Optimal work associated with off-centered harmonic Brownian motion at any friction damping

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There is extensive literature on how to determine the work involving a Brownian particle interacting with an external field and submerged in a thermal reservoir. However, the information supplied is essentially theoretical without specific calculations to show how this property changes with the system parameters and initial conditions. In this article, we provide explicit calculations of the optimal work considering the particle is under the influence of a time-dependent off-centered moving harmonic potential. It is done for all physical values of the friction coefficient. The system is modeled through a more general version of the Langevin equation which encompasses its classical and quasiclassical version. From the equation that defines the work, the external protocol is found through a fairly current extended version of the Euler-Lagrange equation that unifies the local and nonlocal contributions in a simple expression. The protocol is linear and, unlike previous work, not only changes the initial velocity of the particle but also its acceleration. Calculations were done for friction constants γ spanning all possible values. The periodic $\gamma = 1$ shows discontinuities in the optimal work of the interplay of concentration and diffusion processes acting periodically in the dynamics. For higher values work appears to be as a smooth function of time, while the truly overdamped, where the inertial effect can be discarded, agrees with the analytical result up to a time where the numerical overdamped algorithm provides a different solution due to its inability to discard entirely the inertial effect.

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I. INTRODUCTION

In the search for time-dependent controllable external means to optimize the work extraction of a Brownian particle, the so-called protocols, there has been significant progress in this direction. Schmiedl and Seifert [1] analyzed the classical overdamped Langevin equation (LE) in a parabolic potential. They determined the optimal protocol (OP) which minimizes the work done by the field in both the moving harmonic potential and that with a time-dependent stiffness, without any restriction but the system equation of motion. The nonlocal work functional of the former is cast in a local functional of the square of the mean velocity while for the latter in terms of the variance of the particle position. They applied the Euler-Lagrange equation to determine it. Thereafter, Then and Engel [2] analyzed the importance of the nonlocality of the work functional for the systems of Ref. [1]. They derived the nonlocal integrodifferential equation of the OP along the particle trajectory occurring with a given probability which in fact is a functional of the protocol. By applying a second time derivative to this equation, the results of Schmiedl and Siefert are recovered. Similarly for the time-dependent stiffness potential, the authors use Lie symmetry to decompose the OP and solve the nonlocal Euler-Lagrange formalism to match the aforementioned results of Ref. [1]. They ascribe the linearity of the protocol as the cause for the two optimization methods providing the same outcome. They also calculate the OP for a dipole in a thermal bath by a Monte Carlo simulation. Subsequently, Gomez-Marin *et al.* [3] extended the investigation to the underdamped case. They argued that, physically, the protocol forces the velocity to jump instantly at the beginning and reset it to zero at the final time so that the system returns to equilibrium. Although an experimental setup cannot mimic the jumps in the protocol, they suggested that it can be implemented by steeped straight lines instead.

There have been other approaches to study the dynamics involving a harmonic potential with variable stiffness even though they are out of the scope of this article. For instance, Speck [4] looked for the generating function of the work distribution for linear protocols while Plata *et al.* [5] used the alternate Pontryagin's procedure (see references attached) to minimize the work functional.

A further development came from the application of Sekimoto's stochastic energetics approach [6] to attack the work extraction through feedback. Thus, Abreu and Seifert [7] determined the maximum work of an overdamped Brownian particle driven by a potential with a time-dependent stiffness. They addressed the problem by exploiting the information gained from the measurement through a harmonic optical trap for given values of the protocols at the beginning and at the end of the process. Subsequently, Paredes-Altuve *et al.* [8] extended the problem to the underdamped non-Markovian case through the generalized Langevin equation with a moving harmonic potential. As before, the OP depends on its final value.

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There is an important application of optimal protocols such as in the optimization of power and the efficiency of Brownian heat engines in a Carnot cycle. The analysis requires the optimization of the work generated in each stage. The optimization technique for the different potentials is that of Ref. [1]. Schmiedl *et al.* [9] considered a thermodynamic machine in which the particle moves in a harmonic trap with time-dependent strength. The problem requires imposing boundary conditions on the control parameter in order to get the total work produced in the heat engine. Their findings include that the efficiency approaches Carnot's for an infinite cycle time and that at maximum power, it is a universal relation different from the prevailing Curson-Ahlborn efficiency [10]. A further refining of this problem came with the work by Holubec and Ryavob [11] where a new universal efficiency is found by using the results of Ref. [9] and also where the notion of efficiency in heat engines out of equilibrium is extended at a nonzero output power. Furthermore, they show the characteristics of the potential in order to get useful work in the cycle. For instance, in the moving potential most of the energy transferred to the system in the isothermal stages is dissipated so the useful work is zero, coinciding with the results of Ref. [9] about stochastic machines. This result lies in the fact that the output work depends on the position mean value which is independent of the temperature so the output work is unaffected by the thermal reservoir. There is no conversion of heat in work. This is not the case for the time-dependent stiffness potential where the output work depends on the variance, which in turn is temperature dependent.

Esposito and Mukamel [12] derived the basic definitions of quantum work, heat, and fluctuation theorems in terms of the reduced density matrix of the particle without having to refer explicitly to the thermal bath. They obtained simple equations relying on averages over the reduced density matrix of the particle. However, one of the reasons for the unavailability of the quantitative data of the thermodynamic properties for quantum systems, where the initial entanglement is included, is the absence of an expression for the reduced density matrix. In a previous work [13], the quasiclassical LE was used to derive the reduced quasiprobability density associated with the particle, which was proved to be equal to the reduced Wigner function. Hence, it would be interesting to generate quantitative data for thermodynamic properties in the quasiclassical limit when an external field is applied.

The primal objective of this article is to facilitate explicit calculations of the optimal work for all possible values of the damping constant. For this purpose, the definitions of the work of Esposito and Mukamel along with the results of Ref. [13] are used to find out the work is given by the well-known nonlocal functional of the OP. The OP is determined from the work equation through a nonlocal version of the Euler-Lagrange equation described by Eq. (35), which is easier to derive in comparison with the method of Ref. [2]. For the moving harmonic potential our equations reproduce the findings of Ref. [1] in overdamped systems. The first main result of this proposal is condensed in the integral equation for the OP, Eq. (38), whose solution generates a linear OP given by Eq. (41) with distinctive jumps in velocity and acceleration at the beginning. This is the second major result.

The article is structured as follows. In Sec. II, the stochastic dynamics of the system is described through a compendium of the equations of Ref. [13] adapted to the moving harmonic potential. The thermodynamic analysis is done in Sec. III with three sections describing the methodology for the general case in Sec. III A, for overdamped systems in Sec. III B, and an analysis in Sec. III C about the different jumps appearing in the protocol for the various parameter sets used in the numerics. The high-temperature limit is presented in Sec. IV and numerical results for the protocols and work are compiled in Sec. V. The article concludes in Sec. VI with some final remarks. An Appendix is included to show the derivation of the different terms of the nonlocal Euler-Lagrange equation.

II. THE LANGEVIN EQUATION IN A MOVING PARABOLIC POTENTIAL

In general, the dynamics of the position $q(t)$ of a particle of mass M immersed in a thermal reservoir with friction coefficient γ at temperature T and under the influence of $V(q,t)=\omega_0^2[q-\lambda(t)]^2/2$, is controlled by the Ohmic LE,

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

where the dot above a function denotes its time derivative. Constant ω_0^2 is the frequency of the harmonic potential and $\lambda(t)$ is an external controlled function whose value determines the configuration of the system, i.e., an external driving controlling the position of the potential center. The noise depends on the physics in which the equation is applied. In a classical system it is the well-known Gaussian delta-correlated function, while in the semiclassical [14], where the bath is replaced by quantum harmonic oscillators, it is still Gaussian but colored.

The preparation procedure prior to starting the field, that is, for $t\leqslant 0$, requires that the whole system is in equilibrium. It can be achieved by waiting a sufficiently long time before the external field is switched on. Then, the particle density matrix can be safely factorized as the product of the densities of the particle and that of the reservoir, that is, the degrees of freedom of the two subsystems are uncorrelated. The last is the canonical density matrix given in terms of the temperature and bath Hamiltonian. Supposing the field leaves the bath unaltered once it is on, an initial density matrix can be constructed in terms of operators measuring the displacement of the particle by a certain amount. It will depend on the *preparation function* describing the deviation from the equilibrium distribution. This is the starting point of the functional integral approach of Grabert *et al.* [15] from which Eq. (1) is derived in the Ohmic limit. It differs from the theory by Caldeira and Leggett [16] that at $t>0$ a correlation of the initial position with the noise $\xi(t)$ persists, leaving a homogeneous equation of motion instead of the correct nonhomogeneous type as in Ref. [16]. Using the path-integral formalism, the functional approach allows us to write the noise two-time correlation function as

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

Here, $\hbar$ is the Planck constant, $\beta = (k_B T)^{-1}$, k_B is the Boltzmann constant and $\nu = 2\pi(\hbar\beta)^{-1}$.

Unlike the classical Markovian LE, we have to include the extra correlation of the noise with the initial position q_0 because of the preparation procedure mentioned before. It is given by

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

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

Even though the quasiclassical description is Ohmic, that is, the hydrodynamic retardation is proportional to the friction coefficient, the noise $\xi(t)$ is colored unlike in classical Markovian systems. There is no need to resort to a generalized Langevin equation to describe this effect.

Besides the elegance of the functional approach, the assumption of independence between the particle and bath degrees of freedom satisfying Kubo's second fluctuation-dissipation theorem is an approximation. It was addressed in a previous article [17] where the work by Daldrop *et al.* [18] showed that a molecular dynamics simulation of a harmonic Brownian particle shows a noise correlation in terms of a friction coefficient depending on the strength of the field. Moreover, in Refs. [19,20] it was shown that the theorem depends upon the field intensity. These results require one to reformulate the whole theory to include the effect of the field on the bath degrees of freedom. It is out of the scope of this research.

The own quantum nature of the bath leads to the existence of these two correlation functions. According to Ref. [15], the system starts from an equilibrium Gaussian distribution.

The strong friction (overdamped) limit of Eq. (1) is obtained by simply setting the acceleration equal to zero, i.e.,

$$\dot{q}_{\rm ov}(t) = \frac{1}{\gamma}\left(-\omega_0^2[q_{\rm ov}(t) - \lambda(t)] + \frac{1}{M}\xi(t)\right). \tag{4}$$

Any comparison with Eq. (1) for high γ can only be achieved by solving them in the same timescale. Since that of the overdamped is $1/\gamma$, the two LEs become

$$\frac{1}{\gamma^2}\ddot{q}(t) = = -\dot{q}(t) - \omega_0^2[q(t) - \lambda(t)] + \frac{1}{M}\xi(t), \tag{5}$$

$$\dot{q}_{\rm ov}(t) = -\omega_0^2[q_{\rm ov}(t) - \lambda(t)] + \frac{1}{M}\xi(t). \tag{6}$$

From now on, the Langevin equations are reduced by scaling lengths and time by the factors $(M\omega_0/\hbar)^{1/2}$ and ω_0, respectively. The reduced versions and the quasiclassical correlations become

$$\frac{1}{\gamma^2}\ddot{q}(t) = -\dot{q}(t) - q(t) + \lambda(t) + \xi(t), \tag{7}$$

$$\dot{q}_{\rm ov}(t) = -q_{\rm ov}(t) + \lambda(t) + \xi(t), \tag{8}$$

$$\langle \xi(t)\xi(t')\rangle = -\frac{1}{4\pi}\gamma\,\nu\,\sinh^{-2}\left[\frac{1}{2}\nu(t-t')\right], + i\gamma\,\dot{\delta}(t-t'), \tag{9}$$

$$\langle \xi(t) q_0 \rangle = -2\,\gamma\,T^{\star} \sum_{n=1}^{\infty} \frac{\nu_n e^{-\nu_n t}}{(\nu_n + \kappa_1)(\nu_n + \kappa_2)}, \tag{10}$$

where $T^{\star} = 1/(\beta\,\hbar\,\omega_0)$ is the reduced temperature and κ_1 and κ_2 reduce to $\kappa_{1,2} = [\gamma \pm (\gamma^2 - 4)^{1/2}]/2$.

The imaginary term appearing in the two-time noise correlation has two major origins [21]. On one hand, it is a consequence that the quantum operator describing the noise does not commute at two different times. On the other, the linear response theory applied to get the solution of the equation of motion in terms of the dynamic susceptibility of the system leads to an expression in which the imaginary part of the position correlation function determines the energy dissipated by the friction according to Kubo's fluctuation-dissipation theorem.

The solutions of the LEs for the inertial and overdamped modes are achieved by means of the Laplace transform technique. They read

$$\widehat{q}[\lambda](s) = \langle \widehat{q}[\lambda](s)\rangle + \widehat{\varphi}_{\mathbf{q}}(s), \tag{11}$$

$$\widehat{q}_{\rm ov}[\lambda](s) = \langle \widehat{q}_{\rm ov}[\lambda](s)\rangle + \widehat{\varphi}_{\rm ov}(s), \tag{12}$$

where

$$\langle \widehat{q}[\lambda](s)\rangle = v_0\,\widehat{\chi}_{\mathbf{v}}(s) + q_0\,\widehat{\chi}_{\mathbf{q}}(s) + \gamma^2\,\widehat{\chi}_{\mathbf{v}}(s)\widehat{\lambda}(s) \tag{13}$$

$$\langle \widehat{q}_{\rm ov}[\lambda](s)\rangle = \widehat{\chi}_{\rm ov}(s)[q_0 + \widehat{\lambda}(s)], \tag{14}$$

$$\widehat{\varphi}_{\mathbf{q}}(s) = \gamma^2\,\widehat{\chi}_{\mathbf{v}}(s)\widehat{\xi}(s), \tag{15}$$

$$\widehat{\varphi}_{\rm ov}(s) = \widehat{\chi}_{\rm ov}(s)\widehat{\xi}(s), \tag{16}$$

$$\widehat{\chi}_{\mathbf{v}}(s) = \frac{1}{s^2 + \gamma^2(s+1)}, \tag{17}$$

$$\widehat{\chi}_{\mathbf{q}}(s) = \widehat{\chi}_{\mathbf{v}}(s)(s + \gamma^2), \tag{18}$$

$$\widehat{\chi}_{\rm ov}(s) = \frac{1}{s+1}. \tag{19}$$

The notation $\widehat{\psi}[\lambda](s)$ represents the functional dependence of $\widehat{\psi}$ on λ. Inverting Eqs. (11) and (12) [22] gives $q[\lambda](t) = \langle q[\lambda](t)\rangle + \varphi_{\mathbf{q}}(t)$ and $q_{\rm ov}[\lambda](t) = \langle q_{\rm ov}[\lambda](t)\rangle + \varphi_{\rm ov}(t)$. Defining $v[\lambda](t) = \dot{q}[\lambda](t)$ and $v_0 = v(0)$ as the particle velocity and its initial value, respectively, the different terms appearing in $q[\lambda](t)$ and $q_{\rm ov}[\lambda](t)$ are given by

$$\langle q[\lambda](t])\rangle = \chi_{\mathbf{v}}(t)v_0 + \chi_{\mathbf{q}}(t)q_0 + \gamma^2 \int_0^t dx\,\chi_{\mathbf{v}}(t-x)\lambda(x), \tag{20}$$

$$\langle v[\lambda](t)\rangle = \dot{\chi}_{\mathbf{v}}(t)v_0 + \dot{\chi}_{\mathbf{q}}(t)q_0 + \gamma^2 \int_0^t dx\dot{\chi}_{\mathbf{v}}(t-x)\lambda(x), \tag{21}$$

$$\langle q_{\rm ov}[\lambda](t)\rangle = \chi_{\rm ov}(t)q_0 + \int_0^t dx\,\chi_{\rm ov}(t-x)\lambda(x), \tag{22}$$

$$\varphi_{\mathbf{q}}(t) = \gamma^2 \int_0^t dt'\chi_{\mathbf{v}}(t-t')\xi(t'), \tag{23}$$

$$\varphi_{\rm ov}(t) = \int_0^t dt' \chi_{\rm ov}(t-t')\xi(t'), \tag{24}$$

$$\varphi_{\mathbf{v}}(t) = \frac{d}{dt}\varphi_{\mathbf{q}}(t), \tag{25}$$

where the susceptibilities $\chi_{\mathbf{q}}(t)$, $\chi_{\mathbf{v}}(t)$, and $\chi_{\rm ov}(t)$ are

$$\chi_{\mathbf{q}}(t) = e^{-\gamma^2 t/2}\left(\cosh\left[\frac{\omega\gamma\, t}{2}\right] + \frac{\gamma}{\omega}\sinh\left[\frac{\omega\gamma\, t}{2}\right]\right), \tag{26}$$

$$\chi_{\mathbf{v}}(t) = \frac{2}{\omega\,\gamma}e^{-\gamma^2 t/2}\sinh\left[\frac{\omega\,\gamma\, t}{2}\right], \tag{27}$$

$$\chi_{\rm ov}(t) = e^{-t}, \tag{28}$$

with $\omega = \sqrt{\gamma^2 - 4}$. Functions $\chi_{\mathbf{q}}(t)$ and $\chi_{\mathbf{v}}(t)$ are related to each other through [20]

$$\chi_{\mathbf{q}}(t) = 1 - \gamma^2 \int_0^t dt\ \chi_{\mathbf{v}}(s). \tag{29}$$

The full statistical description of the quasiclassical LE requires knowing its probability distribution. In particular, we are not interested in using the distribution in the whole phase space, already derived by Schramm *et al.* [14], but its reduced version in the position space $p(q,t|q_0,t_0)$. The procedure is fully described in a previous work [13] which adapted to the moving harmonic potential gives

$$p(k,t|k_0) = \frac{1}{\sqrt{2\,\pi[\sigma^2(t)]_k}}\exp\left[-\frac{[q - f_k[\lambda](t)]^2}{2[\sigma^2(t)]_k}\right], \tag{30}$$

with $k = \{q, q_{\rm ov}\}$ and for short $f_k[\lambda](t) = \langle k[\lambda](t)\rangle$. All initial velocity states were averaged over the Maxwell distribution. It is also the reduced Wigner function or reduced matrix of the system [13].

The procedure to obtain the standard deviation $[\sigma^2(t)]_k$ is derived in Ref. [13]. It is given as a combination of the different noise correlation functions and becomes independent on the protocol $\lambda(t)$, i.e.,

$$[\sigma^2(t)]_q = 2\int_0^t dt'\Bigg[\int_0^{t'} dt''\langle\varphi_{\mathbf{v}}(t')\varphi_{\mathbf{v}}(t'')\rangle + \chi_{\mathbf{q}}(t')\langle\varphi_{\mathbf{v}}(t')q_0\rangle\Bigg] + T^\star\chi_{\mathbf{v}}^2(t). \tag{31}$$

Function $[\sigma^2(t)]_{q_{\rm ov}}$ is obtained by replacing $\varphi_{\mathbf{v}}$ by $\varphi_{\rm ov}$ and $\{\chi_{\mathbf{q}}, \chi_{\mathbf{v}}\}$ by $\chi_{\rm ov}$.

Having completed the statistical description of the LE, we proceed to analyze the thermodynamics, the optimization of the work, and, finally, the determination of the optimal protocol.

III. OPTIMAL PROTOCOLS

This section will cover in the first place the derivation of the OP for any value of the damping constant. Subsequently, a more general derivation for the underdamped and a brief discussion about the different jumps appearing in the OP are presented.

A. General protocol

The fundamental thermodynamic equations employed here are those of Esposito *et al.* [12] derived in a time-independent basis. They assume that a general external field acts only on the particle and that the bath and interaction Hamiltonians are time independent. This can be justified in the limit where a large number of quantum harmonic oscillators of the bath weakly interact with the particle.

Using the subindex **S** to identify the particle, and according with the first law, the main equation for the work $W_{\mathbf{S}}$ in the time interval $(0, t_{\mathbf{f}})$ in which the protocol is applied is defined as [12]

$$W_{\mathbf{S}} = \int_0^{t_{\mathbf{f}}} dt\left\langle\frac{dH_{\mathbf{S}}(t)}{dt}\right\rangle, \tag{32}$$

where the trace is over the reduced matrix of the system or the position conditional probability distribution.

If the external field is the harmonic moving potential, then the particle Hamiltonian $H_{\mathbf{S}}(t)$ reads

$$H_{\mathbf{S}}(t) = \tfrac{1}{2}[v^2 + [q - \lambda(t)]^2]. \tag{33}$$

Substituting this equation in Eq. (32) and using Eq. (30) to determine the trace gives

$$W_{\mathbf{S}}[\lambda,\dot\lambda] = \int_0^{t_{\mathbf{f}}} dt\ \dot\lambda(t)[\lambda(t) - \langle q[\lambda](t)\rangle], \tag{34}$$

where the functional dependence of $W_{\mathbf{S}}$ on $\lambda(t)$ and its derivative have been written explicitly. This is the central equation from which the optimal protocol is obtained.

The functional given by Eq. (34) has a local $W_{\rm lo}$ contribution depending linearly on the protocol and its derivative and, a nonlocal $W_{\rm nl}$ part through the integral over $\lambda(t)$ contained in $\langle q[\lambda](t)\rangle$. Its first variation has been deducted before [2]. Instead, we use the equivalent version for the functional Lagrange formalism for the time-nonlocal Lagrangian due to Ferialdi and Bassi [23]. It is given as the sum $\delta W_{\mathbf{S}} = \delta W_{\rm lo} + \delta W_{\rm nl}$ of the local and nonlocal contributions. Each one has an integrand involving a conventional Euler-Lagrange equation for the functional under consideration. That is,

$$\delta W_{\mathbf{q}} = \int_0^{t_{\mathbf{f}}} dt\left[\frac{\partial\mathcal{L}_{\mathbf{q}}[\lambda,\dot\lambda,t]}{\partial\lambda} - \frac{d}{dt}\frac{\partial\mathcal{L}_{\mathbf{q}}[\lambda,\dot\lambda,t]}{\partial\dot\lambda}\right]\delta\lambda(t), \tag{35}$$

with $q = \{\rm lo, nl\}$ and

$$\mathcal{L}_{\rm lo}[\lambda,\dot\lambda,t] = \dot\lambda(t)[\lambda(t) - q_0\,\chi_{\mathbf{q}}(t)], \tag{36}$$

$$\mathcal{L}_{\rm nl}[\lambda,\dot\lambda,t] = -\dot\lambda(t)\int_0^t dy\ \chi_{\mathbf{v}}(t-y)\lambda(y). \tag{37}$$

The $[\lambda,\dot\lambda]$ dependence on $W_{\mathbf{q}}$ was suppressed for compactness.

Calculating the corresponding functional derivatives and setting $\delta W_{\mathbf{S}}[\lambda,\dot\lambda] = 0$, it is found that the optimal protocol must comply with the following integral equation (see the Appendix for details of the derivation),

$$\gamma^2\int_0^t dy[\dot\chi_{\mathbf{v}}(t-y) - \chi_{\mathbf{v}}'(y-t)]\lambda(y) = -q_0\,\dot\chi_{\mathbf{q}}(t) + \gamma^2\lambda_{\mathbf{f}}\,\chi_{\mathbf{v}}(t_{\mathbf{f}}-t) - \gamma^2 \times\int_0^{t_{\mathbf{f}}} dy\,\chi_{\mathbf{v}}'(y-t)\lambda(y), \tag{38}$$

where $\chi'_{\mathbf{v}}(y)$ represents the derivative with respect to y. This is the first main result of this proposal.

From the preceding equation, the second functional derivative of W_{s} with respect to $\lambda(t)$ gives $\dot{\chi}_{\mathbf{v}}(0)$ which, according Eq. (27), is equal to 1 because $\dot{\chi}_{\mathbf{v}}(0) = 0$. Therefore, W_{s} reaches a minimum.

Although Eq. (38) is at first sight an intimidating integral equation, its solution can be obtained by taking its Laplace transform.

Defining the functions

$$A_1(t) = q_0 \dot{\chi}_{\mathbf{q}}(t), \tag{39a}$$

$$A_2(t) = \gamma^2 \lambda_{\mathbf{f}} \chi_{\mathbf{v}}(t_{\mathbf{f}} - t), \tag{39b}$$

$$A_3(t, y) = \gamma^2 \chi'_{\mathbf{v}}(y - t), \tag{39c}$$

$$A_4(t - y) = \gamma^2 [\dot{\chi}_{\mathbf{v}}(t - y) - \chi'_{\mathbf{v}}(y - t)], \tag{39d}$$

the Laplace transform of Eq. (38) becomes

$$\widehat{\lambda}(s) = \frac{1}{\widehat{A_4}(s)} \left[\lambda_{\mathbf{f}} \widehat{A}_2(s) - \widehat{A}_1(s) - \int_0^{t_{\mathbf{f}}} dy \, \widehat{A}_3(s, y) \, \lambda(y) \right], \tag{40}$$

which allows us to get the protocol $\lambda(t)$ in the whole interval $t \in [0, t_{\mathbf{f}}]$ by inverting the different products involving the transforms $\widehat{A}_j(s)$ [22]. However, because of the fixed values $\lambda(0) = \lambda_0 = 0$ and $\lambda(t_{\mathbf{f}}) = \lambda_{\mathbf{f}}$, the protocol $\lambda(t)$ becomes a piecewise function. Thus, the inverted transform is restricted to the interval $t \in (0, t_{\mathbf{f}})$ and we can finally write the optimal protocol as given by the function

$$\lambda(t) = \begin{cases} 0, & t \leqslant 0, \\ f(t), & 0 < t < t_{\mathbf{f}}, \\ \lambda_{\mathbf{f}}, & t \geqslant t_{\mathbf{f}}, \end{cases} \tag{41}$$

where $f(t)$ is the result of the inversion of $\widehat{\lambda}(s)$. The former requires us to substitute first $\chi_{\mathbf{q}}(t)$ and $\chi_{\mathbf{v}}(t)$ by their definitions. Making the due symbolic operations [22], the optimal protocol $\lambda(t) = f(t)$ in the interval $t \in [0^+, t_{\mathbf{f}}^-]$ is finally given by

$$\lambda(t) = B_1(t, t_{\mathbf{f}}^-, \lambda_{\mathbf{f}}) + \int_{0^+}^{t_{\mathbf{f}}^-} dy \, B_2(t, y) \lambda(y), \tag{42}$$

where the functions $B_1(t, t_{\mathbf{f}}^-, \lambda_{\mathbf{f}})$ and $B_2(t, y)$ are defined as

$$\begin{aligned} B_1(t, t_{\mathbf{f}}^-, \lambda_{\mathbf{f}}) = {} & \frac{1}{32\gamma^3\omega} \{4\gamma^2 [q_0 \gamma \omega (\gamma^2 - \omega^2) + e^{-\gamma(\gamma+\omega)t_{\mathbf{f}}^-/2} \lambda_{\mathbf{f}} [(\gamma + \omega)^2 e^{\gamma\omega t_{\mathbf{f}}^-} - (\gamma - \omega)^2]] \\ & + \gamma^3 (\gamma^2 - \omega^2) [2\lambda_{\mathbf{f}} e^{-\gamma(\gamma+\omega)t_{\mathbf{f}}^-/2} [(\gamma + \omega) e^{\gamma\omega t_{\mathbf{f}}^-} - \gamma + \omega] - 2q_0 \omega (\gamma^2 - \omega^2)] t + 4\gamma [2\lambda_{\mathbf{f}} e^{-\gamma(\gamma+\omega)t_{\mathbf{f}}^-/2} \\ & \times [\gamma + \omega - (\gamma - \omega) e^{\gamma\omega t_{\mathbf{f}}^-}] - q_0 \omega (\gamma^2 - \omega^2)] \delta(t) + [16\lambda_{\mathbf{f}} (1 - e^{\gamma\omega t_{\mathbf{f}}^-}) e^{-\gamma(\gamma+\omega)t_{\mathbf{f}}^-/2}] \dot{\delta}(t)\}, \end{aligned} \tag{43}$$

$$\begin{aligned} B_2(t, y) = {} & \frac{e^{-\gamma(\gamma_+ + \omega)y/2}}{32\,\gamma^2\,\omega} \{[2\,\gamma^2\,(\gamma^2 - \omega^2)(\gamma + \omega)(e^{\gamma\omega y} - 1)] + [\gamma^3 (\gamma^2 - \omega^2)^2 (e^{\gamma\omega y} - 1)] t \\ & + 4\,\gamma [(\gamma + \omega)^2 - (\gamma - \omega)^2 e^{\gamma\omega y}] \delta(t) + [8[\gamma + \omega - (\gamma - \omega) e^{\gamma\omega y}]] \dot{\delta}(t)\}. \end{aligned} \tag{44}$$

Unlike previous work where the optimal protocol depends on the initial and final particle velocity through the Dirac delta function, it now becomes visible that it also depends on its derivative or equivalently of its acceleration. It is a consequence of the variational optimization carried out on the inertial Langevin equation.

In Eq. (44), the kernel $B_2(t, y)$ appears to be factorized as the sum of the product of a simple pair of functions $M_j(y)$ and $N_j(t)$. This feature will allow us to get the solution of the integral equation, Eq. (42), through the well-known textbook method of separable kernels [24]. After doing this procedure, the optimal protocol can be written for any γ as the general equation

$$\lambda(t) = \begin{cases} 0, & t \leqslant 0, \\ B_1(t, t_{\mathbf{f}}^-, \lambda_{\mathbf{f}}) + \sum_{j=1}^{4} N_j(t) C_j, & 0 < t < t_{\mathbf{f}}, \\ \lambda_{\mathbf{f}}, & t \geqslant t_{\mathbf{f}}, \end{cases} \tag{45}$$

where the constants $C_j = \int_{0^+}^{t_{\mathbf{f}}^-} dy \, M_j(y) \lambda(y)$ obey the linear system of equations $C_i - \sum_j C_j A_{ij} = B_i$ where the matrix elements are $A_{ij} = \int_{0^+}^{t_{\mathbf{f}}^-} dt \, N_j(t) M_i(t)$ and vectors $C_i = \int_{0^+}^{t_{\mathbf{f}}^-} dt \, M_i(t) \lambda(t)$ and $B_i = \int_{0^+}^{t_{\mathbf{f}}^-} dt \, B_1(t, t_{\mathbf{f}}, \lambda_{\mathbf{f}}) M_i(t)$, respectively [24]. This is the second major result.

Special care should be taken on the singularity for the critical case when the frequency $\omega = 0$.

Having determined the OP, Eq. (34) can be integrated by parts to give the general result

$$W_{\mathbf{S}} = \frac{\lambda_{\mathbf{f}}^2}{2} - \lambda_{\mathbf{f}} \langle q(t_{\mathbf{f}}) \rangle + \int_{0^+}^{t_{\mathbf{f}}^-} dt \, \lambda(t) \langle \dot{q}(t) \rangle + \lambda_{\mathbf{f}} \int_{t_{\mathbf{f}}^-}^{t_{\mathbf{f}}} dt \langle \dot{q}(t) \rangle. \tag{46}$$

The equations defining $B_1(t, t_{\mathbf{f}}^-, \lambda_{\mathbf{f}})$, $B_2(t, y)$, and the protocol given by Eq. (45) are linear functions of time. The extra jumps in the velocity and acceleration have no effect in the calculation of $W_{\mathbf{S}}$. This is equivalent to saying that the work calculation requires a protocol with an optimal offset velocity. An experimental optical trap moved at a constant velocity is expected to generate a behavior on the mechanical work with the same characteristics as that described in this article, but it would not be optimum.

B. Overdamped protocol

Applying the nonlocal optimization procedure to the functional work equation, the resulting protocol obeys an integral

equation similar to Eq. (38). It reads as

$$2\lambda^{\rm ov}(t) - \lambda_{\mathbf{f}} e^{-(t_{\mathbf{f}}-t)} - q_0 e^{-t} - \int_{0^+}^{t_{\mathbf{f}}^-} dy e^{(t-y)}\lambda^{\rm ov}(y) + 2\int_{0^+}^{t} dy \sinh(t-y)\lambda^{\rm ov}(y) = 0. \quad (47)$$

It is also almost equal to that of Ref. [2] except for the additional term $q_0\dot{\chi}_{\mathbf{q}}(t)$ which in Ref. [2] has been averaged over the initial position distribution, which in that case is zero. We keep it as it will be discussed in Sec. V. Equation (47) also proves the equivalence of the Euler-Lagrange equations derived by Then and Engel [2] and the one used in this proposal by Ferialdi and Bassi [23].

Instead of solving the integral equation as in Ref. [2] we use again the Laplace transformation method. It gives

$$\widehat{\lambda}^{\rm ov}(s) = \frac{1}{2\,s^2}\left[q_0(s-1) + (s+2) \times \left(\lambda_{\mathbf{f}} e^{-t_{\mathbf{f}}} + \int_0^{t_{\mathbf{f}}} dy\, e^{-y}\,\lambda(y)\right)\right]. \quad (48)$$

Inverting the transform gives $\lambda^{\rm ov}(t)$ [22].Then, adapting the result for $t \in [0^+, t_{\mathbf{f}}^-]$, we have that

$$\lambda^{\rm ov}(t) = \frac{1}{2}\left[q_0 + \lambda_{\mathbf{f}} e^{-t_{\mathbf{f}}} + (\lambda_{\mathbf{f}} e^{-t} - q_0)t + (1+t)\int_{0^+}^{t_{\mathbf{f}}^-} dy\, e^{-y}\lambda^{\rm ov}(y)\right]. \quad (49)$$

Applying the method mentioned before [24] to solve this integral equation, the overdamped optimal protocol is given by

$$\lambda^{\rm ov}(t) = \begin{cases} 0, & t \leqslant 0, \\ \frac{(\lambda_{\mathbf{f}}-q_0)t+\lambda_{\mathbf{f}}+q_0(t_{\mathbf{f}}+1)}{t_{\mathbf{f}}+2} & 0 < t < t_{\mathbf{f}}, \\ \lambda_{\mathbf{f}} & t \geqslant t_{\mathbf{f}}. \end{cases} \quad (50)$$

The result $\lambda^{\rm ov}(t) = t(t_{\mathbf{f}}+1)/(t_{\mathbf{f}}+2)$ of Refs. [1,2] for $0 < t < t_{\mathbf{f}}$ is recovered if $q_0 = 0$.

Substituting Eq. (50) in the derivative of Eq. (22) gives $\langle \dot{q}(t)\rangle$. Using this result into Eq. (46) with the replacement of $\lambda(t)$ by Eq. (50) gives the final analytical expression for the overdamped work, i.e.,

$$W_{\mathbf{S}}^{\rm ov} = \frac{2\,\lambda_{\mathbf{f}}^2 - 4\,q_0\,\lambda_{\mathbf{f}} - q_0^2\,t_{\mathbf{f}}}{2(t_{\mathbf{f}}+2)}. \quad (51)$$

C. Protocol jumps

For the parameter set $\{q_0, \lambda_{\mathbf{f}} \neq q_0, t_{\mathbf{f}}\}$, the numerical solution of Eq. (41) is a linear function of time with initial jumps in the velocity and acceleration. It has the general form $\lambda(t) = a + b\,t + c\,\delta(t) + d\,\dot{\delta}(t)$ with $\{a, b, c, d\}$ being constants. In order to get the final equilibrium state it is necessary to incorporate the delta functions $\delta(t - t_{\mathbf{f}})$ and $\dot{\delta}(t - t_{\mathbf{f}})$ in the protocol. The jumps are asymmetric since $\Delta\lambda_0 = [\lambda(0^+) - \lambda_0]$ and $\Delta\lambda_f = [\lambda_{\mathbf{f}} - \lambda(t_{\mathbf{f}}^-)]$ are different for off-centered initial positions.

Furthermore, the symmetry of the potential leads us to consider a small set of parameters to seize the essence of the problem. For simplicity we choose $q_0 = \{0, 1\}$ and $\lambda_{\mathbf{f}} = \{-1, 0, 1\}$, taking care that the combination $q_0 = \lambda_{\mathbf{f}}$ is excluded. It reduces the analysis to $\{0, 1, t_{\mathbf{f}}\}$, $\{1, -1, t_{\mathbf{f}}\}$, and $\{1, 0, t_{\mathbf{f}}\}$, respectively.

Defining the asymmetric ratio $J = \Delta\lambda_f/\Delta\lambda_i$ and $m = 1$ for $\lambda_{\mathbf{f}} = 1$ and $m = -1$ for $\lambda_{\mathbf{f}} = \{0, -1\}$, then the protocol becomes

$$\lambda(t) = a + b\,t + c[\delta(t) - J\,m\,\delta(t - t_{\mathbf{f}})] + d[\dot{\delta}(t) - J\,m\,\dot{\delta}(t - t_{\mathbf{f}})], \quad 0 < t < t_{\mathbf{f}}. \quad (52)$$

The algorithm applied to the overdamped regime reproduces the analytical jumps $\Delta\lambda_{\mathbf{f}} = (\lambda_{\mathbf{f}} - q_0)/(t_{\mathbf{f}} + 2)$ and $\Delta\lambda_i = [\lambda_{\mathbf{f}} + q_0(t_{\mathbf{f}} + 1)]/(t_{\mathbf{f}} + 2)$. The numerical optimal work is unresponsive to the final jumps.

IV. HIGH-TEMPERATURE LIMIT

It is a fact that the semiclassical LE must reduce to its classical version in the high-temperature limit. Although the equations above can be either applied in the determination of the work for the classical and semiclassical, it is not the case for the heat because it depends on the standard deviation of the distribution [9]. The procedure to get the heat involved is more elaborated and tedious than that of the work. The former involves one to solve the corresponding heat equation described in Ref. [12]. Nonetheless, it is imperative to show first that the well-known classical limit of the position correlation must be obtained from the semiclassical LE. It will serve as indirect proof that the work in the two descriptions is the same, but it would not be the case for the energy change and the heat exchange. This section provides an alternate method to show the explicit derivation of this function and the standard deviation in the prescribed limit when $\lambda(t) = 0$.

Grabert *et al.* [15] showed that the corresponding quasiclassical equation of motion of their functional integral approach is the quasiclassical generalized Langevin equation,

$$\ddot{q}(t) = -\int_0^t dy\,\Gamma(t-y)\dot{q}(y) - \frac{\partial V(q,t)}{\partial t} + \xi(t), \quad (53)$$

where $\Gamma(t)$ is the time-dependent damping kernel of the fluid. At high temperature it is related to the noise spectrum by Kubo's second fluctuation-dissipation theorem $\langle \xi(t)\xi(s)\rangle = T^\star\Gamma(|t-s|)$. It agrees with the classical version of Refs. [25,26].

For the moving harmonic potential, the probability density associated to Eq. (53) is Eq. (30) with $\sigma^2_{\dot{\mathbf{Q}}}(t)$ replaced with the proper definition of the correlation $\langle\varphi_{\mathbf{v}}(t)\varphi_{\mathbf{v}}(s)\rangle$ and setting $\langle\varphi_{\mathbf{v}}(t)q_0\rangle = 0$. The noise correlation function reads

$$\langle\varphi_{\mathbf{v}}(t)\varphi_{\mathbf{v}}(s)\rangle = T^\star\int_0^t dx\,\dot{\chi}_{\mathbf{v}}(t-x)\int_0^s ds\,\dot{\chi}_{\mathbf{v}}(s-y)\Gamma(|x-y|). \quad (54)$$

They are found by replacing γ in the LE's susceptibilities by the Laplace transform $\widehat{\Gamma}(s)$ of the memory kernel as described in Ref. [20].

The noise correlation $\langle\varphi_{\mathbf{v}}(t)\varphi_{\mathbf{v}}(s)\rangle$ can be solved by adapting the procedure developed by Fox [27] to solve the double integral by taking a double Laplace transform. Replacing the

$\chi_{\mathbf{v}}(t)$ appearing in the original by its derivative gives

$$\langle\varphi_{\mathbf{v}}(t)\varphi_{\mathbf{v}}(s)\rangle = T^{\star}[\dot{\chi}_{\mathbf{v}}(t-s) - \dot{\chi}_{\mathbf{v}}(t)\dot{\chi}_{\mathbf{v}}(s) - \chi_{\mathbf{v}}(t)\chi_{\mathbf{v}}(s)]. \tag{55}$$

Then, according Eq. (31), the standard deviation of the probability density function (pdf) reads after some algebra as

$$\sigma^2_{\mathrm{GLE}}(t) = 2\,T^{\star}\int_0^t dt'\,\chi_{\mathbf{v}}(t')\chi_{\mathbf{q}}(t'), \tag{56}$$

where $\chi_{\mathbf{q}}(t) = 1 - \int_0^t ds\,\chi_{\mathbf{v}}(s)$ was used in the derivation. It differs with Eq. (29) in the factor γ^2 because the equation of motion was written in the timescale different from that of Eq. (1).

In the Ohmic case, the classical Markovian pdf is still given by Eq. (30), that is,

$$p_{\mathrm{CL}}(q,t|q_0) = \frac{1}{\sqrt{2\,\pi\,\sigma^2_{\mathrm{CL}}(t)}}\exp\left[-\frac{(q-\langle q[\lambda](t)\rangle)^2}{2\,\sigma^2_{\mathrm{CL}}(t)}\right], \tag{57}$$

with $\langle q[\lambda](t)]\rangle = q_0\,\chi_{\mathbf{q}}(t) + \int_0^t dx\,\chi_{\mathbf{v}}(t-x)\lambda(x)$. It agrees with the findings of Chandrasekhar [28] and Adelman *et al.* [25] letting $\lambda(t) = 0$. The classical standard deviation $\sigma^2_{\mathrm{CL}}(t)$ is given by Eq. (31) which after after the proper substitutions of $\chi_{\mathbf{q}}(t)$ and $\chi_{\mathbf{v}}(t)$ [20] gives

$$\sigma^2_{\mathrm{CL}}(t) = T^{\star}\left[1 - e^{-\gamma t}\left(\cosh\left[\frac{\omega\,t}{2}\right] + \frac{\gamma}{\omega}\sinh\left[\frac{\omega\,t}{2}\right]\right)^2\right], \tag{58}$$

agreeing with previous results [13,29].

This result demonstrates by an alternative method that Langevin's semiclassical Ohmic equation is correctly reduced to the classical one at high temperatures when $\lambda(t) = 0$. Since the equations derived above for the moving harmonic potential are independent of the standard deviation, they are the same regardless of the regime in which they are applied. On the contrary, it would not be the case for the energy change $\Delta E = \langle H_{\mathbf{S}}(t_{\mathbf{f}})\rangle - \langle H_{\mathbf{S}}(0)\rangle$ and the heat $Q = \int_0^{t_{\mathbf{f}}} dt\int_{-\infty}^{\infty} dq\,H_{\mathbf{S}}(t)\,\dot{p}(q,t|q_0)$ [12] because both depend on the standard deviation which is different in the two descriptions.

V. DISCUSSION OF RESULTS

This section will show the results for the mechanical work as a function of the friction coefficient γ and system parameters $\{q_0, \lambda_{\mathbf{f}}\}$. First, we state the importance of the magnitude of γ on the physics behind the calculation of the thermodynamic work, and second, the discussion of the results.

The chosen set of γ values is arbitrary and spans magnitudes above and below of $\gamma = 2$ where ω vanishes. They are those of Ref. [30]. It will allow us to consider the behavior of the optimal protocol and work in the periodic ($\gamma < 2$; ω imaginary), critical ($\gamma = 2$; $\omega = 0$), and $\gamma > 2$ systems.

The critical $\gamma = 2$ defines the limit where the periodic and aperiodic modes meet [31].

The periodic regime presents serious anomalies not found for $\gamma \geqslant 2$. Among others, the diffusion is anomalous [32,33], the mobility can be negative [34], showing poles and discontinuities at specific times [30], a local heating of the particle [35], and the appearance of time oscillatory behavior in the work distribution function for masses larger than a nonzero critical value [36]. These anomalies have an important impact on the behavior of the optimal work for imaginary ω ($\gamma < 2$) in comparison with γ values when ω is real.

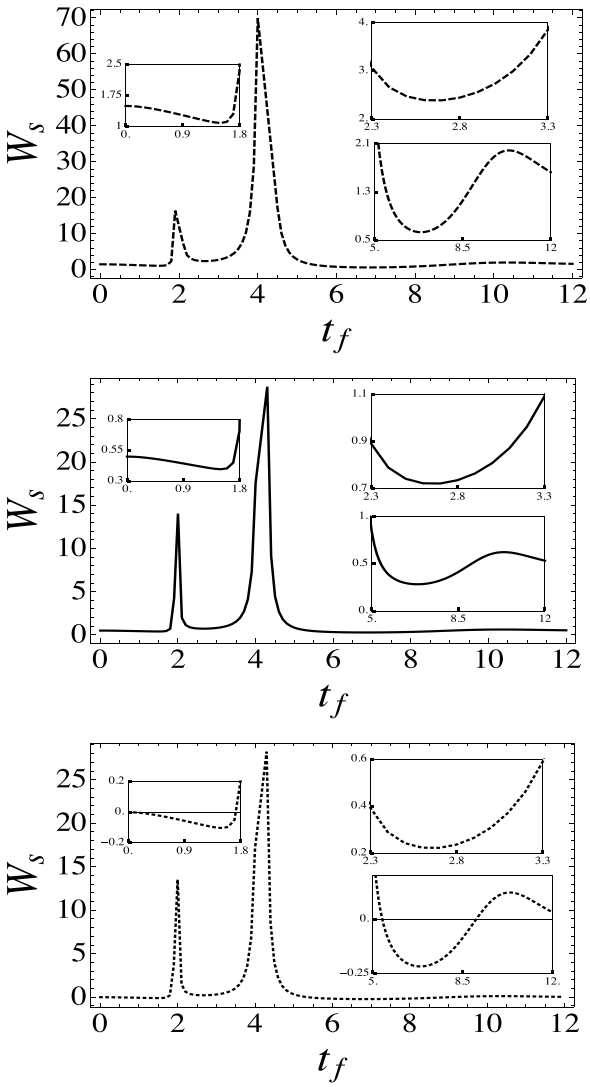

FIG. 1. Optimal work $W_{\mathbf{S}}$ for $\gamma = 1$. Parameter values $\{q_0, \lambda_{\mathbf{f}}\}$ are $\{1,-1\}$ (top dashed), $\{0,1\}$ (middle solid), and $\{1,0\}$ (bottom dotted). The insets show the regions out of the discontinuities.

Figure 1 show the results for $\gamma = 1$ and parameter sets $\{q_0\lambda_{\mathbf{f}}\}$ of $\{1,-1\}$ (top dashed), $\{0,1\}$ (middle solid), and $\{1,0\}$ (bottom dotted) values which, by symmetry considerations, compile all possible combinations of the parameters. The insets amplify the main figure out of the discontinuities.

The effects of the field on a system with the aforementioned anomalies are manifested in the physical properties that depend on them. As the protocol application time increases, the mechanical work shows discontinuities, maxima, and minima. It is not obvious and it is a difficult task to give a specific physical explanation for these behaviors. Instead, we can generally attribute them to the cooperative effects of anomalies in the dynamics without giving any specific physical origin. Despite this, the origin of the discontinuities and extremal points could be explained mathematically since the work depends

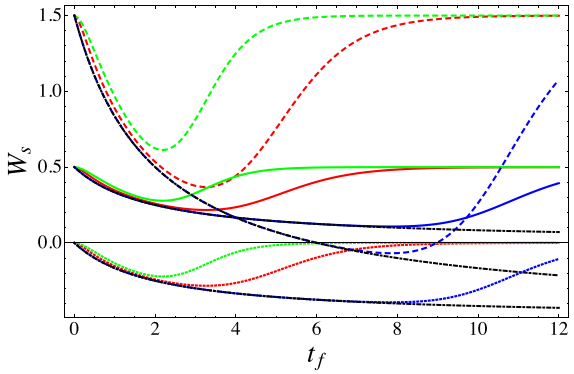

FIG. 2. Optimal work $W_{\mathbf{S}}$ for $\gamma = 2$ (green), $\gamma = 3$ (red), and $\gamma = 30$ (blue). Parameter sets $\{q_0, \lambda_{\mathbf{f}}\}$ are $\{1, -1\}$ (top curve), $\{0, 1\}$ (middle curve), and $\{1, 0\}$ (bottom curve).

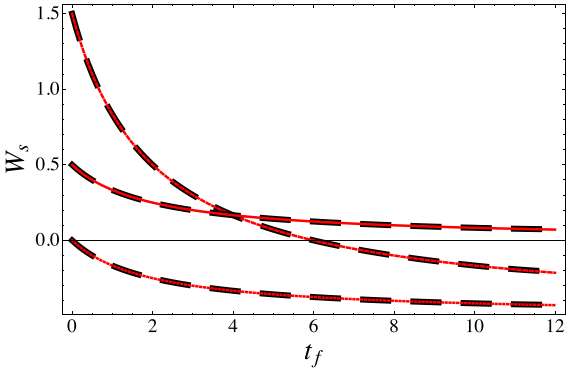

FIG. 3. Overdamped optimal work $W_{\mathbf{S}}$ for $\gamma = 275$ (red) and that from Eq. (51) (black). Parameter values $\{q_0, \lambda_{\mathbf{f}}\}$ the same as in Fig. 2.

on an integral proportional to $\lambda(t)$. The protocol changes its slope at these points with different intensities. Sudden sign slope changes highlight discontinuities, while smooth changes account for the extremal points. It could also be attributed to the direct consequence of the dynamic processes of diffusion and concentration that act periodically on the particle when ω is imaginary. This was demonstrated for the simple harmonic oscillator where the Fokker-Planck equation in the configuration space has a generalized time-dependent diffusion term whose calculation showed periodic sign changes and discontinuities [30]. Although the optimal protocol is independent of the generalized diffusion, it is reasonable to assume that the global dynamics will depend of the conjugation of these two processes.

In general, the work is done by the field except in the $\{1, 0\}$ set that is done by the particle in a restricted time lapse. The last behavior is amplified for higher friction constants, as it will be seen next.

Figure 2 shows the results for real ω. They are $\gamma = 2$ (green), $\gamma = 3$ (red), and $\gamma = 30$ (blue). For a better visualization, the parameter sets are $\{0, 1\}$ (solid), $\{1, -1\}$ (dashed), and $\{1, 0\}$ (dotted). The superimposed dotted-dashed black curve corresponds to the analytical overdamped. It is observed that the agreement of the overdamped improves with the numerical result at short times. From an operational point of view, the overdamped analytical expression could be used as a first approximation at short times. Notice that work can be extracted (dotted red, green, and blue curves) along the protocol application. Apparently there is a violation of the second law. It does not apply in this case because as in Maxwell's demon, information is transformed into work. This comes from the construction of the initial state and not from some measurement made on the system. The latter was rigorously analyzed in Refs. [7,8].

It is an important result than can be experimentally confirmed. In the other cases at short times, the field mainly expends its energy in moving the particle to a location centered in the potential well. Operationally, the overdamped result can be used "with due caution" as an approximation for low damping constants and end times in the range shown by this result. The true nature of the underdamped appears at greater times.

As should be expected, the agreement of the optimal work for $\gamma = 275$ between the numeric LE and Eq. (51) is totally in the overdamped mode, as pointed out by Pan *et al.* in the solution of the extended Kramer's equation including work [31]. It is exemplified in Fig. 3. Although the LE mathematically reduces to the overdamped version for an infinity damping constant, the numerics predicts a minimum such as those of Fig. 2 by increasing the chosen final time, while the overdamped analytic tends to saturate to the value $-q_0^2/2$. This discrepancy at large times shares similarities with the short-time deviation of the mean-squared displacement of a Brownian particle from the classical Einstein relation [37]. The use of the overdamped analytical approach is restricted by this observation, since the numerical result does not converge with the latter for longer end times than those used in the calculations. This theoretical prediction can be evaluated experimentally for γ sufficiently high and appropriate end times.

The choice of the applied protocol is arbitrary. In fact, Albay *et al.* [38] recently made experimental measures on an overdamped classical Brownian particle with a cosine-type driving. They confirm, among other things, the Gaussian character of the pdf along the protocol application and the finding of Li *et al.* [39] that dissipated work done during the driving process always scales with the inverse of the protocol time, a theoretical fact predicted by Schmiedl *el al.* [9] in their work on stochastic engines. So far, experiments have not been performed in the quasiclassical regime.

VI. FINAL REMARKS

Explicit calculations were made for the thermodynamic work of a particle immersed in a thermal fluid that interacts with an off-centered harmonic field without inferring in the heat absorption of the reservoir and its experimental measurement. It was assumed that the external force acts only on the particle and that the potential changes the dynamics, so that the time-dependent configurational pdf is a Gaussian parametrized by the instantaneous mean value of the position, which in turn is a functional of the protocol.

The optimal protocol was consistently derived from the nonlocal Euler-Lagrange approach applied to the work functional. It depends on its final value as an extra parameter.

The Hamiltonians of the thermal reservoir and of interaction are taken as time independents. It could be justified considering a small coupling constant defining the interaction between the Brownian particle and the degrees of freedom of the thermal bath. This is so, because this constant is proportional to the inverse of the volume of the reservoir [40]. In the continuum limit, the friction coefficient is a measure of the system-bath coupling.

In order to further discuss the existence of quantum effects in evaluating W_s one could include the field effects in the Hamiltonian of the bath. This should require the reformulation of both the reduced Wigner function and the general thermodynamic equations, which until now has been an open issue. The information obtained could serve as a basis for the design of experimental measurement protocols. It would also serve as a test of the quasiclassical description to reproduce the classical equations in the high-temperature limit.

Initial states having non-Gaussian initial distributions, whose dynamics do not obey detailed balance and the relative probabilities of microstates are *a priori* unknown, are excluded even in the framework of the path-integral approach used in the derivation of the quasiclassical LE. The work by Wadia *et al.* [41] would give some hints in this respect.

The heat term will largely depend on the theory, be it classical or quasiclassical. The classical Langevin equation is based on position fluctuations assuming a coarse-grained phenomenological noise whose statistical properties are well defined. In contrast, quasiclassical dynamics has the proper unpredictability built into the core of the theory itself. The comprehensive path-integral approach [15] allows us to derive an exact c-number stochastic differential equation in the whole phase space [14] or its reduced version [13]. The Ohmic quasiclassical approach predicts the Langevin equation but with significant differences, namely, the requirement of a quantum entanglement between the noise and the particle initial position, and a random noise function with a colored spectrum even though the friction coefficient of the bath is time independent as in the classical Markovian description. Wigner's function incorporates these facts through its standard deviation and therefore the heat equation will be very different in the two prescriptions.

There are several potential research works on the application of the method described in this article. In the line of the classical Brownian motion analysis, the mean-squared displacement and its relation with the generalized diffusion term [13] appearing in the Fokker-Planck equation associated with Eq. (30) would be studied in the periodic regime. Previous works [32,33] will be essential in the analysis. A second proposal would be the analysis of the effects of the optimal protocol on the work and heat distributions since the protocol is the same regardless of the noise statistics, classical or quasiclassical. Finally, there is a potential application to heat engines. Since the total work depends upon the standard deviation, it could be interesting to study the system with the time-dependent stiffness potential model to compare the protocols obtained by Gomez-Marín *et al.* [3] in the classic LE with those in the quasiclassical regime.

This research, along with Refs. [17,30], is another application of the method developed in Ref. [13] to find the pdf of a particle immersed in an Ohmic quantum thermal reservoir.

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APPENDIX: LOCAL AND NONLOCAL VARIATIONS

The first variation of the nonlocal term of $W_{\mathbf{S}}$ is, according to (37),

$$\delta W_{\rm nl} = -\gamma^2 \int_0^{t_{\mathbf{f}}} dt\, \dot{\lambda}(t) \int_0^t dy\, \chi_{\mathbf{v}}(t-y)\, \delta\lambda(y) - \gamma^2 \int_0^{t_{\mathbf{f}}} dt\, \delta\dot{\lambda}(t) \int_0^t dy\, \chi_{\mathbf{v}}(t-y)\lambda(y).$$

Interchanging the limits of the first double integral and switching $t \leftrightarrow y$,

$$\delta W_{\rm nl} = -\gamma^2 \int_0^{t_{\mathbf{f}}} dt\, \delta\lambda(t) \int_t^{t_{\mathbf{f}}} dy\, \chi_{\mathbf{v}}(y-t)\dot{\lambda}(y) - \gamma^2 \int_0^{t_{\mathbf{f}}} dt\, \delta\dot{\lambda}(t) \int_0^t dy\, \chi_{\mathbf{v}}(t-y)\lambda(y).$$

Integrating by parts the inner term of the first integral it is found

$$\frac{\delta W_{\rm nl}}{\delta\lambda(t)} = \gamma^2\left[-\lambda_{\mathbf{f}}\chi_{\mathbf{v}}(t_{\mathbf{f}}-t) + \int_t^{t_{\mathbf{f}}} dy\, \chi'_{\mathbf{v}}(y-t)\,\lambda(y)\right],$$

and from the second term,

$$\frac{d}{dt}\frac{\delta W_{\rm nl}}{\delta\dot{\lambda}(t)} = -\gamma^2 \int_0^t dy\, \dot{\chi}_{\mathbf{v}}(t-y)\lambda(y).$$

Therefore after splitting the interval $\{t, t_{\mathbf{f}}\}$ gives

$$\frac{\delta W_{\rm nl}}{\delta\lambda(t)} - \frac{d}{dt}\frac{\delta W_{\rm nl}}{\delta\dot{\lambda}(t)} = \gamma^2\left[-\lambda_{\mathbf{f}}\chi_{\mathbf{v}}(t_{\mathbf{f}}-t) + \int_0^{t_{\mathbf{f}}} dy\, \chi'_{\mathbf{v}}(y-t)\,\lambda(y) + \int_0^t dy[\dot{\chi}_{\mathbf{v}}(t-y) - \chi'_{\mathbf{v}}(y-t)]\lambda(y)\right].$$

The local term is just the conventional Euler-Lagrange equation

$$\frac{\partial W_{\rm loc}}{\partial\lambda(t)} - \frac{d}{dt}\frac{\partial W_{\rm loc}}{\partial\dot{\lambda}(t)} = q_0\, \dot{\chi}_{\mathbf{q}}(t).$$

The functional derivative $\delta W_{\rm S}/\delta\lambda(t)$ is the sum of the last two equations. Setting it to zero gives Eq. (38).

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