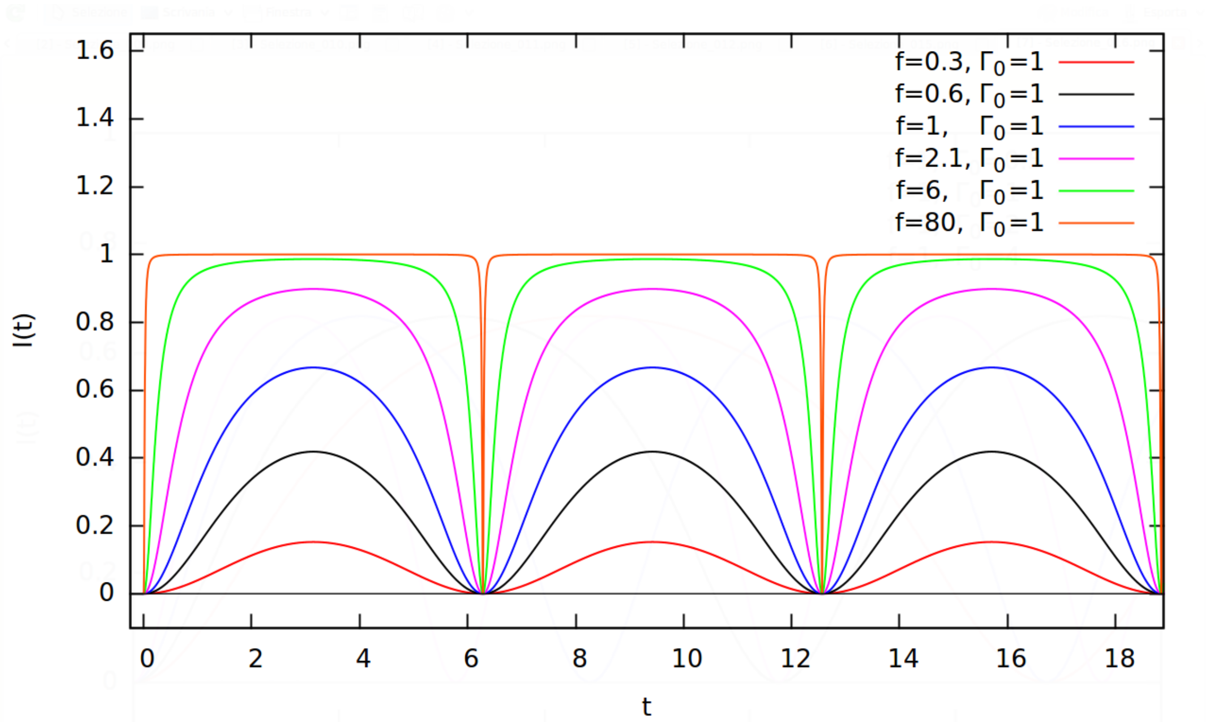


Figure 16: Plot of $I(t)$ for constant memory kernel and constant force with $\Gamma_0 = 1$

Anyway, as we said before, a constant memory kernel must be considered as a (useful) approximation for a short time behaviour of more complicated memory kernel that are analytically very difficult to handle. For this reason we again consider the exponential memory kernel in the case of $\lambda \ll 1$ so that for small times we get:

$$\Gamma(t) = \beta\lambda e^{-\lambda t} \approx \beta\lambda \tag{5.60}$$

that is a constant. Hence for a slowly decaying exponential, at small times we get approximatively a constant and hence in this situation we can identify $\beta\lambda = \Gamma_0$. To make a comparison between the two cases we must match their important parameters, hence (as already made in the previous subsection) we set $\lambda = 0.001$ and $\beta = 100$ so that $\Gamma_0 = 0.1$ both for figure 17 and 18 knowing that a change in these values will only affect the periodicity of the shown pattern. Concerning the value of the force we obviously want the external forces for the two cases to be the same but we have to remember that the dimensionless forces appearing in (5.51) and (5.59) have a different definition. In fact we have that:

$$f_{exp} = \left[\frac{1}{k_B T M \beta^2}\right]^{\frac{1}{2}} F \qquad\qquad f_{const} = \left[\frac{1}{k_B T M \Gamma_0}\right]^{\frac{1}{2}} F \tag{5.61}$$

hence we obtain that:

$$f_{const} = f_{exp}\frac{\sqrt{\Gamma_0}}{\beta} \tag{5.62}$$

with, as already said, $\beta = 100$ and $\Gamma_0 = 0.1$. Hence in figure 17 and 18 it is shown the value of f_{exp} related to the continuous lines and the corresponding f_{const} is obtained through relation (5.62) and it is referred to dashed lines (the colours of the curves such that this relation holds are the same). We observe that, for small times, the behaviour of the curves with same colour is very similar (as expected) and becomes more and more different as time increases.

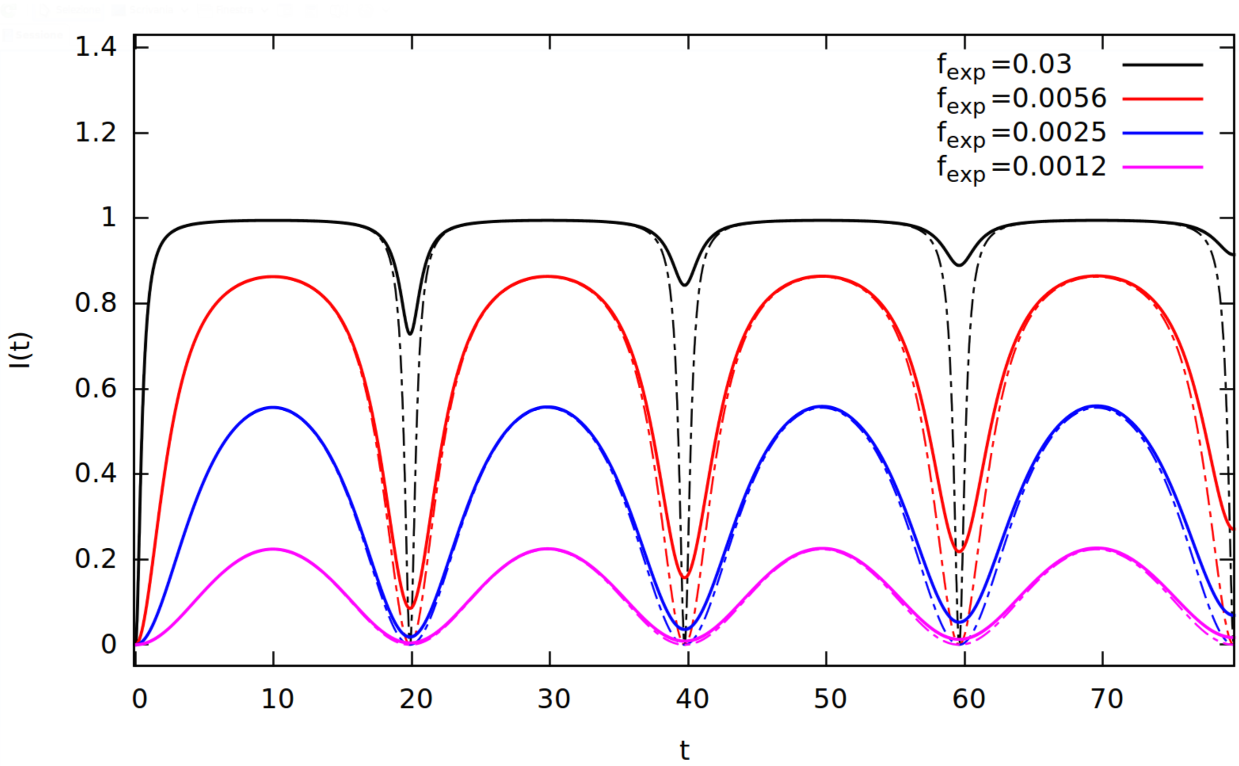


Figure 17: Comparison at short times between $I(t)$ for exponential memory kernel (solid curves) with constant force f_{exp}, $\lambda = 0.001$ and $\beta = 100$ and constant memory kernel (dashed curves) with $f_{const} = f_{exp}\frac{\sqrt{\Gamma_0}}{\beta}$ and $\Gamma_0 = \beta\lambda = 0.1$

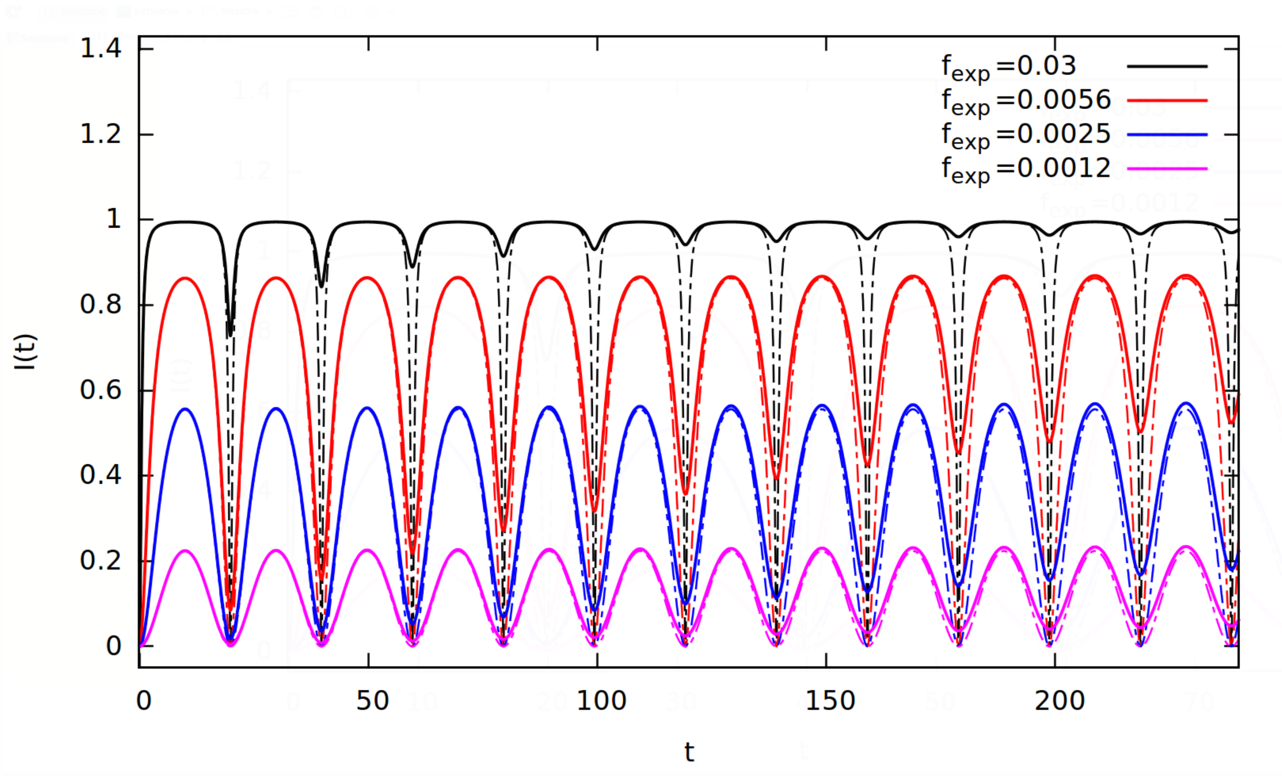


Figure 18: Comparison at greater times between $I(t)$ for exponential memory kernel (solid curves) with constant force f_{exp}, $\lambda = 0.001$ and $\beta = 100$ and constant memory kernel (dashed curves) with $f_{const} = f_{exp}\frac{\sqrt{\Gamma_0}}{\beta}$ and $\Gamma_0 = \beta\lambda = 0.1$. The damping related to the exponential memory kernel is here evident.

It is also interesting to analyse the case of an impulsive force:

$$F(t) = \frac{F\delta(t)}{\Gamma_0}$$

As already said, such a kind of force is an idealisation but can be a good approximation when a strong force is exerted for a small time with respect to the characteristic time of the system, namely the time that the bath needs to respond to the force. Moreover it offers the possibility to do some analytical calculation without too much effort and to observe some more peculiar behaviour with respect to the constant force case.
We need to calculate

$$\widetilde{\chi}_*(t) \approx \chi_*(t) + \alpha\left(\frac{\partial\widetilde{\chi}_*(t)}{\partial\alpha}\Big|_{\alpha=0}\right) \tag{5.63}$$

using the perturbation $\widetilde{\Gamma_0} = (1+\alpha)\Gamma_0$. We obtain

$$\begin{aligned} \widetilde{\chi}_x(t) &\approx \chi_x(t) + \frac{\alpha}{2}\left[t\cos\left(\sqrt{\Gamma_0}t\right) - \frac{\sin\left(\sqrt{\Gamma_0}t\right)}{\sqrt{\Gamma_0}}\right] \\ \widetilde{\chi}(t) &\approx \chi(t) + \alpha\left[\frac{t\sin\left(\sqrt{\Gamma_0}t\right)}{2\sqrt{\Gamma_0}} + \frac{\cos\left(\sqrt{\Gamma_0}t\right) - 1}{\Gamma_0}\right] \end{aligned} \tag{5.64}$$

In order to use equation (5.39) we have to calculate

$$\begin{aligned} \int_0^t ds\left(\frac{\partial\widetilde{\chi}_x(t-s)}{\partial\alpha}\Big|_{\alpha=0}\right)F(s) = \frac{F}{2\Gamma_0}\left(\frac{\partial\widetilde{\chi}_x(t)}{\partial\alpha}\Big|_{\alpha=0}\right) = \\ \frac{F}{4\Gamma_0}\left[t\cos\left(\sqrt{\Gamma_0}t\right) - \frac{\sin\left(\sqrt{\Gamma_0}t\right)}{\sqrt{\Gamma_0}}\right] \end{aligned} \tag{5.65}$$

where we have again used the fact that:

$$\int_0^t dsg(s)\,\delta(s) = \frac{g(0)}{2} \tag{5.66}$$

We use equations (5.64) and (5.65) so that (5.39) becomes:

$$I(t) = \frac{\frac{f^2}{16}\left[t\sqrt{\Gamma_0}\cos\left(\sqrt{\Gamma_0}t\right) - \sin\left(\sqrt{\Gamma_0}t\right)\right]^2}{\frac{f^2}{16}\left[t\sqrt{\Gamma_0}\cos\left(\sqrt{\Gamma_0}t\right) - \sin\left(\sqrt{\Gamma_0}t\right)\right]^2 + \frac{\left[\frac{t\sqrt{\Gamma_0}}{2}\sin\left(\sqrt{\Gamma_0}t\right)+\cos\left(\sqrt{\Gamma_0}t\right)-1\right]^2}{1-\cos\left(\sqrt{\Gamma_0}t\right)}} \leq 1 \tag{5.67}$$

where as before we have set $f = F \cdot (k_B T M \Gamma_0)^{-\frac{1}{2}}$. Again we see that the system exhibits a periodicity which is determined by the Γ_0 parameter as it is shown in figure 19. On the other side, at fixed Γ_0, as we increase f the left hand side (5.67) tends more and more to 1 for almost every time, this is evident in figure 20.
Until now we just focused on the ratio $I(t)$ to extrapolate informations on the system's dynamic, that is to see whether the random or the deterministic component dominates at different times. It is also interesting to see how the single components of equation (5.67) behave and to compare them with the behaviour of $I(t)$. We make this operation in this particular case because, as we have seen, in the constant force case many terms cancel out and hence what we are going to do now would not be so interesting. First of all we remember that (5.67) was originally different as we simplified some terms from the original expression. In fact we had that:

$$I(t) = \frac{\frac{\frac{f^2}{16}\left[t\sqrt{\Gamma_0}\cos\left(\sqrt{\Gamma_0}t\right)-\sin\left(\sqrt{\Gamma_0}t\right)\right]^2}{1-\cos\left(\sqrt{\Gamma_0}t\right)}}{\frac{\frac{f^2}{16}\left[t\sqrt{\Gamma_0}\cos\left(\sqrt{\Gamma_0}t\right)-\sin\left(\sqrt{\Gamma_0}t\right)\right]^2}{1-\cos\left(\sqrt{\Gamma_0}t\right)} + \frac{\left[\frac{t\sqrt{\Gamma_0}}{2}\sin\left(\sqrt{\Gamma_0}t\right)+\cos\left(\sqrt{\Gamma_0}t\right)-1\right]^2}{\left[1-\cos\left(\sqrt{\Gamma_0}t\right)\right]^2}} \leq 1 \tag{5.68}$$

Some constant are still missing because they were used to make F dimensionless but this is no big problem as we will only focus on the functional behaviour of the various components of (5.68).

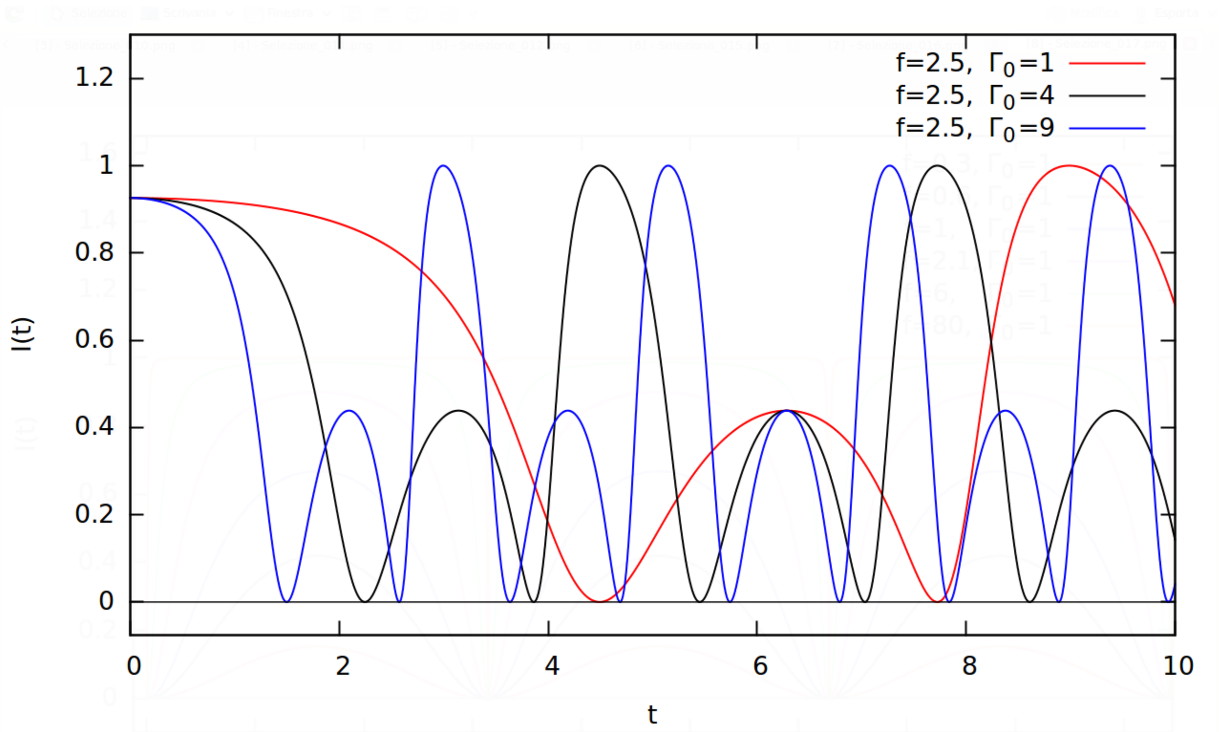


Figure 19: Plot of $I(t)$ for constant memory kernel and impulsive force with $f = 2.5$

Figure 21

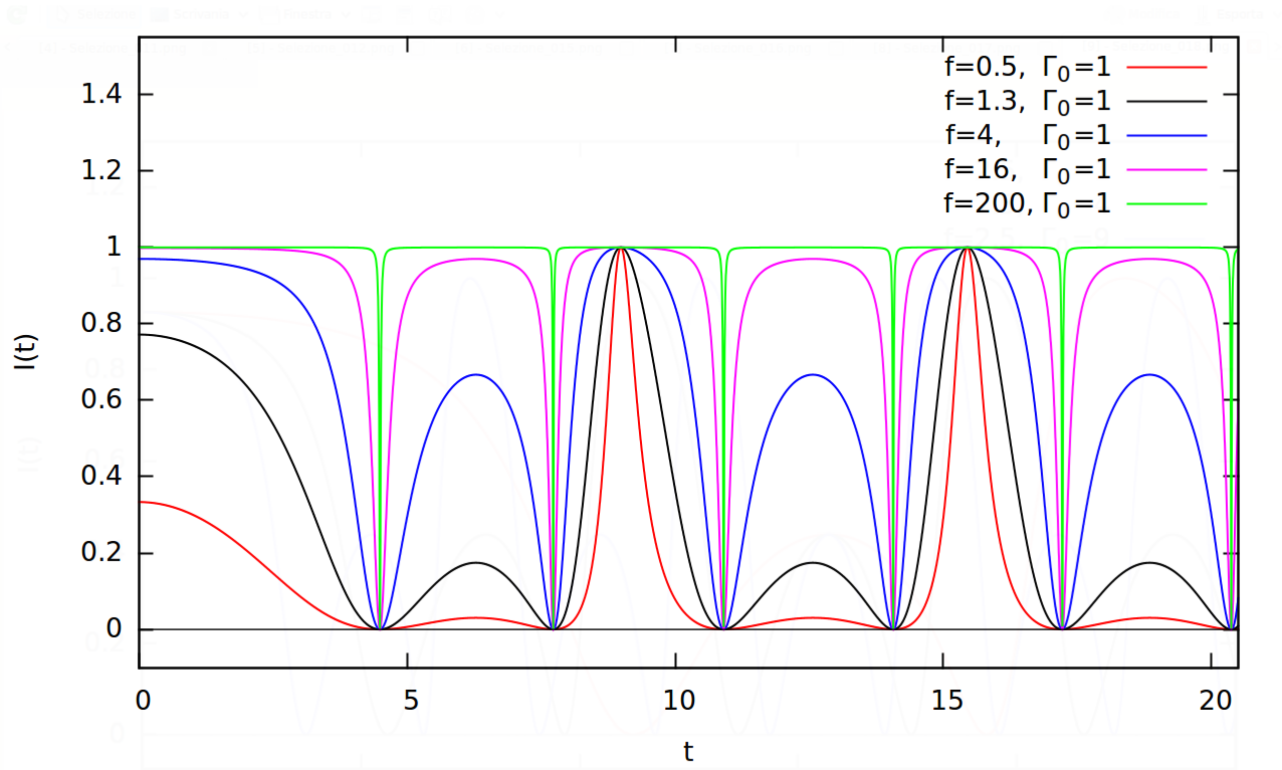


Figure 20: Plot of $I(t)$ for constant memory kernel and constant force with $\Gamma_0 = 1$

For this reason we also set k_B, T , M and Γ_0 equal 1, with this convention we have that $\sigma^2(t) = 2 - 2\cos(t)$ and hence (5.68) becomes:

$$I(t) = \frac{\frac{f^2\left[t\cos(t)-\sin(t)\right]^2}{8\sigma^2(t)}}{\frac{f^2\left[t\cos(t)-\sin(t)\right]^2}{8\sigma^2(t)} + \frac{4\left[\frac{t}{2}\sin(t)+\cos(t)-1\right]^2}{\left[\sigma^2(t)\right]^2}} \leq 1 \tag{5.69}$$

We recognize 2 terms:

$$F(t) = \frac{f^2\left[t\cos(t)-\sin(t)\right]^2}{8\sigma^2(t)} \qquad K(t) = \frac{4\left[\frac{t}{2}\sin(t)+\cos(t)-1\right]^2}{\left[\sigma^2(t)\right]^2} \tag{5.70}$$

The first one is the ratio between the deterministic part given the the external force and the variance while the second one is the term arising from the calculation of the Kullback-Leibler divergence and is a pure random term. Hence we see that if the deterministic part is big so will $F(t)$, this term will then have to compete with the $K(t)$ term which is again purely random. The physical meaning of this last term is yet to be identified. All this competition of terms is well shown in figure 21 ($F(t)$ and $K(t)$ have been displayed attenuated by a factor $\frac{1}{100}$ because of their divergent nature) where we see that $I(t)$ becomes equal to 1 when $K(t)$ becomes equal to zero while when it is that $F(t)$ that becomes 0 so does $I(t)$. Instead, when both $K(t)$ and $F(t)$ diverge the value of $I(t)$ is only determined by the value of f, as previously said as this term becomes bigger $I(t)$ becomes more and more equal to 1.

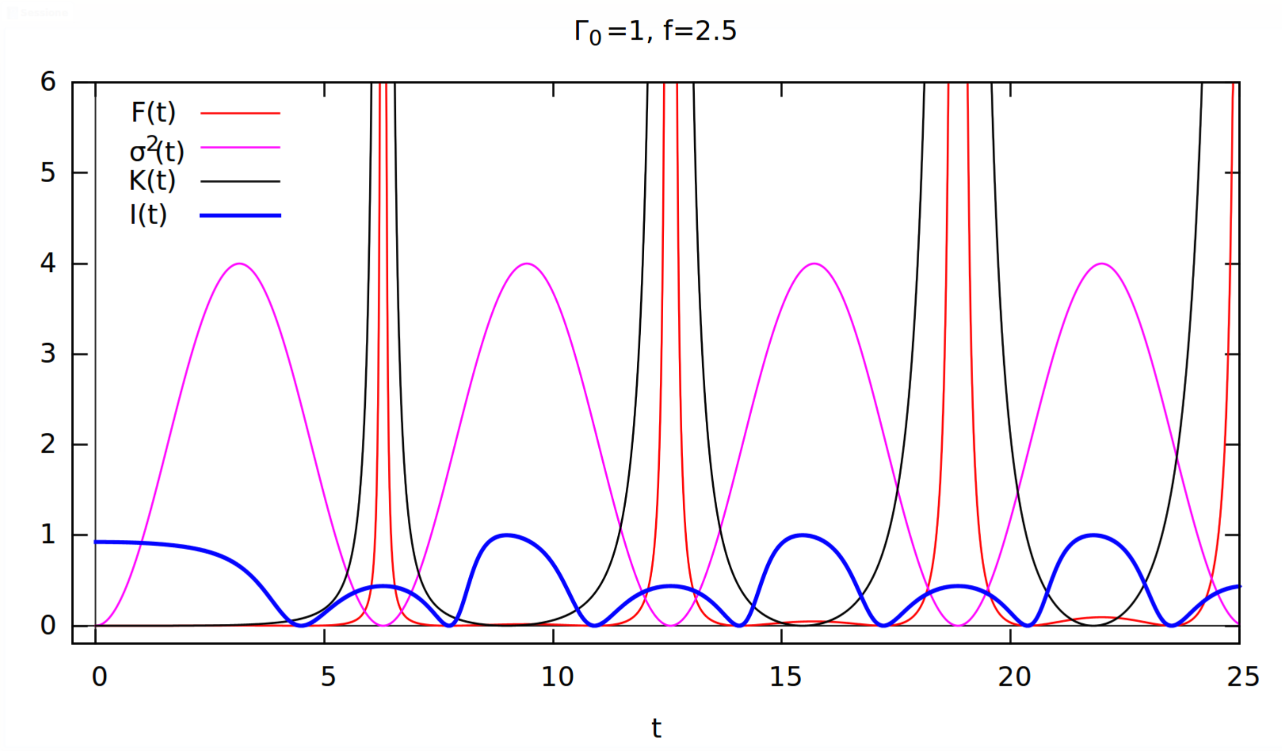


Figure 21: Plot of $I(t)$ for constant memory kernel and impulsive force with $f = 2.5$ along with its components (see definitions above). $F(t)$ and $K(t)$ have been displayed attenuated by a factor $\frac{1}{100}$.

6 Conclusions

In this thesis we used the Kullback-Leibler divergence to obtain general non-equilibrium inequalities for systems modelled by continuous time Markov chains and for some specific Langevin systems. Moreover we have seen that for some particular perturbation performed on the system's dynamic, through which the Kullback-Leibler is calculated, an entropic interpretation of the latter is achieved, hence reobtaining the thermodynamic uncertainty relation described in [1], [2] and [3]. Instead, in this thesis, we have mainly focused on performing some simpler perturbations, calculating the Kullback-Leibler divergences that arise from the latter and on relating the obtained results to other relevant observables of the system. This was done in particular for general jump processes where we performed a linear perturbation of the transition rates obtaining a relation between the variance of a given observable, the time derivative of its mean and the activity of the system, namely the average total number of jumps that the system performed up to time T. As for Brownian motion with time dependent external force, the results obtained involve the variance of a given observable, its susceptibility to the perturbation and of course the Kullback-Leibler divergence that we believe, in this particular situation, to be linked to the dissipation of the system as the perturbations we used involved the friction coefficient and friction kernel respectively in the Markov and non-Markov case. Moreover, using position as observable in the obtained inequalities and plotting the saturation ratio $I(t)$ for these we get interesting informations about the dominant components (deterministic or random) of the dynamics at different times.
The continuation to this thesis will be to find some other perturbation for Brownian systems that make, for example, the susceptibility of the observable proportional to the time derivative of its average and/or that make it possible to interpret the Kullback-Leibler divergence as a physical observable. More generally the objective could be to extend the proposed method to more general Langevin systems driven by a random force that is not Gaussian or for which the dissipation-fluctuation theorems do not hold. In fact the strength of this approach is its generality and its validity in every regime (equilibrium, staedy states and pure non-equilibrium), the only thing needed is that it is possible to define a probability measure and to subsequently calculate the Kullback-Leibler divergence using the formulas showed throughout the thesis.

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