Heat has a kinetic term in overdamped stochastic thermodynamics

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In the derivation of the thermodynamics of overdamped systems, one ignores the kinetic term contribution, since the velocity is a slow variable to the forces. In this paper, we show that the kinetic term needs to be present in the calculation of the heat distribution in order to have a correct correspondence between the underdamped and overdamped cases, meaning that the velocity can not be fully ignored in the thermodynamics of these systems. We emphasize the result for two different systems, the harmonic potential, and the logarithm potential.

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I. INTRODUCTION

The attempt to understand and control heat has been pursued by humanity since before the dawn of modern civilization [1, 2]. Nowadays, we currently understand heat as a disordered form of energy that can be used as a source for thermal machines [3, 4]. With the development of new technologies, we can now manipulate small systems, on the order of nanometers, to the point of building such thermal machines on this scale [5, 6].

On the microscale, thermodynamics has a different character than in the macro-world. Namely, quantities like heat and work now become fluctuating quantities. A lot of attention was devoted to obtaining the probability distribution for these thermodynamic functionals, with experimental [7–10] and theoretical [11–17] calculations. This microscale thermodynamics is now a proper field of research, that is now called stochastic thermodynamics [18–20].

Most of the works in stochastic thermodynamics make use of overdamped models, where one can neglect the inertia of the particle due to the large dissipation from contact with a heat bath. When this is the case, the heat expression lacks the term of kinetic energy in its expression, as opposed to the underdamped case, where we always have this contribution [19]. For the latter, the velocity distribution is stationary, obeying a Boltzmann Gibbs distribution. One example is the distinction between the probability distributions when \( m = 0 \) is taken first, instead of taking \( m/\gamma \to 0 \) after the calculations [21].

However, in [22] it has been shown that for overdamped systems in an isochoric process, the kinetic term can not be ignored. They have shown that the average heat of the overdamped Brownian motion, when there is a temperature protocol, does not correspond to the underdamped case in the large friction limit. At the same time, if no temperature protocol is present the correspondence between the averages is satisfied. The problem is to take the limit in the system dynamics before the calculation of its thermodynamics. While we can ignore the velocity in the dynamics, in the thermodynamics the kinetic term needs to be present.

Another result that breaks the correspondence between underdamped and overdamped systems was obtained by the authors in [23]. We have showed that the heat distribution of the free particle in the underdamped case,

\[
P_u(Q) = \frac{\sqrt{\coth \left( \frac{2\pi}{m} \right)} + 1}{\pi \sqrt{2T}} \text{K}_0 \left(\frac{|Q|\sqrt{\coth \left( \frac{2\pi}{m} \right)} + 1}{\sqrt{2T}}\right),
\]

(1)
does not correspond to the heat distribution of the free particle in the overdamped case

\[
P_o(Q) = \delta(Q),
\]

(2)
in the limit of large friction, where \( \gamma >> m \). The absence of the correspondence manifest the necessity of considering the kinetic term.

In this paper, we show that by considering the kinetic term, the correspondence is satisfied between the heat

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distributions. Different from the conclusions in [22] our result shows that even in an isothermal process, there is the necessity to consider the kinetic term in order to obtain the correct heat distribution of an overdamped system.

The aim of this paper is to show that the presence of the kinetic term is necessary concerning the thermodynamics of overdamped systems, due to the necessity of a correspondence between the heat distribution of an underdamped system and the corresponding overdamped one. We exemplify by calculating explicitly the heat distribution for the free particle case considering the kinetic term. The obtained distribution satisfies the correspondence, therefore is the correct one. Moreover, we also show the necessary modification in the heat distribution for harmonic and logarithm potentials. Both cases serves as illustrations of the changes caused by considering the kinetic term.

In section II, we study the free-particle case. In section III and IV, the heat distribution for the harmonic and logarithmic cases are obtained respectively. In section V, we present our conclusions and discussions.

II. FREE PARTICLE

A free Brownian particle in contact with a heat bath in the overdamped regime obeys the Langevin equation (always assuming \( k_B = 1 \))

\[
\gamma \dot{x}(t) = \eta(t),
\]

(3)

where \( \gamma \) is the friction coefficient, and \( \eta(t) \) is a white noise process, with zero mean and correlation \( \langle \eta(t)\eta(t') \rangle = 2\gamma T \delta(t - t') \), where \( T \) is the temperature of the heat bath.

If one considers the definition of heat given by Sekimoto [19],

\[
Q[x] = \int_0^\tau (\gamma \dot{x} - \eta(t)) \, \dot{x} \, dt,
\]

(4)

which is the definition of the energy exchanged between the Brownian particle and the heat bath, one obtains that \( Q[x] = 0 \) in the free case. One can ask if this result is compatible with our physical intuition. To move, the particle has to receive or lose energy in some way. What \( Q[x] = 0 \) is saying is that there are no fluctuations in the energy exchanged between the particle and the heat bath. Using the definition in equation 4, the heat distribution of the free particle in the overdamped case has a simple formula given by a Dirac delta, as shown in equation 2 which is a deterministic probability (in a sense that there is no fluctuation). In addition, if one calculates the heat distribution of the free particle in the underdamped regime, one obtains equation 1 [23]. The problem is, equation 1 does not correspond to equation 2 in the large friction limit \( \gamma \gg m \). If we take this limit, we obtain

\[
P_o(Q) \xrightarrow{\gamma \gg m} \frac{1}{\pi T} \, K_0 \left( \frac{|Q|}{T} \right).
\]

(5)

What we find is that the solution of this problem is solved by considering the kinetic term in the heat of the overdamped system. For the free particle case, this means that the heat is now

\[
Q[x] = \frac{1}{2} m \left( v_f^2 - v_0^2 \right) = \Delta K,
\]

(6)

where \( v_f \) is the final velocity and \( v_0 \) the initial velocity. By calculating the distribution of this heat we can recover the correspondence. The calculation is easy since we assume that the velocities obey a stationary equilibrium distribution at all times. This means that the initial distribution and transitional distribution of the particle velocities are

\[
P(v_0)P[v_f, \tau|v_0, 0] = \frac{m}{2\pi T e^{-\frac{m}{2T}(v_f^2 + v_0^2)}} e^{-i\lambda \Delta K(v_f^2 - v_0^2)}
\]

(7)

Thus, if we calculate the heat distribution, we will have the characteristic function (see the appendix)

\[
Z(\lambda) = \int dv_0 \int dv_f \frac{m}{2\pi T} e^{-\frac{m}{2T}(v_f^2 + v_0^2)} e^{-i\lambda \Delta K(v_f^2 - v_0^2)} = \frac{1}{\sqrt{1 + \lambda^2 T^2}},
\]

(8)

that can be Fourier transformed to obtain the desired heat distribution

\[
P_o(Q) = \int d\lambda \frac{e^{i\lambda Q}}{2\pi \sqrt{1 + \lambda^2 T^2}} = \frac{1}{\pi T} \, K_0 \left( \frac{|Q|}{T} \right),
\]

(9)

which is the exact heat distribution that one obtains if one calculates the underdamped heat distribution and takes the large friction limit. Also, note that the heat distribution is stationary, due its independence in time.

As a result, to have a correspondence between the heat distributions of the two cases, one needs to take into account the kinetic energy term. Moreover, this means that the definition of heat given by Sekimoto equation 4 is probably not the complete version of the heat in stochastic thermodynamics. Nevertheless, a complete version could be achieved if one can always define the heat according to the first law using the complete energy of the system, i.e., the potential energy plus the kinetic energy. The natural recipe is: firstly defining the work, and then according to the first law using the complete energy of the system, define the heat. Although the distributions in equations 2 and 3 have a similar statistical behavior, both distribution have a singularity in \( Q = 0 \) and gives the same average for the heat \( \langle Q[x] \rangle = 0 \). Furthermore, in the overdamped limit in an isothermal process, where the velocities are in equilibrium, the average kinetic energy is always zero. Explaining why in [22] the average heat in an isothermal process has the correspondence between its overdamped and underdamped cases.
III. HARMONIC SYSTEM

The necessity to include the kinetic term, modifies some results already obtained in the literature. Here, we exemplify the modification using the harmonic potential case that was first calculated (without the kinetic contribution) in [11]. This system obeys the Langevin equation

$$\gamma \dot{x}(t) = kx(t) + \eta(t),$$

(10)

where $k$ is the stiffness of the harmonic potential. We start by noticing that by considering the kinetic term we only add more integrals in the calculation of the characteristic function. That is

$$Z(\lambda) = \int dv_0 \int dv \frac{m}{2\pi T} e^{-\frac{mv^2}{2T}} e^{-i\lambda \left( v_0^2 + v^2 \right)} z(\lambda),$$

(11)

where $z(\lambda)$ is the characteristic function that one obtains if we do not consider the kinetic term. For the harmonic case, this characteristic function is [11, 23]

$$z(\lambda) = \sqrt{\frac{\coth \left( \frac{k\tau}{\gamma} \right) + 1}{\coth \left( \frac{k\tau}{\gamma} \right) + 2\lambda^2 T^2 + 1}}.$$  

(12)

Integrating in the velocities, we obtain the correct characteristic function

$$Z(\lambda) = \frac{1}{\sqrt{1 + \lambda^2 T^2}} \sqrt{\frac{\coth \left( \frac{k\tau}{\gamma} \right) + 1}{\coth \left( \frac{k\tau}{\gamma} \right) + 2\lambda^2 T^2 + 1}},$$

(13)

that, unfortunately, does not allow us to obtain analytically the heat distribution $P(Q)$. Nevertheless, we can integrate it numerically, and the result is showed in figure 1 in comparison with the heat distribution obtained without the kinetic term correction. What we find is that the corrected heat distribution has larger fluctuation tails than the naive distribution. This occurs due to the equilibrium fluctuations of the velocities. Having a greater probability of occurring values of heat far from the mean, it can be exploited in the design of thermal machines [3], where one wants to use the fluctuations to improve the efficiency of these machines.

In the asymptotic time limit of the system, we can recover an analytical solution by noticing that

$$\lim_{\tau \to \infty} Z(\lambda) = \frac{1}{(\lambda^2 T^2 + 1)},$$

(14)

which gives an exponential distribution for the heat distribution

$$\lim_{\tau \to \infty} P_o(Q) = e^{-\frac{|Q|}{2T}}.$$  

(15)

FIG. 1: Heat distribution with and without the kinetic term. The red dashed line it is the case without the kinetic term, while the solid black line is the corrected heat distribution with the kinetic term. All the constants are set to one. We can see that the correct heat distribution allows more fluctuations for the heat due the velocities.

A different result is that the Bessel function obtained in [9], $P_{\text{imp}}(Q) \sim K_0(T^{-1}|Q|).$ Moreover, this asymptotic heat distribution is the same asymptotic distribution of the harmonic case in the underdamped regime [23]. Therefore, in the asymptotic limit, the heat distribution is the same for underdamped and overdamped systems in a harmonic potential.

IV. LOGARITHM SYSTEM

Here we show the modification of another interesting case of the heat distribution in the logarithm potential calculated without correction by one of the authors in [15]. The logarithm potential appears in different stochastic phenomena [24–30]. For the logarithm potential, the Langevin equation is (we take $\gamma = 1$ for simplicity)

$$\dot{x}(t) = \frac{k}{x(t)} + \eta(t),$$

(16)

where now $k$ is the strength of the logarithm potential and now $x(t)$ is defined only in the positive real axis [31], and now the initial distribution of the position is a Dirac delta [15]. Now we will explicitly show the modifications that one have to consider when calculate the heat distribution. This time, without using the characteristic function method, and choosing to illustrate another approach, where instead of the Fourier transform of the Dirac delta, we use its properties.

The heat is shifted with the kinetic correction, therefore we have

$$Q[x] = \Delta K + k \ln \frac{x_t}{x_0},$$

(17)
and thus the heat distribution is
\[ P(Q) = \left( \delta \left( Q - \Delta K - k \ln \frac{x_T}{x_0} \right) \right). \] (18)

If we define \( \bar{Q} = Q - \Delta K \), the calculation can be carried along the same lines in reference [15]. However we will still need to integrate the velocities. Hence, we arrive at the integrals
\[ P(Q) = \int dv_0dv_x \frac{m}{2\pi^2T} e^{-\frac{m}{2T}(v_x^2 + v_0^2)} P(Q - \Delta K), \] (19)
where \( P(Q) \) is the expression of the heat distribution obtained in [15] without the kinetic term. Again we cannot obtain an analytical result for the heat, but it can be solved by numerical integration. It is interesting to note that previous analytical results, when considering the correction of the kinetic term, not give anymore an analytical solution. This suggests that the heat distribution of overdamped systems is way more complex that we think.

\section{V. CONCLUSION}

By considering the kinetic terms, some theoretical works might need to be revisited. Mainly, the works on the fluctuations of the heat in the isothermal process [11,16] might need to be adjusted to include the kinetic term. Moreover, some results in harmonic thermal machines need to be reviewed to properly calculate the fluctuations of the efficiency of such machines. We have shown that the heat distribution with the kinetic term allows more fluctuations for the exchanged heat, a result that can be exploited in the development of thermal machines. Moreover, it ensues that by considering the kinetic term, the calculation of the heat distribution becomes more difficult. Previous analytical results, obtained without the kinetic term, are not possible now, as example here we have showed the harmonic and logarithm potentials.

It will be interesting to see whether there are cases where we can take the overdamped limit before the calculation of the thermodynamic properties. One case was already shown in [24], where the average heat is not affected by taking the overdamped limit before in an isothermal process.

Furthermore, in an active system, it is possible that we might have the same problems as those for an overdamped system and further investigation is necessary.

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\section{Appendix A: Calculating the characteristic function}

The definition of the heat distribution is
\[ P(Q) = \langle \delta(Q - Q[x]) \rangle, \] (A1)
where the average is over the fluctuating degrees of freedom of the system. Here the average is over \( v_0, v_T, x_0, x_T \). Therefore, if the heat depends only on the boundary degrees of freedom we have
\[ P(Q) = \int dv_0dv_xdx_0dx_TP(v_T, v_0, x_T, x_0)\delta(Q - Q[x]). \] (A2)

The joint distribution of the velocities and position can be decomposed as
\[ P(v_T, v_0, x_T, x_0) = P(v_T, v_0)P(x_T, x_0), \] (A3)
since the positions and velocities are independent random variables. And the joint distributions are given by
\[ P(v_T, v_0) = P[v_T, \tau|v_0, 0]P_0(v_0), \] (A4)
\[ P(x_T, x_0) = P[x_T, \tau|x_0, 0]P_0(x_0), \] (A5)
where \( P_0 \) is the initial probability distribution.

In our case, the velocities are assumed to be in an equilibrium stationary distribution at all times, this means that
\[ P[v_T, \tau|v_0, 0]P_0(v_0) = P(v_T)P_0(v_0). \] (A6)

Therefore, the calculation of the heat distribution reduces to
\[ P(Q) = \int dv_0dv_T P_0(v_T)P_0(v_0) \int dx_0dx_T P[x_T, \tau|x_0, 0]P_0(x_0)\delta(Q - Q[x]). \] (A7)

The Dirac delta can be rewritten in terms of its Fourier transform, giving
\[ P(Q) = \int \frac{d\lambda}{2\pi} e^{i\lambda Q} \int dv_0dv_T P_0(v_T)P_0(v_0) \int dx_0dx_T P[x_T, \tau|x_0, 0]P_0(x_0)e^{-i\lambda Q[x]}. \] (A8)

If \( Q[x] \) only depends on the velocity, the integrals in the position reduces to one,
\[ \int dx_0dx_T P[x_T, \tau|x_0, 0]P_0(x_0) = 1, \] (A9)
letting us with
\[ P(Q) = \int \frac{d\lambda}{2\pi} e^{i\lambda Q} \int d\nu_0 d\nu \tau P_0(\nu_\tau) P_0(\nu_0) e^{-i\lambda Q[\nu]}, \]
(A11)

one thus can recognize equation 8. Where the character-

isitifc function is
\[ Z(\lambda) = \int d\nu_0 d\nu \tau P_0(\nu_\tau) P_0(\nu_0) e^{-i\lambda Q[\nu]}. \]
(A12)