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Role of the nature of noise in the thermal conductance of mechanical systems

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Focusing on a paradigmatic small system consisting of two coupled damped oscillators, we survey the role of the Lévy-Itô nature of the noise in the thermal conductance. For white noises, we prove that the Lévy-Itô composition (Lebesgue measure) of the noise is irrelevant for the thermal conductance of a nonequilibrium linearly coupled chain, which signals the independence of mechanical and thermodynamical properties. In contrast, for the nonlinearly coupled case, the two types of properties mix and the explicit definition of the noise plays a central role.

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I. INTRODUCTION

The law of heat conduction, or Fourier's law, i.e., the property by which the heat flux density is equal to the product of the thermal conductivity by the negative temperature gradient [1], is a paradigmatic manifestation of the ubiquitous laws of thermodynamics [2]. Recently, it has stoked a significant amount of work on its explicit derivation for large Hamiltonian systems [3–5]. In this context, models with anharmonic coupling succeed in diffusing energy, but the analytic solutions thereto are very demanding, even for the few cases where that is possible. Since they allow a larger number of exactly solvable cases, small systems are worthwhile [6] and particularly relevant in chemical physics and nanosystems [7]. In the scope of analytical methods, we highlight the time averaging of observables that endure a stationary state [8,9]. This account has several advantages, namely, compared with the Fokker-Planck approach, which cannot be applied to those cases where cumulants of the noise higher than second order are nonvanishing and also significant. This comprises Poissonian [10–12] and other non-Gaussian massive particles [13] as well as other cases where the interaction with a reservoir is described by a process with a nonzero singular part of the measure when a Lévy-Itô (LI) decomposition is applied [14].

Stemming from these facts, we perform a time-averaging study of a small nonequilibrium system composed of two damped coupled oscillators at distinct temperatures and determine the explicit formula of Fourier's law for linear and nonlinear cases. In spite of its simplicity, the former has relevant traits: (i) It is a nonequilibrium system, (ii) its heat flux definition is well known, (iii) it is adjustable to different kinds of reservoirs, (iv) it can be expanded into an infinite chain with a nearly direct application of the results of an $N=2$ block, (v) it represents the result of Langevin colored noises by a renormalization of the masses [8], and (vi) linearity is still a source of important results in many areas [15–18].

II. MODEL

Our problem focuses on solving the set of equations

$$m\frac{dv_i(t)}{dt} = -kx_i(t) - \gamma v_i(t) - \sum_{l=1}^{2} k_{2l-1}[x_i(t)-x_j(t)]^{2l-1} + \eta_i(t), \tag{1}$$

with $v_i(t) \equiv \frac{dx_i(t)}{dt}$, where $(i,j) \in \{1,2\}$ and k_1 and k_3 are the linear and nonlinear coupling constants, respectively. The system is decoupled (linear) for $k_{1\,(3)} = 0$. The transfer flux $j_{12}(t)$ between the two particles reads

$$j_{12}(t) \equiv -\sum_{l=1}^{2} \frac{k_{2l-1}}{2}[x_1(t)-x_2(t)]^{2l-1}[v_1(t)+v_2(t)]. \tag{2}$$

The term $\eta_i(t)$ represents a general uncorrelated Lévy class stochastic process with cumulants

$$\langle \eta_{i_1}(t_1)\cdots\eta_{i_n}(t_n)\rangle_c = \mathcal{A}(t_1,n)\delta_{i_1 i_2}\cdots\delta_{i_{n-1}i_n}\delta(t_1-t_2)\cdots\delta(t_{n-1}-t_n). \tag{3}$$

From Ref. [19] we have either two or an infinite number of nonzero cumulants. The former corresponds to the case in which the measure is absolutely continuous, characterizing a Brownian process. In Eq. (3), $\mathcal{A}(t,n)$ is described by the noise; if it is Wiener-like $W(t) \equiv \int_{t_0}^{t}\eta(t')dt'$, $\mathcal{A}(t,n)$ is time independent and equal to σ^2 for $n=2$ and zero otherwise (σ is the standard deviation of the Gaussian function). Among the infinite nonzero cumulant noises, we can include the Poissonian process for which $\mathcal{A}(t,n)$ equals $\overline{\Phi^n}\lambda(t)$ [20], with Φ being the $p(\Phi)$ independent and identically distributed magnitude and $\lambda(t)$ the rate of shots. Herein $\mathcal{A}$ is time independent without loss of generality. For $k_1 = k_3 = 0$, Eq. (1) is totally decoupled and the solutions to the problem of homogeneous and sinusoidal heterogeneous Poissonian noises can be found in Ref. [10].

III. RESULTS

Laplace transforming $x_i(t)$ and $v_i(t)$ we obtain

$$\tilde{x}_i(s) = \frac{k_1}{R(s)}\tilde{x}_j(s) + \frac{\tilde{\eta}_i(s)}{R(s)} + \frac{k_3}{R(s)} \times \lim_{\alpha\to 0}\iiint \frac{\prod_{n=1}^{3}\frac{dq_n}{2\pi}[\tilde{x}_i(iq_n+\alpha)-\tilde{x}_j(iq_n+\alpha)]}{s-(iq_1+iq_2+iq_3+3\alpha)},$$
$$s\tilde{x}_i(s) = \tilde{v}_i(s) \tag{4}$$

[Re$(s) > 0$], with $R(s) \equiv (ms^2+\gamma s+k+k_1)$. The solutions to Eq. (4) are obtained by considering the relative position $\tilde{r}_D(s) \equiv \tilde{x}_1(s) - \tilde{x}_2(s)$, the midpoint position $\tilde{r}_S(s) \equiv [\tilde{x}_1(s) + \tilde{x}_2(s)]/2$, and the respective noises $\tilde{\eta}_D(s) \equiv \tilde{\eta}_1(s) - \tilde{\eta}_2(s)$ and $\tilde{\eta}_S(s) \equiv [\tilde{\eta}_1(s) + \tilde{\eta}_2(s)]/2$. After some algebra it yields [21]

$$\tilde{r}_D(s) = \frac{\tilde{\eta}_D(s)}{R'(s)} - \frac{2k_3}{R'(s)}\lim_{\alpha\to 0}\int_{-\infty}^{\infty}\frac{\prod_{l=1}^{3}\frac{dq_l}{2\pi}\tilde{r}_D(iq_l+\alpha)}{s-\sum_{l=1}^{3}(iq_l+\alpha)}\tilde{r}_S$$
$$= \frac{\tilde{\eta}_S(s)}{R''(s)}, \tag{5}$$

with $R'(s) \equiv (ms^2+\gamma s+k+2k_1)$ and $R''(s) \equiv (ms^2+\gamma s+k)$. Reverting to Eq. (5), we get $\tilde{x}_1(s)$ and $\tilde{x}_2(s)$. Concomitantly, we must compute the Laplace transforms of η_1 and η_2,

$$\langle\tilde{\eta}_{i_1}(z_1)\cdots\tilde{\eta}_{i_n}(z_n)\rangle_c = \int_0^{\infty}\prod_{j=1}^{n}dt_{i_j}\exp\left[-\sum_{j=1}^{n}z_{i_j}t_{i_j}\right] \times \langle\eta_{i_1}(t_1)\cdots\eta_{i_n}(t_n)\rangle_c = \frac{\mathcal{A}(n)}{\sum_{j=1}^{n}z_{i_j}}\delta_{i_1 i_2}\cdots\delta_{i_{n-1}i_n}, \tag{6}$$

which are employed in the averages over time [8]

$$\overline{\langle x_a^m v_b^n\rangle_c} = \lim_{z\to 0} z\iiint \delta(t-t_1)\delta(t-t_2)e^{-zt} \times \langle x_a^m(t_1)v_b^n(t_2)\rangle_c dt_1 dt_2 dt$$
$$= \lim_{z,\varepsilon\to 0}\int_{-\infty}^{\infty}\prod_{l=1}^{m+n} \times \frac{dq_l}{2\pi}z\frac{\prod_{l'=1}^{n}(iq_{l'}+\varepsilon)\langle\prod_{l=1}^{m+n}\tilde{x}(iq_l+\varepsilon)\rangle_c}{z-\left(\sum_{l'=1}^{m+n}iq_{l'}+(m+n)\varepsilon\right)}. \tag{7}$$

Allowing for a contour that goes along the straight line from $-\rho+i\varepsilon$ to $\rho+i\varepsilon$ and then counterclockwise along a semicircle centered at $0+i\varepsilon$ from $\rho+i\varepsilon$ to $-\rho+i\varepsilon$ ($\rho\to\infty$ and $\varepsilon\to 0$), we realize that one of two situations occurs: The calculation of the residues leads us to either a term such as $\frac{z}{z-w}u$, with $(u,w)\neq 0$, which vanishes in the limit $z\to 0$, or $\frac{z}{z}u$, which is nonzero. The problem solving now resumes with an expansion of Eq. (2) in powers of k_3; actually the expansion is carried out in powers of k_3T/k_1^2 [22]. Hereinafter, besides the results of the Brownian thermostats, which correspond to pure continuous measures, we make explicit the conductance for the Poissonian reservoirs, the epitome of singular measures. Nevertheless, the results for other non-Gaussian noises can be obtained following our methodology, yielding the same qualitative results. In first order the transfer flux reads

$$\overline{\langle j_{12}\rangle} = \overline{\langle j_{12}^{(0)}\rangle} + \overline{\langle j_{12}^{(1)}\rangle} + \overline{\langle j_{12}^{(s)}\rangle} + O(k_3^2), \tag{8}$$

with

$$\overline{\langle j_{12}^{(0)}\rangle} = -\frac{k_1^2}{4}\frac{[\mathcal{A}_1(2)-\mathcal{A}_2(2)]}{mk_1^2+\gamma^2(k+k_1)},$$
$$\overline{\langle j_{12}^{(1)}\rangle} = -\frac{3}{8}\gamma k_1 k_3\frac{(2k+k_1)[\mathcal{A}_1(2)^2-\mathcal{A}_2(2)^2]}{(k+2k_1)\left[\gamma^2(k+k_1)+mk_1^2\right]^2}, \tag{9}$$

and

$$\overline{\langle j_{12}^{(s)}\rangle} = -\frac{27}{2}\gamma^2\frac{k_1k_3}{\lambda}\frac{\mathcal{N}}{\mathcal{D}}\{[\mathcal{A}_1(2)^2-\mathcal{A}_2(2)^2]\} \tag{10}$$

for the Poissonian case and $\overline{\langle j_{12}^{(s)}\rangle} = 0$ for the Brownian case [21]. For the Poissonian case, when $\lambda^{-1} \ll 1$ (keeping the temperature fixed), the weight of the singularity of the noise measure dwindles and $\overline{\langle j_{12}^{(s)}\rangle} \to 0$. The coefficients in Eq. (10) are

$$\mathcal{N} \equiv \gamma^2(5k+3k_1) + m\left(3k_1^2+4k^2+11kk_1\right), \tag{11}$$

$$\mathcal{D} \equiv [\gamma^2(k+k_1)][m(4k+9k_1)^2+6\gamma^2(2k+3k_1)] \times\left[3\gamma^4+m^2k_1^2+4m\gamma^2(k+k_1)\right]. \tag{12}$$

Thence, we are finally in the position to compute the thermal conductance

$$\kappa \equiv -\frac{\partial}{\partial\Delta T}\langle j_{12}\rangle_{\Delta T}, \quad \kappa = -\frac{\overline{\langle j_{12}\rangle}}{T_1-T_2}. \tag{13}$$

Resorting to single-particle results and the equipartition theorem [10], we relate the cumulants of the noise and the proper temperature T_i, namely, $\mathcal{A}_i(2) = 2\gamma T_i$, yielding a thermal conductance $\kappa = \kappa^{(0)} + \kappa^{(1)} + \kappa^{(s)} + O(k_3^3)$. Equations (8)–(10) pave the way to the following assertion: When interacting particles are subject to white reservoirs and coupled in a linear form, the explicit thermal conductance is independent of the specific nature of the noise, namely, the outcome of their Lévy-Itô decomposition, whereas for nonlinear coupling the nature of the measure of the noise (its decomposition) is pivotal. In other words, the linear case is heedless of the measure of the reservoirs and it only takes into consideration their temperatures. Hence $\kappa^{(0)}$ is exactly the same: We have either a Wiener noise (continuous measure), which is the standard noise in fundamental statistical mechanics studies [9,23], or a Poisson noise (paradigmatic case of singular measure). Although the linear coupling result has only been explicitly proved for two particles, it is valid for general N. In fact, for a linear chain, the local energy flow $\langle j_{i,i+1}\rangle$ can be written as a function of the cumulants $\langle\eta_i(z)\eta_1(z')\rangle_c = 2\gamma T_i$ and $\langle\eta_{i+1}(z)\eta_{i+1}(z')\rangle_c = 2\gamma T_{i+1}$, wherein the dependence on the specific nature of the noise is eliminated, except for the respective temperatures. In contrast, if the nature of the noise affects the conductance of the simplest coupling element, the conductance for generic chains is also changed. This result is unexpected since, contrary to single-particle linear cases, wherein the LI nature is already relevant [10,13], for coupled systems the LI composition becomes significant only when the interaction between the elements of the system happens in a nonlinear way. Only in this case do higher-order cumulants of the noise, which can be understood as higher-order sources of energy, influence the result. For the same (k_1,k_3), in decreasing

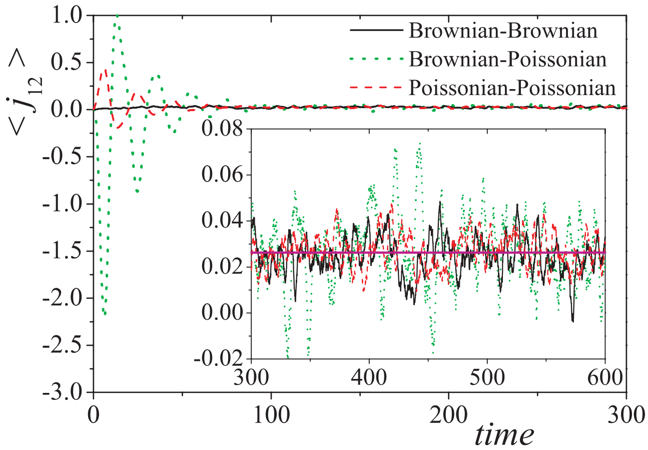

FIG. 1. (Color online) Average exchange flux $\langle j_{12}\rangle$ of a two-massive-particle system for different combinations of paradigmatic types of noise with $T_1 = 10$, $T_2 = 121/10$, $m = 10$, $\gamma = k = 1$, $k_1 = 1/5$, $k_3 = 0$, and $\lambda = 10$ for Poissonian particles. After the transient, κ agrees with the theoretical value, $\kappa = 21/800 = 0.026\,25$, with the fitting curves lying within the line thickness. The averages have been obtained by averaging over $850 \times (5 \times 10^5)$ points. The discretization used is $\delta t = 10^{-5}$ with snapshots at every $\Delta t = 10^{-3}$.

the singularity by soaring λ, the two thermal conductances tally.

To further illustrate these results we have simulated cases of equally massive particles subject to Wiener and Poisson noises at different temperatures T. For the former we have $T = \sigma^2/2$, whereas for the latter we have assumed a homogeneous Poissonian process with a rate of events λ, with a random amplitude Φ exponentially distributed $p(\Phi) \sim \exp[-\Phi/\bar{\Phi}]$, which yields $T = \lambda_0\bar{\Phi}^2/\gamma$ [10]. In Fig. 1 we depict linear coupling. It is visible that after a transient time t^* the system reaches a stationary state and $\langle j_{12}\rangle$ becomes equal to $\overline{\langle j_{12}\rangle}$, whatever the reservoirs. In fact, even more complex models, such as linear chains of oscillators, verify the $\kappa = \kappa^{(0)}$ property. Still, this is valid when each particle is perturbed by different types of noise, e.g., a Brownian particle coupled with a Poissonian particle. The instance where the noises are of different nature gives rise to an apparent larger value of the standard deviation.[1]

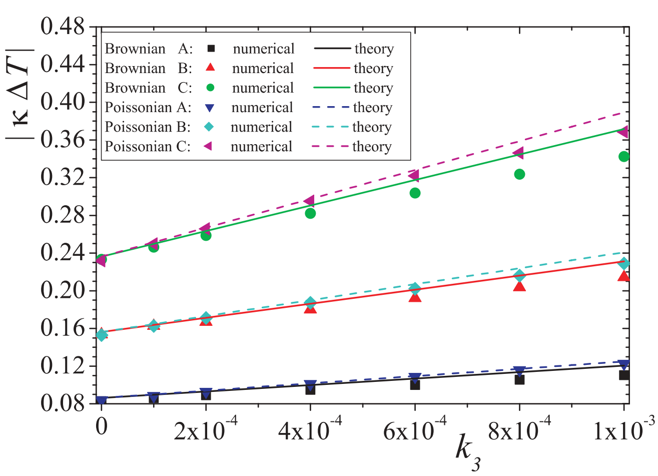

FIG. 2. (Color online) Comparison between numerically obtained values (symbols) and the first-order approximation of thermal conductance from Eqs. (8)–(10) for different temperature pairs, namely, $A = \{10, \frac{169}{10}\}$, $B = \{10, \frac{225}{10}\}$, and $C = \{10, \frac{289}{10}\}$ with $m = 10$, $\gamma = k = 1$, $k_1 = 1/5$, and $\lambda = 1$ for Poissonian particles.

In turning $k_3 \neq 0$ the composition of the measure of the reservoirs comes into play. In Fig. 2 we show the difference between equivalent Brownian and Poissonian particles with good agreement between the averages over numerical realizations and the respective (first-order) approximation. For the same temperature, the larger the value of k_3, the larger the value of the correction on k_3^2, which explains the 10% difference between numerical values of the approximation.

IV. CONCLUSION

To summarize, we have studied the thermal conduction in a paradigmatic mechanical system composed of two coupled damped harmonic oscillators subject to generic noises, which can be understood as a concise way to describe nonequilibrium problems. By averaging in the Laplace space, we have been able to determine the conductance of a linearly coupled system and approximate formulas for nonlinearly coupled particles. We have shown that the conductance of the former is independent of the nature of the (white) noise, namely, its Lévy-Itô decomposition structure. This result is unexpected since the measure of the thermal bath plays a major role for single-particle properties. The dependence on the noise emerges only when there is a transfer of energy in a nonlinear way and higher-order cumulants of the noise enter in the calculations. In the case of Poissonian noises, we show that the difference from Brownian noises becomes negligible when the ratio between the coupling constants and the rate of events is small. Our calculations evidence the independence of the thermodynamical properties of the system from the nature of the reservoirs in linearly coupled systems. In contrast, when the coupling is nonlinear, the nature of the reservoirs affects the conductance, which represents a mixture of mechanic and thermodynamical properties of the system.

Our results have direct implication for the study of the thermal conductance of systems under the influence of noises other than Wiener, for instance, (i) solid state problems wherein shot (singular measure) noise is related to the quantization of the charge [24]; (ii) resistor-inductor-capacitor circuits with injection of power at some rate resembling heat pumps [11]; (iii) surface diffusion and low vibrational motion with adsorbates, e.g., Na/Cu(001) compounds [25]; (iv) biological motors in which shot noise mimics the nonequilibrium stochastic hydrolysis of adenosine triphosphate [12]; and (v) molecular dynamics when the Andersen thermostat is applied. Actually, in molecular dynamics [26], the Langevin reservoir is just one in a large collection of baths represented by our definition of noise (3). In these problems, for nonlinearly coupled elements, the experimentally measured energy flux will be greater than the energy flux given by Langevin reservoirs at the same

[1] Although the computation of $\sigma^2_{j_{12}} \equiv \langle j_{12}^2\rangle - \langle j_{12}\rangle^2$ is possible, we have omitted it as it demands a mathematical *tour de force* likely to yield a lengthy formula with little usable information.

temperatures and equal if coupling is linear. At the theoretical level, the method is worth using to shed light on nonlinear chains as well. Within this context, the feasible approach is once again to consider a perturbative expansion of the nonlinearities in the problem.

Note added. It came to our attention recently that Kanazawa and Coworkers, using a different technique for the noise analysis [27], present an equivalent claim regarding the role of the noise in the conductance of mechanical systems [28].

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