Work and heat distributions of an inertial Brownian particle

Pedro J. Colmenares *

Departamento de Química, Universidad de Los Andes, Mérida 5101, Venezuela

(Received 28 September 2021; revised 10 March 2022; accepted 18 March 2022; published 6 April 2022)

The work and heat distribution densities of a classical Brownian particle immersed in a heat bath and interacting with an external field have been extensively analyzed from different approaches. In this article, a previous method based on basic principles of stochastic dynamics is extended to derive these functions. The starting point is the inertial Langevin equation and the external field is an off-center harmonic potential driven by an external protocol. Unlike previous works where the driving is arbitrary, the so-called optimal protocol that minimizes the mechanical work is used instead. The corresponding work and heat distributions are derived through a procedure based on getting a generic Fokker-Planck equation indistinctly of the variable under consideration. The work distribution is calculated for different initial conditions and values of the friction coefficient of the thermal fluid ranging from the periodic or very low-underdamped mode up to the overdamped regime. It is a Gaussian as that of previous experiments of a particle trapped in an optical tweezers moved at constant velocity. Some aspects about the heat distribution is analyzed in terms of the statistical features of the non-Gaussian noise accompanying its dynamics to give an account of experimental results. It is concluded that the easiness in calculating the work distribution cannot be applied to heat. It requires numerical calculations.

DOI: 10.1103/PhysRevE.105.044109

I. INTRODUCTION

There have been important advances in the determination of the distributions of work (Wd) and heat (Qd) of a classical Brownian particle in a thermal bath and interacting with an external field. They are characterized by the different approaches used in the calculations. Chronologically, a brief review about the development of the different researches on this topic is as follows.

Back in 1999, Mazonka and Jarzynski [1] coupled the overdamped Langevin equation (LE) with a moving harmonic potential and an arbitrary driving force $\lambda(t)$ with the stochastic differential equations of the work W along a trajectory. The Fokker-Planck equation (FPE) associated to the combined pair $\{W, y\}$, where $y = q - \lambda(t)$, with q being the instantaneous position, was deducted from their two first moments by supposing that if at one instant in time the distribution happens to be Gaussian, then it will remain Gaussian for all subsequent times. The Wd was obtained as the marginal distribution of the combined Fokker-Planck density.

This was later confirmed in several works, namely by Speck and Seifert [2] using a projection operator method on the underdamped LE for low but finite driving, by van Zon and Cohen [3] for the two distributions with an approach based on Fourier analysis, and by Imparato and Peliti [4] through path. integrals. Additionally, the Gaussian character of this distribution was later obtained in the overdamped mode for a quadratic potential by Speck and Seifert [5] using the Jarzynski relation [6] and by Taganuchi and Cohen [7] for both distributions in the framework the inertial LE using the more rigorous path integral approach.

Experimental and excellent theoretical prediction on an inertial particle trapped in a laser tweezers moved at constant velocity were done by Imparato *et al.* [8]. They used the method of Ref. [1] for the work and heat distribution and found out that the latter has the form of a Schrödinger-like equation. The former is a Gaussian, while the heat distribution in the long-time limit and a static trap is logarithmic divergent at $Q = 0$ agreeing with van Zon and Cohen [3,9] while is a Gaussian for a finite trap velocity. The experimental Wd and Qd were obtained as histograms from their discrete defining equations in terms of the trajectories. It was found a perfect match with the theoretical prediction. Subsequently, Fogedby and Imparato [10] obtained exact results for the overdamped Qd in a double-well potential. Exact path-integral evaluation of Wd were carried out by Chatterjee *et al.* [11] in the overdamped regime with a harmonic potential finding an exponential distribution. They were unable to determine it for the moving potential. Finally, numerical results for the Wd of a harmonic oscillator with time-dependent strength was analyzed by Speck [12].

An experimental confirmation of the exponential Qd was done by Ciliberto [13] using the torsion pendulum as the experimental set up. Among the different results, he found that in a first approximation Qd is exponential and given by the convolution of the Gaussian Wd and the exponential density of the energy change, observation previously made by Van Zon and Cohen [9] where the latter far outweighs the Gaussian distributed Wd.

Very recently, Paraguassú *et al.* [14] worked out the inertial LE through the path-integral approach. Their distribution agrees with that of Ref. [7] and Ciliberto's [13] for

*Corresponding author: gochocol@gmail.com

the harmonic potential. Recently, Fogedby [15] accounts for the energy exponential density by a heuristic derivation of the previous result found in Ref. [10].

The aim of this research is to determine the heat and work distributions using basic textbook methods of stochastic dynamics [16–18]. To do this, the formalism developed in a previous work [19] and applied elsewhere [20–22] is extended to obtain a FPE associated to a classical Brownian particle immersed in a thermal bath and trapped in a moving harmonic potential. It is done for both probability density functions (pdf). The proposal differs mainly from those currently known, particularly that of Ref. [8] in two aspects. First, the optical trap is moved at an optimal offset velocity in order to minimize the mechanical work [22] and, second, the distributions are determined in terms of the initial parameters of the dynamics. The main result is a generic FPE given by Eq. (27) with time-dependent drift and diffusion terms depending on the variable under consideration. The solutions for the mechanical work is the Gaussian described by Eq. (36). It is solved for all the regimes defined by the coefficient of friction of the thermal fluid and several initial parameters. The heat distribution is formally derived although its solution can only be attainable by numerical methods. In spite of this circumstance, it is done a statistical analysis of the noise accompanying the heat stochastic differential equation to show the complexity of such a distribution.

The paper is structured so that the basic equations on which the distributions densities of work and heat are built is covered in Sec. II. In Sec. III is discussed the numerical results for the work distribution and it is provided an analysis about the outstandingl statistical characteristics of the heat distribution. The paper concludes in Sec. III with some final remarks.

II. BASIC FORMALISM

This section will show the main equations. First, the system is described and the solution of the equation of motion is succinctly shown due to it was deducted in a previous work [22]. Next, the derivation of the Fokker-Planck equations for the work and heat distributions are shown in detail in two separate sections.

A. Equation of motion

The dynamics for the position $q(t)$ of a Brownian particle of mass M submerged in a heat bath of quantum harmonic oscillators at a temperature T with friction damping γ and interacting with a conservative external field $V(q,t)=\omega_0^2[q-\lambda(t)]^2/2$ with stiffness ω_0^2, was analyzed in Ref. [22]. It is governed by the semiclassical inertial Ohmic Langevin equation

$$\ddot{q}(t) = -\gamma\,\dot{q}(t) - \omega_0^2\,(q(t)-\lambda(t)) + \frac{1}{M}\,\xi(t), \tag{1}$$

where the dot above a function denotes its time derivative, $\lambda(t)$ is an external driving or protocol and noise $\xi(t)$ is colored and Gaussian with zero mean and two-time correlation $<\xi(t)\xi(s)>$ given by [23]

$$\langle\xi(t)\,\xi(t')\rangle = -\left(\frac{\gamma M}{2\,\beta}\right)\nu\,\sinh^{-2}\left[\frac{1}{2}\nu(t-t')\right] + i\,\gamma\,M\,\hbar\,\dot{\delta}(t-t'), \tag{2}$$

where $\hbar$ is the Planck constant, $\beta=(k_B T)^{-1}$, k_B is the Boltzmann constant, and $\nu=2\pi(\hbar\,\beta)^{-1}$. Additionally, the quantum origin of this equation requires including an extra correlation between the noise and the initial position due to the initial preparation procedure of the system prior to the switching on the external protocol, i.e.,

$$\langle\xi(t)q_0\rangle = -\frac{2\,\gamma}{\beta}\sum_{n=1}^{\infty}\frac{\nu_n}{(\nu_n+\kappa_1)(\nu_n+\kappa_2)}e^{-\nu_n t}, \tag{3}$$

where frequencies $\kappa_{1,2}=[\gamma\pm(\gamma^2-4\,\omega_0^2/M)^{1/2}]/2$, $\nu_n = n\nu$, and $q_0=q(0)$ [23].

An important feature of this equation is its reduction to the ordinary classical Langevin equation in the continuum limit. There, the initial position-noise correlation is zero and the noise correlation reduces to the delta correlated $2\,\gamma\,T\,\delta(t-s)$ of classical systems. Thus, working on Eq. (1) and scaling time and length by the factors ω_0 and $(M\omega_0/\hbar)^{1/2}$, respectively, the semiclassical equation in the continuum limit reduces to the following dimensionless classical expression [22]

$$\ddot{q}(t) = -\gamma\,\dot{q}(t) - \,(q(t)-\lambda(t)) + \xi(t), \tag{4}$$

where the overdamped limit (strong friction) is obtained by setting to zero the acceleration term. It leads to

$$\dot{q}_{ov}(t) = \frac{1}{\gamma}\{-[q_{ov}(t)-\lambda(t)] + \xi(t)\}. \tag{5}$$

A direct numerical comparison of these two last equations is easier to achieve by writing them in the same timescale. Since that of the overdamped is $1/\gamma$, then the classical Langevin equation can be written as

$$\frac{1}{\gamma^2}\,\ddot{q}(t) = -\dot{q}(t) - (q(t)-\lambda(t)) + \xi(t), \tag{6}$$

where the high-friction limit follows as it is usually used in the literature [24].

Some remarks have to be settled about the correctness of the semiclassical equation. First, it is assumed a large bath so that the interaction coupling between the external field and the Hamiltonian of the reservoir is small. It can be justified by acknowledging the inverse proportionality of the coupling with the volume of the thermal bath [25], which in turn is proportional to the friction coefficient. Second, the interaction and bath Hamiltonians are independent of time and, finally, Kubo's second fluctuation-dissipation theorem is fullfilled. The latter is an approximation because the work by Daldrop, Kowalik, and Netz [26] showed that a molecular dynamics simulation of a harmonic Brownian particle shows a noise correlation depending on the strength of the field. Similarly, Olivares and Colmenares [20] and Lisý and Tóthová [27] also showed that the theorem shows a dependence on this field parameter. These results require reformulating the whole theory to include the effect of the field on the bath degrees of freedom and the Hamiltonian interaction. Despite these considerations and as it was referred before, the classical equation showed a great degree of prediction in its comparison with the experiments of Imparato *et al.* [8] of a overdamped particle in an optical trap. Furthermore, the review of the different theoretical approaches mentioned in the Introduction for a particle in the harmonic potential are based on Eq. (4) setting $\gamma = 1$ in order to recover its natural timescale.

The solution of the inertial Langevin equation is solved in detail in Ref. [22] and reads as:

$$q(t) = \overline{q}(t) + \varphi_q(t), \tag{7}$$

$$\overline{q}(t) = q_0\, \chi_q(t) + v_0\, \chi_v(t) + \gamma^2 \int_0^t dy\, \chi_v(t-y)\, \lambda(y), \tag{8}$$

$$v(t) = \overline{v}(t) + \varphi_v(s), \tag{9}$$

$$\overline{v}(t) = q_0\, \dot{\chi}_q(t) + v_0\, \dot{\chi}_v(t) + \gamma^2 \int_0^t dy\, \dot{\chi}_v(t-y)\, \lambda(y), \tag{10}$$

$$\varphi_q(t) = \gamma^2 \int_0^t dy\, \chi_v(t-y)\, \xi(y), \tag{11}$$

$$\varphi_v(t) = \gamma^2 \int_0^t dy\, \dot{\chi}_v(t-y)\, \xi(y), \tag{12}$$

$$\chi_q(t) = \mathrm{e}^{-\gamma^2 t/2}\Big[\cosh\Big(\frac{\omega\gamma t}{2}\Big) + \frac{\gamma}{\omega}\sinh\Big(\frac{\omega\gamma t}{2}\Big)\Big], \tag{13}$$

$$\chi_v(t) = \frac{2}{\omega\gamma}\mathrm{e}^{-\gamma^2 t/2}\sinh\Big(\frac{\omega\gamma t}{2}\Big), \tag{14}$$

where q_0 and v_0 are the initial position and velocity, respectively, and frequency $\omega = \sqrt{\gamma^2 - 4}$.

The chosen driving protocol is one that minimizes mechanical work. It was determined in a previous work [22] and given by:

$$\lambda(t) = \begin{cases} 0, & t \leqslant 0, \\ f(t), & 0 < t < t_f, \\ \lambda_f, & t \geqslant t_f, \end{cases} \tag{15}$$

where λ_f is the ad hoc final protocol value, t_f the final time application of the driving force, and $f(t) = A_1 + A_2\, t + A_3\, \delta(t) + A_4\, \dot{\delta}(t)$ with constants A_i's depending on $\{\gamma, q_0, \lambda_f, t_f\}$. A distinctive feature of this optimal protocol is its offset linear dependency on time with initial and final jumps in the velocity and acceleration of the particle. They are given by the Dirac delta function and its derivative, respectively. It differs from the nonoptimum experimental protocols where the optical trap is moved at constant velocity.

Since $\varphi_q(t)$ and $\varphi_v(t)$ are Gaussians, any of the two-time correlation functions appearing in the equations shown below are given by:

$$\langle \varphi_i(t)\, \varphi_j(s)\rangle = 2\, T\, \gamma^5 \int_0^{\mathrm{Min}\{t,s\}} dy\, f_i(t-y)\, f_j(s-y), \tag{16}$$

because the noises are delta correlated [18]. The notation $\{i, j\}$ refers to either q or v. Whenever i or j is q then $\{f_i, f_j\} = \chi_v$ and $\dot{\chi}_v$ for v. It emphasizes that the integral of the product of noises has been interpreted as a normal Riemann-Stieljes one.

B. Generic Fokker-Planck equation

The procedure to find the distribution of work and heat shown below is an adaptation of a general functional method derived primarily by Hänggi [28] to find master equations of properties driven by general colored noises. It is based on expanding the system characteristic functional in terms of its cumulants. It has been applied by many authors. A good review can be found in an article by Venturi *et al.* [29]. It should be mentioned that the extended article by Sancho *et al.* [30] for multiplicative noise and by Colmenares in the analysis in of ionic channels [19] inspired the objective of this article.

Without loss of generality let us define the following stochastic differential equation:

$$\dot{f}(t) = a(t) + \phi(t), \tag{17}$$

$$f(t) = \overline{f}(t) + \int_0^t ds\, \phi(s), \tag{18}$$

$$\overline{f}(t) = f_0 + \int_0^t ds\, a(s), \tag{19}$$

where $a(t) = \overline{\dot{f}}(t)$ is the average of $\dot{f}(t)$ over the distribution of the non-Gaussian noise $\phi(t)$ and $f_0 = f(0)$. The benefits of this definition will be important in the determination of the work and heat distribution functions as we will see in the next section.

For now, let $\rho(f, t)$ be the density distribution for a given realization of the general function $f(t)$ under the colored noise $\phi(t)$ which in turn is a functional of $\xi(t)$. According to Kubo [31], the flow of this distribution in f space is given by the stochastic Liouville equation

$$\frac{\partial \rho(f,t)}{\partial t} = -\sum_{j=1}^{n} \frac{\partial}{\partial f}\, \rho\,(f,t)\, \dot{f}(t). \tag{20}$$

Since for a fixed f, $\rho(f,t) = \delta[f(t) - f]$ is a formal solution, then, from the van Kampen lemma [16], the distribution of f is equivalent to take the average of $\delta[f(t) - f]$ over the distribution density of all outcomes of $\phi(t)$, that is,

$$P(f,t) = \langle \delta(f(t) - f)\rangle. \tag{21}$$

Making the substitution of $\dot{f}(t)$,

$$\frac{\partial P(f,t)}{\partial t} = -a(t)\, \frac{\partial P(f,t)}{\partial f} - \frac{\partial}{\partial f}\langle \delta(f(t) - f)\, \phi(t)\rangle. \tag{22}$$

The bracket seems intimidating at first glance because $f(t)$ is itself a function of the noise $\phi(t)$. However, it can be made even more explicit through the generalized Furutzu-Novikov-Donsker (GFND) formula. It was originally derived by Dubkov and Malakhov [32] and found explicitly in Ref. [33]. It was rederived in a better readable form by Hänggi [28] while Venturi *et al.* [29] applied it to a model implying additive and multiplicative noises. It is given by

$$\langle\, \delta(f(t) - f)\, \phi(t)\,\rangle = \langle\, \delta(f(t) - f)\,\rangle \langle \phi(t)\rangle - \frac{\partial}{\partial f}\sum_{n=1}^{\infty}\frac{1}{n!}\int_0^t dt_1 \cdots \int_0^t dt_n \Big\langle \frac{\delta^n \delta(f(t) - f)}{\delta\phi(t_1)\cdots\delta\phi(t_n)}\Big\rangle C_{n+1}(t, t_1, \cdots, t_n), \tag{23}$$

where $C_{n+1}(t, t_1, \cdots, t_n)$ is the multiple-time cumulant of $\phi(t, t_i, \cdots, t_n)$ [18]. Using $\partial\delta(x-y)/\partial x = -\partial\delta(x-y)/\partial y$ and noticing that $\delta f(t)/\delta\phi(t_i) = 1$, the internal average reduces to

$$\left\langle \frac{\delta^n \delta(f(t)-f)}{\delta\phi(t_1)\cdots\delta\phi(t_n)} \right\rangle = (-1)^n \left\langle \frac{\delta^n}{\delta f^n}\,\delta(f(t)-f) \right\rangle = (-1)^n \frac{\partial^n P(f,t)}{\partial f^n}. \tag{24}$$

Therefore, the second term of the right-hand side of Eq. (22) is

$$-\frac{\partial}{\partial f}\langle\,\delta(f(t)-f)\,\phi(t)\,\rangle = -\langle\phi(t)\rangle\frac{\partial P}{\partial f} - \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^{n+1}P(f,t)}{\partial f^{n+1}}\int_0^t dt_1\cdots\int_0^t dt_n\, C_{n+1}(t, t_1, \ldots, t_n). \tag{25}$$

Defining $D_{\phi}^{(n)}(t)$ as a generalized time-dependent diffusion term according to:

$$D_{\phi}^{(n)}(t) = 2\int_0^t dt_1\cdots\int_0^t dt_n\, C_{n+1}(t, t_1, \ldots, t_n), \tag{26}$$

we finally get the FPE,

$$\frac{\partial P(f,t)}{\partial t} = -[\,a(t) + \langle\phi(t)\rangle\,]\frac{\partial P}{\partial f} - \frac{1}{2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}D_{\phi}^{(n)}(t)\,\frac{\partial^{n+1}P(f,t)}{\partial f^{n+1}}. \tag{27}$$

Thus, the approximate solution of the partial differential equation depend on the number of cumulants to be included in the solution. It requires to solve a highly nonlinear PDE.

The generic FPE will be applied next for the work and heat stochastic differential equations.

C. FPE for work

The dynamical equations for the thermodynamic work involved along a single trajectory is [1,34,35]

$$\dot{W}(t) = \dot{\lambda}(t)[\,q(t) - \lambda(t)\,]. \tag{28}$$

There is an important issue to take into account. It is concerned on the dependence of the expressions over v_0. Since the system started from equilibrium, then averaging the equations over the v_0-Maxwell distribution will allow us to get rid of of this initial value.

Working on Eq. (28), we have that after making the appropriate substitutions and proceeding to average over the initial velocity v_0,

$$\dot{W}(t) = \overline{\dot{W}}(t) - \dot{\lambda}(t)\,\varphi_q(t), \tag{29}$$

$$W(t) = \widetilde{W}(t) - \int_0^t ds\,\dot{\lambda}(s)\,\varphi_q(s), \tag{30}$$

$$\widetilde{W}(t) = W_0 + \int_0^t ds\,\widetilde{q}(s)\,\lambda(s), \tag{31}$$

where $\widetilde{q}(t)$ is given by Eq. (8) without the v_0 term.

The resemblance of Eq. (29) with Eq. (17) allows us to make the identifications

$$f(t) = W(t); \qquad a(t) = \overline{\dot{W}}(t),$$
$$\phi(t) = \dot{\lambda}(t)\,\varphi_q(t).$$

Since $\varphi_q(t)$ is Gaussian only the first cumulant is enough in the expansion, the GFND formula reduces to the original FND given by [36–38]

$$\langle\delta(f(t)-f)\,\varphi_q(t)\rangle = \int_0^t ds \left\langle \frac{\delta}{\delta\varphi_q(t)}\delta(f(t)-f) \right\rangle \langle\varphi_q(t)\,\varphi_q(s)\rangle$$
$$= -\frac{\partial P(W,t)}{\partial W}\int_0^t ds\,\langle\varphi_q(t)\,\varphi_q(s)\rangle. \tag{32}$$

Therefore, Eqs. (26) and (27) reduces to

$$D_w(t) = 2\,\dot{\lambda}(t)\int_0^t ds\,\dot{\lambda}(s)\,\langle\varphi_q(t)\,\varphi_q(s)\rangle, \tag{33}$$

$$\frac{\partial P(W,t)}{\partial t} = -\overline{\dot{W}}(t)\,\frac{\partial P}{\partial W} + \frac{1}{2}D_w(t)\,\frac{\partial^2 P}{\partial W^2}, \tag{34}$$

Applying the linear transformation $r(t) = \int_0^t ds\, D_w(s)$ and $y(t) = W - \int_0^t ds\,\overline{\dot{W}}(s)$ gives [39]

$$\frac{\partial P(y,r)}{\partial r} = \frac{1}{2}\frac{\partial^2 P}{\partial y^2}, \tag{35}$$

which is the standard diffusion equation. Its solution with an initial condition $\delta(y-y_0)$ is a Gaussian centered at $y_0 = 0$. In terms of the original variables, the conditional pdf for a given realization W, starting from W_0, is then

$$P(W,t|W_0) = \frac{1}{\sqrt{2\pi\,\sigma_w^2(t)}}\exp\left\{-\frac{\left[W - \widetilde{W}(t)\right]^2}{2\,\sigma_w^2(t)}\right\}, \tag{36}$$

with the mean $\widetilde{W}(t)$ given by Eq. (31) and standard deviation

$$\sigma_w^2(t) = \int_0^t ds\,D_w(s). \tag{37}$$

Having found the Gaussian distribution, then it is pertinent to ask about the FPE associated to it. The procedure was already shown in the Appendix of Ref. [40], which, fitted to Eq. (36), gives the following result:

$$\frac{\partial P(W,t)}{\partial t} = -\Omega(t)\,\frac{\partial}{\partial W}[\,W\,P\,] + \frac{1}{2}D(t)\,\frac{\partial^2 P}{\partial W^2}, \tag{38}$$

$$\Omega(t) = \frac{\dot{\widetilde{W}}(t)}{\widetilde{W}(t)}, \tag{39}$$

$$D(t) = \dot{\sigma_w}^2(t) - 2\,\sigma_w(t)\,\Omega(t). \tag{40}$$

Equation (36) will be solved in Sec. III for different initial parameter sets and values of the damping constant characterizing the regimens ranging from the very low-underdamped up to the noninertial or overdamped. The protocols to be used in the determination of $\widetilde{W}(t)$ are those of Ref. [22].

D. About the heat distribution

The stochastic differential equation for heat is [1,34,35]

$$\dot{Q}(t) = v(t) \circ [\, q(t) - \lambda(t)\,], \tag{41}$$

where the symbol "∘" denotes the Stratonovich-type product, meaning that its integral converges to that of a Reimann-Stieljes kind [41].

Proceeding as before on Eq. (41), its average over the initial velocity gives

$$\langle \dot{Q}(t)\rangle_{v_0} = \langle v(t) \circ [\, q(t) - \lambda(t)\,]\rangle_{v_0}. \tag{42}$$

Making the substitutions of $q(t)$ and $v(t)$, taking into account that from the equipartition theorem $\langle v_0^2\rangle = T$ and that to simplify the writing of the equations the index v_0 is suppressed, we have

$$\dot{Q}(t) = H(t) + \varphi_Q(t), \tag{43}$$

$$H(t) = T\, \dot{\chi}_v(t)\, \chi_v(t) + \widetilde{v}(t)\, G(t), \tag{44}$$

$$\varphi_Q(t) = \widetilde{v}(t)\, \varphi_q(t) + G(t)\, \varphi_v(t) + \varphi_q(t) \circ \varphi_v(t), \tag{45}$$

$$G(t) = \widetilde{q}(t) - \lambda(t), \tag{46}$$

where $\widetilde{v}(t)$ is obtained setting $v_0 = 0$ in Eq. (10). The integration of Eq. (43) with $Q(0) = 0$ gives its mean value $< Q(t) >= \int_0^t ds\, H(s)$.

As before, we make the identifications $f(t) = Q(t)$, $\phi(t) = \varphi_Q(t)$, and $a(t) = H(t)$.

In order to determine the Q distribution, it is imperative to characterize the statistical properties of the noise $\varphi_Q(t)$ defined by Eq. (45). Letting

$$\begin{aligned}
&\varphi_Q(t) = \varphi(t) + \chi(t),\\
&\varphi(t) = \widetilde{\varphi}_q(t) + \widetilde{\varphi}_v(t); \quad \chi(t) = \varphi_q(t)\, \varphi_v(t),\\
&\widetilde{\varphi}_q(t) = \widetilde{v}(t)\, \varphi_q(t); \widetilde{\varphi}_v(t) = G(t)\, \varphi_v(t),\\
&\sigma_q^2(t) = \widetilde{v}^{\,2}(t) \langle \varphi_q^2(t)\rangle; \sigma_v^2(t) = G^2(t) \langle \varphi_v^2(t)\rangle
\end{aligned}$$

the distribution of each noise term appearing in $\phi(t)$ can be analytically deducted. For instance, the joint distribution of the correlated noises $\widetilde{\varphi}_q(t)$ and $\widetilde{\varphi}_v(t)$ is [42]

$$P(\widetilde{\varphi}_q, \widetilde{\varphi}_v, t) = \frac{1}{2\pi\, \sigma_q(t)\, \sigma_v(t) \sqrt{1 - \rho^2(t)}} \exp\left[-\frac{1}{2\,[\,1 - \rho^2(t)\,]} \left[\frac{\widetilde{\varphi}_q^2}{\sigma_q^2(t)} + \frac{\widetilde{\varphi}_v^2}{\sigma_v^2(t)} - \frac{2\,\rho(t)\, \widetilde{\varphi}_q \widetilde{\varphi}_v}{\sigma_q(t)\, \sigma_v(t)} \right] \right], \tag{47}$$

$$\rho(t) = \frac{\langle \varphi_q(t)\, \varphi_v(t)]\rangle}{\sigma_q(t)\, \sigma_v(t)}. \tag{48}$$

Therefore, the distribution of $\varphi(t)$ will be

$$\begin{aligned}
P(\varphi, t) &= \int_{-\infty}^{\infty} d\widetilde{\varphi}_q \int_{-\infty}^{\infty} d\widetilde{\varphi}_v P(\widetilde{\varphi}_q, \widetilde{\varphi}_v, t)\, \delta(\widetilde{\varphi}_q + \widetilde{\varphi}_v - \varphi),\\
&= \frac{\rho(t)}{\sqrt{[\,1 - \rho^2(t)\,]\,[\,\sigma_q^2(t) + \sigma_v^2(t) + 2\,\rho(t)\, \sigma_q(t)\, \sigma_v(t)\,]}} \exp\left[-\frac{\varphi^2}{2\,[\,\sigma_q^2(t) + \sigma_v^2(t) + 2\,\rho(t)\, \sigma_q(t)\, \sigma_v(t)\,]} \right].
\end{aligned} \tag{49}$$

Likewise, the pdf of the correlated product described by $\chi(t)$ is given by [43,44]:

$$P(\chi, t) = \frac{1}{\pi\, \sigma_q(t)\, \sigma_v(t) \sqrt{1 - \rho^2(t)}} \exp\left[\frac{\rho(t)\, \chi}{\sigma_q(t)\, \sigma_v(t)\, [\,1 - \rho^2(t)\,]} \right] K_0\left(\frac{|\chi|}{\sigma_q(t)\, \sigma_v(t)\, [\,1 - \rho^2(t)\,]} \right), \tag{50}$$

where $K_0(\cdot)$ is the modified Bessel function of the second kind of order zero. Unlike the case for uncorrelated variables, the χ distribution is asymmetrical because of the exponential term. From the definitions of $\varphi_q(t)$ and $\varphi_v(t)$ then $\varphi(t)$ and $\chi(t)$ are distributed about zero.

The final task is to find the pdf for $\varphi_Q(t)$ which requires using the statistical method of copula, latin for "link" or "tie," which captures the dependence structure of the distribution of random variables through Sklar's theorem [45]. The article by Zeng *et al.* [46] shows the method to determine it for different marginal distributions.

There is not a route to get the analytical formula for the joint distribution of the random pair $\{\varphi, \chi\}$, but numerical, unlike the analytical result for the copula of the sum of correlated Gaussian random variables given by Eq. (47). This is outside the scope of this research, which leads us to conclude that the proposed method fails to find the analytical heat distribution. However, its associated FPE, substituting f by Q in Eq. (27), is mathematically well defined.

Therefore, without resorting to procedures based on the characteristic function as in previous works, a careful handling *à la* van Kampen [16] of the different noises appearing in the equation that define the heat along the trajectory gives a rather complicated FPE. The key points in the derivation is to recognize that $\widetilde{v}(t)$ and $G(t)$ are nonanticipating functions of the Gaussian $\varphi_q(t)$ and $\varphi_v(t)$ noises, respectively, whose sum along with their product $\varphi_q(t) \circ \varphi_v(t)$ is non-Gaussian. Therefore, the procedure shown above and based on finding the FPE for heat is mathematically justified although its solution cannot be obtained but only numerically.

III. DISCUSSION OF THE RESULTS

This section analyzes the results for the work distribution and an analysis about the complexity of the heat distribution. For presentation, the work distributions for all the regimens defined by γ at specific times and different initial set of parameters are shown in the first subsection. There, the correlation functions were normalized to get manageable magnitudes and calculated assuming $t > s$. Subsequently, the heat distribution is generally discussed and the average heat is calculated at the temperature set to $T = 10$.

A. Work distribution

To numerically calculate the distribution of work, it is essential to know its evolution over time. This requires the knowledge of the external protocol, in which case it could be arbitrary. However, there is no a guaranty that its arbitrariness leads to, for instance, the particle doing work against the external field. This is a crucial property for understanding a Maxwell's demon or the transformation of information into work without violating the second law. We enforce the constraint where the protocol must minimize the mechanical work to check the appearance of the demon. This is the objective of the calculations presented in this proposal.

It was proved in Ref. [22] that the overdamped optimal protocol and work agrees with the calculated from the inertial LE for sufficiently large values of both the friction and final time t_f. For times greater that the chosen t_f, the analytical disagrees with that from the inertial LE because the numerical high-friction limit is not completely achieved. Thus, up to t_f the numerical is consistent with the known analytical overdamped; hence, the two W distributions will be equal.

Calculations were done for all regimens [47]. They are the periodic when $\gamma = 1$ because frequency ω is imaginary, the critical $\gamma = 2$ since $\omega = 0$, the aperiodic for $\gamma \geqslant 2$ or ω real, and the overdamped where $\gamma = 275$. The latter is sufficiently large to assure that numerical inertial effects are sufficiently small up to the chosen final time, such that the agreement is total with the analytical overdamped. In order to check the dependence on the initial condition, only three sets $\{q_0, v_0\}$ compile all possible combinations of q_0 and λ_f because of the potential symmetry [22]. The average work at $t = 0$ for each set is represented by a black vertical line. It corresponds to the adiabatic work calculated in Ref. [22] when the trap is instantaneous moved to the position λ_f and put back to q_0. It is important to mention that in the critical mode, the susceptibilities $\chi_q(t)$ and $\chi_v(t)$ must be obtained in the limit of $\omega = 0$.

The calculation requires knowing the optimal average work. Since they were performed in a previous work [22], they were recalculated for all the cases considered in this article. It is shown in Fig. 1. The results are for the sets $\{1, -1\}$, $\{1, 0\}$, and $\{0, 1\}$ and friction coefficients of 1, 2, 3, and 275 such as indicated. Note that the system behaves like a Maxwell's demon for a specific set of conditions, as seen in the bottom plot of Fig. 1.

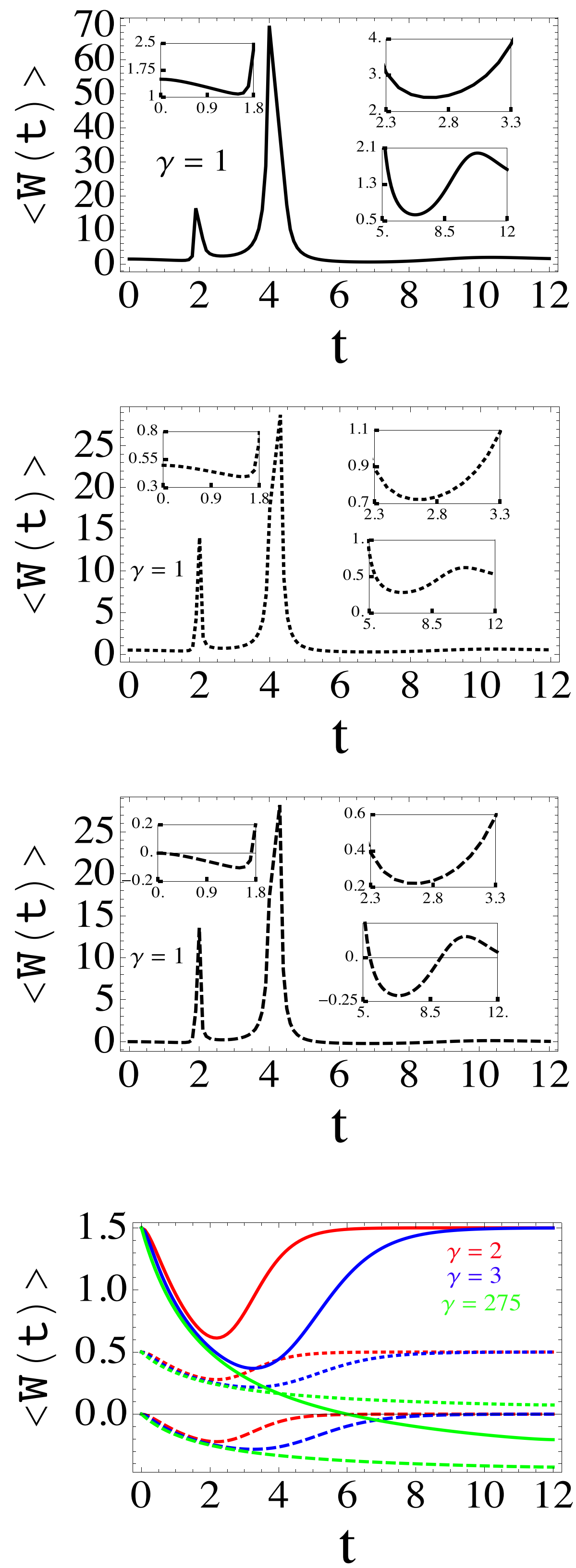

FIG. 1. Effect of the damping constant and initial conditions on the average work. The parameter sets are $\{1, -1\}$ (solid), $\{0, 1\}$ (dotted), and $\{1, 0\}$ (dashed), respectively. The plots were recalculated from Ref. [22].

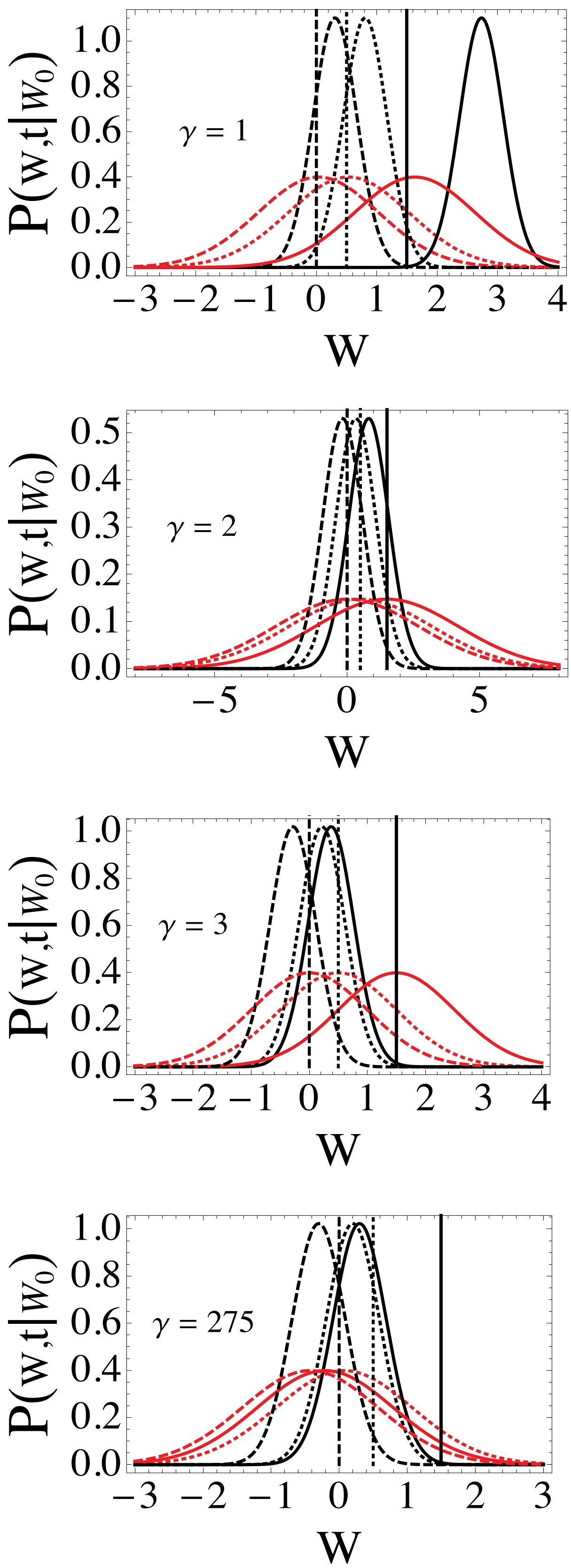

FIG. 2. Effect of the damping constant and initial conditions on the work distribution. The parameter sets are $\{1, -1\}$ (solid), $\{0, 1\}$ (dotted), and $\{1, 0\}$ (dashed). The black vertical lines denote the initial condition W_0. Each curve corresponds to times of 3 (black) and 12 (red).

Figure 2 shows the effect of the friction coefficient and initial conditions on the Wd using the mean work shown in Fig. 1. The initial parameter sets are shown by solid curves for $\{q_0, \lambda_f\} = \{1, -1\}$, dashed for $\{1, 0\}$, and dotted for $\{0, 1\}$ corresponding to times of 3 (black) and 12 (red).

The dynamics of the periodic regimen presents serious anomalies [22]. In particular, the appearance of concentration and diffusion processes acting together in the dynamics [48,49] and a local heating of the Brownian particle [50], among others. This is the reason why the average work shows two discontinuities at two specific times near to the beginning of the protocol application as shown in Fig. 1. Despite this, the work distribution in this regimen appears as a smooth function of W.

As it should be, the distributions for γ of 1, 2, and 3 are centered around their average while in the overdamped is around the center of the trap because the mean work reaches the asymptotic value of $-q_0^2/2$ [22]. For any given γ, the standard deviation and the time-dependent diffusion term are invariants regardless the initial parameter set. Thus, the differences in the distributions are adjudicated to the time-dependent mean work $\widetilde{W}(t)$.

B. Heat: Statistical analysis

As we mentioned before, unfortunately there is no analytical but numerical solution for $P(Q, t)$ given by Eq. (27).

There is no reason to exclude the Gaussian solution that would correspond to $n = 1$ such that the higher-order terms in the summation can be discarded. This will require knowing the joint probability of $\chi(t)$ to asses the magnitude of the cumulants of order greater than two.

In the case that terms involving the distribution of $\chi(t)$ exceed those of $\varphi(t)$, it could happen that the distribution had an important exponential behavior because of the Bessel function. It can be verified if the external field is off. In this case, the particle would be subjected to the potential of an immobile trap, that is, of a simple harmonic potential. Since $\widetilde{v}(t) = G(t) = 0$ because $q_0 = 0$, then $\varphi_Q(t) = \varphi_q(t)\,\varphi_v(t)$ for which its statistics is complete if it is known its joint $P(\chi_1, \dots, \chi_n)$. Furthermore, $\langle Q(t)\rangle = T\, e^{-\gamma^2 t}\,[\cosh(\omega\,\gamma\, t) - 1]/(\gamma^2\,\omega^2)$ resulting to be independent of the initial condition and being a truly exponential for γ sufficiently high. Despite this simplification, it is not possible to delve into more details due to the lack of knowledge of the joint probability, which can only be determined through its copula. As far as is known, there is no explicit literature about this distribution.

Assuming that these two mathematical arguments would be correct, then it would be theoretically reproduced the experimental result of Imparato *et al.* [8], mentioned in the Introduction. Briefly, the set-up consisted of polystyrene microspheres centered in the bottom of an optical tweezers moved at a constant velocity. Their diameter was 2.0 ± 0.05 μm immersed in distilled water at $T = 295$ K. Measuring the trajectories after the equilibration, Wd and Qd were determined. Repeating this process for about 600 runs, the histograms of the two properties were two genuine Gaussians. Furthermore, the heat distribution is a symmetrical exponential for an immobile trap suggesting that the

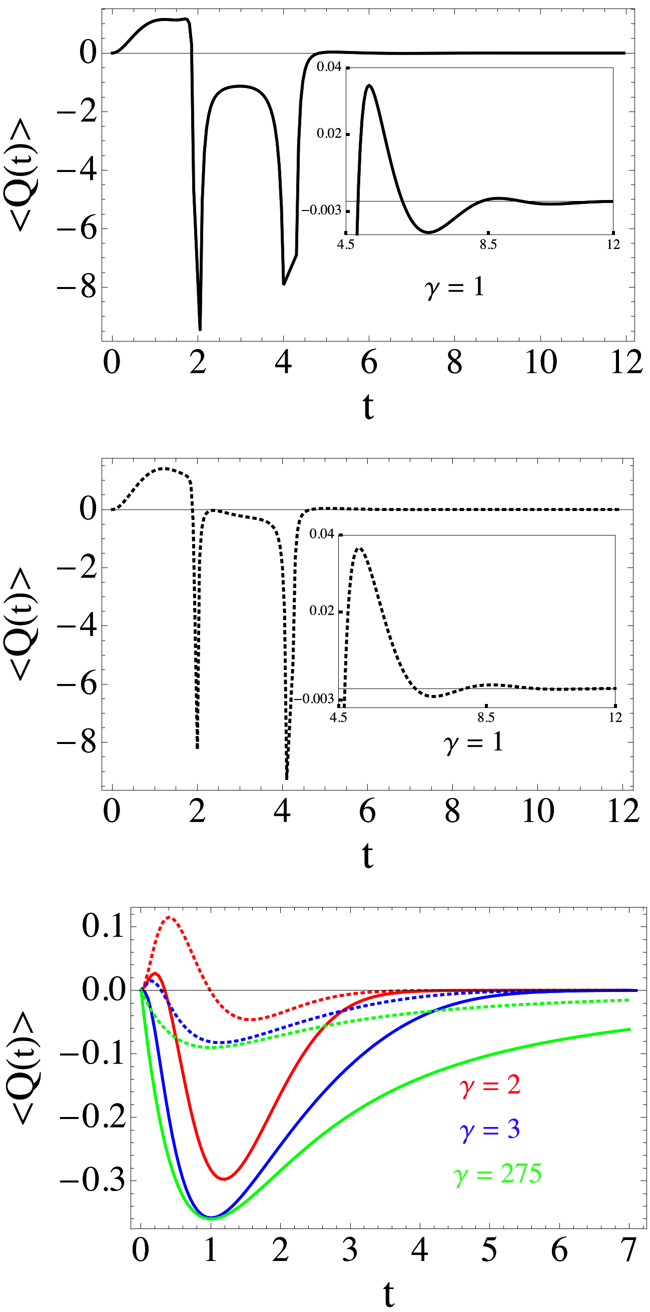

FIG. 3. Effect of the friction coefficient on the mean heat $\overline{Q}(t) = < Q(t) >$ for parameters set $\{1, -1\}$ (solid) and $\{1, 0\}$ (dashed). The set $\{0, 1\}$ superimposed the latter. The inset of the first two panels amplifies the region after $t = 4.5$; $T = 10$.

noise is uncorrelated under the experimental conditions. It will correspond to suppress the exponential term and to let $\rho(t) = 0$ in Eq. (50).

Nevertheless, the mean value $\langle Q(t)\rangle = \int_0^t ds\, H(s)$ when the field is on can be calculated. It is shown in Fig. 3 for the four values of γ and the initial condition sets [47]. It is noticeable that at the beginning there is a brief absorption of heat, being more pronounced in the periodic regime and the critical for the $\{1, 0\}$ set. They last for a brief time and it is when heat is released to the thermal reservoir. Looking at Fig. 2, the particle, except the overdamped one, does mainly adiabatic work at large times. In the latter and in order to keep a constant temperature, the reservoir continually releases heat to the overdamped particle to compensate that from the dissipated by the high value of γ.

IV. FINAL REMARKS

Summarizing, a simple method based on basic stochastic dynamics tools was implemented to determine the Fokker-Planck equation for the optimal work and heat distributions of an inertial Brownian particle interacting with an MHP and a thermal bath.

The work distribution was determined for a variety of initial conditions and friction coefficient values. The resulting equations are easy to manipulate as their numerical implementation. The optimal protocol that minimizes the mechanical work was used instead of the frequently used in the literature involving the displacement of the potential center at a constant velocity. The effect of the latter does not affect the bell shape of the distributions. However, they do not include the effect of the thermodynamic restriction of an optimal protocol on the dynamics.

It should be emphasized that the proposal presented in this article for the moving harmonic potential predicts Gaussian distributions for work and heat without conditions of any kind and based on basic stochastic principles. Unfortunately, the FPE for heat is so complicated that its solution can only be obtained by numerical methods.

The stochastic differential equations describing work and heat averaged over the initial velocity prior to the derivation of their distributions is natural for physical systems starting from equilibrium. Furthermore, keeping the initial position in the final formulas has sense from the mathematical point of view or for comparing the results with simulations.

All the theoretical approaches mentioned in the Introduction are based on considering the external potential as harmonic. The reason is that the experimental potential to optically trap the particle and measure its position and, from it, determine the heat and work distributions by moving it at a constant speed or modifying its intensity for a fixed position, is also of a harmonic type. In this sense, the results of any theoretical scheme used to describe this experiment can be considered general since they describe the same physical phenomenon. They are also singulars depending on the accuracy of the description. This categorization holds for any experimental configuration, such as two traps acting in unison to capture the particle where, in general, the potential loses its harmonic character. Here, the mathematical techniques for obtaining easy-to-compute analytic expressions are more complicated due to underlying nonlinearities. This has already been addressed in a previous work [51] for nonlinear potentials where the response function of the system was the property to be evaluated.

Referring to Ref. [8], the MHP leads to an exponential heat distribution if Eq. (41) is discretized. This is typical for one-step processes [16–18]. Therefore, instead of addressing heat flux as a result of particle diffusion, a potential future investigation would be to use the formalism of the master equation.

ACKNOWLEDGMENTS

The author has benefited from useful discussions with Dr. Oscar Paredes-Altuve of Universidad de Chile. The referees are also thanked for their helpful suggestions.

[1] O. Mazonka and C. Jarzynski, arXiv:cond-mat/9912121.
[2] T. Speck and U. Seifert, Phys. Rev. E **70**, 066112 (2004).
[3] R. van Zon and E. G. D. Cohen, Phys. Rev. E **69**, 056121 (2004).
[4] A. Imparato and L. Peliti, Phys. Rev. E **72**, 046114 (2005).
[5] T. Speck and U. Seifert, Eur. Phys. J. B **43**, 521 (2005).
[6] C. Jarzynski, Phys. Rev. Letts. **78**, 2690 (1997).
[7] T. Taniguchi and E. G. D. Cohen, J. Stat. Phys. **126**, 1 (2007).
[8] A. Imparato, L. Peliti, G. Pesce, G. Rusciano, and A. Sasso, Phys. Rev. E **76**, 050101(R) (2007).
[9] R. van Zon and E. G. D. Cohen, Phys. Rev. Lett. **91**, 110601 (2003).
[10] H. C. Fogedby and A. Imparato, J. Phys. A: Math. Theor. **42**, 475004 (2009).
[11] D. Chatterjee and B. J. Cherayil, Phys. Rev. E **82**, 051104 (2010).
[12] T. Speck, J. Phys. A: Math. Theor. **44**, 305001 (2011).
[13] S. Ciliberto, Phys. Rev. X **7**, 021051 (2017).
[14] P. V. Paraguassú, R. Aquino, and W. A. M. Morgado, arXiv:2102.09115.
[15] H. C. Fogedby, J. Stat. Mech.: Theory Exp. (2020) 083208.
[16] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdan, 1981).
[17] H. Risken, *The Fokker-Planck Equation: Method of Solutions and Applications* (Springer-Verlag, Berlin, 1984).
[18] C. W. Gardiner, *Handbook of Stochastic for Physics, Chemistry and the Natural Sciences*, 2nd ed. (Springer-Verlag, Berlin, 1985).
[19] P. J. Colmenares, J. Theor. Biol. **161**, 175 (1993).
[20] W. Olivares and P. J. Colmenares, Physica A **458**, 76 (2016).
[21] O. Paredes-Altuve, E. Medina, and P. J. Colmenares, Phys. Rev. E **94**, 062111 (2016).
[22] P. J. Colmenares and O. Paredes-Altuve, Phys. Rev. E **104**, 034115 (2021).
[23] P. Schramm, R. Jung, and H. Grabert, Phys. Lett. A **107**, 385 (1985).
[24] T. Schmiedl and U. Seifert, Phys. Rev. Lett. **98**, 108301 (2007).
[25] U. Weiss, in *Series in Modern Condensed Matter Systems*, 3rd. ed, edited by I. Dzyaloshinski and Y. Lu, Vol. 13 (World Scientific, Singapore, 2012).
[26] J. O. Daldrop, B. G. Kowalik, and R. R. Netz, Phys. Rev. X **7**, 041065 (2017).
[27] V. Lisý and J. Tóthová, Results Phys. **12**, 1212 (2019).
[28] P. Hänggi, Z. Physik B **31**, 407 (1978).
[29] D. Venturi, T. P. Sapsis, H. Cho, and G. E. Katniadakis, Proc. R. Soc. A **468**, 759 (2012).
[30] J. M. Sancho, M. S. Miguel, S. L. Katz, and J. D. Gunton, Phys. Rev. A **26**, 1589 (1982).
[31] R. Kubo, J. Math. Phys. **4**, 174 (1963).
[32] A. A. Dubkov and A. N. Malakhov, Academiia Nauk SSRR, Doklady **222**, 793 (1975).
[33] G. N. Bochkov, A. A. Dubkov, and A. N. Malakhov, Radiophys. Quant. Electr. **20**, 276 (1977).
[34] K. Sekimoto, *Stochastic Energetics* (Springer, Heidelberg, 2010).
[35] U. Seifert, Rep. Prog. Phys. **75**, 126001 (2012).
[36] K. Furutzu, Res. Natl. Inst. Stand. Technol. **67D**, 308 (1963).
[37] E. A. Novikov, Zh. Exper. Teor. Fiz. **47**, 1919 (1964) [Sov. Phys. JETP **20**, 1290 (1965)].
[38] M. D. Donsker, in *Analysis in Function Space*, edited by W. T. Martin and I. E. Segal (MIT Press, Cambridge, MA, 1964), pp. 17–30.
[39] R. Ratcliff, J. Math. Psych. **21**, 178 (1980).
[40] P. J. Colmenares, Phys. Rev. E **97**, 052126 (2018), There is a misprint in Eq. (12), $\xi(t)$ must be $\varphi_v(t)$.
[41] A. Budhiraja and G. Kallianpur, Stat. Sin. **7**, 907 (1997).
[42] W. Schneider, arXiv:2107.00007.
[43] S. Nadarajah and T. K. Pogány, C. R. Acad. Sci. Paris, Ser. I **354**, 201 (2016).
[44] G. Cui, X. Yu, S. Iommelli, and L. Kong, IEEE Signal Process. Lett. **23**, 1662 (2016).
[45] R. B. Nelsen, *An Introduction to Copulas*, Springer Series in Statistics, 2nd ed. (Springer, New York, 2005).
[46] X. Zeng, J. Ren, Z. Wang, and S. Marshall, Sign. Process. **94**, 691 (2014).
[47] MATHEMATICA computer package version 8.0.4 was used for the algebraic, numerical and graphics manipulations.
[48] J. Spiechowicz, P. Hänggi, and J. Łuczka, New J. Phys. **21**, 083029 (2019).
[49] P. J. Colmenares, Phys. Rev. E **100**, 052117 (2019), The term inside the summation in Eq. (10 d) must be $(\nu_n \exp[-\nu_n t])[(\nu_n^2 + \lambda_1^2](\nu_n^2 + \lambda_2^2))]^{-1}$.
[50] G. Stolovitzky, Phys. Lett. A **241**, 240 (1998).
[51] P. J. Colmenares, Phys. Rev. E **102**, 062102 (2020).