Test of the Additivity Principle for Current Fluctuations in a Model of Heat Conduction

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The additivity principle allows to compute the current distribution in many one-dimensional (1D) nonequilibrium systems. Using simulations, we confirm this conjecture in the 1D Kipnis-Marchioro-Presutti model of heat conduction for a wide current interval. The current distribution shows both Gaussian and non-Gaussian regimes, and obeys the Gallavotti-Cohen fluctuation theorem. We verify the existence of a well-defined temperature profile associated to a given current fluctuation. This profile is independent of the sign of the current, and this symmetry extends to higher-order profiles and spatial correlations. We also show that finite-time joint fluctuations of the current and the profile are described by the additivity functional. These results suggest the additivity hypothesis as a general and powerful tool to compute current distributions in many nonequilibrium systems.

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Nonequilibrium systems typically exhibit currents of different observables (e.g., mass or energy) which characterize their macroscopic behavior. Understanding how microscopic dynamics determine the long-time averages of these currents and their fluctuations is one of the main objectives of nonequilibrium statistical physics. \[1, 2, 3, 4, 5, 6, 7\]. This problem has proven to be a challenging task, and up to now only few exactly-solvable cases are understood \[1, 2, 3\]. An important step in this direction has been the development of the Gallavotti-Cohen fluctuation theorem \[2, 6\], which relates the probability of forward and backward currents reflecting the time-reversal symmetry of microscopic dynamics. However, we still lack a general approach based on few simple principles. Recently, Bertini and coworkers \[1\] have introduced a Hydrodynamic Fluctuation Theory (HFT) to study large dynamic fluctuations in nonequilibrium steady states. This is a very general approach which leads to a hard optimization problem whose solution remains challenging in most cases. Simultaneously, Bodineau and Derrida \[2\] have conjectured an additivity principle for current fluctuations in 1D which can be readily applied to obtain quantitative predictions and, together with HFT, seems to open the door to a general theory for nonequilibrium systems.

The additivity principle (also referred here as BD theory) enables one to calculate the fluctuations of the current in 1D diffusive systems in contact with two boundary thermal baths at different temperatures, \(T_L \neq T_R\). It is a very general conjecture of broad applicability, expected to hold for 1D systems of classical interacting particles, both deterministic or stochastic, independently of the details of the interactions between the particles or the coupling to the thermal reservoirs. The only requirement is that the system at hand must be diffusive, i.e., Fourier’s law must hold. If this is the case, the additivity principle predicts the full current distribution in terms of its first two cumulants. Let \(P_N(q, T_L, T_R, t)\) be the probability of observing a time-integrated current \(Q_t = q t\) during a long time \(t\) in a system of size \(N\). This probability obeys a large deviation principle \[8, 9\]: \(P_N(q, T_L, T_R, t) \sim \exp[-t \mathcal{F}_N(q, T_L, T_R)]\), where \(\mathcal{F}_N(q, T_L, T_R)\) is the current large-deviation function (LDF), meaning that current fluctuations away from the average are exponentially unlikely in time. The additivity principle relates this probability with the probabilities of sustaining the same current in subsystems of lengths \(N - n\) and \(n\), and can be written as \(\mathcal{F}_N(q, T_L, T_R) = \max_T [\mathcal{F}_N(q, T_L, T) + \mathcal{F}_N(q, T, T_R)]\) for the LDF \[2\]. In the continuum limit one gets \[2\]

\[
\mathcal{G}(q) = -\min_{\mathcal{T}_q(x)} \left\{ \int_0^1 \frac{[q + \kappa \mathcal{T}_q(x)] T_q'(x)^2}{2\sigma[T_q(x)]} \, dx \right\} ,
\]

with \(\mathcal{G}(q) = N \mathcal{F}_N(q)\). We drop the dependence on the baths for convenience, \(x \in [0, 1]\), and where \(\kappa(T)\) is the thermal conductivity appearing in Fourier’s law, \(\langle Q_t \rangle / t = -\kappa(T) \nabla T\), and \(\sigma(T)\) measures current fluctuations in equilibrium \((T_L = T_R)\), \(\langle Q_t^2 \rangle / t = \sigma(T)/N\). The optimal profile \(T_q(x)\) derived from \[1\] obeys

\[
\kappa^2[T_q(x)] \frac{d^2 T_q(x)}{dx^2} = q^2 \left\{ 1 + 2K\sigma[T_q(x)] \right\} ,
\]

where \(K(q^2)\) is a constant which fixes the correct boundary conditions, \(T_q(0) = T_L\) and \(T_q(1) = T_R\). Eqs. \[1\] and \[2\] completely determine the current distribution, which is in general non-Gaussian and obeys the Gallavotti-Cohen symmetry, i.e., \(\mathcal{G}(-q) = \mathcal{G}(q) - E q^2\) with \(E\) some constant defined by \(\kappa(T)\) and \(\sigma(T)\) \[2\].

The additivity principle is better understood within the context of HFT \[1\], which provides a variational principle for the most probable (possibly time-dependent) profile responsible of a given current fluctuation, leading usually to unmanageable equations. The additivity principle, which on the other hand yields explicit predictions,
A Gibbs distribution at the corresponding temperature baths whose energy is randomly drawn at each step from chosen nearest neighbors. In addition, boundary sites through random energy exchanges between randomly-chosen nearest neighbors. is defined on a 1D open lattice with principal in a particular system: the 1D Kipnis-Marchioro-Peliti model. This method yields the Legendre transform of the current LDF, $\mu(\lambda) \equiv N^{-1} \max_{q} [G(q) + \lambda q]$. The function $\mu(\lambda)$ can be viewed as the conjugate potential to $G(q)$, with $\lambda$ the parameter conjugate to the current $q$, a relation equivalent to the free energy being the Legendre transform of the internal energy in thermodynamics, with the temperature as conjugate parameter to the entropy.

We applied the method of Giardinà et al to measure $\mu(\lambda)$ for the 1D KMP model with $N = 50$, $T_L = 2$ and $T_R = 1$, see Fig. 1. The agreement with BD theory is excellent for a wide $\lambda$-interval, say $-0.8 < \lambda < 0.45$, which corresponds to a very large range of current fluctuations. Moreover, the deviations observed for extreme current fluctuations are due to known limitations of the algorithm, so no violations of additivity are observed. In fact, we can use the Gallavotti-Cohen symmetry, $\mu(\lambda) = \mu(-\lambda - E)$ with $E = (T_R^{-1} - T_L^{-1})$, to bound the range of validity of the algorithm. The inset to Fig. 1 shows that this symmetry holds in the large current interval for which the additivity principle predictions agree with measurements, thus confirming its validity in this range. However, we cannot discard the possibility of an additivity breakdown for extreme current fluctuations due to the onset of time-dependent profiles [1], although we stress that such scenario is not observed here.

The additivity principle leads to the minimization of a functional of the temperature profile, $T_q(x)$, see eqs. (1) and (2). A relevant question is whether this optimal profile is actually observable. We naturally define $T_q(x)$ as the average energy profile adopted by the system during a large deviation event of (long) duration $t$ and time-integrated current $q$, measured at an intermediate time $1 < \tau < t$. Top panel in Fig. 2 shows $T_q(x)$ measured in standard simulations for small current fluctuations, and the agreement with BD predictions is again very good. This confirms the idea that the system modifies its temperature profile to facilitate the deviation of the current.

To obtain optimal profiles for larger current fluctuations we may use the method of Giardinà et al [11]. This method naturally yields $T_{\lambda}^{\text{meas}}(x)$, the average energy profile at the end of the large deviation event ($\tau = t$), which can be connected to the correct observable $T_{\lambda}(x)$ by noticing that KMP dynamics obeys the local detailed balance condition [2], which guarantees the time reversibility of microscopic dynamics. This condition implies a symmetry between the forward dynamics for a current fluctuation and the time-reversed dynamics for the negative fluctuation [13] that can be used to derive the following.

**FIG. 1:** (Color online) Main: $\mu(\lambda)$ for the 1D KMP model. Fluctuations are Gaussian for $\lambda \approx 0$, but non-Gaussian in the tails. Inset: Test of the Gallavotti-Cohen fluctuation relation.
This agreement shows that corrections to LE are weak in the KMP model, though we show below that these small corrections are present and can be measured.

An important consequence of eq. 3 is that $P_{\lambda}(C) = P_{-\lambda,E}(C)$, or equivalently $P_{\lambda}(C) = P_{-\lambda}(C)$, so midtime statistics does not depend on the sign of the current. This implies in particular that $T_q(x) = T_q(-x)$, but also that all higher-order profiles and spatial correlations are independent of the current sign.

As another test, BD theory predicts for $q \approx (\epsilon) = \frac{1}{2}$ the limiting behavior

$$T_q(x) - T_{st}(x) = \frac{1}{2q-1} x (1-x)(5-x) + \mathcal{O}(2q-1).$$

The inset to Fig. 2 confirms this scaling for $T_q(x)$ and many different values of $q$ around its average.

We can now go beyond the additivity principle by studying fluctuations of the system total energy, for which current theoretical approaches cannot offer any prediction. An exact result by Bertini, Gabrielli and Lebowitz [14] predicts that $m_2(e,q) = m_2^{LE}(e,q) + \frac{1}{12}(T_L - T_R)^2$, where $m_2(e,q)$ is the variance of the total energy, $m_2^{LE}$ is the variance assuming a local equilibrium (LE) product measure, and the last term reflects the correction due to the long-range correlations in the nonequilibrium stationary state [14]. In our case, $m_2^{LE} = (T_L^2 + T_L T_R + T_R^2)/3 \approx 2.3333$, while $m_2 = 29/12 \approx 2.4166$. Fig. 3 plots $m_2(e,q) = N [(\epsilon^2(q) - \langle \epsilon \rangle^2)]$ measured in standard simulations, showing a non-trivial, interesting structure for $m_2(e,q)$ which both BD theory and HFT cannot explain. One might obtain a theoretical prediction for $m_2(e,q)$ by supplementing the additivity principle with a LE hypothesis, i.e. $P_{\lambda}(C) \approx \Pi_{i=1}^{N} \exp[-e_i/T_{\lambda}(x)]$, which results in $m_2^{LE}(e,q) = \int_0^1 dx T_q(x)^2$. However, Fig. 3 shows that $m_2^{LE}(e(q)) \approx 2.33$ as corresponds to a LE picture, and in contrast to the exact result $m_2(e,q) \approx 2.4166$. This proves that, even though LE is
In summary, we have confirmed the additivity principle in the 1D KMP model of heat conduction for a large current interval, extending its validity to joint current-profile fluctuations. These results strongly support the additivity principle as a general and powerful tool to compute current distributions in many 1D nonequilibrium systems, opening the door to a general approach based on few simple principles. Our confirmation does not discard however the possible breakdown of additivity for extreme current fluctuations due to the onset of time-dependent profiles, although we stress that this scenario is not observed here and would affect only the far tails of the current distribution. In this respect it would be interesting to study the KMP model on a ring, for which a dynamic phase transition to time-dependent profiles is known to exist \[.\] Also interesting is the possible extension of the additivity principle to low-dimensional systems with anomalous, non-diffusive transport properties \[,\] or to systems with several conserved fields or in higher dimensions.

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