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A large deviation analysis on the near-equivalence between external and internal reservoirs

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HIGHLIGHTS

- Mapping external into internal reservoirs can yield equivalent entropy production.
- Only heat fluctuation can distinguish an external from an internal reservoir.
- The best approximation to coloured reservoirs is its white-noise analogue.

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ABSTRACT

Within the spirit of van Kampen's "Langevin approach", we discuss the limits of validity of rephrasing the non-equilibrium problem of a particle subject to an external (work) reservoir – a system where the fluctuation–dissipation relation is not verified – into the simpler case with an internal (heat) reservoir for which the fluctuations and the dissipation arise from the same source. Using a convenient mapping of the thermomechanical parameters we show that, counter-intuitively, such approach is not only valid for steady state time independent quantities, but also for time dependent thermostatistical quantities, namely the injected and dissipated fluxes. We connect this result with the problem of large deviations and conclude that, in this context, we can only distinguish reservoirs by analysing the "fluctuations of accumulated fluctuations". As a by-product, we learn that the best reference approximation to the large deviation functions of a non-Markovian external reservoir system is not the respective internal reservoir limit – as often assumed and suggested by the Langevin approach – but its internal reservoir analogue system obtained from the mapping of the original thermomechanical parameters.

1. Introduction

One of the most typical ways of tackling a problem in Physics – and get the solution thereto – is to cast the respective model in a simpler way by redefining the variables/parameters or introducing a phenomenological approach which preserves the backbone of the problem. Concerning the latter, the use of models inspired in the Langevin Equation (LE) is one of the most employed methods [1,2]; it has a widespread field of applications and has played a relevant role in surveys over the thermostatistical properties of systems far from the thermodynamic limit [3]. Perhaps, the most striking feature of the LE is that in problems of non-equilibrium statistical mechanics, it permits the direct (statistical) characterisation of the position, $x = x(t)$, and velocity, $v = v(t) \equiv \mathrm{d}x/\mathrm{d}t$, as well as probing the relation between the fluctuation and dissipation in

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the system, which is the upshot of the fluctuation–dissipation theorem [4]. The way the two physical effects are connected (or not) dictates the nature of the reservoir. According to [1], a reservoir is:

- *internal* (IntRes) if it allows establishing the dissipation as a property of the reservoir, the fluctuation–dissipation relation is verified and the corresponding theorem as well;
- *external* (ExtRes) if the effects of dissipation and fluctuation that are taking place have different origins and thus the fluctuation–dissipation relation is not verified.

The quintessential IntRes corresponds to the diffusion problem of Brownian motion as treated by Einstein, where the water acts as the reservoir. The random impacts of the water molecules in the pollen grain are the cause of both the dissipation and the fluctuations. Furthermore, since a pollen grain is weightier than water molecules,[2] the noise correlation function falls off very rapidly (typically 10^{-8} s) and thus the noise, η, that is responsible for the fluctuation is nicely reproduced by a white noise,

$$\langle \eta\,(t_2)\,\eta\,(t_1)\rangle_c = 2\,\gamma\,T\,\delta\,(t_2 - t_1)\,, \tag{1}$$

where γ is the dissipation coefficient and T is the temperature of the bath (throughout this paper $k_B = 1$). For a significantly dense medium, η is Gaussian as well. Thence, if we consider a system composed of a particle with mass, m, that is subject to a confining potential, $V = V(x)$, we get a dynamics is ruled by,

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\gamma\,\frac{\mathrm{d}x}{\mathrm{d}t} - \frac{\mathrm{d}V}{\mathrm{d}x} + \eta\,(t)\,. \tag{2}$$

Later, Mori and Kubo [5] surveyed the problem of a reservoir the particles of which have got a mass of the same order of magnitude of the focal particle. In that case, the fluctuations cannot be white noise, but they have the same source as dissipation still. In order to square such type problem within the IntRes scenario, Eq. (2) was generalised to,

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\int_{t_0}^{t} \kappa\left(t - t'\right)\left(\frac{\mathrm{d}x}{\mathrm{d}t'}\right)\mathrm{d}t' - \frac{\mathrm{d}V}{\mathrm{d}x} + \xi\,(t)\,. \tag{3}$$

For this non-Markovian problem, the fluctuations – which although Gaussian are now represented by $\xi(t)$ – and the dissipation are defined by,

$$\langle \xi\,(t_2)\,\xi\,(t_1)\rangle_c = \frac{\gamma}{\tau}T\exp\left[-\frac{|t_1 - t_2|}{\tau}\right], \qquad \kappa\,(t_1 - t_2) = \frac{\gamma}{\tau_\kappa}\exp\left[-\frac{|t_1 - t_2|}{\tau_\kappa}\right], \tag{4}$$

with $\tau_\kappa = \tau$, which guarantees that both spectra scale equally. In the limit ($\tau \to 0$, $\tau_\kappa \to 0$), Eq. (4) reads,

$$\langle \xi\,(t_2)\;\xi\,(t_1)\rangle = 2\,\gamma\,T\,\delta\,(t_2 - t_1)\,, \qquad \int_{t_0}^{t} \kappa\left(t - t'\right)\left(\frac{\mathrm{d}x}{\mathrm{d}t'}\right)\mathrm{d}t' = \gamma\,\frac{\mathrm{d}x}{\mathrm{d}t} \tag{5}$$

and Eq. (2) matches with Eq. (3) [$\eta(t) \equiv \xi_{\tau\to 0}(t)$].

It is not hard to grasp that when $\tau \neq \tau_\kappa$, the source of the fluctuations has nothing to do with the origin of the dissipation, resulting in an ExtRes situation. The simplest ExtRes situation corresponds to $\tau \neq 0$ and $\tau_\kappa \to 0$,

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\gamma\,\frac{\mathrm{d}x}{\mathrm{d}t} - \frac{\mathrm{d}V}{\mathrm{d}x} + \xi\,(t)\,, \tag{6}$$

and Eq. (4) keeps on being valid for $\xi(t)$.

The definitive instance of a system described by Eq. (6) is a particle in a frictional medium subject to a coloured random force [6–8]. This can be set up, *e.g.*, by inserting a charged particle in liquid helium (above superfluid phase though) – or any other situation where thermal noise is negligible in comparison with the fluctuations due to the external source – and applying a coloured Gaussian electric field to it. Additionally, we can refer to experiments with dye lasers [9] and laser gyroscopes [10] where this type of reservoir emerges as well as models for biological processes such as neuronal dynamics [11].

The description of IntRes and ExtRes cases helps understand that the two types of reservoirs are often distinguishable by the way they affect the energy of the system: while the IntRes is always a heat reservoir, the ExtRes frequently corresponds to a work reservoir, *i.e.*, it changes the energy of the system by performing work on it.

Herein, an important point pertains to calling the quantity T (Eq. (4)) the temperature of the ExtRev system (6). Although its properness might be disputed within a cautious Thermodynamical parlance, we will use that terminology upholding our decision on the fact that T has energy units ($k_B = 1$) and provides us with a typical scale of the fluctuations of velocity and position induced by the ExtRes (*e.g.*, in the form of positive/negative work performed on the system). Such broad understanding of the concept of temperature has been recently employed in the statistics of vortices in superconductors whence an athermal formalism – absolutely analogous to standard Thermodynamics – was derived [12]. Moreover, alternative definitions of temperature concurring with equipartition and fluctuation–dissipation relations were introduced in the field of stochastic dynamics with non-Gaussian reservoirs as well [13].

[2] A typical pollen grain is 10^4 times as weighty as a molecule of water.