Heat leakage in overdamped harmonic systems

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We investigate the occurrence of heat leakages in overdamped Brownian harmonic systems. We exactly compute the underdamped and overdamped stochastic heats exchanged with the bath for a sudden frequency or temperature switch. We show that the underdamped heat reduces to the corresponding overdamped expression in the limit of large friction for the isothermal process. However, we establish that this is not the case for the isochoric transformation. We microscopically derive the additionally generated heat leakage and relate its origin to the initial relaxation of the velocity of the system. Our results highlight the limitations of the overdamped approximation for the evaluation of the stochastic heat in systems with changing bath temperature.

I. INTRODUCTION

Stochastic thermodynamics offers a general framework for the study of the thermodynamic properties of small systems whose dynamics is dominated by thermal fluctuations [1, 2]. It successfully extends the concepts of macroscopic thermodynamics, such as work, heat, energy and entropy, to the level of single random trajectories [3, 4]. This framework has been widely used in theoretical and experimental investigations [11–14]. An important application of stochastic thermodynamics is the analysis of Brownian heat engines that cyclically transform heat into mechanical work. Two broad classes of stochastic heat engines are usually distinguished: i) motors with a static confining potential in the overdamped limit. However, an asymptotic analysis of the Klein-Kramers equation for the evolution is described by the Langevin equation [21],

\[ \dot{v} = -\gamma v - \omega^2 x + \sqrt{\frac{2\gamma kT}{m}} F(t), \quad \dot{x} = v, \]  

(1)

where \( F(t) \) is a centered Gaussian white noise obeying \( \langle F(t)F(t') \rangle = \delta(t-t') \), \( k \) the Boltzmann constant, \( T \) the temperature of the bath and \( \gamma \) the friction coefficient. Because of the linearity of Eq. (1), the dynamics may be equivalently described in terms of the position and velocity variances, \( \sigma_x = \langle x^2 \rangle \) and \( \sigma_v = \langle v^2 \rangle \), leading to,

\[ \dot{\sigma}_v = -2\gamma \sigma_v - \omega^2 \sigma_x + \frac{2\gamma kT}{m}, \]  

(2)

\[ \dot{\sigma}_x = 2\sigma_v - \gamma \sigma_x - 2\omega^2 \sigma_x. \]  

(3)

In the overdamped limit, \( \dot{\sigma}_v = 0 \), the above equations decouple and the Langevin equation reduces to,

\[ \dot{\sigma}_x = -2\frac{\omega^2}{\gamma} \sigma_x + \frac{2kT}{\gamma m}. \]  

(4)

The solutions of the above equations for constant frequency and temperature are given in the appendix.

The stochastic heat along an individual trajectory is respectively defined for small and large friction as [11–12],

\[ Q_u = \int_0^t dt' \langle [m\dot{v}v(t') + \partial_x V(x,t')]v(t') \rangle, \]  

(5)

\[ Q_o = \int_0^t dt' \langle \partial_x V(x,t')v(t') \rangle. \]  

(6)

II. HEAT FOR A HARMONIC PARTICLE

We consider a Brownian particle with position \( x \), velocity \( v \) and mass \( m \) confined in the harmonic potential \( V(x) = m\omega^2 x^2/2 \) with frequency \( \omega \). Its underdamped evolution is described by the Langevin equation [21],

\[ \dot{v} = -\gamma v - \omega^2 x + \sqrt{\frac{2\gamma kT}{m}} F(t), \quad \dot{x} = v, \]  

(1)

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(6)
The underdamped expression (5) contains a kinetic term that accounts for the relaxation of the velocity degree of freedom. In the limit of strong friction, this thermalization is almost instantaneous and the velocity is assumed to always have its stationary value. However, this does not necessarily imply that there is no heat flow associated with the velocity relaxation (17). In the harmonic case, the stochastic heats (5) and (6) can be directly expressed in terms of the position and velocity variances $\sigma_x$ and $\sigma_v$,

$$Q_u = \gamma kT t - \gamma m \int_0^t dt' \sigma_v,$$
$$Q_o = \frac{m}{2} \omega^2 \int_0^t dt' \dot{\sigma}_x. \quad (7)$$

These two equations form the basis of our study of heat leakages in stochastic harmonic systems.

### III. Isothermal Process

We begin by investigating isothermal processes during which the frequency of the potential is varied at constant temperature. We assume that the oscillator is initially at thermal equilibrium at $t = 0$ with frequency $\omega_0$. The corresponding initial conditions for the variances are $\sigma_{v0} = kT/m$, $\sigma_{x0} = kT/m\omega_0^2$ and $\sigma_{x0} = 0$ due to the equipartition theorem. We drive the system by instantaneously changing its frequency to $\omega_1$ at time $t = t_0$,

$$\omega(t) = \omega_0 + (\omega_1 - \omega_0) \Theta(t - t_0), \quad (9)$$

where $\Theta(t)$ denotes the Heavyside function.

The corresponding underdamped position and velocity variances can be obtained from Eq. (11). Introducing

$$\omega' = \sqrt{4\omega_1^2 - \gamma^2}$$

and $
\tau = t - t_0$, we find,

$$\sigma_x = \begin{cases} \frac{kT}{m\omega_0^2} & 0 \leq t < t_0 \\ \frac{kT}{m\omega_1^2} \left[ 1 + \left( \frac{\omega_1^2 - \omega_0^2}{\omega_0^2} \right) \frac{e^{-\gamma\tau}}{\omega_1^2} \left( 2\omega_1^2 - \gamma^2 \cos(\omega'\tau) + \gamma \omega' \sin(\omega'\tau) \right) \right] & t \leq t \\ \frac{kT}{m} \left( 1 + \frac{2\omega_1^2}{\omega_0^2} \left( \frac{\omega_1^2}{\omega_0^2} - 1 \right) e^{-\gamma\tau} \sin(\omega'\tau) \right) & t_0 \leq t. \end{cases} \quad (10)$$

$$\sigma_v = \begin{cases} \frac{kT}{m} & 0 \leq t < t_0 \\ \frac{kT}{m} \left( 1 + \frac{2\omega_1^2}{\omega_0^2} \left( \frac{\omega_1^2}{\omega_0^2} - 1 \right) e^{-\gamma\tau} \sin(\omega'\tau) \right) & t \leq t \end{cases} \quad (11)$$

The time dependence of the variances $\sigma_x$ and $\sigma_v$ is shown in Fig. 1 for increasing values of the friction coefficient $\gamma$. We observe a qualitatively different behavior in the underdamped and overdamped regimes. For small friction, the position and velocity variances settle to their respective equilibrium values, $\sigma_{x1} = kT/m\omega_1^2$ and $\sigma_{v1} = kT/m$, in a slow oscillatory fashion. We note that these oscillations are out of phase, revealing the continuous conversion of kinetic to potential energy and vice versa. By contrast, for strong friction, the position variance reaches its new equilibrium value exponentially fast, while the velocity variance remains quasi constant at its initial value. We additionally emphasize that the relaxation time first decreases with increasing $\gamma$, before it starts increasing for higher values of the friction coefficient.

We next compute the underdamped heat (7) using the variance (10) and the overdamped heat (8) using
The last point may be confirmed analytically by Taylor expanding Q_u using \( \omega' = i\gamma \sqrt{1 - \alpha} \approx i\gamma (1 - \alpha/2) \) with \( \alpha = 4\omega^2/\gamma^2 \ll 1 \). For an isothermal process, we may thus take the large friction limit either before or after evaluating the heat.

**IV. ISOCHORIC PROCESS**

Let us now turn to the isochoric process where the temperature is modified at constant frequency. We assume that the oscillator is initially at thermal equilibrium at temperature \( T_0 \) and frequency \( \omega \). The corresponding initial conditions for the variances are accordingly \( \sigma_{v0} = kT_0/m \), \( \sigma_{x0} = kT_0/m\omega^2 \) and \( \dot{\sigma}_{x0} = 0 \). We thermally drive the system by instantaneously switching the temperature to the value \( T_1 \) at \( t = t_0 \).

\[
T(t) = T_0 + (T_1 - T_0) \Theta(t - t_0).
\]

The undamped position and velocity variances may be calculated as in the previous section. We obtain with \( \omega' = \sqrt{4\omega^2 - \gamma^2} \),

\[
\sigma_x = \begin{cases} 
0, & 0 \leq t < t_0 \\
\frac{kT_0}{m\omega^2}, & t \geq t_0 \\
\frac{kT_1}{m} \left(1 + \frac{T_0}{T_1} - 1\right) e^{-\gamma\tau} \frac{4\omega^2 - \gamma^2}{\omega^2 - \gamma^2} \left[\gamma^2 \cos(\omega'\tau) + \gamma \omega' \sin(\omega'\tau)\right], & t_0 \leq t < t_0 \\
\frac{kT_1}{m} \left(1 + \frac{T_0}{T_1} - 1\right) e^{-\gamma\tau} \frac{4\omega^2 - \gamma^2}{\omega^2 - \gamma^2} \left[\gamma^2 \cos(\omega'\tau) - \gamma \omega' \sin(\omega'\tau)\right], & t_0 \leq t.
\end{cases}
\]

Equations (15) and (16) are shown in Fig. 3 as a function of time for increasing friction. The position variance \( \sigma_x \) reaches its new equilibrium value, \( \sigma_{x1} = kT_1/m\omega^2 \), exponentially with a decay time that first decreases before it increases with larger \( \gamma \). On the other hand, the velocity variance \( \sigma_v \) exhibits two different behaviors; for small friction, it slowly equilibrates to \( \sigma_{v1} = kT_1/m \), whereas it jumps almost instantaneously to that value for high friction. The assumption that the velocity variance is quasi constant in the overdamped limit is therefore verified for both isothermal and isochoric processes. However, in the latter case, it displays an initial sudden jump induced by the temperature variation, which is neglected in the overdamped approximation. This initial jump may be physically understood by noting that the system adjusts instantly to the heat bath in the overdamped limit, while it adjusts immediately to changes of the external potential in the opposite underdamped limit.

We may next compute the undamped and overdamped heats in analogy to the previous section and get,

\[
Q_u = \begin{cases} 
0, & 0 \leq t < t_0 \\
\frac{k(T_1 - T_0)}{2} \left[1 - \frac{4\omega^2 - \gamma^2}{\omega^2 - \gamma^2} \times e^{-\gamma\tau} \cos(\omega'\tau)\right], & t_0 \leq t \\
0, & 0 \leq t < t_0 \\
\frac{k(T_1 - T_0)}{2} \left(1 - e^{-\frac{4\omega^2 - \gamma^2}{\gamma^2} \tau}\right), & t_0 \leq t.
\end{cases}
\]

The two heat expressions are represented in Fig. 4 as a function of time for increasing friction. We first notice that the undamped and overdamped heats differ by exactly a factor two in the long-time limit, \( Q_u \to 2Q_o \), although the work done on the system is identically zero in both situations. The equipartition theorem provides an explanation for this discrepancy. In the overdamped regime, there is only one relevant degree of freedom (the velocity being frozen). As a result, the total
energies of the oscillator before and after the temperature switch are respectively $kT_0/2$ and $kT_1/2$. Since no work is done on the system, the total energy change is $\Delta E = k(T_1 - T_0)/2 = Q_o(t \to \infty)$. The same argument applies to the underdamped regime with now two relevant degrees of freedom (position and velocity). Consequently, $\Delta E = k(T_1 - T_0) = Q_o(t \to \infty)$.

The quick relaxation of $\sigma_v$ immediately after $t_0$ thus causes a large heat flux during this short period of time, leading to the sudden jump of $Q_o$ in Fig. 4. The ensuing heat flux is mostly induced by the much slower relaxation of $\sigma_x$, when $\sigma_o$ is mostly constant. A lowest-order Taylor expansion of Eq. (17) for $\gamma \gg \omega$ further yields,

$$Q_u \simeq Q_o + \frac{k(T_1 - T_0)}{2}. \tag{20}$$

The second term in Eq. (20) is the heat leakage associated with the initial relaxation of the velocity. Its origin may be traced to the inertial term $m\ddot{x}$ in the Langevin equation (1). This term is neglected in the overdamped approximation. However, the heat leakage remains finite even for arbitrarily strong friction. This again follows from the fact that the oscillator reacts instantaneously to temperature changes in the overdamped regime.

**V. SUMMARY**

We have investigated the occurrence of heat leakages in harmonic systems which are known to significantly reduce the efficiency of Brownian heat engines. Due to the conceptual simplicity of these systems, we were able to analyze the physical origin of these heat leakages in detail and to compute their exact expression for a sudden temperature switch in an isochoric process. Our results emphasize the fact that the overdamped limit can be taken before or after calculating the stochastic heat for the case of a constant temperature. However, this is no longer true when the temperature changes in time, as the initial fast velocity relaxation will induce heat leakages which are not captured by the overdamped approximation. These findings complement those obtained for a spatial temperature variation in Ref. [17]. In these situations, heat should be evaluated before taking the overdamped limit.
Appendix A: Solutions for the variances

We here provide for convenience the solutions of the equations (2)-(4) for the position and velocity variances for constant frequency and temperature. The under-damped equations (2) and (3) may be solved with the help of the Laplace transformation\cite{23}. We obtain,

\[ \sigma_v = \frac{kT}{m} + D_1 e^{-\gamma t} + D_2 e^{(-\gamma + \omega^*) t} + D_3 e^{(-\gamma - \omega^*) t}, \]

\[ \sigma_x = \frac{kT}{m\omega^2} + \frac{1}{\omega^2} e^{-\gamma t} \left[ D_1 + \frac{\gamma + \omega^*}{4\omega^2} D_2 e^{\omega^* t} + \frac{(\gamma - \omega^*)^2}{4\omega^2} D_3 e^{-\omega^* t}\right], \]

(A1) where we have defined the following quantities,

\[ \omega^* = \sqrt{\gamma^2 - 4\omega^2} = i\omega, \]

\[ D_1 = \frac{\omega^2}{\omega^*} \left( 4 \frac{kT}{m} - 2\sigma_{x0} - 2\omega^2\sigma_{x0} - \gamma\sigma_{x0} \right), \]

\[ D_2 = -\frac{1}{2\omega^*} \left( \frac{2kT}{m} \left( \gamma - \omega^* \right) + \left( 2\omega^2 - \gamma^2 + \gamma\omega^* \right) \sigma_{x0} \right) - 2\omega^4\sigma_{x0} + \omega^2 \left( -\gamma + \omega^* \right) \sigma_{x0}, \]

\[ D_3 = \frac{1}{2\omega^*} \left( -\gamma + \omega^* \right) + \left( 2\omega^2 - \gamma^2 + \gamma\omega^* \right) \sigma_{x0} + 2\omega^4\sigma_{x0} + \omega^2 \left( \gamma + \omega^* \right) \sigma_{x0}, \]

(A2)

and the initial values \( \sigma_{v0}, \sigma_{x0} \) and \( \sigma_{x0} \). On the other hand, the solution of the overdamped equation (4) is given by,

\[ \sigma_x = \frac{kT}{m\omega^2} - \left( \frac{kT}{m\omega^2} - \sigma_{x0} \right) e^{-2\omega^* t} \]

(A3) with the initial condition \( \sigma_{x0} \).

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