

## Integral fluctuation theorem for the housekeeping heat

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## LETTER TO THE EDITOR

**Integral fluctuation theorem for the housekeeping heat****T Speck and U Seifert**

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Online at [stacks.iop.org/JPhysA/38/L581](http://stacks.iop.org/JPhysA/38/L581)**Abstract**

The housekeeping heat  $Q_{\text{hk}}$  is the dissipated heat necessary to maintain the violation of detailed balance in nonequilibrium steady states. By analysing the evolution of its probability distribution, we prove an integral fluctuation theorem  $\langle \exp[-\beta Q_{\text{hk}}] \rangle = 1$  valid for arbitrary-driven transitions between steady states. We discuss Gaussian limiting cases and the difference between the new theorem and both the Hatano–Sasa and the Jarzynski relation.

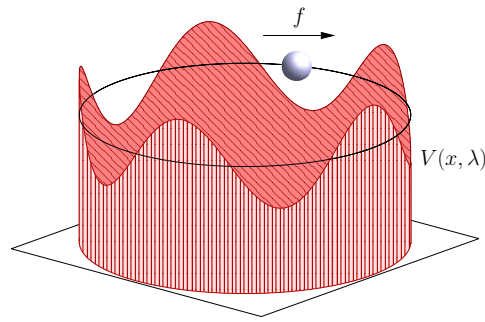
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**Introduction**

Steady-state thermodynamics provides a framework for describing transitions between different nonequilibrium steady states using terms familiar from ordinary thermodynamics [1–3]. As a crucial concept, the division of the total heat dissipated in such transitions into two contributions, a housekeeping heat  $Q_{\text{hk}}$  and an excess heat  $Q_{\text{ex}}$ , has emerged. The housekeeping heat is the one permanently dissipated while maintaining a nonequilibrium steady state at fixed external parameters  $\alpha$ . The excess heat is the one associated with a transition between different steady states caused by changing  $\alpha$ . For transitions between equilibrium states, the housekeeping heat vanishes and the total heat reduces to the excess heat. These concepts have been made explicit in the model of a colloidal particle driven along a one-dimensional coordinate described by a Langevin equation [2, 4]. In particular, it was shown that the excess heat  $Q_{\text{ex}}$  obeys a fluctuation theorem

$$\langle \exp[-\beta Q_{\text{ex}} - \Delta\phi] \rangle = 1, \quad (1)$$

where  $\phi(x, \alpha) \equiv -\ln p_s(x, \alpha)$  with  $p_s$  the steady-state probability distribution for fixed external parameters  $\alpha$ . The brackets  $\langle \cdot \cdot \cdot \rangle$  denote an average over many different realizations of the process in a surrounding heat bath of inverse temperature  $\beta \equiv 1/k_B T$ . Since the average  $\langle \Delta\phi \rangle$  can be identified as the change in generalized system entropy  $\Delta S$ , the relation  $\Delta S \geq -\beta \langle Q_{\text{ex}} \rangle$  following from equation (1) corresponds to a generalization of the second law to transitions between two different steady states [2]. An experimental test of this fluctuation



**Figure 1.** A periodic potential  $V(x, \lambda)$  with period  $L = 2\pi$ , where  $x$  is the angular position of a driven colloidal particle moving through a viscous fluid representing the surrounding heat bath. Depth and shape of the potential depend on the externally controlled parameter  $\lambda$ . A force  $f$  can be applied directly to the particle.

(This figure is in colour only in the electronic version)

theorem was realized using laser tweezers dragging a colloidal particle through a viscous fluid [5]. In this letter, we prove a similar fluctuation theorem for the housekeeping heat

$$\langle \exp[-\beta Q_{\text{hk}}] \rangle = 1 \quad (2)$$

valid for arbitrarily driven systems described by such a Langevin equation.

Integral fluctuation theorems of the type  $\langle \exp[-A] \rangle = 1$  have been derived and the corresponding probability distribution  $P(A = a)$  has been discussed for a variety of systems showing an underlying stochastic dynamics [6–14]. The most prominent example is the Jarzynski relation [6], where  $A$  is the dissipated work spent driving the system from one equilibrium state to another. Crucial for the Jarzynski relation proper is the fact that the system obeys detailed balance for fixed external parameters  $\alpha$ . However, even if this is not the case, by applying the same reasoning a Jarzynski-like relation

$$\langle \exp[-\beta Q_{\text{tot}} - \Delta\phi] \rangle = 1 \quad (3)$$

can be derived, which differs from equation (1) by using the total heat  $Q_{\text{tot}}$  as shown below. It is crucial to appreciate that all three relations (1–3) are genuinely different and require a different derivation.

Such integral fluctuation theorems should be distinguished from the detailed fluctuation theorem  $P(-a)/P(+a) = e^{-a}$  valid for a probability distribution  $P(a)$  in steady states at constant external parameters. Such a theorem was discussed first for entropy production in sheared two-dimensional fluids [15, 16] and later generalized to chaotic and stochastic dynamics [17–20]. It even holds for periodically driven systems as demonstrated experimentally using a single two-level system [21].

### The model

As a paradigm, we will focus on driven diffusive motion of a single colloidal particle in one dimension. The potential  $V(x, \lambda) = V(x + L, \lambda)$  is spatially periodic with period  $L$  and depends on an external parameter  $\lambda$ , see figure 1. The Langevin equation for the position  $0 \leq x(t) < L$  of the particle becomes

$$\gamma \dot{x} = -V' + f + \eta, \quad (4)$$

where  $V' \equiv \partial V/\partial x$  and  $f(t)$  is a time-dependent nonconservative force. The thermal noise  $\eta$  obeys the usual correlations  $\langle \eta(t)\eta(t') \rangle = 2(\gamma/\beta)\delta(t-t')$  with friction coefficient  $\gamma$ . The externally controllable parameters of the system are  $\alpha \equiv (\lambda, f)$ . A transition from  $\alpha_0 \equiv \alpha(0)$  to  $\alpha_t \equiv \alpha(t)$  occurs along the path  $\alpha(\tau)$  through parameter space.

Following Sekimoto [4], we write the total exchanged heat between system and reservoir in the time interval  $0 \leq \tau \leq t$  as the functional

$$Q_{\text{tot}}[x(\tau); \alpha(\tau)] \equiv \int_0^t d\tau \dot{x}(\tau)[f(\tau) - V'(x(\tau), \lambda(\tau))]. \tag{5}$$

We take the sign of the heat to be positive when energy flows out of the system into the heat bath.

In the case of genuine nonequilibrium states where  $p_s(x, \alpha)$  violates detailed balance at fixed  $\alpha$  (in our model for  $f \neq 0$ ), it makes sense to split up the total heat into the housekeeping heat, i.e., the part needed to maintain the violation of detailed balance

$$Q_{\text{hk}}[x(\tau); \alpha(\tau)] \equiv \gamma \int_0^t d\tau \dot{x}(\tau) v_s(x(\tau), \alpha(\tau)), \tag{6}$$

and the excess heat  $Q_{\text{ex}} \equiv Q_{\text{tot}} - Q_{\text{hk}}$  [2]. The function  $v_s$  is the local mean velocity of the particle in the steady state at fixed  $\alpha$ ,

$$v_s(x, \alpha) \equiv \frac{j_s(\alpha)}{p_s(x, \alpha)}, \tag{7}$$

where  $j_s$  is the steady-state probability current.

**Evolution equation**

In the definition (6) of the housekeeping heat the singular velocity  $\dot{x}$  appears, which requires a regularization. We therefore introduce the momentum  $p = m\dot{x}$  of the particle with mass  $m$  as an additional degree of freedom, even though we are considering the overdamped case. Then the coupled Langevin equations become

$$\dot{x} = p/m, \tag{8}$$

$$\dot{p} = f - V' - (\tilde{\gamma}/m)p + \zeta \quad \text{with} \quad \langle \zeta(t)\zeta(t') \rangle = 2(\tilde{\gamma}/\beta)\delta(t-t'), \tag{9}$$

$$\dot{q} = (\gamma/m)p v_s. \tag{10}$$

In equation (10),  $\dot{q}$  is the dissipation rate of the housekeeping heat (6) with  $\dot{x}$  replaced by  $p$ . The joint probability  $\bar{\rho}(x, p, q, t)$  to find the particle at position  $x$  with momentum  $p$  and to have spent a housekeeping heat  $q$  up to time  $t$  obeys the generalized Fokker-Planck equation

$$\partial_t \bar{\rho} = \left[ -\frac{p}{m} \partial_x + (V' - f) \partial_p + \varepsilon \partial_p p + \varepsilon \frac{m}{\beta} \partial_p^2 - \frac{\gamma}{m} p v_s \partial_q \right] \bar{\rho}. \tag{11}$$

Since  $Q_{\text{hk}}$  was defined for overdamped motion, we fix the friction coefficient  $\gamma$  and use  $\varepsilon \equiv \tilde{\gamma}/m$  as expansion parameter to recover the appropriate dynamics for  $Q_{\text{hk}}$  in the limit of large  $\varepsilon$ .

Adiabatic elimination of fast variables is a standard technique in stochastic dynamics [22]. To simplify the notation, we introduce the two differential operators

$$\mathcal{L}_p \equiv \partial_p [p + (m/\beta) \partial_p], \tag{12}$$

$$\mathcal{A} \equiv (p/m) \partial_x - (V' - f) \partial_p + (\gamma/m) p v_s \partial_q, \tag{13}$$

where we use the usual convention that a differential operator like  $\partial_x$  acts on all factors placed to its right. Using these operators, we rewrite equation (11) as

$$\partial_t \bar{\rho} = [\varepsilon \mathcal{L}_p - \mathcal{A}] \bar{\rho}. \quad (14)$$

Further we define a projector by

$$\mathcal{P} \psi(x, p) \equiv \psi_0(p) \int dv \psi(x, p), \quad (15)$$

where the Maxwell distribution  $\psi_0(p) = \sqrt{\beta/2\pi m} e^{-\beta p^2/2m}$  is the stationary solution of  $\mathcal{L}_p \psi_0 = 0$ . This ensures the two important properties

$$\mathcal{P} \mathcal{L}_p = \mathcal{L}_p \mathcal{P} = 0, \quad \mathcal{P} \mathcal{A} \psi_0 = 0 \quad (16)$$

of the projector  $\mathcal{P}$ . Now we decompose the joint probability  $\bar{\rho} = \bar{\rho}_0 + \bar{\rho}_1$  into a part ‘parallel’ to the stationary distribution

$$\bar{\rho}_0 \equiv \mathcal{P} \bar{\rho} = \rho \psi_0 \quad (17)$$

and a part perpendicular,  $\bar{\rho}_1 \equiv (1 - \mathcal{P}) \bar{\rho}$ . The function

$$\rho(x, q, t) = \int dp \bar{\rho}(x, p, q, t) \quad (18)$$

is the probability distribution we are looking for. Physically, this scheme corresponds to a decomposition into a part for which position  $x$  and momentum  $p$  are uncorrelated and into a deviation  $\bar{\rho}_1$ . For uncorrelated stochastic variables, the joint probability decays to the simple product (17).

Taking advantage of the properties (16), the coupled equations of motion become

$$\partial_t \bar{\rho}_0 = -\mathcal{P} \mathcal{A} \bar{\rho}_1, \quad (19)$$

$$\partial_t \bar{\rho}_1 = \varepsilon \mathcal{L}_p \bar{\rho}_1 - \mathcal{A} \bar{\rho}_0 - (1 - \mathcal{P}) \mathcal{A} \bar{\rho}_1. \quad (20)$$

The second equation (20) can be expanded into powers of  $\varepsilon^{-1}$ , yielding up to the first order  $\bar{\rho}_1 \simeq \varepsilon^{-1} \mathcal{L}_p^{-1} \mathcal{A} \bar{\rho}_0$ . Putting this back into equation (19), we finally arrive at

$$\partial_t \rho = -\varepsilon^{-1} \left[ \int dp \mathcal{A} \mathcal{L}_p^{-1} \mathcal{A} \psi_0 \right] \rho. \quad (21)$$

For the calculation, we insert definition (13) and note that  $\mathcal{L}_p^{-1} p \psi_0 = -p \psi_0$ . Gaussian integration then leads straightforwardly to the evolution equation

$$\partial_t \rho = \left[ \mathcal{L} + \left( 2\partial_x v_s - \frac{v_s^2}{D} \right) \frac{\partial_q}{\beta} + \frac{v_s^2}{D} \frac{\partial_q^2}{\beta^2} \right] \rho, \quad (22)$$

where we have set  $\tilde{\gamma} = \gamma$  and used the Einstein relation  $D = 1/\gamma\beta$ . The operator

$$\mathcal{L} \equiv \partial_x [(V' - f)/\gamma + D \partial_x] \quad (23)$$

is the usual Fokker–Planck operator. The probability distribution of the housekeeping heat

$$P(q, t) = \int dx \rho(x, q, t) \quad (24)$$

can then be calculated simply by integrating over  $x$ . Since we start in a steady state, the initial condition needed to solve equation (22) is  $\rho(x, q, 0) = p_s(x, \alpha_0) \delta(q)$ .

## Proof of the fluctuation theorem 2

In the time derivative

$$\partial_t \langle \exp[-\beta Q_{\text{hk}}] \rangle = \int dx dq e^{-\beta q} \partial_t \rho(x, q, t), \quad (25)$$

we insert the equation of motion (22) and get rid of the partial derivatives with respect to  $q$  by integration by parts with vanishing boundary terms. We then have

$$\partial_t \langle \exp[-\beta Q_{\text{hk}}] \rangle = \int dx dq e^{-\beta q} \rho(x, q, t) [-v_s^2 + v_s^2] / D = 0. \quad (26)$$

Therefore, the average over trajectories of length  $t$  becomes

$$\langle \exp[-\beta Q_{\text{hk}}] \rangle_t = \langle \exp[-\beta Q_{\text{hk}}] \rangle_0 = 1, \quad (27)$$

since for  $t = 0$  we start with  $Q_{\text{hk}} = 0$ . This proof of the fluctuation theorem 2 for any time-dependence  $\alpha(\tau)$  is the central result of this letter.

## Mean and variance

In order to obtain an explicit expression for the mean of  $Q_{\text{hk}}$ , we integrate equation (22) with  $\int dx dq q$  and obtain after integration by parts with respect to  $q$

$$\partial_t \langle Q_{\text{hk}} \rangle = \gamma \int dx v_s^2(x, \alpha) p(x, t) = \gamma \langle v_s^2(\alpha) \rangle \geq 0 \quad (28)$$

and hence

$$\langle Q_{\text{hk}} \rangle = \gamma \int_0^t d\tau \langle v_s^2(\alpha(\tau)) \rangle \geq 0. \quad (29)$$

In general, the average over  $v_s^2$  has to be taken using the time-dependent probability  $p(x, t)$  of the position  $x$ . However, in a steady state we have  $p(x, t) = p_s(x, \alpha)$  and the mean becomes

$$\langle Q_{\text{hk}} \rangle = \gamma \langle v_s^2 \rangle t = \gamma \left[ j_s^2 \int dx p_s^{-1} \right] t, \quad (30)$$

leading to a constant mean dissipation rate.

Applying the same scheme to the second moment leads to a variance

$$\sigma^2 = 2\gamma \int_0^t d\tau \langle v_s^2(\alpha(\tau)) Q_{\text{hk}}(\tau) \rangle + (2/\beta) \langle Q_{\text{hk}} \rangle - \langle Q_{\text{hk}} \rangle^2. \quad (31)$$

The variance thus involves weighting the housekeeping heat with the square velocity  $v_s^2$  in the first term. This recursive scheme can be continued to obtain any moment or cumulant as a function of all previous moments or cumulants and the weight function  $v_s^2$ .

## Limiting cases

In the limiting case  $V' \ll f$  which corresponds to the situation where  $f$  is large such that the particle hardly 'feels' the underlying potential, we can solve equation (22) exactly. Then the stationary distribution becomes uniform and  $v_s(\tau) \approx f(\tau)/\gamma$ . By integrating over  $x$  in equation (22), we get for the probability distribution  $P(q, t)$  the evolution equation

$$\partial_t P = -\gamma^{-1} f^2 \partial_q P + D f^2 \partial_q^2 P. \quad (32)$$

This is a diffusion-like equation and its solution is a Gaussian with mean

$$\langle Q_{\text{hk}} \rangle = \gamma^{-1} \int_0^t d\tau f^2(\tau) \quad (33)$$

and variance  $\sigma^2 = (2/\beta)\langle Q_{\text{hk}} \rangle$ , which obviously obeys the integral constraint implied by the fluctuation theorem 2.

In the opposite case  $V' \gg f$  for  $\dot{\alpha} = 0$  the local mean velocity  $v_s$  is small, which we make explicit by  $v_s \rightarrow \varepsilon \bar{v}_s$ . Now a time scale separation using  $\varepsilon$  as a small parameter becomes possible. The fast time variable is simply  $t$  whereas the slow time variable  $s \equiv \varepsilon t$  is given by the ‘hopping time’, i.e., the mean time the particle needs to complete one period. Switching to the slow time scale  $\rho(x, q, s)$ , equation (22) becomes

$$\partial_s \rho = \left[ \varepsilon^{-1} \mathcal{L} + \left( 2\partial_x \bar{v}_s - \varepsilon \frac{\bar{v}_s^2}{D} \right) \frac{\partial_q}{\beta} + \varepsilon \frac{\bar{v}_s^2}{D} \frac{\partial_q^2}{\beta^2} \right] \rho. \quad (34)$$

In order to eliminate  $x$  for small  $\varepsilon$ , we apply exactly the same scheme developed above for elimination of the momentum  $p$  for large friction  $\gamma$ . Again dividing the distribution  $\rho$  into a part parallel to the stationary distribution  $\rho_0(x, q, s) = P(q, s)p_s(x)$  and into a part  $\rho_1$  perpendicular, we see that  $\rho_1$  is of order  $\varepsilon^2$ . If we take into account only terms of order  $\varepsilon$  and restore the original variables, we get the evolution equation

$$\partial_t P = -\gamma \langle v_s^2 \rangle \partial_q P + (\gamma/\beta) \langle v_s^2 \rangle \partial_q^2 P. \quad (35)$$

Its solution again is a Gaussian with mean (30) and variance  $\sigma^2 = (2/\beta)\langle Q_{\text{hk}} \rangle$ .

### Relation to other fluctuation theorems

Finally, we discuss the connection between the new integral fluctuation theorem 2 and the Hatano–Sasa relation (1) as well as the Jarzynski-like relation (3). For a transition along  $\alpha(\tau)$ , the latter two involve the dimensionless functional

$$Y[x(\tau); \alpha(\tau)] \equiv \int_0^t d\tau \dot{\alpha}(\tau) \frac{\partial \phi}{\partial \alpha}(x(\tau), \alpha(\tau)), \quad (36)$$

for which Hatano and Sasa show  $\langle \exp[-Y] \rangle = 1$  [2]. With the boundary term

$$\Delta \phi \equiv \phi(x(t), \alpha_t) - \phi(x(0), \alpha_0) \quad (37)$$

and  $Y = \beta Q_{\text{ex}} + \Delta \phi$  this leads to relation (1).

Relation (3) follows by applying the same reasoning used for deriving the original Jarzynski relation [6–8] to the present case of broken detailed balance. The ratio of the probability of the trajectory  $x(\tau)$  to the probability of the time-reversed trajectory  $\tilde{x}(\tau) \equiv x(t - \tau)$  under the time-reversed protocol  $\tilde{\alpha}(\tau) \equiv \alpha(t - \tau)$  is given by

$$R[x(\tau); \alpha(\tau)] \equiv \ln \frac{\text{prob}[x(\tau); \alpha(\tau)] p_s(x(0), \alpha_0)}{\text{prob}[\tilde{x}(\tau); \tilde{\alpha}(\tau)] p_s(\tilde{x}(0), \tilde{\alpha}_0)} = \beta Q_{\text{tot}} + \Delta \phi. \quad (38)$$

Here,  $\text{prob}[x(\tau); \alpha(\tau)]$  is the probability of a single trajectory  $x(\tau)$  under the protocol  $\alpha(\tau)$  starting in microstate  $x(0)$ . It is easy to show  $\langle \exp[-R] \rangle = 1$  and hence relation (3) follows.

Isothermal nonequilibrium processes are therefore characterized by the two trajectory-dependent functionals  $Y$  and  $Q_{\text{hk}}$ , and a boundary term  $\Delta \phi$ . Both functionals and their sum

$$R = Y + \beta Q_{\text{hk}} = \beta Q_{\text{tot}} + \Delta \phi \quad (39)$$

obey an integral fluctuation theorem as summarized in table 1. However, there are two special cases in which two of the three become identical and the third one trivial. First,

**Table 1.** A classification of isothermal nonequilibrium processes and the corresponding integral fluctuation theorems 1–3. Here,  $Y = \beta Q_{\text{ex}} + \Delta\phi$  and  $R = \beta Q_{\text{tot}} + \Delta\phi$ . The second column holds for transitions  $\alpha(\tau)$  where for fixed  $\alpha$  the system is in a detailed balanced state (DBS). The third column holds in nonequilibrium steady states (NESS) with broken detailed balance.

		DBS	NESS
General		$Q_{\text{hk}} = 0, R = Y = \beta W_{\text{dis}}$	$Y = 0, R = \beta Q_{\text{hk}}$
(1)	$\langle \exp[-Y] \rangle = 1$	$\langle \exp[-\beta W_{\text{dis}}] \rangle = 1$	$1 = 1$
(2)	$\langle \exp[-\beta Q_{\text{hk}}] \rangle = 1$	$1 = 1$	$\langle \exp[-\beta Q_{\text{hk}}] \rangle = 1$
(3)	$\langle \exp[-R] \rangle = 1$	$\langle \exp[-\beta W_{\text{dis}}] \rangle = 1$	$\langle \exp[-\beta Q_{\text{hk}}] \rangle = 1$

if for any fixed  $\alpha$  reached along the transition  $\alpha(\tau)$  the system obeys detailed balance we have  $Q_{\text{hk}} = 0$ . The stationary distribution then is simply the Boltzmann distribution with  $\phi(x, \alpha) = \beta[H(x, \alpha) - F(\alpha)]$ , where  $H(x, \alpha)$  is the Hamiltonian of the system and  $F(\alpha)$  is the free energy. Inserting this  $\phi$  into equation (36), we find that  $Y$  is the dissipated work

$$R = Y = \beta[W - \Delta F] \equiv \beta W_{\text{dis}} \quad (40)$$

and the relations (1) and (3) become the Jarzynski relation [6]. Second, in a nonequilibrium steady state with  $\dot{\alpha} = 0$  we have  $Y = 0$  and  $R = \beta Q_{\text{hk}}$ , and the relations (2) and (3) become identical. In such a steady state,  $R = \beta Q_{\text{hk}}$  can also be interpreted as total entropy production, which then obeys a detailed fluctuation theorem  $P(-R)/P(R) = e^{-R}$  even for finite times [13].

## Summary

We have derived and discussed a new integral fluctuation theorem 2 for the housekeeping heat valid under arbitrary time-dependent driving. Even though we focused on one-dimensional motion, it is obvious how to generalize our approach to coupled Langevin equations describing interacting systems. It would be interesting to test experimentally all three integral fluctuation theorems and to measure the corresponding probability distributions, in particular, in nonharmonic time-dependent potentials, where *a priori* one does not expect Gaussian distributions.

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