Optimization of an active heat engine

Giulia Gronchi [1] and Andrea Puglisi [1,2]
[1] *Dipartimento di Fisica, Università di Roma Sapienza, Piazzale Aldo Moro 2, 00185 Rome, Italy*
[2] *Istituto dei Sistemi Complessi, CNR, Piazzale Aldo Moro 5, 00185 Rome, Italy*

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Optimization of heat engines at the microscale has applications in biological and artificial nanotechnology and stimulates theoretical research in nonequilibrium statistical physics. Here we consider noninteracting overdamped particles confined by an external harmonic potential, in contact with either a thermal reservoir or a stochastic self-propulsion force (active Ornstein-Uhlenbeck model). A cyclical machine is produced by periodic variation of the parameters of the potential and of the noise. An exact mapping between the passive and the active model allows us to define the effective temperature $T_{\rm eff}(t)$, which is meaningful for the thermodynamic performance of the engine. We show that $T_{\rm eff}(t)$ is different from all other known active temperatures, typically used in static situations. The mapping allows us to optimize the active engine, regardless of the values of the persistence time or self-propulsion velocity. In particular, through linear irreversible thermodynamics (small amplitude of the cycle), we give an explicit formula for the optimal cycle period and phase delay (between the two modulated parameters, stiffness and temperature) achieving maximum power with Curzon-Ahlborn efficiency. In the quasistatic limit, the formula for $T_{\rm eff}(t)$ simplifies and coincides with a recently proposed temperature for stochastic thermodynamics, bearing a compact expression for the maximum efficiency. A point, which has been overlooked in recent literature, is made about the difficulty in defining efficiency without a consistent definition of effective temperature.

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I. INTRODUCTION

In Ref. [1] Feynman envisioned a microscopic motor working at small scales, even at the single-atom level. Such a motor would be the first step required to achieve the ability of "manipulating and controlling things on a small scale." Sixty years later, Feynman's idea has been realized in several experiments and its theoretical implications have been deeply analyzed [2–4].

A motor is a device that delivers mechanical work, for instance, by pushing a weight in a given direction. Work is obtained by converting a fraction of energy taken from reservoirs; such a fraction represents the motor's efficiency. In the microscopic world, the list of available energy reservoirs is not substantially different from the macroscopic scale, i.e., mainly chemical or electrochemical reservoirs or chemically induced heat reservoirs.[1] In physics of course the choice of heat reservoirs is the one that better stimulates theoretical research as it involves translating principles of thermodynamics to small scales, far from the thermodynamic limit [5]. The challenge with microscopic heat engines is to achieve optimal control of thermal fluctuations, which not only are involved as the energy source and sink (as in macroscopic heat engines) but also spoil the stability and reliability of the delivered work. Microscopic work, and therefore efficiency, is in fact a highly fluctuating quantity [6,7]. The effect (also beneficial) of fluctuations on motor efficiency is one of the most intriguing recent discoveries in the field of stochastic thermodynamics [8].

A. Passive microscopic heat engine

Microscopic heat engines have been at the center of theoretical and experimental research in the past decade. They have been realized with colloidal particles in optical traps, for instance, in Stirling cycles with isochoric and isothermal transformations [2] and Carnot cycles with adiabatic and isothermal transformations [4]. The realization of adiabatic passages (which would require complete isolation of the Brownian particle) is obtained through a protocol, proposed first in theoretical works [9], where both the characteristic volume and temperature of the system are changed in such a way that the entropy of the system is conserved. Heat engines have also been realized at the atomic scale, by manipulating a trapped ion [10]. The exploitation, at the single-atom level, of so-called quantum squeezed states has also been proposed as a way to circumvent the Carnot limit in efficiency [3]. The theoretical research on small-scale engines has involved also the possibility of designing specific cycles with optimal power or efficiency [11]. An important challenge in this field is going beyond the single-particle limit and achieving control or design of systems made of a small number (e.g., 100–1000) of particles, which can be meaningful for biophysical applications [12].

[1] The macroscopic world has additional sources of energy, unfortunately (for our environment) of minor importance for the moment, such as those related to natural macroscopic flows, e.g., air and water.

A severe limitation against a straightforward experimental realization of a heat engine stems from the difficulty of controlling the temperature with due precision, plagued by the unwanted development of gradients and the presence of long relaxation times [5]. A typical work-around is to replace the high-temperature reservoir with a source of noise, e.g., an applied noisy voltage as in [2,4]. A different fascinating possibility is to consider engines made of a different kind of working substances which stay at an *effective temperature* different (typically higher) than the environment or solvent [13]. This can be achieved by means of active particles, i.e., particles which are self-propelled, for instance, bacteria or sperms or active colloids (e.g., Janus particles) [14].

B. Active heat engines

Every active particle has its own internal motor which induces, in the presence of a viscous solvent, a typical speed v_0. Of course v_0 is unrelated to the thermal speed, that is, $v_0 \neq \sqrt{k_B T/m}$, where T is the temperature of the environment, k_B is the Boltzmann constant, and m is the mass of the particle. Most importantly, considering that active microswimmers move through overdamped kinematics, their unconfined diffusivity D_a is typically much larger than molecular diffusivity D, $D_a = \tau_a v_0^2 \gg D = k_B T/\gamma$, with τ_a the active persistence time and γ the viscous drag of the particle [14]. This consideration leads naturally to the definition of a diffusivity-based active temperature $T_D = \gamma D_a/k_B \gg T$. The equilibrium limit $\tau_a \to 0$ is typically taken in such a way that $T_D \to T$, which requires $v_0^2 \to D/\tau_a$.

Early studies and experiments demonstrating the possibility of converting random self-propulsion into directed motion or work have been realized in the realm of active ratchets [15–19], which are autonomous engines. In the most recent years several proposals of cyclical heat engines have been done and in a few cases also experimentally realized.

In [20] an early example of a Stirling engine (two isotherms and two isochores) was obtained, where bacteria were involved as the bath and the central system was made of a trapped colloidal particle: An external control of the solvent temperature was reflected in a variation of the average speed (activity) of the bacteria, measured through tracking the position fluctuations of the colloidal particles. The authors verified that isothermal transformations (compressions and expansions) were also isoactive, i.e., activity did not depend appreciably upon the trap stiffness. The advantage of such a bacterial bath was to achieve a much larger range of effective (active) temperatures than in the passive case.

The concept of an active Stirling engine was investigated in a more recent theoretical study [21]. The authors showed that the performances of the engine depend upon the temperature which is kept fixed during the isothermal transformations: The two candidates considered (here we set $k_B = 1$) are $T_{\rm var} = k\langle x^2\rangle$, as chosen in [20], related to the energy in a harmonic potential of stiffness k, and the diffusion temperature T_D defined above, as proposed in [22]. At equilibrium (i.e., for thermal particles at temperature T) of course $T_{\rm var} = T_D = T$. The authors consider several different models for the bacterial bath (including non-Gaussian effects and/or temporal correlations, i.e., persistence), concluding that if $T_{\rm var}$ is kept constant in isothermal transformations then the equilibrium limit for efficiency (given by the Carnot value) cannot be surpassed, while different things may happen if T_D is adopted for the isothermal branches of the cycle.

Other authors [23] have considered a different theoretical model where the central particle is a self-propelled particle (pushed by a random force with exponentially decaying autocorrelation, with typical time τ_a, as in the active Ornstein-Uhlenbeck particle model, discussed below) immersed in a bath of passive particles. The authors consider both Stirling-type engines (cyclical modulation of temperature and stiffness at fixed τ_a) and engines with modulation of τ_a and stiffness, at fixed temperature. Of course the second case does not have a passive counterpart and therefore there is no direct way to compare performances. It is important to stress that the authors here have decided to connect the thermal bath temperature to the self-propulsion speed, similarly to [20], making it more difficult to disentangle their contributions.

In [24] a new heat engine was proposed where a passive particle is trapped in a harmonic potential with time-dependent stiffness and is put in contact with a thermal bath in the first half of the cycle and with an active bath (time-persistent noise) in the second half. In this paper the relevance of $T_{\rm var}$ as a sort of effective temperature and a general equation for its evolution, for a broad class of choices of the driving noise, were shown (an equation discussed in greater detail in [25]).

In [26] a Stirling engine was considered where the central substance is a particle that changes its nature during the cycle itself, i.e., it is passive for three of the four steps and is an active Ornstein-Uhlenbeck particle (AOUP) during the fourth step, which is isothermal compression. In this paper a higher efficiency (with respect to the passive case) was claimed when activity is present, a fact which evidently depends upon the chosen definition of efficiency.

In [27] the authors considered a model with many active Brownian particles (ABPs), i.e., such that their self-propulsion velocity has fixed magnitude and diffusing orientation. The external potential (which also act on the propulsion's orientation) has many parameters that can be varied. The presence of many of the potential's parameters allows one to design cycles without changing other properties (such as bath temperature or properties of the activity). Efficiency appears to be proportional to the extracted power and both are optimal together.

We conclude this overview of the recent literature with [25], where the authors proposed a general mapping from an active heat engine to a passive heat engine. The mapping can be made explicit when the confining potential is harmonic, and this can be done for whatever model of self-propulsion is proposed: Only the autocorrelation of the self-propulsion affects the evolution of the effective temperature. The authors gave explicit examples of their formalism using an ABP in a harmonic trap, where a Stirling-like cycle is operated by tuning the stiffness, temperature, and parameters of activity (both speed and persistence time). The important point raised by the authors, also relevant for the interpretation of the experiments in [20], is that the effective temperature may change also during the (apparently) isothermal transformations, because it depends upon all the system's parameters.

TABLE I. Main definitions of effective temperatures used in the context of active particle models (in one dimension). We recall that γ is the viscous drag coefficient and k_B the Boltzmann constant, both set to 1 throughout the paper.

Name	Definition	Application
T_D	$\gamma D_a/k_B$	free diffusion [14]
T_{var}	$k\langle x^2\rangle/k_B$	steady states [20]
T_{kin}	$m\langle v^2\rangle/k_B$	steady states with inertia [40]
$T_a(t)$	$\frac{\gamma}{k_B}\frac{v_0^2(t)\tau_a}{[1+\tau_a k(t)]^2}$	dynamical UCNA [38]
$T_{Cl}(t)$	$\frac{\gamma}{k_B}\frac{v_0^2(t)\tau_a}{1+\tau_a k(t)}$	Clausius relation [28,29](and $\lim_{\omega\to 0} T_{\mathrm{eff}}(t)$)
$T_{\mathrm{eff}}(t)$	see Eq. (19)	heat engines [25]

C. The present paper

Here we propose a study which is complementary to that done in [25]. We consider AOUPs which have a natural mapping to passive systems with an active temperature $T_a(t)$, which in fact depends upon the potential's parameters, in the low persistence limit. A recent study of entropy production for AOUPs also revealed the existence of a Clausius relation that connects entropy changes with an active heat flow divided by a temperature $T_{Cl}(t)$ [28,29]. Our main point is that the proper effective temperature $T_{\mathrm{eff}}(t)$, relevant for the thermodynamic behavior of the engine, can be quite different from $T_a(t)$ and $T_{Cl}(t)$, as well as from other temperatures such as T_{var}, T_D, and T_a. Later, in Table I, we summarize some of the most used definitions of temperatures in this context.

The knowledge of the correct effective temperature is crucial to optimize the engine's performance, for instance, of its delivered power. As an explicit application of this concept, we show how to achieve maximum power by tuning T_{eff} through the control of self-propulsion speed, a possibility which has been experimentally realized recently with light-controlled bacteria [17,30] and colloids [31].

Let us summarize the structure of the paper. In Sec. II we introduce a few standard thermodynamic tools which are useful for finite-size and finite-time thermodynamics (i.e., when models are stochastic and the period of a cyclic transformation is not infinite). In this section we briefly discuss the definition of heat flow coming from the high-temperature thermostat, which is important for nonactive systems and becomes even more important for active heat engines where the temperature is not directly under control. In Sec. III we present the passive and active models investigated in the paper, showing the mapping that makes them equivalent from the point of view of heat engine performances [25]. In Sec. IV we study the periodic heat engine model with only passive particles, particularly in the limit of linear irreversible thermodynamics, deriving a few results which are complementary to those given for the same model in [32]. In Sec. V we show how to transfer the knowledge of the passive engine to optimize the active one. In Sec. VI we summarize and provide conclusions and perspectives for future work.

II. WORK AND HEAT FOR MICROSCOPIC (PASSIVE) HEAT ENGINES

In the context of microscopic engines, basic thermodynamic concepts, such as heat and work, need a definition in terms of stochastic quantities, even if only averages are needed. For simplicity we consider models with a single (passive or active) particle in a solvent fluid which is viscous enough to make inertia negligible. The particle therefore obeys dynamical equations which result from some external potential $\mathcal{H}(\mathbf{x}, \lambda_t)$, thermal fluctuations, and self-propulsion (in the active case). An external agent can control the parameters λ_t of the potential and also the properties of the thermal bath and the active self-propulsion; in doing so, it performs or extracts work. In stochastic thermodynamics the definition of the stochastic work injection rate (or injected power) is related to the variation of the external potential [33,34], i.e.,

$$\dot{W} = \sum_i \frac{\partial \mathcal{H}}{\partial \lambda_i}\dot{\lambda}_i = \frac{\partial \mathcal{H}}{\partial t}. \tag{1}$$

Instantaneous (stochastic) heat exchange is defined for complementarity from work [35], i.e.,

$$\dot{Q} = \frac{dH}{dt} - \dot{W}, \tag{2}$$

so the first principle is guaranteed. When the parameters λ_t are tuned according to a cyclical protocol, i.e., $\lambda_{t+t_{\mathrm{cycle}}} = \lambda_t$ with t_{cycle} the machine period, most of the models and the initial conditions lead to a limit cycle where averages are periodic with the same period t_{cycle}. It is then meaningful to consider the average work integrated in a period

$$W_p = \int_{t_0}^{t_0+t_{\mathrm{cycle}}} dt\,\langle \dot{W}\rangle, \tag{3}$$

where t_0 is a time large enough to consider the system in the limit cycle. We recall that, in our notation, W_p must be negative to have a working machine.

A. Adsorbed heat

For the purpose of computing the engine's efficiency, it is crucial to define a measure of energy consumption through heat

$$Q_h = \int_{t_0}^{t_0+t_{\mathrm{cycle}}} dt\, w_{\mathrm{ads}}(t)\langle \dot{Q}\rangle, \tag{4}$$

where $w_{\mathrm{ads}}(t) \in [0, 1]$ is a (periodic) weighting function that discriminates how much heat is to be considered as energy gain, while the remaining fraction $1 - w_{\mathrm{ads}}(t)$ is to be considered as dissipation. We believe that a good choice (and a good understanding) of $w_{\mathrm{ads}}(t)$, even in the framework of passive, not active, particles, deserves a brief discussion, since it seems that there is not unanimous agreement about it in the literature, even in recent works. In Carnot's original heat engine, there are two well-defined thermostats, i.e., one at high temperature T_h and one at low temperature T_c, with adiabatic connections; then heat is only adsorbed when in contact with T_h and is only released when at T_c. This means that one can safely set

$$w_{\mathrm{ads}}(t) = \Theta(\langle \dot{Q}\rangle(t)), \tag{5}$$

where Θ is the Heaviside Theta function [4,36]. However, in more general cases, the definition (5) has drawbacks. For instance, the Stirling engine, even in the quasistatic limit, exchanges heat during the isochoric branches of the cycle, when in contact with intermediate values $T_c < T(t) < T_h$: If

Eq. (5) is adopted, then Q_h receives a contribution also from one of the isochores and the quasistatic efficiency is in general smaller than the Carnot one [2,21]. Such a definition is also problematic from the conceptual point of view, since Q_h should be related to heat flowing from a thermostat to a different one. However, Eq. (5) gives $Q_h > 0$ also when there is a single thermostat, i.e., when Q_h comes from the same thermostat which, considering the whole transformation, dissipates heat. This happens in several examples with a time-dependent Hamiltonian (periodically modulated potential energy) at a constant temperature. Notwithstanding these drawbacks, the definition (5) is frequently adopted [2,20,21,23].[2]

An alternative recipe was offered in [12,32], adopted by us in the present study,

$$w_{\rm ads}(t) = \frac{\beta(t) - \beta_c}{\beta_h - \beta_c}, \tag{6}$$

where $\beta(t) = 1/T(t)$ and $\beta_{c(h)} = 1/T_{c(h)}$. This definition weighs more heat (whatever its sign) coming from higher temperature. Equation (6) is justified by splitting the entropy production into two contributions that depend upon two different thermodynamic forces, one related to the variation of potential energy (which generates work) and one related to the variation of temperature (which generates a heat flux Q_h going through the system from high to low temperature) [32]. Such a recipe also guarantees that in the quasistatic limit the Carnot efficiency $\eta_c = 1 - T_c/T_h$ is always reached, including the Stirling engine.[3] Once work and adsorbed heat are defined, one can define the average power

$$P = \frac{W_p}{t_{\rm cycle}} \tag{7}$$

and the average efficiency

$$\eta = -\frac{W_p}{Q_h}. \tag{8}$$

B. Active-passive equivalence

A fundamental observation can be made for harmonic potentials, i.e., when

$$\mathcal{H}(t) = \tfrac{1}{2}k(t)x^2(t). \tag{9}$$

For such a choice, the average work (and average total heat, which is the opposite of average work, in a period) is known through the knowledge of $\sigma(t) = \langle x^2\rangle$ and $k(t)$ only [25]:

$$W_p = \int_{t_0}^{t_0+t_{\rm cycle}} dt \frac{1}{2}\dot{k}(t)\sigma(t). \tag{10}$$

The same holds true for the instantaneous total heat $\langle\dot{Q}\rangle$; see Eq. (2) as well for its integral over a period. On the contrary and at variance with what was concluded in [25], adsorbed heat

$$Q_h = \int_{t_0}^{t_0+t_{\rm cycle}} dt\, w_{ads}(t)\frac{1}{2}k(t)\dot{\sigma}(t) \tag{11}$$

in general *does not* depend only upon $\sigma(t)$ and $k(t)$, since the definition of $w_{ads}(t)$ could depend upon other parameters; for instance, in the definition adopted by us, Eq. (6), it depends upon $T(t)$.

III. PARTICLE MODELS

In this section we discuss the model of active (and passive) particles and the adopted cycle for the heat engine we want to study. We stick to a harmonic potential with time-dependent stiffness and we adopt the AOUP model for self-propulsion.

A. Passive model

As a reference, we consider first an overdamped passive particle with time-dependent diffusivity $D(t) = \frac{k_B T(t)}{\gamma}$. We choose units such that the viscous drag γ and the Boltzmann constant k_B are both set to 1. The model then reads

$$dx(t) = -k(t)x(t)dt + \sqrt{2T(t)}dw(t), \tag{12}$$

where $x(t)$ is particle's position at time t, $k(t)$ is the time-dependent harmonic stiffness, and $dw(t)$ is the infinitesimal increment of the Wiener process. The model has been studied in detail in [11]. The model has a Gaussian propagator and in the absence of drifts and initial displacements its dynamics is fully described by the variance of the position $\sigma(t)$, which obeys

$$\dot{\sigma}(t) = -2k(t)\sigma(t) + 2T(t). \tag{13}$$

In the quasistatic limit of $t_{\rm cycle} \to \infty$, one can change the time variable in Eq. (13), defining $s = \frac{t}{t_{\rm cycle}}$ (so that in s the period is 1) and obtaining

$$-2k(s)\sigma(s) + 2T(s) = O(1/t_{\rm cycle}), \tag{14}$$

which of course in the limit $t_{\rm cycle} \to \infty$ gives $\sigma(t) = \frac{T(t)}{k(t)}$.

B. AOUP active model

The AOUP model is considered a good description of a colloid in a bath of swimmers such as bacteria [38]. This model has some properties in common with the ABP model, for instance, the exponentially decaying time correlation of the Cartesian components of the self-propulsion force (but the ABP model has non-Gaussian fluctuations and therefore it is more complicated to get analytical results). The AOUP model has the advantage of being more accessible to calculations; in particular, it has a very well studied approximation in the passive limit (discussed below), where, in the case of constant parameters, it is mapped into a passive model. We will see,

[2]A different definition for Q_h has been proposed recently in the context of active engines coupled with both a steady active bath and a steady thermal bath, which are of course at different temperatures [37]. In that case a cyclical engine can be obtained by tuning in time *two* parameters of the external potential and the proposed definition of adsorbed heat is all the heat exchanged with the active bath, which is positive on average.

[3]With this definition, the entropies produced in a period due to work and heat flux are equal to $S_{{\rm prod},W} = \beta_c W_p$ and $S_{{\rm prod},h} = Q_h(\beta_c - \beta_h)$, respectively [32], so that $\eta = -W_p/Q_h = S_{{\rm prod},W}(\beta_h - \beta_c)/(S_{{\rm prod},h}\beta_c)$. In the quasistatic limit $S_{{\rm prod},W}/S_{{\rm prod},h} = -1$, which leads to the Carnot efficiency $\eta = 1 - \beta_h/\beta_c = \eta_c$.

however, how this mapping is not the proper one to understand the performance of this model as a heat engine.

We consider noninteracting AOUPs (in one dimension) in the hypothesis of large viscosity, that is, inertia is neglected and the dynamics is overdamped. We also neglect the thermal noise (which has a small effect with respect to activity), writing

$$dx(t) = [-k(t)x(t) + f_a(t)]dt,$$
$$df_a(t) = -\frac{1}{\tau_a} f_a(t)dt + \frac{2D_a{}^{1/2}}{\tau_a} dw(t). \tag{15}$$

The role of self-propulsion is played by $f_a(t)$, which is a colored noise with exponentially decaying time correlation (with $t \geqslant s$)

$$\langle f_a(t) f_a(s)\rangle = \frac{D_a}{\tau_a} e^{-(t-s)/\tau_a}, \tag{16}$$

modeling a force which remains persistent for a time of order τ_a. The self-propulsion model has two parameters: the persistence time τ_a and the active diffusivity D_a. In the absence of external potential and if D_a is constant, at large times $t \gg \tau_a$, the particle displays normal diffusivity with coefficient D_a. From it one can define the average self-propulsion speed $v_0(t) = \sqrt{D_a(t)/\tau_a}$. The passive model is recovered taking $\tau_a \to 0$ and $v_0(t) \to \infty$ with $D_a \to D$. The more general case we consider is a time-dependent $D_a(t)$ or $v_0(t)$, a situation which has been demonstrated experimentally, for instance, in [17].

The model in Eqs. (15), being the external potential harmonic, is again a Markovian diffusive model with Gaussian propagator in two variables [39]. Again, in the absence of drifts and initial displacements, the dynamics is fully described by the entries of the covariance matrix that obey the following system of coupled equations:

$$\frac{d\langle f_a^2\rangle}{dt} = -\frac{2}{\tau_a}\langle f_a^2\rangle + \frac{2v_0^2}{\tau_a}, \tag{17a}$$
$$\frac{d\langle x f_a\rangle}{dt} = \langle f_a^2\rangle - \frac{1+\tau_a k}{\tau_a}\langle x f_a\rangle, \tag{17b}$$
$$\frac{d\langle x^2\rangle}{dt} = \dot{\sigma} = -2k\langle x^2\rangle + 2\langle x f_a\rangle. \tag{17c}$$

The latter is equivalent to Eq. (15) of [25] and for a direct comparison with Eq. (13) defines the effective temperature

$$T_{\text{eff}}(t) = \langle x f_a\rangle(t), \tag{18}$$

which is the temperature of the passive system which gives the same $\sigma(t)$ and therefore the same delivered work or power. Remarkably, this expression of T_{eff} is directly proportional to the kinetic temperature $T_{\text{kin}} = m\langle v^2\rangle/d$ (where d is the dimensionality) recently calculated in a static harmonic potential for an inertial AOUP model [40]. Interestingly, it is also proportional to the so-called swim pressure [41,42].

In the present case, $T_{\text{eff}}(t)$ obeys quite a simple differential equation [from combining Eqs. (17a) and (17b)]

$$\ddot{T}_{\text{eff}} + \left(\frac{3+\tau_a k(t)}{\tau_a}\right)\dot{T}_{\text{eff}} + \left[\dot{k}(t) + 2\frac{1+\tau_a k(t)}{\tau_a^2}\right]T_{\text{eff}}(t) - 2\frac{v_0^2(t)}{\tau_a} = 0, \tag{19}$$

which represents a central result of this paper. In the passive limit $\tau_a \to 0$ with $\tau_a v_0^2(t) \to D_a(t)$ Eq. (19) gives the correct expectation $T_{\text{eff}}(t) \to T_D(t)$. However, already at first order in τ_a, one has $T_{\text{eff}}(t) \neq T_D$.

When the parameters are constant or vary very slowly ($\omega = 2\pi/t_{\text{cycle}} \to 0$ as in Eq. (14)), the system reaches a (steady or quasistatic) state where

$$\langle f_a^2\rangle(t) = v_0^2(t), \tag{20a}$$
$$\langle x f_a\rangle(t) = T_{\text{eff}}(t) = \frac{v_0^2(t)\tau_a}{1+\tau_a k(t)}, \tag{20b}$$
$$\langle x^2\rangle(t) = \sigma(t) = \frac{v_0^2(t)\tau_a}{k(t)[1+\tau_a k(t)]} = \frac{T_{\text{eff}}(t)}{k(t)}. \tag{20c}$$

It is useful to stress that, even in the quasistatic limit (very slow transformations), $T_{\text{eff}}(t) \neq T_D(t)$ if $\tau_a > 0$, i.e., if the system is active. In other terms, even with very slow transformations, an active system has a different thermodynamics with respect to a passive one. Interestingly, in the recent literature a temperature equal to T_{eff} in the quasistatic limit, $T_{Cl} = \frac{v_0^2\tau_a}{1+\tau_a k}$, has shown to bear thermodynamic properties, as it underlies a Clausius relation for the entropy change of active particles [28,29].

We conclude this section by summarizing the meaning of the *dynamical* effective temperature introduced here, $T_{\text{eff}}(t)$: It is the temperature which, replacing $T(t)$ in the passive model (12), gives the same evolution of $\sigma(t)$ in the presence of the same protocol $k(t)$, which guarantees that work, heat, and power are exactly the same. We also remark that the equation governing $T_{\text{eff}}(t)$ [Eq. (19)] is valid for this particular case where the external potential is harmonic and the self-propulsion is of the Ornstein-Uhlenbeck type, so the full system is linear. For other models of self-propulsion, effective temperatures can be more difficult to compute but, provided the potential is harmonic, a definition for the purpose of engine thermodynamics exists and always takes the implicit form (18), as discussed in [25]. Generalization to nonharmonic potentials is under investigation. For purposes different from engine thermodynamics, nevertheless, the concept of effective temperature can be more elusive (see, for instance, [13,43]).

C. Approximation for small persistence

It is easy to show [38] that the model in (15) can be mapped, without any approximation to a Klein-Kramers model with an effective mass τ_a, a harmonic force with an effective stiffness $\dot{k} + \frac{k}{\tau_a}$, and a viscous bath with effective drag coefficient $1+\tau_a k(t)$,

$$dx = v dt,$$
$$dv = -\frac{\Gamma(t)}{\tau_a} v dt - \left(\dot{k} + \frac{k}{\tau_a}\right) x dt + \sqrt{\frac{2v_0^2(t)}{\tau_a}} dw, \tag{21}$$

with

$$\Gamma(t) = 1 + \tau_a \partial_x^2 \mathcal{H} = 1 + \tau_a k(t). \tag{22}$$

Again, the model has a Gaussian propagator and its dynamics is described by the coefficient of the covariance matrix

$$\frac{d\langle v^2\rangle}{dt} = -\frac{2\Gamma(t)}{\tau_a}\langle v^2\rangle + 2\frac{\tau_a\dot{k}+k}{\tau_a}\langle xv\rangle + \frac{2v_0^2}{\tau_a},$$
$$\frac{d\langle xv\rangle}{dt} = \langle v^2\rangle + \frac{\Gamma(t)}{\tau_a}\langle xv\rangle - \frac{\tau_a\dot{k}+k}{\tau_a}\langle x^2\rangle, \tag{23}$$
$$\frac{d\langle x^2\rangle}{dt} = 2\langle xv\rangle,$$

whose steady (or quasistatic) state reads

$$\langle v^2\rangle(t) = \frac{v_0^2(t)}{\Gamma(t)} = \frac{T_{Cl}(t)}{\tau_a},$$
$$\langle xv\rangle = 0, \tag{24}$$
$$\langle x^2\rangle(t) = \frac{v_0^2(t)\tau_a}{k(t)\Gamma(t)} = \frac{T_{Cl}(t)}{k(t)}.$$

In the limit of $\tau_a \to 0$, the model in Eqs. (21) can be approximated by a heuristic procedure, equivalent to *overdamping*, where inertia (i.e., dv) is neglected. This procedure generalizes to the case of time-dependent parameters the so-called unified colored noise approximation (UCNA) expansion [44,45] and (for the case of a harmonic potential) gives

$$dx = -\frac{\tau_a\dot{k}+k}{1+\tau_a k} x dt + \sqrt{\frac{2v_0^2\tau_a}{(1+\tau_a k)^2}} dw. \tag{25}$$

For simplicity, in the rest of the paper we call this model the dynamical UCNA. We notice that it is equivalent to the passive model (12) and therefore has variance satisfying Eq. (13), with $k(t)$ and $T(t)$ replaced by

$$k_a(t) = \frac{\tau_a\dot{k}(t)+k(t)}{1+\tau_a k(t)}, \tag{26a}$$

$$T_a(t) = \frac{v_0^2(t)\tau_a}{[1+\tau_a k(t)]^2}. \tag{26b}$$

We highlight that $T_a(t) \neq T_{\rm eff}(t)$, even at first order in τ_a. Of course in the passive limit ($\tau_a \to 0$ and $v_0^2(t)\tau_a \to D_a(t)$) both temperatures $T_a(t)$ and $T_{\rm eff}(t)$ go to $T_D(t)$.

In the steady or quasistatic regime (constant or very slowly varying $k(t)$ and $v_0(t)$), $T_a(t)$ and $T_{\rm eff}(t)$ are still different, even at first order in τ_a:

$$T_{\rm eff}(t) \approx \tau_a v_0^2\left[1 - k(t)\tau_a + O\left(\tau_a^2\right)\right], \tag{27a}$$

$$T_a(t) \approx \tau_a v_0^2\left[1 - 2k(t)\tau_a + O\left(\tau_a^2\right)\right]. \tag{27b}$$

TABLE II. Three important physical limits which can be considered when discussing an active heat engine (the definition of cycle amplitudes ϵ_k, ϵ_T, and ϵ are given in Sec. IV A).

Limit	Definition
passive	$\tau_a \to 0$, $v_0 \to \infty$, $\tau_a v_0^2 \to D_a$
quasistatic	$t_{\rm cycle} \to \infty$ $(\omega \to 0)$
linear	cycle amplitude ϵ, ϵ_k, $\epsilon_T \to 0$

However, $\sigma(t) = T_a(t)/k_a(t)$ coincides with that in Eq. (20c). For small τ_a, it takes the form

$$\sigma = \frac{v_0^2\tau_a}{k}(1 - \tau_a k) + O\left(\tau_a^3\right). \tag{28}$$

It is important to understand that the passive problem with parameters $k_a(t)$ and $T_a(t)$ is not *thermodynamically* equivalent to our original active problem, since the work (and therefore power) of the original problem must be evaluated against the original stiffness $k(t)$ and not against $k_a(t)$. Therefore, the analogy appearing in Eq. (25) cannot be immediately used for optimization purposes. In Table I we summarize the main definitions of the temperatures used in this paper. We also summarize, in Table II, the important physical limits which can be considered when discussing active heat engines.

D. Possible strategies for optimizing the active heat engine

We have shown that the active engine with the parameters τ_a, $k(t)$, and $v_0(t)$ is equivalent, for the purpose of both the evolution of $\sigma(t)$ and the computation of work, to a passive engine model defined in Eq. (12) with the parameters $k(t)$ and $T_{\rm eff}(t)$ obeying Eq. (19). Such an equivalence allows us to transfer results from the study of the passive model to the active heat engine.

Note that the passive model has maximum efficiency [using for $w_{ads}(t)$ the definition of [32], that is, Eq. (6)] given by the Carnot efficiency in the quasistatic limit

$$\eta \leqslant \eta_c = 1 - \frac{T_{\min}}{T_{\max}}, \tag{29}$$

where $T_{\min}$ and $T_{\max}$ are the minimum and maximum of $T(t)$, respectively. In the active case this limit holds for the equivalent efficiency, but one must take $T_{\min}$ and $T_{\max}$ as the minimum and maximum of $T_{\rm eff}(t)$ given by Eq. (19). The efficiency of an active heat engine, however, is not a univocal concept. It depends, through Eq. (8), upon the definition of Q_h, which is already ambivalent for passive particles (see the discussion at the end of Sec. II) and is even more ambivalent for active ones, since it could rely on the adopted choice of effective temperature. Our point of view is that the choice of $T_{\rm eff}$ for reference temperature, together with the choice illustrated in [32] for Q_h (which is using Eq. (6), detailed in Sec. IV B), guarantees that η reaches the Carnot efficiency in the quasistatic limit, for any choice of the other parameters (including activity). Therefore, it is a meaningful figure of merit, in the sense that it makes clear how far the machine is from the maximum deliverable power. Of course a more severe measure of efficiency could be considered, where Q_h includes the energy spent to feed the active particles, but this is of course beyond the scope of the present paper (see the discussion in [25]).

IV. DISCUSSION OF THE PASSIVE HEAT ENGINE

The optimization of the passive model was first studied in [11], where specific Carnot-like protocols (two isothermal and two adiabatic) were considered and optimization was done towards the maximum power at fixed minimum and maximum σ. A study of the same model within the framework of linear irreversible thermodynamics [46,47] was presented in [32]. In that study the Onsager coefficient relative to the passive model for cyclical protocols $k(t)$ and $T(t)$ (undergoing small variations) was given, with a formula for the efficiency and power as a function of the parameters of the model. Optimization is done by fixing the efficiency and the temperature protocol and looking for the optimal stiffness protocol producing maximum power. In this section we consider a class of harmonic protocols with phase shift (between stiffness and temperature), investigating the more common question of the efficiency at maximum power with, in this protocol class, results equivalent to the Curzon-Ahlborn formula [48].

In this paper we consider $k(t)$ and $T(t)$ to be periodic functions with period $t_{\rm cycle}$ corresponding to an angular frequency $\omega = 2\pi/t_{\rm cycle}$. The maximum variations of $k(t)$ and $T(t)$ are proportional to ϵ_k and ϵ_T, respectively. In some situations we consider $\epsilon_k \propto \epsilon_T \propto \epsilon$.

Equation (13) has a formal solution

$$\sigma(t) = \left[\int_0^t e^{K(t')} 2T(t')dt' + \sigma(0)\right] e^{-K(t)}, \qquad (30)$$

where $\dot{K}(t) = 2k(t)$. In general, whatever the initial variance $\sigma(0)$, given the periodic protocols described above, we observe a relaxation of Eq. (30) towards a limit cycle. We assume that this relaxation is achieved within a time t_0 (typically a few periods are sufficient). The power and efficiency of the model are computed through integration of Eqs. (10) and (11) with $\sigma(t)$ given by the solution in (30). This task can be nontrivially processed analytically, even for simple protocols such as sinusoidal functions. We resort to numerical integration of differential equations[4] for $\sigma(t)$, W_p, and Q_h and, to get analytical formula, to the linear response regime, i.e., when the amplitudes of variations of $k(t)$ and $T(t)$ are small.

A. Qualitative picture of cycle thermodynamics

To get a first qualitative picture it is useful to set the protocols equal to simple sinusoidal functions (with the same relative amplitude)

$$k(t) = k_0 + \epsilon_k \sin \omega t, \qquad (31)$$

$$T(t) = T_c + \epsilon_T \frac{1 - \cos \omega t}{2}. \qquad (32)$$

The protocol is illustrated in Fig. 1. The stiffness and temperature variations are out of phase by a fourth of a period: The temperature maximum is synchronized with the instant where the expansion (decreasing stiffness) is fastest. This choice is inspired by the classical idealized Stirling engine. In the discussion of the linear response regime below we show that this choice is not optimal (i.e., a slightly different lag between temperature and stiffness can be found to increase delivered power), a fact rarely discussed.

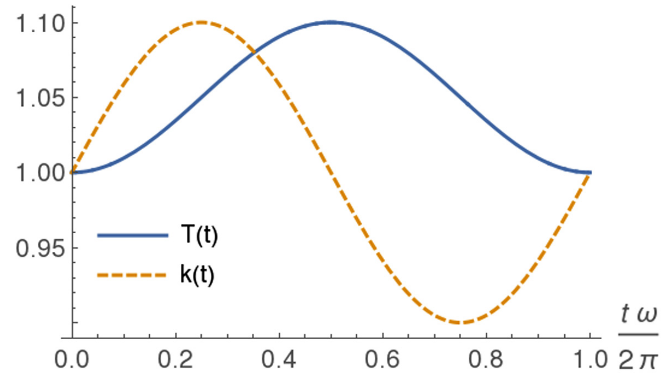

FIG. 1. Sketch of the stiffness and temperature protocols used in Sec. IV A. In Sec. IV B we consider a phase shift (denoted by ϕ) with respect to the case shown in the figure, for $T(t)$, which can be adjusted to optimize the delivered power. In this plot we have chosen $T_c = k_0 = 1$ and $\epsilon_k = \epsilon_T = 0.1$.

In Fig. 2 we summarize the behavior of the passive heat engine with the protocol given by Eq. (31). Figure 2(a) shows the total work per cycle W_p as a function of ω for $\epsilon_k = 0.1$ (with $k_0 = 1$ and $T_c = 1$). The blue curve is for $\epsilon_T = 0$, i.e., when the temperature does not change during the cycle (it is constant at $T = T_c$); the work in a period is never negative, a fact which is consistent with expectation from thermodynamics, i.e., there is no way to extract work from a single thermostat. Moreover, in the quasistatic limit $\omega \to 0$ one has $\sigma(t) = T/k(t)$ at each time. In this limit one gets $W_p = 0$ because the curve in the k-σ plane goes back and forth along the same route and the enclosed area is empty. As soon as a temperature variation is introduced, as shown by the yellow curve computed for $\epsilon_T = 0.1$, the work may become negative, i.e., there can be a positive power output so that the system behaves as a heat engine. This occurs at small frequencies (including the limit $\omega \to 0$), while at high frequency the work returns to being positive and the machine stops acting as an engine. In Figs. 2(b) and 2(c) we show what happens in the k-σ plane. It is seen directly from Eq. (10) that a negative (produced) work occurs when the limit cycle in that plane is swept in the counterclockwise direction, as it is observed for low frequencies [Fig. 2(b)] and opposite to high frequencies [Fig. 2(c)].

The facts observed above can be understood analytically in the small perturbation limit, computing an approximate expression for $\sigma(t)$, even before going to the full linear response treatment discussed in the next section. For this purpose we consider two simplified situations: (i) a situation where only the stiffness is perturbed so that $\epsilon_k = k_0\epsilon$ and $\epsilon_T = 0$ and (ii) a situation where we assume that the two perturbations (stiffness and temperature) are similar; more precisely, we set $\epsilon_k = k_0\epsilon$ and $\epsilon_T = \epsilon T_c$. In both cases we set $\sigma(t) = \sigma_0(t) + \epsilon\sigma_1(t)$

[4]Our numerical scheme is a classical fourth-order Runge-Kutta integrator with time step $dt = 10^{-3}$ for the passive system and $dt = 10^{-4}$ for the active one.

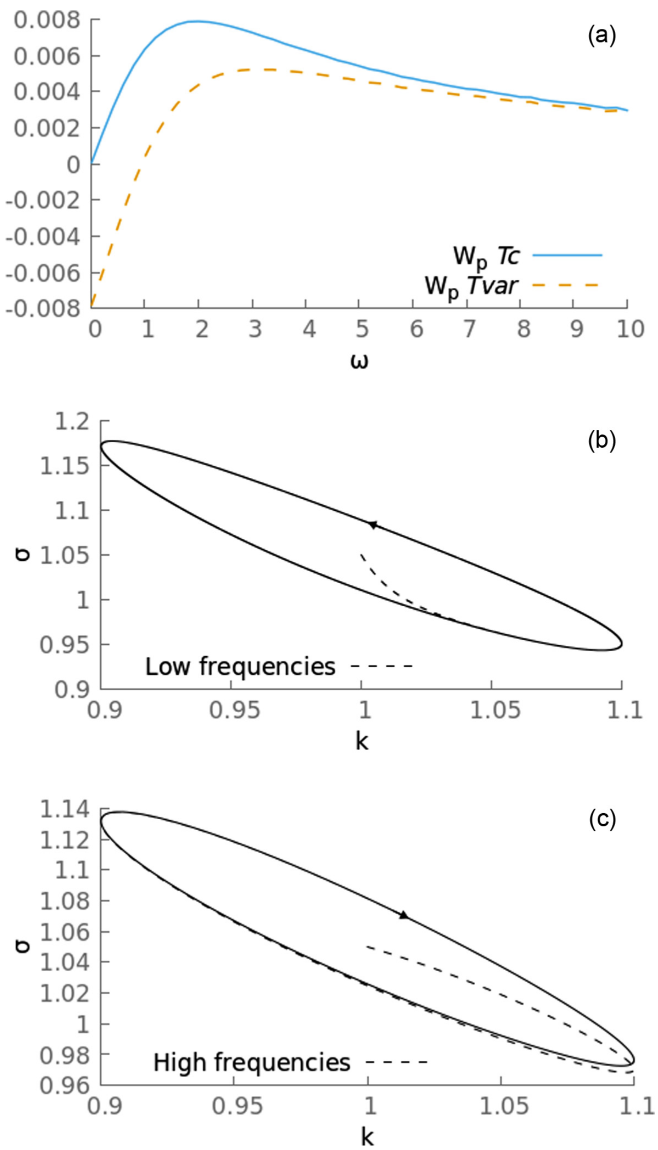

FIG. 2. Study of the passive engine. (a) Work per cycle W_p in the cases at $\epsilon_T = 0.1$ [blue curve, constant $T(t) = T_c$] and at $\epsilon_T = 0.1$ (yellow curve, variable temperature). Also shown is the Clapeyron plane and the different senses of rotation for two different frequencies of the engine cycle: (b) $\omega = 0.2$ and (c) $\omega = 2$. In all plots the parameters are $k_0 = 1$, $\epsilon_k = 0.1$, and $T_c = 1$.

and then replace it in the expanded Eq. (13), equating equal powers in ϵ, concluding by dropping terms with powers of ϵ larger than 1.

In the first situation ($\epsilon_k = k_0\epsilon$ and $\epsilon_T = 0$) we get

$$\frac{\sigma}{\sigma_s} = 1 + \epsilon \frac{2k_0}{\omega^2 + 4k_0^2}[-2k_0 \sin(\omega t) + \omega \cos(\omega t)], \quad (33)$$

where we have defined the static variance $\sigma_s = T_c/k_0$ (the formula given here is valid if $0 < \sigma_s < \infty$). Power adsorbed in this case reads

$$P = \epsilon^2 k_0 T_c \frac{\omega^2}{2(4k_0^2 + \omega^2)}, \quad (34)$$

which is always non-negative, meaning that with $\epsilon_T = 0$ this machine cannot do useful work, but only adsorb it.

In the second situation ($\epsilon_k = k_0\epsilon$ and $\epsilon_T = \epsilon T_c$) instead we get

$$\frac{\sigma}{\sigma_s} = 1 + \epsilon\left\{\frac{1}{2} + k_0 \frac{2(\omega - k_0)\cos(\omega t) - (4k_0 + \omega)\sin(\omega t)}{\omega^2 + 4k_0^2}\right\}. \quad (35)$$

Integration of Eq. (10) with the latter approximated expression of $\sigma(t)$ gives, for the average power,

$$P = \frac{\omega}{2} k_0 T_c \epsilon^2 \frac{\omega - k_0}{\omega^2 + 4k_0^2}. \quad (36)$$

Such a formula is consistent with the observation of a critical frequency separating a regime (at low frequency) where the model produces work, i.e., $P < 0$, and a regime (at high frequency) where it adsorbs work, i.e., $P > 0$; in this small-ϵ limit the critical frequency is $\omega^* = k_0$. Efficiency is more complicated to get, since it requires integrating the heat on the heat-adsorbing part of the cycle. In the next section we calculate the heat and efficiency, again in the linear regime, following a more powerful approach, i.e., recalling the study of Onsager coefficients done in [32] and discussing the possible optimization strategies for the passive engine with the chosen protocols.

B. Linear irreversible thermodynamics

In order to exploit general results obtained in [32], we consider here the choices of the parameter time dependence

$$k(t) = k_0 + \epsilon_k \gamma_w(t), \quad (37a)$$

$$T(t) = \frac{T_c T_h}{T_h - \epsilon_T \gamma_q(t)} \approx T_c + \epsilon_T \gamma_q(t), \quad (37b)$$

with the cold temperature T_c, the hot temperature $T_h = T_c + \epsilon_T$, and $\gamma_w(t)$ and $\gamma_q(t)$ two adimensional periodic functions with period t_{cycle} oscillating the first between +1 and −1 and the second between 0 and 1. The new temperature protocols then oscillate with the same period between T_c and $T_c + \epsilon_T$. With such a protocol one may easily see that the weighting function for adsorbed heat, needed in Eq. (4), according to the recipe in Eq. (6), is $w_{ads}(t) = \gamma_q(t)$. Here we adopt the choice $\gamma_w(t) = \sin \omega t$ and $\gamma_q = \frac{1}{2}(1 - \cos \omega t + \phi)$. With such a choice for small ϵ, the protocol for $\phi = 0$ is identical to the protocol discussed in the preceding section. The advantage of the form (37b) is the possibility of inheriting all the results presented in [32] where the linear thermodynamics study of the same model was discussed broadly.

Linear thermodynamics [47] is a framework where there are thermodynamic fluxes J_w and J_q, proportional to the power and rate of adsorbed heat, respectively, and conjugate thermodynamic forces F_w and F_q, proportional to maximal variations of stiffness and temperature (ϵ_k and ϵ_T), respectively. More precisely, one sets

$$J_w = \frac{P}{T_c F_w}, \quad (38)$$

$$J_q = \frac{Q_h}{t_{\text{cycle}}}, \quad (39)$$

$$F_w = 2\frac{\epsilon_k}{k_0}, \tag{40}$$

$$F_q = \frac{1}{T_c} - \frac{1}{T_c + \epsilon_T} \approx \frac{\epsilon_T}{T_c^2} \tag{41}$$

for the fluxes and the forces, respectively. We stress that, in our definitions, work and power are positive when adsorbed, so J_w has the same sign as P, which is different from the definition in [32]. When forces are small $F_w \ll 1$ and $F_q \ll 1$ it is possible to write linear relations between fluxes and forces, through the introduction of so-called Onsager coefficients $L_{\alpha\beta}$, with α and β indices that take the value w or q:

$$J_w = L_{ww}F_w + L_{wq}F_q + O(F^2), \tag{42}$$

$$J_q = L_{qw}F_w + L_{qq}F_q + O(F^2). \tag{43}$$

This immediately gives expressions for power, heat, and efficiency:

$$P = T_c F_w (L_{ww}F_w + L_{wq}F_q), \tag{44}$$

$$\frac{Q_h}{t_{cycle}} = L_{qw}F_w + L_{qq}F_q, \tag{45}$$

$$\eta = -\frac{T_c F_w (L_{ww}F_w + L_{wq}F_q)}{L_{qw}F_w + L_{qq}F_q} \tag{46}$$

(recall that the machine does useful work when $P < 0$ and $\eta > 0$).

The coefficients are given by Eqs. (72) of [32], which we rewrite with our notation:

$$L_{\alpha\beta} = -\frac{2T_c^2 \xi_\alpha \xi_\beta}{t_{cycle}} \int_0^{t_{cycle}} dt[\dot{\gamma}_\alpha(t)\gamma_\beta(t) - \dot{\gamma}_\alpha(t)\Gamma_{\alpha\beta}(t)], \tag{47}$$

$$\Gamma_{\alpha\beta}(t) = \int_0^\infty d\tau \dot{\gamma}_\beta(t-\tau)e^{-2k_0\tau}, \tag{48}$$

$$\xi_w = \frac{1}{4T_c}, \quad \xi_q = -\frac{1}{2}. \tag{49}$$

For the present case (i.e., chosen harmonic potential and chosen temporal protocols), direct calculations give

$$L_{ww}(k_0, \omega) = \frac{k_0\omega^2}{8(4k_0^2 + \omega^2)}, \tag{50a}$$

$$L_{qq}(k_0, \omega) = \frac{k_0\omega^2 T_c^2}{8(4k_0^2 + \omega^2)}, \tag{50b}$$

$$L_{wq}(k_0, T_c, \omega, \phi) = -\frac{k_0\omega T_c[2k_0\cos(\phi) + \omega\sin(\phi)]}{8(4k_0^2 + \omega^2)} \tag{50c}$$

$$L_{qw}(k_0, T_c, \omega, \phi) = -L_{wq}(k_0, T_c, \omega, -\phi). \tag{50d}$$

The positivity of L_{ww} confirms that, in the absence of temperature variation, the work is always positive, i.e., it is always adsorbed. The relation between the off-diagonal coefficients L_{wq} and L_{qw} is consistent with reciprocity, which is expected from the assumption of the underlying time-reversible dynamics (when in the absence of thermodynamic forces), which here takes the form $L_{wq}[k(t), T(t)] = L_{qw}[k(-t), T(-t)]$ [32].

From the expressions (50) one gets the expressions for power, heat, and efficiency as functions of the model's parameters

$$P = \frac{\omega\epsilon_k}{4k_0}\,\frac{2\epsilon_k\omega T_c - \epsilon_T k_0 f_+(\phi, k_0, \omega)}{4k_0^2 + \omega^2}. \tag{51a}$$

$$\frac{Q_h}{t_{cycle}} = \frac{\omega}{8}\frac{\epsilon_T k_0 \omega + 2\epsilon_k T_c f_-(\phi, k_0, \omega)}{4k_0^2 + \omega^2}, \tag{51b}$$

$$\eta = 2\frac{\epsilon_k}{k_0}\,\frac{-2\frac{\epsilon_k}{k_0}\omega + \frac{\epsilon_T}{T_c} f_+(\phi, k_0, \omega)}{\frac{\epsilon_T}{T_c}\omega + 2\frac{\epsilon_k}{k_0} f_-(\phi, k_0, \omega)}, \tag{51c}$$

where we have introduced the two phase-dependent frequencies $f_\pm(\phi, k_0, \omega) = 2k_0\cos(\phi) \pm \omega\sin(\phi)$. Note that the efficiency is always lower than the Carnot efficiency, which is reached when $\omega \to 0$:

$$\eta(\omega > 0) \leqslant \eta(\omega = 0) = \frac{\epsilon_T}{T_c} \approx 1 - \frac{T_c}{T_h} = \eta_c. \tag{52}$$

Power is negative (i.e., the machine produces work) only in a range of (non-negative) frequencies, at given ϕ, defined by

$$\frac{\omega}{k_0} < r(\phi) = \eta_c \frac{2\cos\phi}{2\frac{\epsilon_k}{k_0} - \eta_c\sin\phi}, \tag{53}$$

which implies that valid frequencies can be found only for ranges of ϕ such that $r(\phi) \geqslant 0$ (such ranges depend upon η_c and ϵ_k/k_0).

In formula (51a) we find interesting the role of ϕ, which seems to be overlooked in the literature. At constant ω one can get relevant improvement in power or efficiency by tuning ϕ: It is sufficient to consider, for instance, that at $\phi = 0$ the range of working frequencies is $\omega < k_0\eta_c\frac{k_0}{\epsilon_k}$, but in general such a range extends to higher frequencies when ϕ is increased.

In conclusion, we also report the expressions for power and efficiencies for the case of proportional thermodynamic forces, i.e., $\epsilon_T/T_c = \epsilon_k/k_0 = \epsilon$:

$$P = \frac{\omega\epsilon^2 k_0 T_c}{4}\frac{2\omega - f_+(\phi, k_0, \omega)}{4k_0^2 + \omega^2}, \tag{54a}$$

$$\eta = 2\epsilon\frac{-2\omega + f_+(\phi, k_0, \omega)}{\omega + 2f_-(\phi, k_0, \omega)}. \tag{54b}$$

We note that the power for $\phi = 0$ has the same expression as in (36).

C. Optimization of power

In Fig. 3 we show the surface $-P$ as a function of ω and ϕ, with given $k_0 = T_c = 1$ and $\epsilon_T = \epsilon_k = 0.1$. As a general feature, the surface has a positive part in the low-ω and low-$|\phi|$ region.

Now we find the optimal phase and frequency to get the maximum delivered power $-P$ at given ϵ_T, ϵ_k, k_0, and T_c. This maximum is obtained by imposing the simultaneous conditions $\partial_\phi P = 0$ and $\partial_\omega P = 0$ and excluding solutions with $\omega \leqslant 0$. The result of the procedure is the following formula for the optimal values ω^* and ϕ^* and the corresponding values

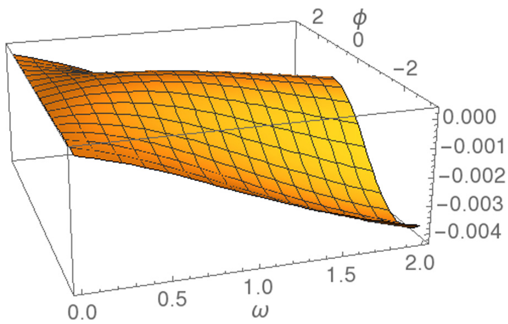

FIG. 3. Delivered power $-P$ as a function of ω and ϕ, with $k_0 = T_c = 1$ and $\epsilon_T = \epsilon_k = 0.1$.

of power and efficiency:

$$\omega^* = 2k_0 \frac{\epsilon_T k_0}{\sqrt{(4\epsilon_k T_c)^2 - (\epsilon_T k_0)^2}}, \tag{55a}$$

$$\phi^* = \arctan \frac{\omega^*}{2k_0}, \tag{55b}$$

$$-P(\phi^*, \omega^*) = \frac{k_0 \epsilon_T^2}{32 T_c}, \tag{55c}$$

$$\eta(\phi^*, \omega^*) = \frac{\epsilon_T}{2T_c} \approx 1 - \sqrt{\frac{T_c}{T_h}}. \tag{55d}$$

Several comments are in order after looking at those formula. First of all, we notice that the optimal frequency exists only if $\epsilon_T/T_c < 4\epsilon_k/k_0$. Second, we confirm the interesting role of ϕ which must be tuned consistently to achieve maximum power. Finally, we underline that the efficiency at maximum power is given by the Curzon-Ahlborn formula (approximated for small ϵ_T) [48].

V. ACTIVE HEAT ENGINE

In this section we analyze how the previous results obtained for the passive engine model can be exploited to get an optimal active heat engine. In Sec. V A, for the purpose of a knowledge of all possibilities, we discuss what can be done using the dynamical UCNA (small τ_a) elaborated in Sec. III C (and frequently used in the literature for problems with constant parameters). Such an approximation is useful to get an initial idea of when an active machine can do useful work; however, it is not obvious how it can be optimized. In contrast, in Sec. V B we discuss the result of the exact equivalence between the active model and a passive one, with temperature obeying Eq. (19), exploiting the optimization strategies of the passive model.

A. Small-τ_a limit and the role of active temperature in the dynamical UCNA

As discussed in Sec. III C, the dynamical UCNA obtained in a weak active regime ($\tau_a \to 0$) constitutes an alternative mapping of an active AOUP system into a passive one, with active stiffness $k_a(t)$ and temperature $T_a(t)$ given by Eqs. (26). The fact that in the dynamical UCNA the active temperature is spontaneously time dependent even when the characteristic energy v_0^2, dictated by the active speed, is constant leads us to argue that it is in principle possible that a thermic machine is at work by modulating in time $k(t)$ only; this would be a remarkable results, in view of the fact that for passive particles it is forbidden (see Sec. IV A) and that it would be a great advantage for experiments, where modulating v_0 in time can be complicated.

To test this hypothesis we plug our simple protocol $k(t)$ [Eq. (31)] in the equation for the variance, obtaining $T_a(t)$. Then, similarly to what we did with the passive heat engine, we look for a formal solution of $\sigma(t)$ [by replacing k with k_a and T with T_a in the expression (30)]. Given the difficulty in writing this form explicitly, we move as usual to the linear response regime and to a numerical approach.

The numerical integration betrays our expectations showing that work in a cycle is positive at any frequency ω [Fig. 4(a)]. This is furthermore verified by the small perturbation in ϵ. We proceed as in Sec. IV A, expanding $\sigma(t) = \sigma_0(t) + \epsilon\sigma_1(t)$ and computing an approximate expression for k_a and T_a to be inserted in (13),

$$k_a = \frac{k_0}{\Gamma_0} + \epsilon \frac{k_0}{\Gamma_0^2}(\Gamma_0 \omega \tau_a \cos \omega t + \sin \omega t), \tag{56a}$$

$$T_a = \frac{v_0^2 \tau_a}{\Gamma_0^2}\left[1 - \epsilon \frac{2\tau_a k_0}{\Gamma_0} \sin \omega t\right], \tag{56b}$$

where we have used $\Gamma_0 = 1 + \tau_a k_0$.

The related work $W_p = \epsilon^2 (v_0^2 \tau_a) \frac{k_0}{2\Gamma_0} \frac{\omega^2}{4k_0^2 + (\Gamma_0 \omega)^2}$ is positive and does not cross 0 for any frequency value $\omega > 0$. Note that in the passive limit we recover the expression for the power (34).

The fact that the pure modulation of $k(t)$, i.e., keeping v_0 constant, does not produce a working machine in the small-τ_a limit can be understood on a more general ground, i.e., independently of the small-ϵ limit and of the choice of the protocol $k(t)$. In fact, following the qualitative discussion given in Sec. IV, we suggest that the form of $T_a(t)$ with v_0 constant does not meet the requirement of a working Stirling engine: The expansions ($\dot{k}_a < 0$) are not in phase with the maximum temperature T_a (see Fig. 4(b) for an example). Given the positivity of k, it is straightforward to see that the following constraints are never satisfied at the same time:

$$\dot{T}_a = 0, \quad \ddot{T}_a > 0, \\ \dot{k}_a < 0. \tag{57}$$

The presence of a lag between stiffness and temperature, such that the temperature maximum is in the expansion phase of the confining potential, is decisive in the realization of a working engine, similarly to the passive case. We need to let $v_0(t)$ vary in time in order to force $T_a(t)$ to take the required form.

For small τ_a note that $k_a \to k$ and $T_a \to T_D = v_0^2 \tau_a$, so it is natural to propose a v_0 which resembles the passive temperature in (31). We take

$$v_0^2(t) = u^2 + \epsilon_u \frac{1 - \cos \omega t}{2}. \tag{58}$$

This intuition is qualitatively right: The active AOUP model with a time-dependent typical velocity is able to produce work, as we can see in Fig. 4(c). Along with the numeri-

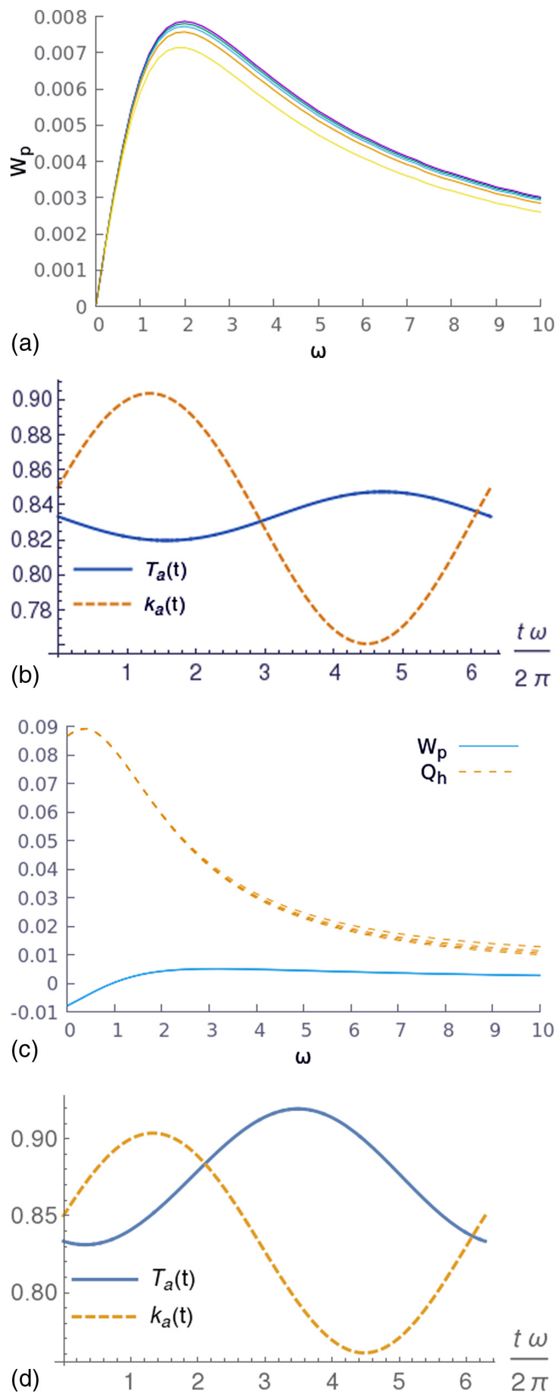

FIG. 4. Study of thermodynamics for the AOUP model at small τ_a. (a) Work per cycle W_p as a function of ω in the case of constant self-propulsion speed v_0; no work is produced for $\tau_a = 0.01$ (higher curve) and -0.1 (lower curve). (b) Active stiffness and temperature (in the case with $\tau_a = 0.1$ and $\omega = 1$) when $v_0^2\tau_a = 1$ is constant; the maxima of $T_a(t)$ are always in phase with the minima of $k_a(t)$, failing to meet a working machine condition. (c) Work W_p and adsorbed heat Q_h per cycle when $v_0(t)$ is time dependent. (d) Active stiffness and temperature (with $\tau_a = 0.2$ and $\omega = 1$) in the time-dependent $v_0(t)$ case. The time modulation of v_0 in (c) and (d) occurs with the parameters $\tau_a u^2 = 1$ and $\epsilon_u = 0.1u^2$. In all plots $k_0 = 1$ and $\epsilon_k = 0.1$.

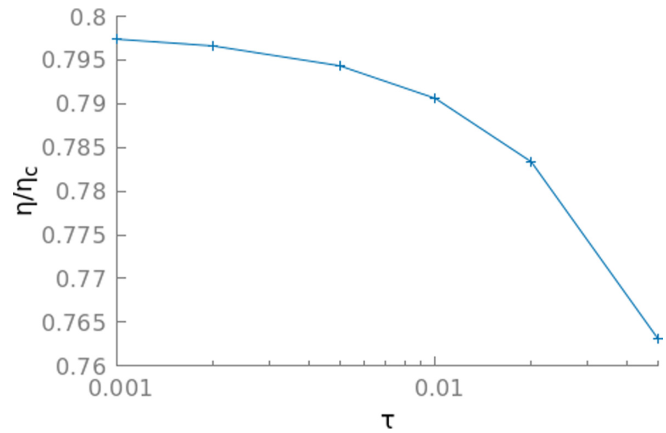

FIG. 5. Efficiency rescaled by the Carnot efficiency in the passive limit $\eta_c = \epsilon_u/u^2 = 0.1$ in the small-τ_a AOUP model when $v_0(t)$ follows the protocol in Eq. (58), inspired by the dynamical UCNA. The efficiency decreases with activity. The parameters are $\omega = 0.1$, $\epsilon_k = 0.1$, $k_0 = 1$, $u^2 = 1/\tau_a$, and $\epsilon_u = 0.1u^2$.

cal result, it is possible to repeat our linearization strategy for $\sigma(t)$ and show that the power, obtained with the correct approximation for T_a, is $P = \epsilon^2(v_0^2\tau_a)\frac{k_0}{2\Gamma_0}\frac{\omega(\omega-k_0)}{4k_0^2+(\Gamma_0\omega)^2}$. We note a regime change for $\omega = k_0$ and the agreement with the expression (36) in the passive limit. In order to evaluate the efficiency of this working machine, in particular its behavior with τ_a, we resort to numerical integration of adsorbed heat and work. For adsorbed heat we use the definition (6) for $w_{ads}(t)$, using $T_D(t) = \tau_a v_0^2(t)$ in place of $T(t)$. The results for efficiency are represented in Fig. 5: We emphasize that it is maximum in the quasistatic and in the passive limits. The effect of self-propulsion within this approach seems to decrease efficiency, but this is basically due to the fact that the chosen protocol is not sensitive to τ_a and $k(t)$, while the real effective temperature $T_{\rm eff}$ is. Changing τ_a without adapting the protocol degrades the efficiency.

In the next section we explore the aforementioned passive-active equivalence, which gives the possibility to adjust the protocol when τ_a is varied, in order to control the power and efficiency of the engine.

B. Optimization by passive equivalence

The idea of exploiting passive-active equivalence is the following. Whatever particular optimization procedure is applied to the passive model, one gets optimal passive protocols $k^*(t)$ and $T^*(t)$. At that point the mapping equation (19) can be used to derive the corresponding protocols for the active models; such protocols will give exactly the same power and the same efficiency and therefore will be optimal in that particular set of protocols. Note that, if the passive engine is optimized in the family of protocols $k(t)$ and $T(t)$ given by Eq. (37a), with the parameters k_0, T_c, ϵ_k, ϵ_T, ω, and ϕ, the family of protocols which is spanned in the optimization procedure is given by the same $k(t)$ and a function $v_0(t)$ which satisfies Eq. (19) with $T_{\rm eff} = T(t)$. Putting Eq. (37a) into Eq. (19), we get the corresponding family of protocols for $v_0(t)$,

$$\begin{aligned} v_0^2(t)\tau_a = {} & T(t) + \tau_a k(t) T(t) \\ & + \frac{3}{4}\omega\tau_a\epsilon_T \sin(\omega t + \phi) \\ & + \frac{\omega\tau_a^2}{2}\left[\epsilon_k \cos(\omega t) T(t) + \frac{\epsilon_T}{2}\sin(\omega t + \phi) k(t)\right] \\ & + \frac{\omega^2\tau_a^2\epsilon_T}{4}\cos(\omega t + \phi), \end{aligned} \tag{59}$$

which is parametrized by k_0, T_c, ϵ_k, ϵ_T, ω, ϕ, and τ_a.

Summing up, if τ_a and $k(t)$ are imposed by the experiment and one looks for an optimal $v_0(t)$, the task is relatively easy, i.e., one may (a) choose arbitrary values for T_c and small ϵ_T (discussed below) and then (b) directly find the optimal ω^* and ϕ^* for the passive problem (in the family of sinusoidal passive protocols given by Eq. (37a)), i.e., the formula in Eqs. (55), and finally (c) use formula (59) to get the corresponding active optimal protocol for $v_0(t)$, which guarantees the maximum possible power and a corresponding Curzon-Ahlborn efficiency, whatever the value of τ_a. Given that ϵ_T/T_c must be small and therefore it is not really a free number (reasonable values are 0.1 or smaller), some freedom remains in choosing T_c, which can be exploited in two ways: One may (i) set the desired optimal frequency ω^* (based upon possible experimental requirements) and then invert Eq. (55a) to get the corresponding T_c or, alternatively, (ii) observe that Eq. (19) is invariant for common rescaling of $T_{\rm eff}$ (and therefore T_c) and v_0^2, that is, one may meet any experimental upper or lower limit for v_0^2 by accordingly rescaling T_c.

In Fig. 6 we show the optimal protocols for a given choice of T_c, k_0, ϵ_T, and ϵ_k. As anticipated, there is an important difference between the optimal protocol for $\tau_a v_0^2(t)$ and $T_{\rm eff}(t)$. We underline that, following this strategy, if one spans a range of τ_a, keeping the same $k(t)$, the optimal effective temperature $T_{\rm eff}(t)$ is not changed. What is changed is the corresponding protocol for $v_0(t)$; if one follows it, whatever the value of τ_a, the power and the efficiency of the engine will always be the same. Also for this reason it is useless to show a plot with efficiencies as a function of τ_a. The constancy of power and efficiency as a function of τ_a demonstrates the superiority of this approach with respect to other approaches not informed with the correct formula for $T_{\rm eff}$ (for instance, the one of the preceding section, where the efficiency decays with τ_a (see Fig. 5)).

The situation is more complicated if τ_a and $v_0(t)$ are imposed by the experiment and one wants to look for the optimal $k(t)$. In such a case, a possible strategy is to use Eq. (19) to get a functional constraint between $k(t)$ and $T_{\rm eff}(t)$; thereafter, one needs to solve the passive problem with a variation of the coupled protocols $k(t)$ and $T_{\rm eff}(t)$ with the given constraint.

Strategies of passive-to-active equivalence are substantially simplified if very slow transformations are considered, i.e., in the limit of large period t_{cycle}, more precisely by taking $\tau_a/t_{cycle} \ll 1$. In this limit Eq. (19) is considerably simpler, as it reduces to the identity (valid for any magnitude of forces ϵ_k and ϵ_T)

$$T_{\rm eff}(t) = \frac{\tau_a v_0^2(t)}{1 + k(t)\tau_a}. \tag{60}$$

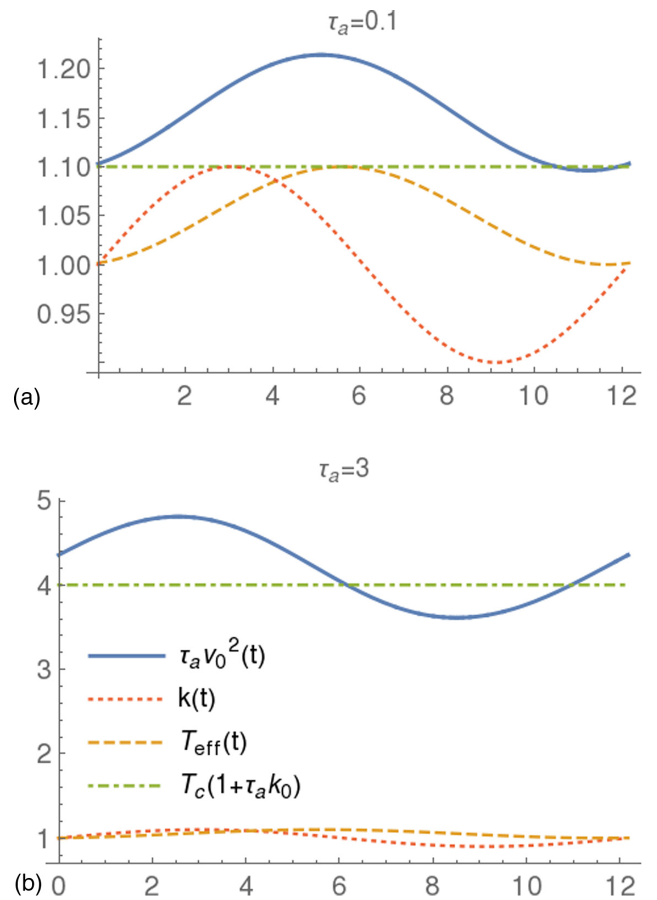

FIG. 6. Examples of the optimal protocol $\tau_a v_0^2(t)$ for an active engine to achieve maximum power when $k_0 = T_c = 1$, $\epsilon_T = \epsilon_k = 0.1$ (which, according to formula (55), give $\omega^* \approx 0.52$ and $\phi^* \approx 0.25$), and $\tau_a = 0.1$. Two values are considered: $\tau_a = 0.1$ and $\tau_a = 3$. We underline that in both cases the engine gives the same maximum power approximately equal to 3×10^{-4} and the same Curzon-Ahlborn efficiency approximately equal to 0.05. The blue curve is $\tau_a v_0^2(t)$ and the red curve is $k(t)$. For reference we also include $T(t) = T_{\rm eff}(t) = T_c + \epsilon_T \frac{1}{2}[1 - \cos(\omega^* t + \phi^*)]$ (yellow dashed curve) and the constant $T_c(1 + \tau_a k_0)$ (green dashed curve), which is the approximation of Eq. (59) at zeroth order in ω, ϵ_k, and ϵ_T.

As mentioned, in this limit $T_{\rm eff}(t)$ is still different from $T_a(t)$, even at first order in τ_a (see Eq. (27a)). We underline that the same problem discussed above (see the discussion above Eqs. (57)) occurs for the expression of $T_{\rm eff}(t)$ in formula (60): If $v_0(t)$ is taken constant, the resulting effective temperature is always in opposition of phase with $k(t)$ (i.e., maxima of k correspond to minima of $T_{\rm eff}$ and vice versa). Several empirical attempts by numerical integration of W_p for a wide range of choices of all the parameters convinced us that such a situation always leads to $W_p \geqslant 0$, i.e., a machine that does not produce work. We recall that this is rigorously proven in the linear forcing regime (see Sec. IV B and formula (51a), where the opposition of phase between $k(t)$ and $T(t)$ corresponds to $\phi = -\pi/2$).

Equation (60) gives an estimate of the maximum efficiency (to be attained in the $\omega \to 0$ limit, that is, at vanishing power), i.e.,

$$\eta_c = 1 - \min\left\{\frac{v_0^2(t)}{1+\tau_a k(t)}\right\} \max\left\{\frac{v_0^2(t)}{1+\tau_a k(t)}\right\}^{-1}, \qquad (61)$$

which is striking evidence of the nontrivial relation between the two thermodynamic forces (for temperature and volume forces) in shaping the efficiency of active heat engines. Equation (60) can be also used to find the shape of $v_0(t)$ to get any desired efficiency η_c (at vanishing power $\omega \to 0$). This is achieved by imposing that $\eta_c = \epsilon_T/(T_c + \epsilon_T)$ and recalling the nonlinear expression for $T(t)$ (see (37b)). Then we obtain

$$v_0^2(t) = \frac{T_c}{\tau_a}\frac{1+\tau_a k(t)}{1-\eta_c \gamma_q(t)} \xrightarrow{\tau_a \to \infty} \frac{T_c k(t)}{1-\eta_c \gamma_q(t)}. \qquad (62)$$

We warn, however, that Eq. (60) only guarantees that the passive model with temperature $T_{\rm eff}(t)$ gives the same evolution for $\sigma(t)$ and therefore produces or adsorbs the same work, but is not necessarily a heat engine. The positivity of work production (which in our notation corresponds to $W_p < 0$) depends upon the phase shift between $T_{\rm eff}(t)$ and $k(t)$. Therefore, in Eq. (62) one needs to put the proper $k(t)$ and $\gamma_q(t)$, i.e., the correct choices of ω, k_0, and ϕ; the desired efficiency is reached provided the machine does useful work. We know, however, that for small ϵ_k and ϵ_T (as demonstrated by Eq. (54a) in the $\omega \to 0$ limit) such a condition is satisfied for $\phi \in (-\pi/2, \pi/2)$.

VI. CONCLUSION

A well defined thermostat temperature is a crucial ingredient for definitions of basic thermodynamic tools (e.g., adsorbed heat and efficiency) as well as to transfer known results valid for thermal systems: For a lack of such a well defined temperature, active heat engines elude intuition and expectation in stochastic thermodynamics. Here, building upon an important observation made in [25], we have shown an example where such a temperature can be defined and gives important advantages, useful also in experiments.

The effective temperature for this particular model satisfies Eq. (19) and is different from all other temperatures based upon particular, usually static, configurations (e.g., T_D related to unconfined diffusion, $T_{\rm var}$ related to equilibrium steady states, and T_a related to the small-τ_a limit). It represents, exactly, the thermostat of an equivalent passive model which gives, in the presence of the same external harmonic potential, the same position variance and therefore the same power and the same total heat exchanged. An observation about the definition of adsorbed heat (see the discussion at the end of Sec. II) suggests that the equivalence noted in [25] may be extended to efficiency only for a particular definition of adsorbed heat, which comes at the price of losing the simplicity and generality of the Carnot bound. In fact, such an extension gives an efficiency that in the quasistatic limit depends not only upon the maximum and minimum temperatures of the system but also upon other parameters. We suggested a different definition of adsorbed heat, considering the efficiency of the equivalent passive model and following [32] for the adsorbed heat definition: Since it is designed to give a Carnot efficiency $\eta_c = 1 - T_c/T_h$ in the quasistatic limit, whatever the values of the other parameters, one can use it as a proper figure of merit for the purpose of evaluating the performance of the machine.

The active-passive equivalence (19), which contains time derivatives of $T(t)$ and $k(t)$, suggests the study of the optimization of a passive model with smooth protocols, which is different from what is usually done with piecewise linear modulations (for Carnot-like or Stirling-like engines). Therefore, we have extended previous studies to a family of smooth protocols where the lag (between temperature and stiffness modulation) is varied to improve efficiency. In the linear approximation of fluxes we have found the optimal frequency and phase lag (Eqs. (55a) and (55b)) that produce maximum power output (and correspondingly Curzon-Ahlborn efficiency, roughly half of Carnot efficiency), a result which is readily translated to active engines through Eq. (19). This equivalence equation also immediately gives the Carnot efficiency of an active engine (see Eq. (61)), which is valid for any activity time τ_a (i.e., also far from the passive limit) and any amplitude of the protocols (i.e., also far from the linear regime), but of course can be attained only in the quasistatic limit, that is, at vanishing power.

Future investigations may concern the possibility of extending, through suitable approximations, the results of our study to nonharmonic potentials [25], as well as to other active particle models. It would also be interesting to consider fluctuations of the relevant quantities, such as power or efficiency, which constitute an important ingredient of microscopic engines. Finally, a promising direction of research would be to consider bunches of active particles with interactions in order to probe the effect of collective behavior on the performance of such kinds of heat machines.

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