Asymmetric fluctuation-relaxation paths in FPU models

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Abstract

A recent theory by Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim predicts a temporal asymmetry in the fluctuation-relaxation paths of certain observables of nonequilibrium systems in local thermodynamic equilibrium. We find temporal asymmetries in the fluctuation-relaxation paths of a form of local heat flow, in the nonequilibrium FPU-β model of Lepri, Livi and Politi.

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I. INTRODUCTION

In Refs. [1, 2], Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim proposed a generalization of Onsager-Machlup’s theory [3] to the large fluctuations around nonequilibrium steady states. This theory predicts temporal asymmetries between fluctuation and relaxation paths of certain observables, and includes the results of Derrida, Lebowitz and Speer [4], and of Bodineau and Derrida [5] as special cases. In particular, the theory of [1, 2] concerns stochastic lattice gases, which admit the hydrodynamic description

$$\partial_t \rho = \nabla \cdot \left[ \frac{1}{2} D(\rho) \nabla \rho - \chi(\rho) \nabla E \right] \equiv D(\rho), \quad \rho = \rho(u,t),$$

where $\rho$ is the vector of macroscopic observables, $u$ and $t$ are the macroscopic space and time variables, $D$ is the Onsager diffusion matrix, $\chi$ is the linear response conductivity, and $\nabla E$ is the external driving force. For such models, Refs. [1, 2] prove that the spontaneous fluctuations out of a steady state most likely follow an adjoint hydrodynamic equation:

$$\partial_t \rho = D^*(\rho), \quad \text{with} \quad D^*(\rho) = D(\rho) - 2A,$$

where $D$ has been decomposed as

$$D(\rho) = \frac{1}{2} \nabla \cdot \left( \chi(\rho) \nabla \frac{\delta S}{\delta \rho} \right) + A,$$

and $A$ is a vector field orthogonal to the thermodynamic force, i.e. to the functional derivative of the entropy with respect to the state $\delta S/\delta \rho$. The fact that $A$ is orthogonal to the thermodynamic force implies that it does not contribute to the entropy production: $A$ is the non-dissipative part of the dynamics.

Because the theory of [1, 2] is developed for stochastic processes, the question arises whether its predictions can be observed in the dynamics of time reversal invariant, deterministic, particle systems, such as those of nonequilibrium molecular dynamics (NEMD) [6]. Indeed, the stochastic description of a given system is often thought to be a reduced representation of the microscopic deterministic dynamics of its particles. One difficulty in addressing this question is that not all reductions of a microscopic dynamics to a mesoscopic (stochastic) one are equivalent, and it is not always easy to identify the stochastic counterparts of the observables of deterministic systems.

A nonequilibrium steady state requires at least two reservoirs at different thermodynamic states, in contact with the system of interest, and NEMD provides techniques to avoid the...
simulations of the reservoirs. However, present day NEMD simulations cannot be performed
with sufficiently many particles, and for sufficiently long times to achieve the mesoscopic
level of description. Therefore, in Ref. [7] the simplest of particle systems, the nonequilibrium
Lorentz gas, was investigated, but no temporal asymmetry was found in the fluctuation-
relaxation paths (FRPs) of its current. Here, we consider the FRPs of the local heat flux
of a more realistic model: the nonequilibrium FPU-β model of Lepri, Livi and Politi [8, 9],
and we observe that they are asymmetric in time. The model consists of the usual FPU-β
chain with \(N\) anharmonic oscillators of equal masses \(m\), located at \(x_j, j = 1, \ldots, N\), and
with two Nosé-Hoover “thermostats” at different temperatures acting on the first and the
last oscillator. The interaction potential and the internal energy are thus given by

\[
V(q) = \frac{q^2}{2} + \beta \frac{q^4}{4}; \quad \text{and} \quad H = \sum_{j=0}^{N} \frac{1}{2} m q_j^2 + V(q_{j+1} - q_j),
\]

where \(q_j = x_j - ja\) is the displacement of the \(j\)-th oscillator from its equilibrium position,
and \(a\) is the equilibrium distance between two nearest neighbours. The equations of motion
take the form

\[
\ddot{q}_1 = F(q_1 - q_0) - F(q_2 - q_1) - \zeta r \dot{q}_1, \quad \ddot{q}_N = F(q_N - q_{N-1}) - F(q_{N+1} - q_N) - \zeta r \dot{q}_N
\]

\[
\ddot{q}_j = F(q_j - q_{j-1}) - F(q_{j+1} - q_j), \quad \text{for} \ j = 2, \ldots, N - 1
\]

where \(F(q) = -V'(q)\), and the terms \(\zeta_r, \zeta_r\) obey

\[
\dot{\zeta}_r = \frac{1}{\theta_r^2} \left( \frac{\dot{q}_r^2}{T_r} - 1 \right), \quad \dot{\zeta}_r = \frac{1}{\theta_r^2} \left( \frac{\dot{q}_r^2}{T_r} - 1 \right),
\]

with the boundary conditions \(q_0 = q_{N+1} = 0\). We take \(\beta = 0.1\) and \(m = \theta_r = \theta_\ell = 1,\)
as in [8]. Equations (5) and (7) constitute the Nosé-Hoover thermostats at “temperatures”
\(T_r\) and \(T_\ell\), with response times \(\theta_r\) and \(\theta_\ell\). This nonequilibrium FPU-β model is dissipative
[11], but time reversal invariant [12]. Note that in our context \((T_r - T_\ell)\) is just a parameter
expressing the distance from the equilibrium state, and not a real temperature gradient.

Let \(L\) be a number of contiguous oscillators in a sublattice \(L = \{j_1, \ldots, j_L\}\) of the chain,
whose center coincides with the center of the chain, and let \(\eta = L/N\) be the fraction of the
chain occupied by \(L\). The instantaneous local heat flux \(F\) is defined by [9]:

\[
F = \frac{1}{L} \sum_{j=j_1}^{j_L} \frac{1}{2} (x_{j+1} - x_j)(\dot{q}_{j+1} + \dot{q}_j)F(q_{j+1} - q_j) + \dot{q}_jh_j,
\]
where
\[ h_j = \frac{1}{2} m \dot{q}_j^2 + \frac{1}{2} [V(q_{j+1} - q_j) + V(q_j - q_{j-1})], \]
and \( F(q) = -V'(q) \). There is another definition of local heat flux, which could be considered:

\[ f = \frac{1}{L} \sum_{j=n}^{j_L} \frac{1}{2} a F(q_j - q_{j-1})(\dot{q}_j + \dot{q}_{j-1}) + \frac{1}{2L} a (\dot{q}_{j_1} F(q_{j_1+1} - q_{j_1}) + \dot{q}_{j_L} F(q_{j_L+1} - q_{j_L})) \, , \]  
(9)

The first term of \( f \) is the average over \( L \) of the heat flux in the limit of small (compared to the lattice spacing \( a \)) oscillations as in \[9\], while the second term gives the flux through the boundary of \( L \). The quantities \( F \) and \( f \) are supposed to be equivalent in the limit of small oscillations and long chains. Therefore, for the sake of brevity, in this paper we do not study the properties of the FRPs of \( f \), which will be considered in a future paper \[10\], along with the FRPs of other observables.

Because of the large difference between the mesoscopic level of description, and the microscopic level simulated by us, it is not obvious that our FRPs are directly related to those of \[1, 2\]; if they are not, their temporal asymmetry is a feature of their dynamics which, to the best of our knowledge, has not been studied before in microscopic deterministic dynamics. However, the fact that our results do not change qualitatively with the growth of \( N \) suggests a relation between our results and the asymmetries of the large deviations of Refs. \[1, 2\], and indicates how the theory of \[1, 2\] may extend to the microscopic level of description.

II. DETERMINISTIC FLUCTUATION-RELAXATION PATHS

Given the observable \( \mathcal{F} : \mathcal{M} \to \mathbb{R} \), the identification of a FRP around its steady state (expected) value \( \mathcal{E}(\mathcal{F}) \) requires some care. Indeed, the time series of \( \mathcal{F} \) looks very noisy, and takes the value \( \mathcal{E}(\mathcal{F}) \) only at discrete instants of time. Similarly, the fluctuation values selected to be observed are also achieved only at discrete instants of time. Averaging over many particles, and over many microscopic times, stabilizes the signal, but makes negligible the frequency of the FRPs, to the point that it becomes impossible to assess their statistical properties.

By analogy with the notation of \[1\], we denote by \( \mathcal{F}_t \) the quantity \( \mathcal{F}(S^t \Gamma) \), if \( \Gamma \) is the initial point of the trajectory in \( \mathcal{M} \), and \( S^t : \mathcal{M} \to \mathcal{M} \) is the time evolution operator. We want to identify the most likely FRP, according to the SNS probability distribution, starting
at \( \mathcal{F}_i = \mathbb{E}(\mathcal{F}) \), reaching the fluctuation value \( \mathcal{F}_T = \mathcal{T}(\mathcal{F}) \), and returning to \( \mathcal{F}_f = \mathbb{E}(\mathcal{F}) \) after a certain time. To assess the dependence of the phenomenon on \( N \), we consider two kinds of fluctuation values:

\[
T_s^*(\mathcal{F}) = \mathbb{E}(\mathcal{F}) + s \sigma(\mathcal{F}), \quad \text{and} \quad T_s^{(N)}(\mathcal{F}) = \mathbb{E}(\mathcal{F}) + \frac{1}{s} \sigma(\mathcal{F}) \sqrt{N}; \quad s = 1, 2, 3...
\]

with \( \sigma(\mathcal{F}) \) the standard deviation of \( \mathcal{F} \) (which depends on \( N \)), and we introduce the following definition of FRP:

**Definition 1.** Let \( \mathcal{F} \) take the value \( \mathcal{T}(\mathcal{F}) \) at time \( \hat{t} \), with \( [d\mathcal{F}_i/dt]_i > 0 \). Let \( \bar{t} \) be the smallest time after \( \hat{t} \) such that \( \mathcal{F}_\bar{t} = \mathcal{T}(\mathcal{F}) \). Choose a time \( \tau_0 > 0 \), representing the expected duration of the fluctuation path. The union \( \{\mathcal{F}_{\hat{t} - \tau}, \ \tau \in [0, \tau_0]\} \cup \{\mathcal{F}_{\hat{t} + \tau}, \ \tau \in [0, \tau_0]\} \) of the trajectory segments of duration \( \tau_0 \) preceding \( \hat{t} \), and following \( \hat{t} \), is called an FRP.

Numerically, the time \( \hat{t} \) can be identified testing the condition

\[
(\mathcal{F}_{(t+h)} - \mathcal{T})(\mathcal{F}_t - \mathcal{T}) < 0, \quad \text{where} \ h = \text{time step}, \ \mathcal{T} = \text{fluctuation value}. \quad (11)
\]

Whenever a FRP is obtained, we shift it in order to have \( \hat{t} = 0 \). Given \( n \) FRPs, we collect them in the set \( \{(\tau, \mathcal{F}_\tau^{(s)})\}, \ s = 1, 2, \ldots, n \}, \) and build a histogram by partitioning the rectangle \( [-\tau_0, \tau_0] \times [\min_{r,s} \mathcal{F}_\tau^{(s)}, \ max_{r,s} \mathcal{F}_\tau^{(s)}] \) with small rectangular bins, and evaluating the frequency of visitation of each bin. The number of temporal intervals in which \( [-\tau_0, \tau_0] \) is subdivided is denoted by \( b_\tau \), while the number of bins of \( \min_{r,s} \mathcal{F}_\tau^{(s)}, \ max_{r,s} \mathcal{F}_\tau^{(s)} \) is denoted by \( b_\mathcal{F} \). The area of each rectangular bin \( \Delta_{p,q} \), with \( p = 1, \ldots, b_\tau, \ q = 1, \ldots, b_\mathcal{F} \), is \( \Delta = 2\tau_0[\max_{r,s} \mathcal{F}_\tau^{(s)} - \min_{r,s} \mathcal{F}_\tau^{(s)}]/(b_\tau b_\mathcal{F}) \), and the corresponding histogram is a two-dimensional surface, whose “crest”, defined by

\[
C(p) = ((2\tau_0 + 1)n\Delta)^{-1} \max_{q=1,\ldots,b_\mathcal{F}} \sharp\{(\tau, \mathcal{F}_\tau^{(s)}) \in \Delta_{p,q}, \ s = 1, 2, \ldots, n\}, \quad p = 1, \ldots, b_\tau, \quad (12)
\]

with \( \sharp\{\ldots\} \) the number of FRPs in \( \{\ldots\} \), represents the most likely FRP in the sample. To assess the asymmetries of the FRPs, and of the corresponding crests, we introduce the following definition:

**Definition 2.** Let \( \mathcal{T} \) be the fluctuation value chosen for \( \mathcal{F} \). If \( \mathcal{F}(\hat{t}, \bar{t}, \tau_0) = \{\mathcal{F}_{\hat{t} - \tau}, \ \tau \in [0, \tau_0]\} \cup \{\mathcal{F}_{\hat{t} + \tau}, \ \tau \in [0, \tau_0]\} \) is an FRP; its asymmetry coefficient is given by

\[
\alpha(\mathcal{F}(\hat{t}, \bar{t}, \tau_0)) = \frac{1}{\tau_0(\mathcal{T} - \mathbb{E}(\mathcal{F}))} \sum_{0 \leq \tau \leq \tau_0} (\mathcal{F}_{\hat{t} + \tau} - \mathcal{F}_{\hat{t} - \tau}). \quad (13)
\]
Let $C : \{1, \ldots b_\tau\} \to \mathbb{R}$ be the crest obtained from the given sample of FRPs; the asymmetry coefficient of $C$ is given by

\[
\alpha_c(C) = \frac{2}{b_\tau(T - \mathbb{E}(F))} \left( \sum_{p=\frac{b_\tau}{2}+1}^{b_\tau} C(p) - \sum_{p=1}^{\frac{b_\tau}{2}} C(p) \right). \tag{14}
\]

The asymmetry coefficient $\alpha$ of a single FRP is defined in the same way, replacing the values $C(p)$ with the corresponding values of the FRP. A FRP or a crest is symmetric if its asymmetry coefficient vanishes.

Observe that the asymmetry coefficients can take positive as well as negative values, because the differences which define them are not taken in absolute value. This is motivated by the fact that random oscillations of a fluctuation path around its symmetric relaxation path should result in a vanishing asymmetry coefficient.

### III. NUMERICAL RESULTS

We deal with an observable which is odd under the time reversal operation. Unfortunately, the crests obtained from our simulations are strongly noisy, as evidenced by Fig.1 in one of the cases considered, and their asymmetry coefficient $\alpha_c$ is not particularly meaningful. Therefore, we study the statistics of the asymmetry coefficient $\alpha$ of the single FRP, considered as a random variable which takes different values on the different paths. Our results are summarized in Tables I and II, in which the fraction of oscillators over which the averages are computed to the total number of oscillators are fixed, but the other parameters defining the model vary. We conclude that the most likely FRP, which is the object of the theory of [1, 2], is hard to assess directly, because the crest obtained for each different case is highly noisy and not sharp: indeed, the supports and the variances of the marginal probability distributions, for fixed $\tau$ in the flux space, are quite wide (cf. Tables I and II).

On the other hand, all the data Tables I and II indicate that the FR paths of $F$ have a positive asymmetry, like those of $f^{[10]}$. A positive asymmetry of the FRPs is testified not only by the fact that the mean asymmetry is a positive number, but especially by the fact that the probability of being positive is well above $1/2$. Furthermore, the dependence on the various parameters defining the model is rather weak.

Therefore, we have found evidence of a new phenomenon in the nonequilibrium FPU-$\beta$ model of Lepri, Livi and Politi, which shows how irreversible phenomena can be obtained
FIG. 1: Crest of the observable $F$, with $N = 100, \eta = 0.16, T_\ell = 200, T_r = 20$, $\mathbb{E}(f) \simeq 24.741$, and $T_3^* \simeq 1738$. The asymmetry coefficient of the crest, computed according to (13), is $\alpha_c(C) = 0.0142$.

| $N$ | $\mathbb{E}(F)$ | $\sigma(F)$ | $P(\alpha > 0)$ ; $T_3^*$ | $\mathbb{E}(\alpha)$ ; $T^*$ | $P(\alpha > 0)$ ; $T_4^{(N)}$ | $\mathbb{E}(\alpha)$ ; $T_4^{(N)}$ |
|-----|-----------------|-------------|---------------------------|-----------------------------|-------------------------------|-------------------------------|
| 25  | 49.2262         | 1449.5949   | 0.7001                    | 0.0254                      | -                             | -                             |
| 50  | 37.3129         | 777.1178    | 0.6316                    | 0.0336                      | -                             | -                             |
| 100 | 26.4482         | 569.0022    | 0.6354                    | 0.0391                      | 0.6200                        | 0.0447                        |
| 150 | 21.3395         | 405.9141    | 0.6121                    | 0.0492                      | 0.6103                        | 0.0483                        |
| 200 | 18.2231         | 355.5294    | 0.6142                    | 0.0478                      | 0.6074                        | 0.0410                        |
| 250 | 15.7638         | 309.9113    | 0.6122                    | 0.0481                      | 0.6075                        | 0.0388                        |
| 300 | 14.7470         | 295.3437    | 0.5987                    | 0.0410                      | 0.5951                        | 0.0384                        |
| 350 | 12.9422         | 271.1457    | 0.5865                    | 0.0350                      | 0.5845                        | 0.0386                        |
| 400 | 12.1784         | 249.9643    | 0.5960                    | 0.0347                      | 0.5732                        | 0.0319                        |

TABLE I: Mean and standard deviation of $F$, probability of positive asymmetry with different fluctuation values, and mean of its single FRPs, as functions of $N$. Here, $\eta = 0.16, T_\ell = 200, T_r = 20$, and $\tau_0 = 15$.

out of (dissipative) reversible dynamics. Furthermore, the weak dependence of our results on $N$ suggests that the asymmetries may survive in the large $N$ limit, with growing fluctuation values, although at present it is not possible to test directly very large $N$’s and $T$’s. If the asymmetries really survive, our results constitute a first (partial) verification of the predictions of Refs. [1, 2] (originally obtained for nonequilibrium stochastic systems), in the
\begin{tabular}{|c|c|c|c|c|}
\hline
$N$ & $\mathbb{E}(\mathcal{F})$ & $\sigma(\mathcal{F})$ & $P(\alpha > 0)$ & $\mathbb{E}(\alpha)$ \\
\hline
250 & 25.8539 & 564.2185 & 0.5840 & 0.0305 \\
300 & 23.8107 & 558.0274 & 0.6082 & 0.0334 \\
350 & 24.0250 & 571.7431 & 0.6219 & 0.0484 \\
400 & 20.3576 & 554.6692 & 0.6480 & 0.0430 \\
350(*) & 40.6265 & 1117.7722 & 0.6297 & 0.0474 \\
400(*) & 41.4094 & 1099.1702 & 0.6131 & 0.0473 \\
\hline
\end{tabular}

TABLE II: Same as Table I, for $T_4^{(N)}$ only, with $T_\ell = 300$. The cases with a (*) have $T_\ell = 500$.

context of time reversal invariant, deterministic dissipative particle systems.

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[11] The time average of the divergence of the equations of motion, $-\langle \zeta_r \rangle - \langle \zeta_\ell \rangle$, is negative.

[12] There is an involution $i: \mathcal{M} \to \mathcal{M}$, $i(q, p, \zeta) = (q, -p, -\zeta)$, $p = m\dot{q}$, on the phase space $\mathcal{M}$, which anticommutes with the time evolution: $iS^t = S^{-t}i$, where $S^t: \mathcal{M} \to \mathcal{M}$ is the time evolution.