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Heat fluctuations in Brownian transducers

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The heat fluctuation probability distribution function in Brownian transducers operating between two heat reservoirs is studied. We find, both analytically and numerically, that the recently proposed fluctuation theorem for heat exchange [C. Jarzynski and D. K. Wojcik, Phys. Rev. Lett. **92**, 230602 (2004)] has to be applied carefully when the coupling mechanism between both baths is considered. We also conjecture how to extend such a relation when an external work is present.

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Nonequilibrium systems are receiving much attention from a theoretical point of view through the derivation of the so-called fluctuation theorems. The theoretical approach is based on microscopic reversibility and elegant analytical properties for the probability distribution of the entropy generated are derived [2]. From these rigorous results, corollaries such as a statistical derivation of the second law can be achieved. Moreover, they hold for systems arbitrarily far away from equilibrium and are not restricted to the linear regime. There are different fluctuation relations depending on the dynamics that they apply to, the magnitudes they relate to, or the state of the system they refer to. Amongst the most relevant one finds the Gallavoti-Cohen fluctuation theorem [3], the Jarzynski equality [4], the formalism for steady-state thermodynamics [5], an extension of the fluctuation theorem [6], and an integral fluctuation theorem [7]. Apart from their intrinsic value to theoretical physics, a vast number of experimental applications based on such results have been developed [8]. The benchmark of these theorems is nanosystems such as molecular motors [9]. Nearly all of such relations focus on work fluctuations [10–12]. In contrast, not much attention has been paid to heat fluctuations. There are only a few contributions to the topic [6,13,14], in which only one thermal bath is considered. Recently, Jarzynski and Wojcik [1] derived a fluctuation theorem for heat exchange (denoted as XFT) between two systems initially prepared at different temperatures T_1 and T_2, then placed in thermal contact with one another for a certain time and, finally, separated again. The theorem states that the probability distribution $p(Q)$ of the heat exchange Q satisfies

$$\ln \frac{p(+Q)}{p(-Q)} = \Delta\beta Q, \qquad (1)$$

where $\Delta\beta = 1/T_1 - 1/T_2$, and $k_B = 1$ is taken for simplicity from now on. Both systems must be prepared in equilibrium and then placed in thermal contact with one another, for an arbitrary period of time t_0, during which a net heat Q is transferred. This is a very interesting result because, in the first place, it focus on heat fluctuations and, secondly, because of its universal character: the prediction depends only on the two temperatures and not on any characteristic of the systems. Nevertheless, the theorem was derived for the presence of heat exchange only, without considering other sources of energy such as external work or the energy involved in the connecting mechanisms. Then, it is supposed that the heat lost by one system has exactly compensated the amount of energy gained by the other. However, any two bodies put in contact need a mechanism that connects them and therefore an interaction term should be considered and its relevance and effects studied. We may also notice that when work comes into play, the transfer of heat must be revised because, according to the second law, both baths interchange different amounts of heat.

The purpose of this work is to study the predictions and applicability of the XFT in specific models, such as Brownian motors. For a simple mechanical system that allows a heat exchange between two baths, we show that Eq. (1) is modified and we present an analytical calculation of such a modification, which does not depend on the details of the connecting mechanism. We also propose an extension for the case in which external work is present.

Brownian motors are a set of particularly peculiar machines that make use of thermal fluctuations of the environment they are immersed in to perform useful work [15]. There are many different models being the Feynman ratchet and the pawl device [16], the paradigm. In general, Feynman-like Brownian motors are built from two subsystems immersed, respectively, in two thermal baths at different temperatures and connected by some mechanism. These engines, such as the motor in Ref. [17], fit perfectly the study of heat fluctuations from the point of view of the setting of the XFT. Let us consider the transducer in Fig. 1. It has two degrees of freedom, x and y, at different temperatures $T_1 < T_2$ and is connected through a spring. Note that in the colder bath there is a saw-toothed wheel which acts as a ratchet potential. The Langevin equations of motion of this

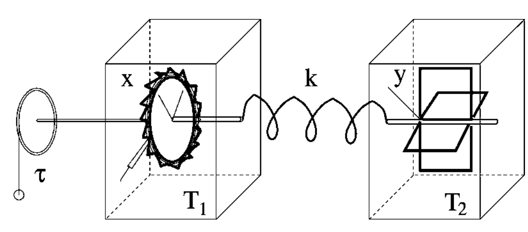

FIG. 1. Ratchet, pawl, and spring Brownian motor.

device in the overdamped limit, when setting the friction equal to 1, are

$$\dot{x} = -\partial_x V_c(x,y) - V_r'(x) + \tau + \xi_1(t), \quad (2)$$

$$\dot{y} = -\partial_y V_c(x,y) + \xi_2(t), \quad (3)$$

where $V_c(x,y)=(k/2)(x-y)^2$ is a harmonic coupling, $V_r(x)$ is the ratchet potential in [17], and τ is an external load. $\xi_1(t)$ and $\xi_2(t)$ are independent Gaussian white noises of correlation $\langle \xi_i(t)\xi_j(t')\rangle = 2T_i\delta_{ij}\delta(t-t')$.

Heat will flow from one bath to the other through the spring. We call Q the heat outcoming from the reservoir at T_2. Note that due to the internal energy stored in the spring, in the ratchet potential and due to the mechanical work, Q is not equal to the heat dissipated in the thermal bath at T_1. From Sekimoto's energetics scheme [18] one can obtain Q as

$$Q = \int_{y(0)}^{y(t_0)} [\xi_2(t) - \dot{y}(t)]dy(t) = k\int_0^{t_0} [y(t) - x(t)]\dot{y}(t)dt. \quad (4)$$

Before a formal approach to the analytic properties of this central quantity, let us perform a numerical study of it. A numerical computation of the stochastic heat Q is easily done by simulating the dynamics of the motor and performing the above integral numerically, once the steady state has been reached. Then we can get a collection of values of the total heat Q transferred during a fixed time interval t_0, with which histograms can be built. This is not exactly the situation described in the derivation of the XFT. According to Ref. [1], both subsystems are initially in equilibrium, then connected for a time period t_0 and, finally, separated again. However, in our simulations and calculations the transient regime hardly contributes compared to the steady-state state. Preliminary simulations in the nonlinear Brownian transducer at nonzero external work conditions show that, in the limit $kt_0 \gg 1$, heat histograms are very well fitted by Gaussian distributions. For smaller kt_0 distributions deviate from Gaussianity (see Fig. 2). Several numerical explorations performed with different values of the parameters involved, measuring the kurtosis and the skewness of the histograms and checking the tails of the distributions reveal a wide range of the parameter space in which the Gaussian approximation is justified. Therefore, in an appropriate and also physical limit, we can write

$$p(Q) = \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-(Q-\langle Q\rangle)^2/2\sigma^2} \quad (5)$$

and, accordingly, the XFT (1) can be expressed as,

$$\ln\frac{p(+Q)}{p(-Q)} = Q\frac{2\langle Q\rangle}{\sigma^2}. \quad (6)$$

This is a very interesting situation because, if we were able to calculate the quantities $\langle Q\rangle$ and $\sigma^2 = \langle \Delta Q^2\rangle$ for any specific model, then we could test the XFT prediction on a nonideal case. This cannot be done analytically for the nonlinear models (2) and (3) but it is possible if we simplify it by taking $V_r=0$. In particular, for this passive Brownian transducer and in the absence of external load ($\tau=0$) we find

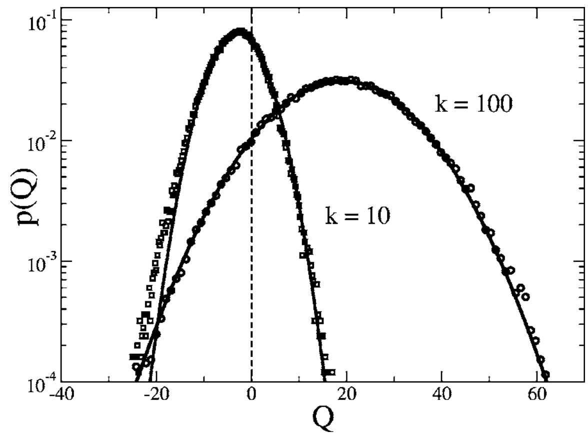

FIG. 2. Histograms of the heat transfer Q for the models (2) and (3) at nonzero external torque for a Gaussian and a non-Gaussian case. The parameters are $\tau=5$, $V_0=1$, $d=12$, $t_0=1$, $T_1=1$, and $T_2=1.5$. The continuous lines are Gaussian fits.

$$\langle Q\rangle = t_0\frac{k}{2}(T_2 - T_1), \quad (7)$$

which is indeed Fourier's law for the thermal conductivity (see Refs. [19,20]) and, in the limit $kt_0 \gg 1$, the second moment is [21]

$$\sigma^2 = t_0\frac{k}{4}(T_2 + T_1)^2. \quad (8)$$

Note that the mean value and variance are extensive in t_0 and they are also linear in k. The above results yield to

$$Y(Q) \doteq \ln\frac{p(+Q)}{p(-Q)} = \Delta\beta Q(1-\gamma), \quad (9)$$

where

$$\gamma = \left(\frac{T_2 - T_1}{T_2 + T_1}\right)^2. \quad (10)$$

This is one of the main results of this work. The expression does not depend on any detail of the coupling mechanism. We obtain that the XFT holds for small $\Delta\beta (T_2 \simeq T_1)$ but an important correction of order $\Delta\beta^3$ appears. In Fig. 3 we plot the XFT (1), the new prediction for the passive Brownian transducer (9), and results from numerical simulations, exploring the T_2 dependence. The symbols correspond to numerical data and deserve a careful explanation. The circles are obtained at $kt_0=100$. For white circles, $Y(Q)$ has been obtained by direct analysis of the probability distribution functions of heat. Around $T_2>2$, negative values ($Q<0$) are rarer events and therefore the tails are very difficult to observe directly. Black circles are obtained assuming a Gaussian behavior of the tails, though it is important to note that the distributions are still checked to be fitted reasonably well by a Gaussian. The higher the temperature T_2, the worse the Gaussian supposition is and so, for $T_2 \gtrsim 6$, we cannot conclude anything about $Y(Q)$. Finally, diamonds correspond to data at $kt_0=10$ from which $Y(Q)$ is directly measured from the histograms. This case is also very instructive because the

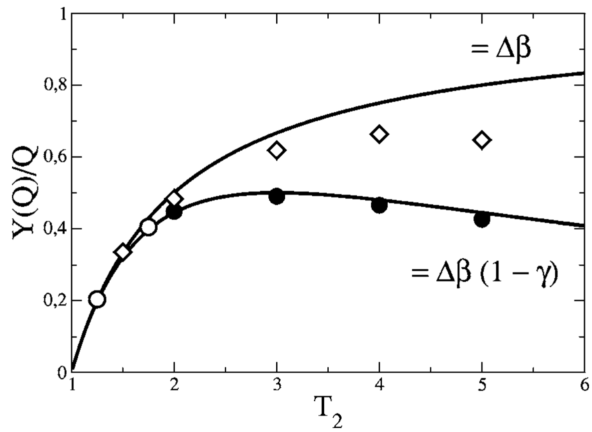

FIG. 3. Prediction of the XFT [Eq. (1)] and the correction found due to the coupling mechanism [Eq. (9)] in the Gaussian approximation. The symbols are obtained from numerical data through different procedures (see text). The device considered is the passive Brownian transducer at $\tau=0$ and $T_1=1$.

distributions observed are non-Gaussian (see Fig. 2). The prediction (9) has also been checked satisfactorily (data not shown) in the nonlinear Brownian motor for $kt_0=100$, $V_0=1$ and $d=12$. Then our simulations indicate that, despite the rapidly increasing difficulty to test the theorem, important and systematic deviations do appear.

The γ factor modifying the XFT is a signature of the important role of the coupling between both systems. This points out the applicability of the theorem for large $\Delta\beta$, which strongly depends on the approximation made in the XFT derivation. It consists of neglecting the interaction term coupling the two bodies [1] by assuming that the energy involved in the coupling mechanism is much smaller than the typical energy change in both systems. When comparing in our model the typical energy of the coupling mechanism (the mean value of the potential energy of the spring $\langle V_c\rangle=[(T_2+T_1)/4]$, and the typical energy change in every subsystem (the mean heat released $\langle Q\rangle$), for the parameter values $k=100$, $t_0=1$, $T_2=5$, and $T_1=1$, we find $\langle V_c\rangle/\langle Q\rangle\sim 0.0075$. Therefore, we must remark here that, albeit the interaction energy can be negligible, its consequences are not.

The second point we study is the effect of an external work into the system. We want to explore the possibility of an extension of the relation (9) for this case. Taking $\tau\neq 0$ in (2), discarding the nonlinear ratchet potential and proceeding as before for these type of calculations, the quantity $\langle Q\rangle$ is

$$\langle Q\rangle = t_0\frac{1}{2}k(T_2-T_1) - t_0\tau^2/4 = \langle Q\rangle_c - \frac{\langle W\rangle}{2}, \qquad (11)$$

where $\langle Q\rangle_c$ is the mean heat conducted and $\langle W\rangle=t_0\tau^2/2$ is the mean work. Remember that $\langle Q\rangle$ is the mean heat released by the heat bath a T_2, so we are studying the fluctuations of this quantity, while heat exchanged at bath T_1 is different. The Fourier heat is conducted to the cold bath but also the hotter bath receives heat from the colder due to the external work. In fact, each bath dissipates half of the total work. It is worth remarking that the sign of $\langle Q\rangle$ can be reversed for

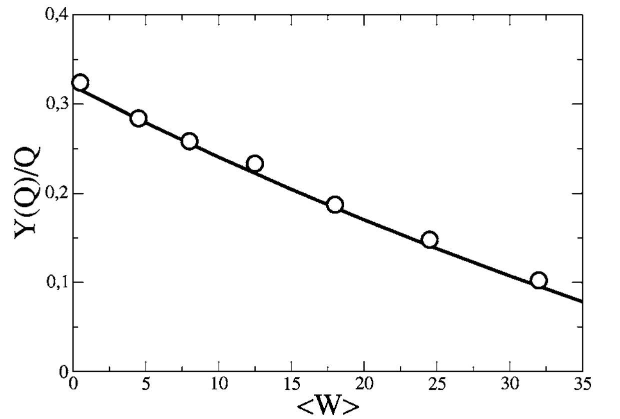

FIG. 4. Numerical simulations (dots) and analytical predictions (line) of Eq. (13) for the relation of heat fluctuations versus the mean value of the work in the Brownian motor model defined in Eqs. (2) and (3). The agreement is very good, even for this nonlinear system. The data are obtained by a direct measurement of the slope of $Y(Q)$. The parameters used are $T_1=1$, $T_2=1.5$, $d=12$, $V_0=1$, $t_0=1$, and $k=100$.

$\langle W\rangle > 2\langle Q\rangle_c$, reversing the heat flux, now from the cold bath to the hot one. The calculus of the variance is more involved but we find

$$\sigma^2 = t_0\frac{k}{4}(T_2+T_1)^2 + \langle W\rangle T_1. \qquad (12)$$

Using these results and defining the ratio of the two (model dependent) energies involved, $\mathcal{R}=\langle W\rangle/\langle Q\rangle_c$, the generalized relation for heat fluctuations is

$$\ln\frac{p(+Q)}{p(-Q)} = \Delta\beta Q(1-\gamma)\frac{1-\mathcal{R}/2}{1+f(T_1,T_2)\mathcal{R}}, \qquad (13)$$

where

$$f(T_1,T_2) = \frac{2T_1(T_2-T_1)}{(T_2+T_1)^2}. \qquad (14)$$

The above extension depends on the mechanisms involved. Nevertheless, although expression (13) has been derived for a linear model, we can apply it to the nonlinear case obtaining a very good agreement, as it is shown in Fig. 4. This means that we have found the terms that gather the most relevant features and which work even for general nonlinear devices. Notice that the torque used is, in general, beyond the stall torque of the motor performance. This is so because for very small loads, thus the ones that this motor is able to lift, it is very difficult to observe changes in the distributions of Q. We must also stress that our analytical prediction does not involve any adjustable parameter and, as a consequence, it could be confronted against other types of conducting and working devices.

One can derive similar results if the heat interchanged by the cold bath at T_1 is considered instead of the heat transferred from the bath at T_2. In this case, we have found (not shown here) that the relation (9) is unchanged when we deal with the fluctuations of the energy dissipated in the cold bath. Nevertheless for the $\tau \neq 0$ case, the expressions vary but one can find the corresponding relations following the same type of calculations. With respect to the conditions of our approach, we stress that it could be possible to obtain analytical expressions for the statistical moments of Q in the transient regime, after putting both systems initially in contact. Transient corrections of order e^{-kt_0} appear which, in the limit $kt_0 \gg 1$, can be discarded. Thus the transient regime is negligible compared to the steady-state contribution. Therefore, all the calculations in this Rapid Communication are done in the steady state and in the long t_0 limit (or big coupling). This is, indeed, of a great advantage because it makes it possible to derive analytically the most dominant contributions of the first and second moments. What is more, in such limit, although $p(Q)$ is not rigorously Gaussian because $Q(t)$ as defined in (4) is a nonlinear functional of a Gaussian Orstein-Uhlenbeck process, our main results are dominated by the Gaussian-like property of the distribution. As a byproduct we have shown in a linear model that heat fluctuations relative to the mean value $\sigma^2/\langle Q\rangle$ are system independent. It would be worthy to explore this result for other nonlinear models.

This work is a preliminary application and test of the XFT [1] to a nonideal system, in the sense that the effects of the system-environment coupling energy cannot be neglected. We have checked the sensitivity of the hypothesis of a small interaction term in Ref. [1] for simple Brownian devices. Quite surprisingly the XFT works better when the heat conducted is of the order of the energy stored in the coupling device but not when it is larger. It is worth emphasizing that any attempt to write a model that consists on two bodies interchanging heat needs a connection and, therefore, the observations mentioned above are encountered. Hence, one can neglect the energy stored in the connecting mechanism but its fluctuations have relevant consequences. However, in order to understand in more detail the role of heat, work, and coupling energy, it would be very interesting to address these questions from a more general theoretical point of view. The applicability of such results in theoretical models and in experiments is of great importance for discovering and understanding nonequilibrium statistical mechanics principles.

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[21] The calculation of the moments of Q is tedious. We rewrite Eq. (4) and as a functional of $Y=y$-x and white noises. Then, making use that $Y(t)$ is an Ornstein-Uhlenbeck process $[\dot{Y}=-2kY-\tau+\xi_2(t)-\xi_1(t)]$, $\langle Q\rangle$ and σ^2 can be evaluated from the moments and correlations of $Y(t)$ and $\xi(t)$.