Thermostatistics of small nonlinear systems: Gaussian thermal bath

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We discuss the statistical properties of small mechanothermodynamic systems (one- and two-particle cases) subject to nonlinear coupling and in contact with standard Gaussian reservoirs. We use a method that applies averages in the Laplace-Fourier space, which relates to a generalization of the final-value theorem. The key advantage of this method lies in the possibility of eschewing the explicit computation of the propagator, traditionally required in alternative methods like path integral calculations, which is hardly obtainable in the majority of the cases. For one-particle equilibrium systems we are able to compute the instantaneous (equilibrium) probability density functions of injected and dissipated power as well as the respective large deviation functions. Our thorough calculations explicitly show that for such models nonlinearities are irrelevant in the long-term statistics, which preserve the exact same values as computed for linear cases. Actually, we verify that the thermostatistical effect of the nonlinearities is constricted to the transient towards equilibrium, since it affects the average total energy of the system. For the two-particle system we consider each element in contact with a heat reservoir, at different temperatures, and focus on the problem of heat flux between them. Contrarily to the one-particle case, in this steady state nonequilibrium model we prove that the heat flux probability density function reflects the existence of nonlinearities in the system. An important consequence of that it is the temperature dependence of the conductance, which is unobserved in linear(harmonic) models. Our results are complemented by fluctuation relations for the injected power (equilibrium case) and heat flux (nonequilibrium case).

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I. INTRODUCTION

Prompted by several results and applications in engineering and biology [1], particularly at the nanometric scale, the thermodynamical description of small dynamical systems in contact with heat reservoirs has been in the limelight and ultimately acted as one of the cornerstones of the so-called stochastic thermodynamics [2]. Besides the interest piqued by the smorgasbord of applications, most of the theoretical interest resides in the fact that due to its the intrinsic finiteness, fluctuations can be crucial to their statistical features, especially when the system is in a state of nonequilibrium giving rise to deviations from standard thermodynamical results, which were established within a macroscopic context [3].

Considering nonequilibrium, the instance of a mechanical system in contact with two reservoirs at different temperatures is perhaps the quintessential heat dissipative problem [4] allowing the emergence of a steady (nonequilibrium) state with heat flowing through the system and permits a long-term treatment based on time averaging. Looking at the way the elements of the system interact, the problem has been mainly set forth in terms of either linear or nonlinear coupling. On the one hand, linear coupling presents several simplifying advantages, namely, (1) it defines a pure nonequilibrium system; (2) it has its heat flux definition completely established; (3) it is adaptable to different kinds of reservoirs; (4) it can be easily expanded into an infinite chain with a nearly direct application of the results of $N = 2$ block; (5) it might represent results of Langevin colored noises by a renormalization of the masses; and last but not least (6) linearity is still widely assumed in problems of statistical mechanics and condensed matter [5]. On the other hand, higher dimensional anharmonic (i.e., nonlinear) coupling might be able to better diffuse energy and enlarge the scope of any enquiry. Nonetheless, the range of exact analytical solutions thereto behaves the other way around, exhibiting a sharp decrease of its broadness [6,7], which is plainly counterbalanced by its experimental relevance (see, e.g., Ref. [8]).

At this point it is worth stressing it is systematically forgotten that, conceptually, probability distributions in statistical physics represent a mathematical tool for obtaining quantities, commonly limited the first statistical moments, that act as predictions to match with measurements made on a system [9]. In other words, we can reckon the probability distribution as a compact way of presenting the statistical information about an ensemble. For these reasons, methods pinpointed at the description of the statistical moments or cummulants are manifestly the most convenient approach as they enable a straightforward comparison of the theoretical prediction with experimental results, e.g., mean first-passage times and temperatures as averages of kinetic energy of particles among many others.

In experiments, we are often interested in analyzing the behavior of a single sample system that is assumed in a

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steady state[1] and for which a reliable empirical distribution function is unlikely. In that case, the steady state condition makes a time-averaging procedure utterly valid, nay, adequate and outperforming in opposition to the standard (statistical) probabilistic mechanics framework [10–13].

The present work aims at introducing a comprehensive description of thermostatistical laws for small nonlinear mechanical models in contact with heat reservoirs. Our account is split into two main parts: first, the analysis of the one-particle problem in contact with a reservoir, which after some time attains a state of equilibrium, is made in Sec. II. We center our efforts on carrying out a statistical description of power and heat in their injected and dissipated forms, performing calculations in the Laplace-Fourier space, and using diagrammatic representations as well. In addition, we describe the response of thermostatistical quantities to variations of mechanical and thermal parameters of the problem. In Sec. III we survey a two-particle nonequilibrium steady state, namely, the statistics and probabilistics the heat flux between elements of the system. Finally, we dedicate Sec. IV to the comparison of the effect of nonlinearities in the thermostatistical features of equilibrium and nonequilibrium problems.

II. ONE-PARTICLE CASE

Let us first assume the following model of a single particle in contact with a heat reservoir at temperature T. The position, x, and velocity, $v \equiv \dot{x}$, of the particle are governed by the stochastic differential equations

$$\begin{aligned} \dot{x}(t) &= v(t), \\ m\,\ddot{x}(t) &= -k_1\,x(t) - k_3 x^3(t) - \gamma\,\dot{x}(t) + \eta(t), \end{aligned} \tag{1}$$

where the initial conditions can be set to $x(t=0)=0$ and $v(t=0)=0$ without any loss of generality. The stochastic variable η is a proxy for the interaction of system with the reservoir, which must be statistically defined beforehand. Doing it in terms of its cumulants, it is well known that a stochastic variable is specified by either its first two cumulants altogether or else all of them are needed [14]. The present paper studies the former, distinguishing the Gaussian noise and which defines a Wiener-like (Brownian) process $dW(t) \equiv \int_t^{t+dt} \eta(t')$. The latter, which has a wide field of applicability as well, will be scrutinised in a subsequent paper. A driftless Gaussian noise, which leads to a Lévy-Itô continuous measure process [15], is described in terms of its cumulants as

$$\begin{aligned} \langle \eta(t_1)\cdots\eta(t_n)\rangle_c &= 0 \quad (\text{if } n \neq 2), \\ \langle \eta(t_1)\,\eta(t_2)\rangle_c &= 2\,\gamma\,T\,\delta(t_1-t_2). \end{aligned} \tag{2}$$

As we shall see shortly, the Laplace transform of the cumulants,

$$\begin{aligned} &\langle \tilde{\eta}(s_1)\cdots\tilde{\eta}(s_n)\rangle_c \\ &\quad = \prod_{i=1}^{n} \int_0^\infty \exp\left[-\sum_{i=1}^{n} s_i\,t_i\right] \langle \eta(t_1)\cdots\eta(t_n)\rangle_c\,, \end{aligned} \tag{3}$$

plays a central role in obtaining the results. Accordingly, for the present case we have

$$\langle \tilde{\eta}(s_1)\tilde{\eta}(s_2)\rangle_c = \frac{2\,\gamma\,T}{s_1+s_2}, \tag{4}$$

and zero otherwise. In applying the aforementioned initial conditions, the Laplace transform of Eq. (1) is expressed in a recursive form as

$$\begin{aligned} \tilde{x}(s) &= \frac{\tilde{\eta}(s)}{R(s)} - \frac{k_3}{R(s)} \lim_{\epsilon\to 0^+} \int_{-\infty}^{+\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{+\infty} \frac{dq_2}{2\pi} \\ &\quad \times \int_{-\infty}^{+\infty} \frac{dq_3}{2\pi}\, \frac{\tilde{x}(\mathrm{i}\,q_1+\epsilon)\,\tilde{x}(\mathrm{i}\,q_2+\epsilon)\,\tilde{x}(\mathrm{i}\,q_3+\epsilon)}{s-(\mathrm{i}\,q_1+\mathrm{i}\,q_2+\mathrm{i}\,q_3+3\epsilon)}, \\ \tilde{v}(s) &= s\,\tilde{x}(s), \end{aligned} \tag{5}$$

where

$$R(s) \equiv m\,s^2 + \gamma s + k_1 = m\,(s-\zeta_+)(s-\zeta_-), \tag{6}$$

the zeros of which are

$$\zeta_\pm = -\frac{\theta}{2} \pm \frac{i}{2}\sqrt{4\,\omega^2-\theta^2}, \tag{7}$$

where $\theta = \gamma/m$ and $\omega^2 = k_1/m$. The recursive structure can be best understood looking at Fig. 1 where we depict Eq. (5) in a diagrammatic way.

A. Energy considerations

We start by conducting an energy analysis of the system, which shows that in solving the problem from the exact dynamics of the system standard statistical mechanical averages are recovered. Recall that because the system reaches an equilibrium state it is clear the long-term values could be obtained using the Boltzmann distribution. Yet, we shall tackle the computations differently; seeing that we will need the time dependence of the equations further ahead, in order to keep

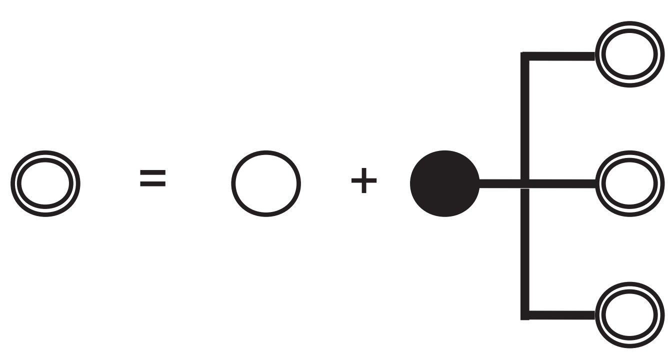

FIG. 1. Diagrammatical representation of Eq. (5). Here double circles depict a $\tilde{x}$ term, which make the fork represent the triple integral, and the simple circles picture the term η/R.

[1]Within this context equilibrium can be regarded as the utmost steady state. That is to say, in a general steady state there is entropy production to keep the probability current constant, whereas in a equilibrium state the average overall entropy production cancels out.

a uniform approach we resort to a final-value theorem which brackets the Laplace transform with time averages [16]

$$\lim_{z\to 0} z\,\tilde{A}(z) = \bar{A}, \tag{8}$$

where

$$\bar{A} \equiv \lim_{T\to\infty} \frac{1}{T}\int_0^T A(t)\,dt \tag{9}$$

and

$$A(t) = \lim_{\epsilon\to 0}\int_{-\infty}^{\infty}\frac{dq}{2\pi}\,e^{(i\,q+\epsilon)t}\,\tilde{A}(i\,q+\epsilon). \tag{10}$$

With Eqs. (5) and (8) on hand we can compute the average values of v^2, x^2, and x^4, which are related to the average kinetic,

$$\overline{\mathcal{K}} = \tfrac{1}{2}m\overline{v^2},$$

and potential energy of the particle,

$$\overline{\mathcal{V}} = \tfrac{1}{2}k_1\overline{x^2} + \tfrac{1}{4}k_3\overline{x^4}.$$

Explicitly, for the kinetic energy we read

$$\begin{aligned}\overline{\mathcal{K}} &= \frac{m}{2}\lim_{z,\,\epsilon\to 0}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\,\frac{z}{z-(i\,q_1+i\,q_2+2\epsilon)}\\ &\quad\times\langle\tilde{v}(i\,q_1+\epsilon)\,\tilde{v}(i\,q_2+\epsilon)\rangle\\ &= \frac{m}{2}\lim_{z,\,\epsilon\to 0}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\,\frac{z}{z-(i\,q_1+i\,q_2+2\epsilon)}\\ &\quad\times(i\,q_1+\epsilon)\,(i\,q_2+\epsilon)\,\langle\tilde{x}(i\,q_1+\epsilon)\,\tilde{x}(i\,q_2+\epsilon)\rangle\,. \end{aligned}\tag{11}$$

Plugging Eq. (5) into Eq. (11) we verified that only the zeroth order in k_3 yields a result different to zero, and therefore we have

$$\begin{aligned}\overline{\mathcal{K}} &= \frac{m}{2}\lim_{z,\,\epsilon\to 0}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\,\frac{z}{z-(i\,q_1+i\,q_2+2\epsilon)}\\ &\quad\times\frac{(i\,q_1+\epsilon)\,(i\,q_2+\epsilon)}{R(i\,q_1+\epsilon)\,R(i\,q_2+\epsilon)}\,\langle\tilde{\eta}(i\,q_1+\epsilon)\,\tilde{\eta}(i\,q_2+\epsilon)\rangle\end{aligned}\tag{12}$$

$$= \frac{T}{2}. \tag{13}$$

This result should not be unexpected; by the time-averaging we obtain predictions for the values of the observables in the long-term steady (equilibrium) state. In such a state the velocity must be Gaussian irrespective of the form of either potential of the spring.

The verification of the equipartition theorem obviously does not occur for the time average of the nonquadratic potential energy. Making explicit the potential energy we have

$$\begin{aligned}\overline{\mathcal{V}} &= \frac{k_1}{2}\lim_{z\to 0}\lim_{\epsilon\to 0}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\,\frac{z}{z-(i\,q_1+i\,q_2+2\epsilon)}\\ &\quad\times\langle\tilde{x}(i\,q_1+\epsilon)\tilde{x}(i\,q_2+\epsilon)\rangle + \frac{k_3}{4}\lim_{z\to 0}\lim_{\epsilon\to 0}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\dots\\ &\quad\times\int_{-\infty}^{\infty}\frac{dq_4}{2\pi}\,\frac{z}{z-(i\,q_1+i\,q_2+i\,q_3+i\,q_4+4\epsilon)}\\ &\quad\times\langle\tilde{x}(i\,q_1+\epsilon)\,\tilde{x}(i\,q_2+\epsilon)\,\tilde{x}(i\,q_3+\epsilon)\,\tilde{x}(i\,q_4+\epsilon)\rangle\,,\end{aligned}\tag{14}$$

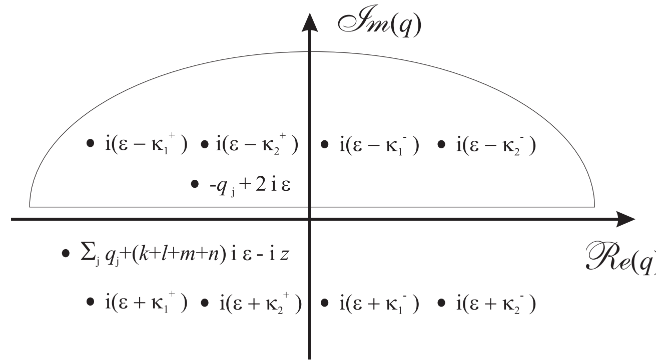

FIG. 2. Path of integration for the q variables.

whence, once again, a recursive relation is obtained by replacing the transforms $\tilde{x}$ by their expression from Eq. (5). At this stage, we make use of the previous equation to address two important points: First, the only contributing terms are those for which the successive integration over distinct q_j make $\sum_{j=1}^{l}(i\,q_j+\epsilon)$ in the factor $z/[z-\sum_{j=1}^{l}(i\,q_j+\epsilon)]$ to vanish. If not, these contributions zero out when the limit $z\to 0$ is evaluated; second, in representing the integration contour diagrams, the noise averages such as $\langle\tilde{\eta}(i\,q_1+\epsilon)\,\tilde{\eta}(i\,q_2+\epsilon)\rangle$ represent contractions on the diagrams, which allow representing the contributing terms as simple residue integrations on the path given in Fig. 2. Hereinafter, we represent the contraction involving two noises in the Laplace space $\tilde{\eta}(i\,q_1+\epsilon)$ and $\tilde{\eta}(i\,q_2+\epsilon')$ as $(q_1 \diamond q_2)$.

Our task is thus to compute these integrals in order to obtain the leading contributions that ultimately allow finding the function for which the terms correspond to the elements of the generating function. In this case that calculation is very much simplified by the Gaussian nature of the reservoirs and the direct application of the Isserlis-Wick theorem [17]. In the Supplemental Material [18] we show the computations related to the first terms of $\overline{\mathcal{V}}$. The same procedure dare be used to compute any order of $\overline{x^n v^m}$ $(n,m \geqslant 0)$. Up to second order in k_3 the potential energy reads

$$\begin{aligned}\overline{\mathcal{V}} &= \sum_{n=0}^{\infty}k_3^n\,\overline{\mathcal{V}}_n\\ &= \frac{1}{2}T - \frac{3}{4}\frac{k_3\,T^2}{k_1^2} + 6\frac{k_3^2\,T^3}{k_1^4} + O\left[\left(\frac{k_3\,T}{k_1^2}\right)^3\right],\end{aligned}\tag{15}$$

which gives $V = T/2$ for the standard harmonic case ($k_3 = 0$) and according to equilibrium statistics. This expansion enables identifying the dimensionless argument $\Lambda \equiv \frac{k_3\,T}{k_1^2}$ that characterizes the order of the expansion. The average total energy of the system easily yields

$$\begin{aligned}\overline{\mathcal{E}} &= \overline{\mathcal{K}} + \overline{\mathcal{V}}\\ &= T - \frac{3}{4}\frac{k_3\,T^2}{k_1^2} + 6\frac{k_3^2\,T^3}{k_1^4} + O\left[\left(\frac{k_3\,T}{k_1^2}\right)^3\right].\end{aligned}\tag{16}$$

It is important to stress that Eq. (16) is exact; exact in the sense that no simplifying argument nor Edgeworth expansion have been used. If we are interested in getting higher order contributions of Λ, it is only necessary to continue applying the Isserlis-Wick theorem.

We have hitherto shed light on a main statistical property of the system which can directly link to measurements in experiments, but what if we were interested in the probabilistic properties? Is this method capable of providing us with distribution? The answer to this question is yes. That is to say, should we be concerned with the probabilistic steady state behavior of the system? Instead, all we have to do is to assume that our quantity $A(t)$ is nothing but

$$p(x,v,t) = \langle \delta(y(t)-x)\,\delta(u(t)-v)\rangle. \tag{17}$$

Introducing the last equation in $A(t)$ and using the Fourier representation of the Dirac δ we can write the equilibrium distribution as

$$p_{eq}(x,v) = \sum_{n,m=0}^{\infty}\int_{-\infty}^{+\infty}\frac{dQ}{2\pi}\frac{dP}{2\pi}e^{\mathrm{i}(Q\,x+P\,v)} \times \frac{(-i\,Q)^n}{n!}\frac{(-i\,P)^m}{m!}\overline{\langle y^n u^m\rangle}, \tag{18}$$

where we anew use the time-averaging technique to compute $\overline{\langle x^n v^m\rangle}$. That approach has proven worthwhile in a variety of cases, especially when a Fokker-Plank approach does not hold [12,13]. The first terms of $\overline{\langle x^n v^m\rangle}$ we computed to obtain the average energy concur with the expected probability equilibrium distribution $p_{eq}(x,v) = Z^{-1}\exp[-(m\,v^2/2 + m\,x^2/2 + m\,x^4/4)/T]$.

B. Energy fluctuations and thermostatistical greeks

Let us now turn our attention to the other main statistical moment of the energy, the variance,

$$\sigma_{\mathcal{E}}^2 \equiv \overline{(\mathcal{E}-\overline{\mathcal{E}})^2} = \overline{\mathcal{K}^2} + \overline{\mathcal{V}^2} - \overline{\mathcal{K}}^2 - \overline{\mathcal{V}}^2,$$

which up to second order in k_3^2 gives

$$\sigma_{\mathcal{E}}^2 = T^2 - \frac{3}{2}\frac{k_3}{k_1^2}T^3 + 18\frac{3}{4}\frac{k_3^2}{k_1^4}T^4 + O\left(\frac{k_3^3}{k_1^6}T^5\right).$$

Assuming standard relation between the energy fluctuations and the heat transferred to the particle we can explicit the specific heat of the nonlinear particle, $\sigma_{\mathcal{E}}^2 = C_x\,T^2$ where

$$C_x = 1 - \frac{3}{2}\frac{k_3}{k_1^2}T + 18\frac{k_3^2}{k_1^4}T^2 + O\left(\frac{k_3^3}{k_1^6}T^3\right), \tag{19}$$

up to second order in $k_3\,T/k_1^2$. It is easily understood that the nonlinear particle has got a smaller specific heat because the first anharmonic correction is negative. What is the rationale beyond that? By introducing a small higher-order positive term in the expression defining the energy of the spring we are implicitly augmenting its stiffness and thus turning it less elastic, or in other words, diminishing the response function, C_x, to energy fluctuations caused by the contact with the thermostat. In respect of Eq. (19) two further observations can be made: (1) in the limit $T \to 0$, $C_x = 1 \neq 0$, thus violating the third law of thermodynamics, as characteristically done by classical systems; (2) the specific heat of the nonlinear classical Brownian particle is a function of the temperature only when the system in anharmonic. These features underscore the mixing between mechanical properties of a system and the thermal properties of the reservoir conveyed in Ref. [13], which are absent when the system is of a linear(harmonic) nature.

In analyzing the response of the (average) total energy of the system we can go farther afield borrowing the concept of Greeks used in option pricing. Originally, these quantities were introduced to quantify the sensitivity of the appraised value of an option, V, with respect to the parameters used to price it (for further details please consult, e.g., Ref. [19]). In the present case we set forth the following Greeks:

$$\begin{aligned}
\nu &\equiv \frac{\partial\overline{\mathcal{E}}}{\partial T} \approx 1 - \frac{3}{2}\frac{k_3}{k_1^2}T^2 + 18\frac{k_3^2}{k_1^4}T^4,\\
\rho &\equiv \frac{\partial\overline{\mathcal{E}}}{\partial k_1} \approx \frac{3}{2}\frac{k_3}{k_1^3}T^2 - 24\frac{k_3^2}{k_1^5}T^3 + \frac{891}{2}\frac{k_3^3}{k_1^7}T^4,\\
\varrho &\equiv \frac{\partial\overline{\mathcal{E}}}{\partial k_3} \approx -\frac{3}{4}\frac{T^2}{k_1^2} + 12\frac{k_3}{k_1^4}T^3 - \frac{891}{4}\frac{k_3^2}{k_1^6}T^4,\\
\upsilon &\equiv \frac{\partial\overline{\mathcal{E}}}{\partial\gamma} = 0,\\
\Gamma &\equiv \frac{\partial\overline{\mathcal{E}}}{\partial m} = 0,
\end{aligned} \tag{20}$$

(all up to second order in k_3) wherewith we intend to describe the sensitivity of the mean energy with respect to the parameters of the problem. Let us elaborate upon these results. From ν, ρ, and ϱ, we can grasp once again the relevance of the anharmonicity in the blending of thermal and mechanical properties of the problem. In other words, in the linear case we verify that ν is constant, hence independent of T, respecting the classical theory, whereas for anharmonic systems we have a temperature-dependent response. Additionally, ρ clearly shows that the value of the average energy depends on the value of k_1 when nonlinearities exist and that ν and ϱ show smaller and negative sensitivity of $\overline{\mathcal{E}}$ when $k_3 \neq 0$. Last, we verify $C_x = \nu$ as expected. In both cases, we have smaller values for $k_3 \neq 0$ than the harmonic instance. This is explained by observing that as we increase the stiffness of the spring we are making the system more inefficient in terms of transfer of energy between the bath and the particle. With respect to other response measures we can still introduce the displacement coefficient,

$$\alpha \equiv (\overline{x^2})^{-\frac{1}{2}}\frac{\partial\sqrt{\overline{x^2}}}{\partial T} = \frac{1}{2T} - \frac{3}{2}\frac{k_3}{k_1^2} + \frac{39}{2}\frac{k_3^2}{k_1^4}T,$$

which signals the decreasing of the amplitude of movement in stiffening the spring.

C. Power considerations

As is well known, the energy of a particle at time Θ is related to the balance between the injected and dissipated heat fluxes [2], $\mathcal{J}_I(\Theta)$ and $\mathcal{J}_D(\Theta)$, respectively,

$$\mathcal{E}(\Theta) \equiv \mathcal{J}_I(\Theta) + \mathcal{J}_D(\Theta) = \int_0^\Theta \eta(t)\, v(t)\, dt - \gamma \int_0^\Theta v(t)^2\, dt. \tag{21}$$

In the long term (large Θ), because the system reaches an equilibrium state, it is expected that

$$\lim_{\Theta \gg \theta} \langle \mathcal{J}_I(\Theta) + \mathcal{J}_D(\Theta) \rangle = \langle \mathcal{E} \rangle = \overline{\mathcal{E}}, \tag{22}$$

as the problem becomes ergodic after the transient.

Applying the Laplace method we have verified that for the injected heat flux,

$$\lim_{\Theta \gg \theta} \langle \mathcal{J}_I(\Theta) \rangle = \frac{\gamma}{m} T\, \Theta.$$

This result arises from the zeroth order contribution in k_3,

$$\begin{aligned} \langle \mathcal{J}_{I,0}(\Theta) \rangle &= \lim_{\Theta \gg \theta} \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} \frac{\exp[(i\,q_1 + i\,q_2 + 2\epsilon)\,\Theta]}{(i\,q_1 + i\,q_2 + 2\epsilon)} (i\,q_1 + \epsilon) \frac{1}{R(i\,q_1 + \epsilon)} \langle \tilde{\eta}(i\,q_1 + \epsilon)\, \tilde{\eta}(i\,q_2 + \epsilon) \rangle , \\ &= \frac{\gamma}{m} T\, \Theta \end{aligned} \tag{23}$$

and from the fact that $\langle \mathcal{J}_{I,n}(\Theta) \rangle = 0$ for any other order of the expansion in k_3. As regards to the dissipated flux we have obtained a different picture where the terms $\langle \mathcal{J}_{D,n}(\Theta) \rangle$ do not vanish ($n > 0$). However, the only term which exhibits time dependence is the zeroth order term, namely,

$$\begin{aligned} \langle \mathcal{J}_{D,0}(\Theta) \rangle &= -\lim_{\Theta \gg \theta} \lim_{\epsilon \to 0} \gamma \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} \frac{\exp[(i\,q_1 + i\,q_2 + 2\epsilon)\,\Theta] - 1}{(i\,q_1 + i\,q_2 + 2\epsilon)} \frac{(i\,q_1 + \epsilon)(i\,q_2 + \epsilon)}{R(i\,q_1 + \epsilon)\, R(i\,q_2 + \epsilon)} \langle \tilde{\eta}(i\,q_1 + \epsilon)\, \tilde{\eta}(\mathrm{i}\,q_2 + \epsilon) \rangle \\ &= -\frac{\gamma}{m} T\, \Theta + T, \end{aligned} \tag{24}$$

and, for the sake of conciseness, we just show here the first order contribution yielding

$$\begin{aligned} \langle \mathcal{J}_{D,1}(\Theta) \rangle &= \lim_{\Theta \gg \theta} \lim_{\epsilon \to 0} \lim_{\epsilon' \to 0} \frac{2\,\gamma\, k_3}{m^5} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \cdots \int_{-\infty}^{+\infty} \frac{dq_5}{2\pi} \frac{\exp[(i\,q_1 + i\,q_2 + 2\epsilon)\,\Theta] - 1}{(i\,q_1 + i\,q_2 + 2\epsilon)} \\ &\quad \times \frac{1}{R(i\,q_1 + \epsilon)\, R(i\,q_2 + \epsilon) \prod_{l=3}^{5} R(i\,q_l + \epsilon')} (i\,q_1 + \epsilon)(i\,q_2 + \epsilon) \frac{\langle \tilde{\eta}(i\,q_2 + \epsilon)\, \tilde{\eta}(i\,q_3 + \epsilon')\, \tilde{\eta}(i\,q_4 + \epsilon')\, \tilde{\eta}(i\,q_5 + \epsilon') \rangle}{(i\,q_1 + \epsilon) - (i\,q_3 + i\,q_4 + i\,q_5 + 3\epsilon')} \\ &= -\frac{3}{4} \frac{k_3\, T^2}{k_1^2}. \end{aligned} \tag{25}$$

The subsequent computation of higher order terms in k_3 allows verifying Eq. (22). Interpreting the results of Eqs. (23)–(25) we learn that modifying the linearity of the model only implies changes in the transient time average behavior of the system, i.e., after reaching equilibrium. In other words, for an arbitrarily large time Θ the constant terms of the total injected and dissipated energy, which add up to define the average total energy of the system, will be arbitrarily small and thus negligible.

The fact that the problem becomes ergodic after a transient tells us very little about modifications in the distributions. In order to check it, we compute the remaining moments and get the probability distribution for the total injected and dissipated heat which matches the large deviation function of the power [20] . Since it has to do with the product of different quantities, namely, $\tilde{\eta}$ by $\tilde{v}$, the case of the injected power turns out easier by adopting a diagrammatic representation of all the integrals involved to get each raw moment $\langle \mathcal{J}_I^n(\Theta) \rangle$. Let us focus on second order moment,

$$\begin{aligned} \left\langle \mathcal{J}_I^2(\Theta) \right\rangle &= \lim_{\Theta \gg \theta} \lim_{\epsilon \to 0} \int_0^\Theta dt \int_0^\Theta dt' \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dq_4}{2\pi} \exp[(i\,q_1 + i\,q_2 + 2\epsilon)\,t + (i\,q_3 + i\,q_4 + 2\epsilon)\,t'] \\ &\quad \times \frac{(i\,q_2 + \epsilon)(i\,q_4 + \epsilon)}{\prod_{l=1}^{2} R(i\,q_{2l} + \epsilon)} \langle \tilde{\eta}(i\,q_1 + \epsilon)\, \tilde{\eta}(i\,q_2 + \epsilon)\, \tilde{\eta}(i\,q_3 + \epsilon)\, \tilde{\eta}(i\,q_4 + \epsilon) \rangle , \end{aligned} \tag{26}$$

as an illustrative example.

Applying the Isserlis-Wick theorem we can split the 4-q correlation into three different products of two-q correlations, namely:$(q_1 \diamond q_2)$ $(q_3 \diamond q_4)$, which represents $\langle \mathcal{J}_I(\Theta) \rangle^2$, and $(q_1 \diamond q_3)$ $(q_2 \diamond q_4)$ and $(q_1 \diamond q_4)$ $(q_2 \diamond q_3)$, which yield the cumulant of second order. The diagrammatic representation, depicted Fig. 3 for $n = 2$ and $n = 3$ works as follows: bearing in mind the factorisation in time of the exponential term in the integral, we assume a number n of nodes, representing j_I in Laplace space, that can connect to the other nodes in three different ways:

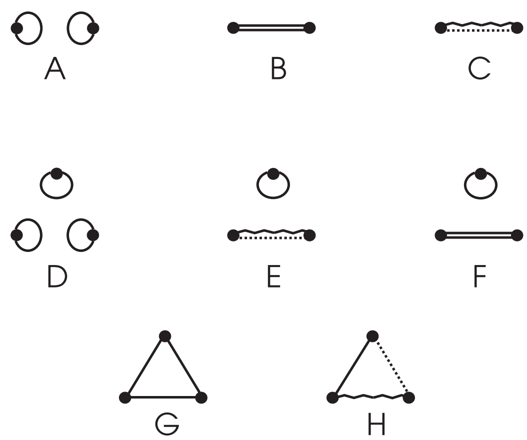

FIG. 3. Diagrammatic representation of the integrals involved in the calculation of the second and third order cumulants.

(1) By full straight links, when the pair of $\tilde{\eta}$s is composed of one $\tilde{\eta}$ coming from the pure noise and the other from the velocity, independent of the time [e.g., $(q_1 \diamond q_2)$ or $(q_1 \diamond q_4)$ for $\langle \mathcal{J}_I^2(\Theta)\rangle$];

(2) By dotted links, when the pair is composed of $\tilde{\eta}$s coming from the pure noise [e.g., $(q_1 \diamond q_3)$ for $\langle \mathcal{J}_I^2(\Theta)\rangle$];

(3) By wavy links, when the pair is composed of $\tilde{\eta}$s coming from the the velocity [e.g., $(q_1 \diamond q_3)$ for $\langle \mathcal{J}_I^2(\Theta)\rangle$].

A node can have two full straight lines, but if one of the links is a dotted (wavy) line the other must be a wavy (dotted) or straight line. The nodes can self-connect creating a loop; in this case the value is $\gamma T\,\Theta/m$ for every of them. When all the nodes are only connected by straight lines forming a closed chain the result of such diagram is equal to zero. Last, the cumulant of order n, which must be linear in Θ so that one we recover the key extensive property of the cumulants, is defined by the diagrams that form closed chains with $n-2$ links. Accordingly we have

$$\begin{aligned}\left\langle \mathcal{J}_I^2(\Theta)\right\rangle &= \mathsf{A}+\mathsf{B}+\mathsf{C}\\ &= \left(\frac{\gamma}{m}T\,\Theta\right)^2 + 0 + 2\frac{\gamma}{m}T^2\Theta \end{aligned} \tag{27}$$

and

$$\begin{aligned}\left\langle \mathcal{J}_I^3(\Theta)\right\rangle &= \mathsf{D}+3\times\mathsf{E}+3\times\mathsf{F}+6\times\mathsf{G}+2\times\mathsf{H}\\ &= \left(\frac{\gamma}{m}T\,\Theta\right)^3 + 6\frac{\gamma^2}{m^2}T^3\Theta^2 + 0 + 0 + 12\frac{\gamma}{m}T^3\Theta, \end{aligned} \tag{28}$$

where in each term we have preserved the leading term in Θ, which rules its long-term behavior. The computations are carried on for higher moments of the injected energy flux until the respective moment-generating function (MGF) is identified with the help of tabulated series [21]

$$\begin{aligned}\mathcal{M}_{\mathcal{J}_I(\Theta)}(\lambda) &\equiv \langle \exp[\lambda\,\mathcal{J}_I(\Theta)]\rangle\\ &= \exp\left[\frac{\gamma\,\Theta}{2\,m}\left(1-\sqrt{1+4\,T\,\lambda}\right)\right]. \end{aligned} \tag{29}$$

Since we can identify the total injected(dissipated) heat as the large deviation variable of the respective powers the distribution is finally obtained making use of the Gärtner-Ellis Theorem [20,22], which by means of a Legendre transform relates $\mathcal{M}_{\mathcal{J}_I(\Theta)}(\lambda)$ to the large deviation function, $L(\mathcal{J}_I)$, and thus,

$$L(\mathcal{J}_I) \sim H(\mathcal{J}_I)\exp\left[-\frac{(\mathcal{J}_I-\gamma\,T\,\Theta/m)^2}{4\,T\,\mathcal{J}_I}\right], \tag{30}$$

where we scrapped the time dependence of $\mathcal{J}_I$ and $H(x)$ denotes the Heaviside function. Heed that in this case we do not explicit the propagator as in calculations based on path integration [6,23]. That results in a clear advantage when we deal with problems associated with non-Gaussian reservoirs. In the case of the absolute dissipated power, $|\mathcal{J}_D|$, we did not manage to establish a diagrammatic representation yet. Nevertheless, a monotonous calculation of the first terms shows that they equal those obtained for $\mathcal{J}_I$, as expected and depicted in Fig. 4 where we reckon that the distributions coincide. Additionally, it becomes intuitive to think that nonlinear effects are most stressed during the transient when the particle is building up energy towards its average equilibrium value. This is again plain in Fig. 5, after the transient $\tau \sim 10$, the systems attains a linear regime of injection and dissipation of energy independently of the value of k_3.

Despite the equality of $L(\mathcal{J}_{I(D)})$, it is quite clear from the respective definitions that the injected and the dissipated powers cannot have the same distribution. Actually, they must be quite different because $j_D \equiv -\gamma\,v^2$ is nonpositive defined, whereas $j_I \equiv \eta\,v$ assumes any real value. In respect of the dissipated power distribution, $p(|j_D|)$, we use the Gaussian nature, with variance $T/(2\,m)$, of the velocity in equilibrium and applying the law of the probability conservation under changes of variable we obtain

$$p(|j_D|) = \sqrt{\frac{m}{2\pi\,\gamma\,T\,|j_D|}}\exp\left[-\frac{m}{2\gamma T}\,|j_D|\right], \tag{31}$$

which is reminiscent of a χ-squared distribution with one degree of freedom. Regarding the injected power distribution,

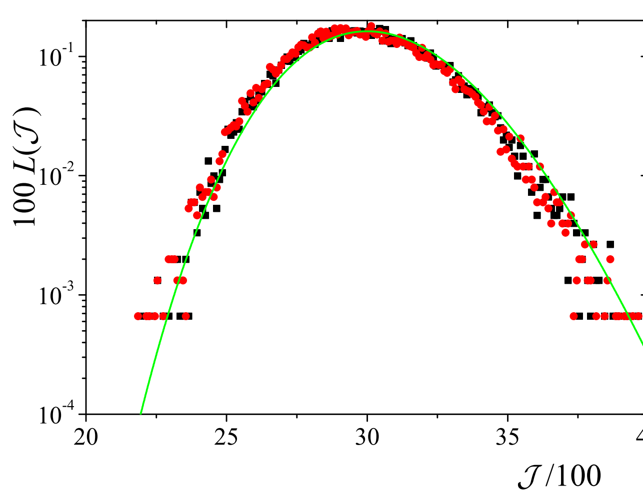

FIG. 4. (Color online) Long-term distribution function of the total injected (black squares) and dissipated (red circles) heats vs total injected(dissipated) heat. The green line is given by Eq. (30). The parameters used are $\Theta = 300$, $k_1 = 1$, $k_3 = 2/100$, $m = 1$, $\gamma = 1$, and $T = 10$.

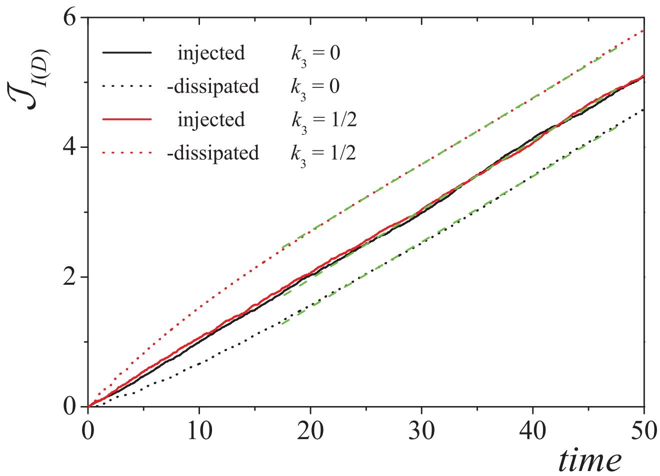

FIG. 5. (Color online) Injected and dissipated heats vs time. The parameters used are the following $k_1 = 1$, $m = 1$, $\gamma = 1/10$ and $T = 1$, and $k_3 = 0$ or $k_3 = 1/2$, i.e., significantly nonlinear. It is clear that after the transient both heats grow at a rate $\gamma\, T/m = 1/10$, which agrees with the slopes of the dashed green lines. N.B.: In order to obtain a greater separation between the curves we have set slightly different initial conditions, namely, $x = 1$.

$p\,(j_I)$, the calculation is more complex. Let us start by computing the correlation function between the stochastic term η and the velocity in equilibrium. This gives

$$\begin{aligned} C_{\eta\, v}(\tau) &\equiv \overline{\langle \eta\,(t)\, v\,(t+\tau)\rangle} - \overline{\langle \eta\,(t)\rangle \langle v\,(t)\rangle} \\ &= 2T\frac{\gamma}{m}\exp\left[-\frac{\gamma}{2\,m}\tau\right]\left\{\cos\left[\sqrt{\frac{k}{m}-\left(\frac{\gamma}{2\,m}\right)^2}\,\tau\right]\right. \\ &\quad \left. -\frac{\gamma}{m}\left[4\frac{k}{m}-\left(\frac{\gamma}{m}\right)^2\right]^{-\frac{1}{2}}\sin\left[\sqrt{\frac{k}{m}-\left(\frac{\gamma}{2\,m}\right)^2}\,\tau\right]\right\} \\ &\quad \times (\tau > 0) \end{aligned} \tag{32}$$

and

$$\overline{\langle \eta\,(t)\, v\,(t+\tau)\rangle} = 0, \qquad (\tau < 0). \tag{33}$$

In the limit $\tau \to 0$ we obtain $C_{\eta\, v}\,(0) = T\frac{\gamma}{m}$, and it coincides with the average injected power.[2] With this result we can assume that, for equilibrium probabilistic purposes, the velocity is given by the sum

$$v = c\,\eta + f\,\xi, \tag{34}$$

where $c = C_{\eta\, v}(0)/\sigma^2$, $\sigma^2 = 2\,\gamma\, T\,\delta(0)$, $f = \sqrt{1 - \frac{m}{T}(\frac{C_{\eta\, v}(0)}{\sigma})^2}$. The variable ξ is Gaussian and independent of η with a variance $\langle \xi^2\rangle = \omega^2 = \frac{T}{m}$. Accordingly, the injected power PDF

[2]It must be noted that $C_{\eta v}\,(0)$ is not simply obtained by assuming $\tau = 0$. In the respective calculation the value $\tau = 0$ implies that the Jordan's lemma becomes invalid, and we must take into consideration the result of the integration in the upper semicircle.

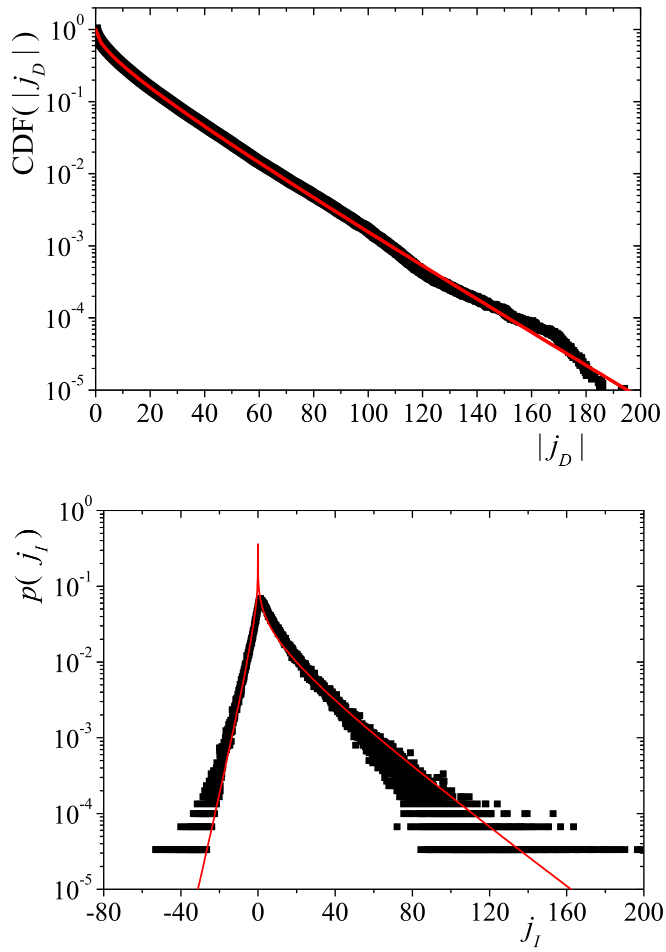

FIG. 6. (Color online) Upper panel: Cumulative distribution of dissipated power vs dissipated power. Lower panel: Probability density function of injected power (empirically obtained using the Savitzky-Golay filter) vs injected power. In both cases the parameters are the following: $m = 1$, $\gamma = 1$, $k = 1$, $k_3 = 2/100$, and $T = 10$. The last part of the curves are naturally affected by finite size effects.

reads

$$\begin{aligned} p(j_I) &= \iint \frac{1}{2\,\pi\,\sigma\,\omega}\exp\left[-\frac{\eta^2}{2\sigma^2} - \frac{\xi^2}{2\,\omega^2}\right]\delta(j_I - \eta\, v) \\ &\quad \times \delta\,(v - c\,\eta - f\,\xi)\; d\eta\, d\xi \\ &= \frac{2\,c}{\pi\, f\,\sigma\,\omega}\exp\left[\frac{c}{f^2\omega^2}j_I\right]K_0\left[\frac{\sqrt{(c\,\sigma)^2 + f^2\omega^2}}{f^2\omega^2\,\sigma}|j_I|\right]. \end{aligned} \tag{35}$$

This distribution is different from Eq. (31) and compared with numerical implementation results in Fig. 6. It must be taken into consideration that since j_I is actually a noise in its strictest sense, the numerical computation of that quantity is quite sensitive and thus prone to erroneous results. The way to circumvent this obstacle is to smoothly differentiate $\mathcal{J}_I$ for which we used the Savitzky-Golay filter [24]. Taking into account this point Eq. (35) can be deemed a good approach. Furthermore, the assumption (34) allows understanding the large deviation function if we make $f = 0$. In that case Eq. (35)

becomes

$$p\,(j_I) = \int_{-\infty}^{+\infty} d\eta \frac{1}{\sqrt{4\pi\gamma T}} \exp\left[-\frac{\eta^2}{4\gamma T}\right] \delta\left(j_I - \frac{1}{2m}\eta^2\right) = \sqrt{\frac{m}{2\pi\,\gamma\,T\,j_I}} \exp\left[-\frac{m}{2\gamma T} j_I\right] H\,(j_I)\,, \tag{36}$$

which has the same functional form as $p\,(|j_D|)$. Thence, we comprehend that the large deviation limit of the injected power is dominated by the correlation between the velocity of the particle and the action of the reservoir. On the other hand, the fluctuations introduced by ξ give rise to negative values that act on the energy of the particle as a dissipative contribution. The imperative positive skew of $p\,(j_I)$ is provided by the exponential factor, whence we can establish the fluctuation relation

$$\lim_{\Theta\to\infty} \frac{p\,(|\,j_I\,|)}{p\,(-\,|\,j_I\,|)} = \exp\left[2\frac{c}{f^2\omega^2}\,|\,j_I\,|\right]. \tag{37}$$

III. TWO-PARTICLE CASE

Having surveyed the thermostatistical properties of an equilibrium nonlinear particle let us move on to a nonequilibrium steady state apt system, the dynamics of which is ruled by the following equations:

$$\begin{aligned} \dot{x}_1 &= v_1 \\ \dot{x}_2 &= v_2 \\ m\,\ddot{x}_1 &= -k\,x_1 - k_1(x_1 - x_2) - k_3(x_1 - x_2)^3 - \gamma\dot{x}_1 + \eta_1 \\ m\,\ddot{x}_2 &= -k\,x_2 - k_1(x_2 - x_1) - k_3(x_2 - x_1)^3 - \gamma\dot{x}_2 + \eta_2. \end{aligned} \tag{38}$$

The current system is still (broadly) ergodic in the sense that after the transient averages over time and averages over samples do agree. The noise reservoir-mimicking functions are again assumed as white and Gaussian,

$$\begin{aligned} \langle\eta_\alpha(t_1)\rangle &= 0 \\ \langle\eta_\alpha(t_1)\eta_\beta(t_2)\rangle &= 2\,\gamma\,T_\alpha\,\delta(t_1 - t_2)\,\delta_{\alpha\,\beta}, \end{aligned} \tag{39}$$

and the initial conditions are set to $x_1(0) = v_1(0) = x_2(0) = v_2(0) = 0$.

The Laplace transforms read

$$\tilde{v}_1(s) = s\tilde{x}_1(s), \tag{40}$$

$$\tilde{v}_2(s) = s\tilde{x}_2(s). \tag{41}$$

Using

$$R(s) = (m\,s^2 + \gamma\,s + (k + k_1)) = m(s - \kappa_+)(s - \kappa_-),$$

where

$$\kappa_\pm = -\frac{\theta}{2} \pm \frac{i}{2}\sqrt{4\omega^2 - \theta^2}$$

and

$$\begin{aligned} R'(s) &= (m\,s^2 + \gamma\,s + (k + 2\,k_1)) = m(s - \kappa_{1+})(s - \kappa_{1-}), \\ R''(s) &= (m\,s^2 + \gamma\,s + k) = m(s - \kappa_{2+})(s - \kappa_{2-}), \end{aligned}$$

with

$$\begin{aligned} \kappa_{1\pm} &= -\frac{\theta}{2} \pm \frac{i}{2}\sqrt{4\omega_1^2 - \theta^2}, \\ \kappa_{2\pm} &= -\frac{\theta}{2} \pm \frac{i}{2}\sqrt{4\omega_2^2 - \theta^2}, \end{aligned}$$

we can rewrite the dynamical evolution of the system in terms of the difference between the positions,

$$\begin{aligned} \tilde{r}_D &= [\tilde{x}_1(s) - \tilde{x}_2(s)] \\ &= \frac{\tilde{\eta}_1(s) - \tilde{\eta}_2(s)}{R'(s)} - \frac{2\,k_3}{R'(s)} \lim_{\epsilon\to 0} \int_{-\infty}^{+\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{+\infty} \frac{dq_2}{2\pi} \int_{-\infty}^{+\infty} \frac{dq_3}{2\pi} \\ &\quad \times \frac{[\tilde{x}_1(\mathrm{i}\,q_1 + \epsilon) - \tilde{x}_2(\mathrm{i}\,q_1 + \epsilon)]\,[\tilde{x}_1(\mathrm{i}\,q_2 + \epsilon) - \tilde{x}_2(\mathrm{i}\,q_2 + \epsilon)][\tilde{x}_1(\mathrm{i}\,q_3 + \epsilon) - \tilde{x}_2(\mathrm{i}\,q_3 + \epsilon)]}{s - (\mathrm{i}\,q_1 + \mathrm{i}\,q_2 + \mathrm{i}\,q_3 + 3\epsilon)}, \end{aligned} \tag{42}$$

and the average position of the system,

$$\tilde{r}_S = \frac{[\tilde{x}_1(s) + \tilde{x}_2(s)]}{2} = \frac{\tilde{\eta}_1(s) + \tilde{\eta}_2(s)}{2\,R''(s)}. \tag{43}$$

Inverting the last two equations we can retrieve the positions in the Laplace space,

$$\begin{aligned} \tilde{x}_1(s) &= \tilde{r}_S + \frac{\tilde{r}_D}{2}, \\ \tilde{x}_2(s) &= \tilde{r}_S - \frac{\tilde{r}_D}{2}. \end{aligned} \tag{44}$$

Similarly, we can define the difference and the average of the noise as

$$\begin{aligned} \tilde{\eta}_S(s) &= \frac{\tilde{\eta}_1\,(s) + \tilde{\eta}_2\,(s)}{2}, \\ \tilde{\eta}_D(s) &= \tilde{\eta}_1\,(s) - \tilde{\eta}_2\,(s)\,, \end{aligned} \tag{45}$$

the Laplace transforms of which are

$$\begin{aligned} \langle\tilde{\eta}_D(s_1)\tilde{\eta}_D(s_2)\rangle_c &= 2\,\gamma\,\frac{T_1 + T_2}{s_1 + s_2}, \\ \langle\tilde{\eta}_S(s_1)\tilde{\eta}_S(s_2)\rangle_c &= \frac{\gamma}{2}\,\frac{T_1 + T_2}{s_1 + s_2}, \\ \langle\tilde{\eta}_S(s_1)\tilde{\eta}_D(s_2)\rangle_c &= \gamma\,\frac{T_1 - T_2}{s_1 + s_2}. \end{aligned} \tag{46}$$

Finally we express the recurrence relations for the new variables,

$$\begin{aligned} \tilde{r}_D(s) &= \frac{\tilde{\eta}_D(s)}{R'(s)} - \frac{2\,k_3}{R'(s)} \lim_{\epsilon\to 0} \lim_{\epsilon'\to 0} \int_{-\infty}^{+\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{+\infty} \frac{dq_2}{2\pi} \\ &\quad \times \int_{-\infty}^{+\infty} \frac{dq_3}{2\pi} \frac{\tilde{r}_D(\mathrm{i}\,q_1 + \epsilon')\,\tilde{r}_D(\mathrm{i}\,q_2 + \epsilon')\,\tilde{r}_D(\mathrm{i}\,q_3 + \epsilon')}{s - (\mathrm{i}\,q_1 + \mathrm{i}\,q_2 + \mathrm{i}\,q_3 + 3\epsilon')}, \\ \tilde{r}_S &= \frac{\tilde{\eta}_S\,(s)}{R''(s)}. \end{aligned} \tag{47}$$

A. Heat conductance

As provided by Eq. (38), for this two-particle system the force $F_{1\to 2}$ exerted by particle 1 on particle 2 is defined by

$$F_{1\to 2} = -k_1(x_1 - x_2) - k_3(x_1 - x_2)^3. \tag{48}$$

Accordingly, the power transmitted from one particle to another is given by the instantaneous power difference [10],

$$J_{1\to 2} = \frac{dW_{1\to 2} - dW_{2\to 1}}{2\,dt} = \frac{F_{1\to 2}v_2 - F_{2\to 1}v_1}{2}. \tag{49}$$

In this respect, our approach revolves around deriving a systematic expansion for the time-averaged moments of $J_{1\to 2}$ in the steady state,

$$\begin{aligned}\langle \overline{J^n_{1\to 2}}\rangle &= \left\langle \overline{\left(\frac{F_{1\to 2}v_2 - F_{2\to 1}v_1}{2}\right)^n}\right\rangle \\ &= \left\langle \overline{\left\{[-k_1(x_1 - x_2) - k_3(x_1 - x_2)^3]\frac{v_1 + v_2}{2}\right\}^n}\right\rangle,\end{aligned} \tag{50}$$

where we have applied the condition that in steady state $< x^n_\alpha v_\alpha = 0$ [10]. The last representation is particularly valid because it easily allows us to write the the moments $\langle \overline{J^n_{1\to 2}}\rangle$ by means of the average velocity and the position difference. The average value is traditionally expressed as

$$J_Q = \langle J_{1\to 2}\rangle \equiv \kappa_T\,(T_2 - T_1), \tag{51}$$

where κ_T is the *conductance* of the model. Heeding Eqs. (42)–(47) we get

$$\begin{aligned}J_Q = &-k_1 \lim_{z\to 0}\lim_{\epsilon\to 0}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\,\frac{z}{z-(\mathrm{i}\,q_1+\mathrm{i}\,q_2+2\epsilon)}(\mathrm{i}\,q_2+\epsilon)\ \langle\tilde r_D(\mathrm{i}\,q_1+\epsilon)\,\tilde r_S(\mathrm{i}\,q_2+\epsilon)\rangle \\ &- k_3 \lim_{z\to 0}\lim_{\epsilon\to 0}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\int_{-\infty}^{\infty}\frac{dq_3}{2\pi}\int_{-\infty}^{\infty}\frac{dq_4}{2\pi}\,\frac{z}{z-(\mathrm{i}\,q_1+\mathrm{i}\,q_2+\mathrm{i}\,q_3+\mathrm{i}\,q_4+2\epsilon)} \\ &\times\{(\mathrm{i}\,q_4+\epsilon)\ \langle\tilde r_D(\mathrm{i}\,q_1+\epsilon)\,\tilde r_D(\mathrm{i}\,q_2+\epsilon)\,\tilde r_D(\mathrm{i}\,q_3+\epsilon)\,\tilde r_S(\mathrm{i}\,q_4+\epsilon)\rangle\}\,.\end{aligned} \tag{52}$$

We now proceed to expand the heat flow (per unit time) in powers of k_3 and obtain the respective statistical moment. Let us first concentrate our focus on the linear coupling case, $k_3 = 0$. Having computed the heat flux moments we understood that it would be best to introduce a cumulant representation rather than the statistical moment representation for which we inferred the following equation:

$$\kappa_n = \sum_{k=0}^{n}(n-1)!\binom{n}{2k}A^{n-2k}B^k, \tag{53}$$

with

$$A = -\frac{1}{2}\frac{\gamma\,k_1^2}{k_1^2 m + (k+k_1)\,\gamma^2}\,(T_1 - T_2)\,, \tag{54}$$

$$B = \frac{1}{4}\frac{k_1^2}{m\,\gamma\,(k+2k_1)}\,(T_1 + T_2)^2\,, \tag{55}$$

whence we determine the cumulant generating function,

$$\begin{aligned}\mathcal{G}_{J_{1\to 2}}(\lambda) &\equiv \sum_{n=1}^{\infty}\kappa_n\frac{\lambda^n}{n!} \\ &= \ln\frac{1}{\sqrt{[1-(A+\sqrt{B})\lambda][1-(A-\sqrt{B})\lambda]}}.\end{aligned} \tag{56}$$

Since $\mathcal{G}_{J_{1\to 2}}(\lambda)$ is nothing but $\ln \mathcal{M}_{J_{1\to 2}}(\lambda)$ we straightforwardly identify the moment-generating function,

$$\mathcal{M}_{J_{1\to 2}}(\lambda) = \frac{1}{\sqrt{[1-(A+\sqrt{B})\lambda][1-(A-\sqrt{B})\lambda]}}. \tag{57}$$

Unfortunately, to the best of both our knowledge there is no analytical inversion of this equation. Yet we can consider some limit situations for which the characteristic function, $\mathcal{C}_{J_{1\to 2}}(\lambda) \equiv \mathcal{M}_{J_{1\to 2}}(i\,\lambda)$, is invertible. Particularly, we identify $A \pm \sqrt{B}$ as the maximal and minimal typical values of $J_{1\to 2}$. In the limit of $T_1 \to T_2$, we have $A = 0$ that yields

$$p_0\,(J_{1\to 2}) = \frac{1}{\pi\,\sqrt{B}}K_0\left[\frac{|J_{1\to 2}|}{\sqrt{B}}\right], \tag{58}$$

where $K_\cdot\,(\cdot)$ represents the modified Bessel function of second kind. Mind that when $A = 0$ the system reaches an equilibrium state where the flux is both symmetrical and, from Eq. (58), its distribution shows exponential decay. To obtain the full distribution we avail ourselves of a Gram-Charlier series (also known as Edgeworth expansion) to compute an approximation for that. Specifically, within this approach an unknown probability distribution, $p\,(\cdot)$ can be written as a function of some other (close) known reference distribution, $p_0\,(\cdot)$, and the difference between the cumulants of both distributions,

$$\delta\kappa_n \equiv \kappa'_n - \kappa_n, \tag{59}$$

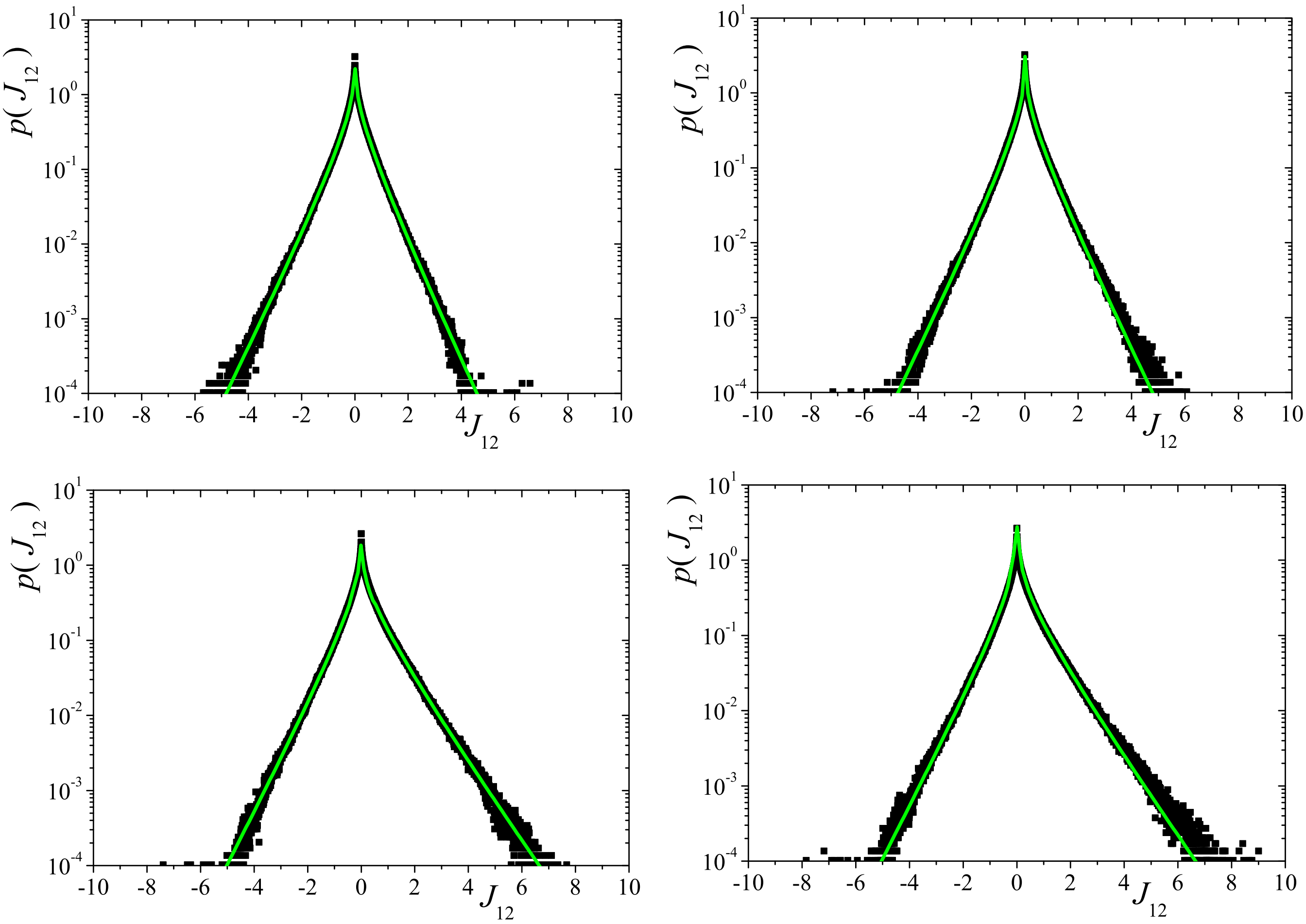

FIG. 7. (Color online) $p\,(J_{1\to 2})$ vs $J_{1\to 2}$. In all the panels $m=1$, $\gamma=1$, $k=1$, $k_1=1$. The symbols were obtained from numerical realisations of the model (38), and the green line given by Eq. (61). In the upper panels we have used the temperature pairs $T_1=1, T_2=1.05$, and in the lower panels $T_1=1, T_2=1.3$. Regarding the nonlinear parameters $k_3=0$ (left panels) $k_3=0.02$ (right panels).

according to the relation

$$\mathcal{C}_{J_{1\to 2}}(\lambda) = \exp\left[\sum_{n=1}^{\infty}\delta\kappa_n\frac{(i\,\lambda)^n}{n!}\right]\mathcal{C}_{0,J_{1\to 2}}(\lambda) \tag{60}$$

or, equivalently,

$$p\,(J_{1\to 2}) = \exp\left[\sum_{n=1}^{\infty}\delta\check{\kappa}_n\frac{(-1)^n}{n!}\frac{\partial^n}{\partial J_{1\to 2}^n}\right]p_0\,(J_{1\to 2}). \tag{61}$$

Defining

$$\mathcal{N} \equiv m\,k_1^2\,(k_1-k) + \gamma^2\left(k^2 + k\,k_1 + k_1^2\right),$$
$$\mathcal{D}_1 \equiv k + 2k_1,$$
$$\mathcal{D}_2 \equiv k\,\gamma^2 + k_1^2\,m + k_1\,\gamma^2,$$

we have

$$\check{\kappa}_1' = A + A_1 \tag{62}$$

$$= A - \frac{3}{2}k_3\gamma\frac{\mathcal{N}_1}{\mathcal{D}_1\,\mathcal{D}_2}(T_1-T_2)(T_1+T_2) + O\left(k_3^2\right). \tag{63}$$

Additionally, we can always set $\delta\check{\kappa}_2 = 0$ by making $\check{\kappa}_2' = \check{\kappa}_2 = B$ when $k_3 = 0$ or replacing the linear case value with

$$\check{\kappa}_2' = \check{\kappa}_2 = B'$$
$$= B + B_{1a} + B_{1b} + A^2 - (\check{\kappa}_1')^2, \tag{64}$$

where

$$B_{1a} = \frac{3}{2}\,k_3\,k\,\frac{(3\,k+2\,k_1)}{m\,\mathcal{D}_1^3}\,(T_1+T_2)^3 + O\left(k_3^2\right), \tag{65}$$

$$B_{1b} = 3k_3\,k\,k_1\,\gamma^2\frac{\mathcal{N}}{\mathcal{D}_1\,\mathcal{D}_1}\,(T_1-T_2)^2\,(T_1+T_2) + O\left(k_3^2\right). \tag{66}$$

The remaining orders $\delta\kappa_n$ are obtained from the difference between κ_n given by Eq. (53) plus the nonlinear corrections and the cumulants of the reference distribution $p_0\,(J_{1\to 2})$.

In Fig. 7 we show a comparison between $p\,(J_{1\to 2})$ obtained by numerical simulation, using Eq. (61) in two situations: A slightly different from 0 (upper panels) and Λ less, but not significantly less, than 1 (lower panels). In the same figure it is noticeable the skewness of $p\,(J_{1\to 2})$ reflecting the second law of thermodynamics, in the Clausius statement, within a nonequilibrium steady state context.

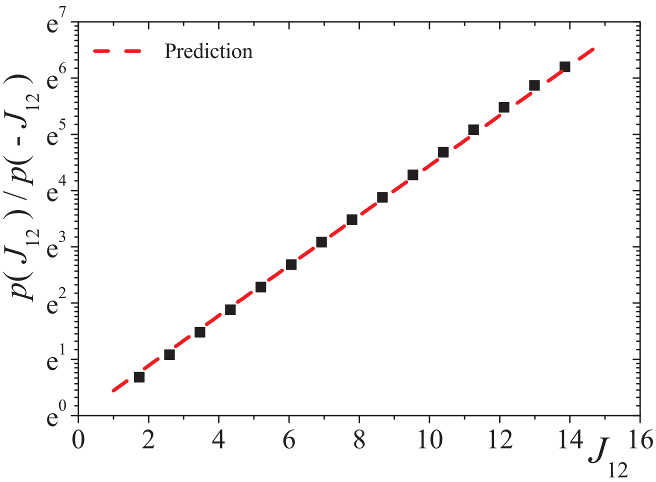

FIG. 8. (Color online) Numerical verification of Eq. (68) (dashed red line) where the points were obtained by numerically inverting $\mathcal{M}_{J_{1\to 2}}$ in a log-linear scale. The points span the interval between 2 and 16 standard deviations. The parameters used are the following: $k = 1, k_1 = 1, m = 1, \gamma = 1, T_1 = 1$, and $T_2 = 2$.

For the sake of simplicity let us now consider a first order approximation of $p(J_{1\to 2})$ in the linear case, which reads

$$p(J_{1\to 2}) \approx p_0(J_{1\to 2}) + \frac{A}{\pi B}\frac{J_{1\to 2}}{|J_{1\to 2}|}K_1\left[\frac{|J_{1\to 2}|}{\sqrt{B}}\right]. \quad (67)$$

Bearing in mind the modified Bessel functions of the second kind has the same asymptotic we can write the ratio between positive and negative values of the heat flux for $|A| \ll \sqrt{B}$ as

$$\lim_{|J_{1\to 2}|\to\infty, |A|\ll\sqrt{B}} \frac{p(|J_{1\to 2}|)}{p(-|J_{1\to 2}|)} = \frac{1 + A/\sqrt{B}}{1 - A/\sqrt{B}} \approx 1 + 2\frac{A}{\sqrt{B}} + \frac{A^2}{B} + O\left[\left(\frac{A}{\sqrt{B}}\right)^3\right], \quad (68)$$

the right-hand side of which, up to second order, matches $\exp[2\frac{A}{\sqrt{B}}]$. Moreover, if we remember that $J_{1\to 2}$ acts in the form of injected power on the colder particle, and paying attention to the fact that according to the conditions of Eq. (68) we are analyzing deviations $J_{1\to 2}$ not too far away from from $p(J_{1\to 2} = 0) = 1$, we finally get the following fluctuation relation:

$$\lim_{|J_{1\to 2}|\to\infty} \frac{p(|J_{1\to 2}|)}{p(-|J_{1\to 2}|)} = \exp\left[2\frac{\overline{J_{1\to 2}}}{\sigma^2_{J_{1\to 2}}}|J_{1\to 2}|\right], \quad (69)$$

which is appraised in Fig. 8.

IV. FINAL REMARKS

In this paper using techniques of time averaging over the noise that link with the final-value theorem, we studied the impact of nonlinearities in the limit of small perturbations $\frac{k_3 T}{k_1^2} \ll 1$ (where T is the temperature k_1 and k_3 are the harmonic and anharmonic constants, respectively) on the long-term thermostatistical properties of massive one- and two-particle systems in contact with Gaussian reservoirs and friction.

For one-particle systems, we mainly computed the values of the average total energy, injected and dissipated heat, and the respective probability distributions as well as the injected and dissipated power distributions. At first sight and somewhat surprisingly, we verified that the nonlinearities essentially affect the values of the energy of the particle and do not alter the statistics of the long-term injected and dissipated heat. Putting it differently, within a thermostatistical context the nonlinearities just bear upon the transient when the system is adjusting its total energy to the equilibrium value. After reaching equilibrium, the velocity of the particle is Gaussian, and thus both the injected and the dissipated heat, which are functions of the velocity [see Eq. (21)], are not modified by such deviations from linearity and continue growing as a first order function of the elapsed time. In addition, we noticed that not only the average values of the long-term injected and dissipated heat are equal but their distributions as well [6]. In solving the case of the injected heat, we used a diagrammatic representation of the contributing terms. Looking into the heat derivatives, i.e., the injected and dissipated powers, and making use of probabilistic arguments we were able to confirm that the distributions for these quantities are different; Whereas the dissipated power distribution is one sided, the injected power, j_I, can have both signs. Nevertheless, $p(j_I)$ is positively skew, a consequence of the correlation between the velocity and the action of the reservoir on the system, η, so that dissipation is set off. From an assumption about the relation between v and η we also introduced a relation between positive and negative values of j_I with the same absolute value resembling a fluctuation relation. We computed the response functions of the equilibrium energy with respect to changes in the thermomechanical parameters. Our computations have shown that with the introduction of nonlinearities the specific heat becomes temperature dependent, breaking the standard classical relation. In particular, we have noted that in the first order the specific heat decreases. This effect is understood bearing in mind that in analyzing the confining potential as a spring; adding a nonlinear term, we are increasing efficiency of the energy transfer between particles. Moreover, from the response functions $\frac{\partial\overline{\mathcal{E}}}{\partial k_1}$ and $\frac{\partial\overline{\mathcal{E}}}{\partial k_3}$ we have recovered the role of nonlinearities in coupling mechanical and thermal properties of the systems.

In the case of a two-particle system we have extended our previous results on the average heat flux [13] to the cumulant of any order. This result has permitted us to obtain the exact generating function of the distribution of the heat flux, $p(|J_{1\to 2}|)$. When the temperatures of both reservoirs are the same we get a symmetrical distribution, which is functionally equal to a modified Bessel function of second kind, non-Gaussian though, in the linear coupling case. Interestingly, this is the distribution of a variable that results from the product of two Gaussian random variables. Thus, taking into consideration the definition of $J_{1\to 2}$ we induce that the relative displacement $x_1 - x_2$ and the velocity of the center of mass $(v_1 + v_2)/2$ are Gaussian distributed. For the heat flux it is possible to compute the same Greek functions as well. In doing that we can learn that the introduction of nonlinearities turns $\overline{J_{1\to 2}}$ dependent on the effective temperature of the system $T_e \equiv (T_1 + T_2)/2$, i.e., $\nu_{1\to 2} \equiv \frac{\partial\overline{J_{1\to 2}}}{\partial T_e} \neq 0$, whereas in the linear case $\nu_{1\to 2} \equiv \frac{\partial \overline{J_{1\to 2}}}{\partial T_e} = 0$. Once again, this underpins the blending of the mechanical and thermal properties of the system in the presence of nonlinearities [13] and also explains why the expansions are carried out considering $\frac{k_3 T}{k_1^2}$ as the perturbation onto linearity instead of simply considering the values of k_3. Such conjoining can also be understood when computing $\rho_{1\to 2} \equiv \frac{\partial \overline{J_{1\to 2}}}{\partial k_1}$ and $\varrho_{1\to 2} \equiv \frac{\partial \overline{J_{1\to 2}}}{\partial k_3}$. In the former case, we find dependence on $T_d \equiv (T_1 - T_2)$ for $k_3 = 0$, while we find dependence on both T_d and T_e for $k_3 \neq 0$ and in addition $\varrho_{1\to 2}$. Last, there is an important difference between the Greeks υ and Γ of $\overline{\mathcal{E}}$ and $\overline{J_{1\to 2}}$: in the latter case they are always different from zero, even in the linear case.

In applying a Gram-Charlier (or Edgeworth) expansion to $p\,(J_{1\to 2}; k_3 = 0)$ we have succeeded in obtaining an approximative representation of the distribution of heat flux for nonlinear cases, whence it has become clear that the skew $p\,(J_{1\to 2})$ is a consequence of the temperature gap. From the ratio between positive and negative values of $|J_{1\to 2}|$ we have conjectured another fluctuation relation, this time for the heat flux.

Regarding the possible experimental corroboration of our results this can be carried out in three ways: (1) using analog electronic circuits (RLC-type) in the spirit of Refs. [25]; (2) thermostatistical behavior of gas droplets in nucleation phenomena (after molecular dynamics results reported in Ref. [26]); and (3) analysis of small magnetic systems along the lines of Refs. [8,27].

Finally, we would like to call attention to the fact many problems are badly represented by Gaussian reservoirs [28]. In recent work of ours and other authors [13,29], it was shown that the assumption of Poissonian (singular measure [15]) reservoirs can introduce sharp changes in the thermostatistical features of a mechanical system. In a subsequent paper we will convey results concerning the change of measure.

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