



Brief paper

Stochastic thermodynamic engines under time-varying temperature profile[☆]

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ABSTRACT

A recently developed stochastic control formalism (Stochastic Thermodynamics) has opened for the first time the possibility to quantify energy exchange and entropy production in finite-time thermodynamic transitions, based on Langevin models for mesoscopic thermodynamic systems. Within this framework we quantify power output and efficiency of overdamped stochastic thermodynamic engines that are powered by a heat bath with temperature that varies periodically with time. Our setting is in contrast to most of the existing literature that considers the Carnot paradigm, alternating contact with heat baths having different fixed temperatures, hot and cold. Specifically, we consider a periodic and bounded but otherwise arbitrary temperature profile and derive explicit bounds on the power and efficiency achievable by a suitably controlling potential that couples the thermodynamic engine to the external world – the time-varying potential represents the control input to the system. A standing assumption in our analysis is that the norm of the gradient of the potentials is bounded – in the absence of any such constraint on the control input, the physically questionable conclusion of arbitrarily large power can be drawn.

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1. Introduction

The classical model of a thermodynamic engine involves an ensemble of particles (e.g., confined gas molecules) that is brought in contact with two heat baths of different temperatures, hot (T_h) and cold (T_c), in periodic succession. Based on such a model, in the foundational treatise (Carnot, 1986), Sadi Carnot established the ultimate limit on the efficiency in transforming heat into mechanical work. The Carnot bound was later expressed by Thomson (Lord Kelvin) in terms of the ratio of absolute temperatures of the two heat baths as $\eta = 1 - \frac{T_c}{T_h}$, and is known as *Carnot efficiency* – it represents a “holy grail” in thermodynamic energy transduction. A salient property in Carnot’s analysis was the reversibility of thermodynamic transitions, which necessitated infinitely slow operation, thereby delivering zero power.

For more than one hundred years, classical thermodynamics (Callen, 1998; Lebon, Jou, & Casas-Vázquez, 2008) did not succeed in addressing questions that pertain to the maximal power that can be delivered during finite-time transitions – the main obstacle stemming from the difficulty in modeling dissipation during fast transitions. The quest to comprehend far-from-equilibrium thermodynamic transitions, and to quantify the maximal power output of thermodynamic engines, ultimately led to the development of fluctuation theorems and stochastic thermodynamics (Brockett, 2017; Lebon et al., 2008; Schmiedl & Seifert, 2007b; Seifert, 2008, 2012; Sekimoto, 2010). This emerging framework, that broadly falls within the field of stochastic control (Åström, 2012), allows describing thermodynamic transitions at the level of individual particles and small ensembles, and as such, it has been applied to the study of biological molecular machines and nano-scale engineering devices.

Early work on power and efficiency of microscopic thermodynamic systems focused on Carnot-like heat engines operating between two thermal heat baths of constant temperature, in the overdamped (Schmiedl & Seifert, 2007a) and low friction (Dechant, Kiesel, & Lutz, 2017) regimes. Recently, the framework has been applied to continuous and periodic temperature profiles in the linear response regime (Bauer, Brandner, & Seifert,

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2016; Brandner & Saito, 2020; Brandner, Saito, & Seifert, 2015; Frim & DeWeese, 2022; Fu, Miangolarra, Taghvaei, Chen, & Georgiou, 2020; Yuan, Ma, & Sun, 2022), the standing assumption being that of small perturbations and linearized dynamics. Under a low-friction assumption, explicit bounds on maximal power have also been obtained in the nonlinear regime (Miangolarra, Fu, Taghvaei, Chen, & Georgiou, 2021).

The aim of the present work is to analyze thermodynamic systems that remain in contact with a single thermal bath periodically time-varying temperature profile. The work we present below focuses on the fully nonlinear regime, removing the low friction assumption to study overdamped systems. It generalizes our previous work (Fu, Taghvaei, Chen, & Georgiou, 2021) in which we studied a Carnot-like heat engine in contact with two heat baths with prespecified hot and cold temperatures. Thus, in the present, we develop formulae for achievable power and efficiency when the thermodynamic engine operates in contact with a heat bath of periodically varying temperature.

The paper is organized as follows. Section 2 provides background on stochastic thermodynamics as a formalism within stochastic control. Section 3 explains the conceptualization of a cyclic operation on a thermodynamic manifold – the space of probability distributions metrized by the Wasserstein metric, and gives geometric expressions for power and dissipation along with some illustrative examples. Section 4 contains the main results on achievable power for an arbitrary periodic temperature profiles of the thermal bath, under suitable constraints on the Fisher information of the thermodynamic states and the gradient of the controlling potential. Section 5 recaps the main ideas and discusses future research directions.

2. Background on stochastic energetics

A thermodynamic system that is immersed in a heat bath is thought of as an ensemble of particles that obey Langevin dynamics, following Einstein and Smoluchowski (Sekimoto, 2010, page17). For the purposes of the present work, we will consider only overdamped dynamics.¹

The state of the thermodynamic ensemble is identified with the probability density of the stochastic process X_t and is denoted by $\rho(t, x)$. It represents the likelihood of a particle residing at location $x \in \mathbb{R}^n$ at time t , and is governed by the Fokker-Planck equation

$$\frac{\partial \rho}{\partial t}(t, x) = -\nabla_x \cdot (\rho(t, x)v(t, x)), \text{ with} \quad (2a)$$

$$v(t, x) = -\frac{1}{\gamma} [\nabla_x U(t, x) + k_B T(t) \nabla_x \log \rho(t, x)]. \quad (2b)$$

Note that by substituting the effective velocity field v into (2a) (which is written as a continuity equation) brings out the familiar form with the Laplace operator $\Delta_x = \nabla_x \cdot \nabla_x$, in that, $\partial_t \rho = \frac{1}{\gamma} \nabla_x \cdot (\rho \nabla_x U) + \frac{k_B T}{\gamma} \Delta_x \rho$.

Variations in the potential energy $U(t, X_t)$ of the particles mediate transference of heat between the particles and the heat

bath, and exchange of work between the particles and the externally controlled potential $U(t, \cdot)$. Specifically, the rates of heat and work that are being transferred are²

$$dQ = \nabla_x U(t, X_t) \circ dX_t, \quad (3a)$$

$$dW = \frac{\partial U}{\partial t}(t, X_t) dt, \quad (3b)$$

where \circ represents Stratonovich integration (Oksendal, 2013). Note that these definitions for heat and work ensure validity of the first law of thermodynamics at the level of individual particle, $dU(t, X_t) = dW + dQ$.

Collectively, at the level of the ensemble, the averaged³ $d\mathcal{E}(\rho, U) = dQ + dW$ at the level of the ensemble, with the internal energy of the ensemble being

$$\mathcal{E}(\rho, U) = \int_{\mathbb{R}^n} U(t, x) \rho(t, x) dx. \quad (5)$$

Two additional thermodynamic quantities of great importance to thermodynamic transitions are the entropy \mathcal{S} and the free energy \mathcal{F} . The familiar Shanon entropy (rate)

$$\mathcal{S}(\rho) = -k_B \int_{\mathbb{R}^n} \log(\rho) \rho dx, \quad (6a)$$

represents information while the free energy

$$\begin{aligned} \mathcal{F}(\rho, U, T) &= \mathcal{E}(\rho, U) - T\mathcal{S}(\rho) \\ &= k_B T \int_{\mathbb{R}^n} \rho \log(\rho/\rho_B) dx \end{aligned} \quad (6b)$$

represents relative entropy of the ensemble state from the unnormalized Boltzmann distribution $\rho_B := \exp(-U/(k_B T))$. Intuitively, the free energy represents a thermal potential that is steering the dynamics (see Owen, 2012; Parrondo, Horowitz, & Sagawa, 2015 and especially Jordan, Kinderlehrer, & Otto, 1998).

In the sequel, our goal is to quantify the maximal power that can be drawn from a thermodynamic ensemble by way of a control input $-\nabla_x U$, with the ensemble powered by the time-varying temperature gradient of a heat bath, with period t_f . That is, we seek a time-varying control that takes advantage of variations in temperature to extract work, and does so optimally, to maximize power of the cycle that is dictated by periodicity of the temperature.

3. Cyclic operation: power and dissipation

We assume that the temperature of the heat bath oscillates with period t_f , and that a periodic control is applied to the thermodynamic system in the form of a driving potential $U(t, \cdot) | t \in [0, t_f]$. Under these conditions, we assume that the thermodynamic state $\rho(t, \cdot)$ settles to a closed orbit with the same period. Over this cycle we seek to optimize the average of the work drawn from the thermodynamic system by way of our control $-\nabla_x U$. The thermodynamic system is powered by the temperature gradients, and thereby, energy is drawn out of the heat bath and into the coupling to the externally controlled potential.

¹ Overdamped dynamics are widely used to model the motion of colloidal particles in an ambient heat bath (Peliti & Pigolotti, 2021; Seifert, 2012). expressed via the stochastic differential equation

$$\gamma dX_t = -\nabla_x U(t, X_t) dt + \sqrt{2\gamma k_B T(t)} dB_t. \quad (1)$$

The stochastic process $X_t \in \mathbb{R}^n$ represents the position of a single particle in the ensemble, and resides in the n -dimensional ambient space. The constant coefficient γ models dissipation, the time-varying potential $U(t, x)$ exerts an externally controlled force $\nabla_x U(t, x)$ at location x that represents our control input, k_B denotes the Boltzmann constant, and $T(t)$ the temperature of the thermal heat bath that generates stochastic excitation modeled by the n -dimensional standard Brownian motion B_t .

² d indicates that the corresponding integral is path-dependent, i.e., not a function of the terminal conditions, in contrast to d .

³ $\mathbb{E}\{\cdot\}$ denotes expectation rates of heat and work ($dQ := \mathbb{E}\{dQ\}$, $dW := \mathbb{E}\{dW\}$) are leading to (with $\langle v_1, v_2 \rangle = v_1^T v_2$ denoting the standard inner product in \mathbb{R}^n)

$$dQ = \left[\int_{\mathbb{R}^n} \langle \nabla_x U(t, x), v(t, x) \rangle \rho(t, x) dx \right] dt, \quad (4a)$$

$$dW = \left[\int_{\mathbb{R}^n} \frac{\partial U}{\partial t}(t, x) \rho(t, x) dx \right] dt, \quad (4b)$$

consistent with the first law of thermodynamics (energy invariance).

Averaging the work drawn over a cycle, the mean power that is gained is

$$\mathcal{P} = -\frac{1}{t_f} \int_0^{t_f} \int_{\mathbb{R}^n} \frac{\partial U}{\partial t}(t, x) \rho(t, x) dx dt. \quad (7)$$

In general, potential and temperature profiles can be discontinuous in time, but need to abide by the periodic boundary condition, e.g., $U(0^+, \cdot) = U(t_f^+, \cdot)$ and the same for the temperature. Throughout we assume that $U(t, x)$ is differentiable in x , while both $T(t)$ and $U(t, x)$ are piecewise differentiable in t . Under these assumptions we seek to maximize \mathcal{P} .

3.1. Dissipation along thermodynamic paths

A serendipitous connection between thermodynamics and the so-called Wasserstein geometry of probability distributions was discovered by Aurell, Mejía-Monasterio, and Muratore-Ginanneschi (2011) (see also our work in Chen, Georgiou, & Tannenbaum, 2019), in that the dissipation along a path of the thermodynamic state can be expressed as the traversed geometric length. To this end, we briefly describe the basic elements (Villani, 2003) that are essential for our exposition.

3.1.1. The Wasserstein space $\mathcal{P}_2(\mathbb{R}^n)$

The space of probability distributions on \mathbb{R}^n with finite second-order moments, denoted by $\mathcal{P}_2(\mathbb{R}^n)$, or \mathcal{P}_2 here for short, assumes a Riemannian-like structure. Our interest in this space, as noted, is due to the fact that it serves as state space for our thermodynamic system (2a) and, in addition, it is normed in a way that the length of trajectories equals the dissipation generated during the corresponding thermodynamic transition of ensembles. Thus, \mathcal{P}_2 is a natural choice.

The structure of \mathcal{P}_2 is inherited by the so-called Wasserstein metric⁴

$$W_2(\rho_0, \rho_f) := \sqrt{\inf_{\pi \in \Pi(\rho_0, \rho_f)} \int_{\mathbb{R}^n \times \mathbb{R}^n} \|x - y\|^2 \pi(x, y) dx dy},$$

for $\rho_0, \rho_f \in \mathcal{P}_2$. The optimization in the above expression is over probability distributions π on the product space $\mathbb{R}^n \times \mathbb{R}^n$ having ρ_0, ρ_f as marginals; $\Pi(\rho_0, \rho_f)$ denotes the set of distributions on the product space with this property, i.e., having the specified marginals.

A tangent displacement $\delta\rho$ about a given density $\rho(\cdot)$ can be identified with a vector field $v(\cdot)$ that effects the infinitesimal perturbation via the continuity equation $\delta\rho = -(\nabla_x \cdot (\rho v)) \delta t$. The most “economical” v , by Helmholtz decomposition, can be selected curl-free and, thereby, as the gradient of suitable (unique modulo a constant) scalar potential function ϕ , i.e., $v(x) = \nabla_x \phi(x)$, see Villani (2003, Section 8.1.2, p. 246–247). As a consequence, we can formally identify $\delta\rho/\delta t$, ϕ , v , as alternative representations of tangent directions linked bijectively in pairs (modulo a constant in the choice of ϕ) via the Poisson equation $\delta\rho/\delta t + \nabla_x \cdot (\rho \nabla_x \phi) = 0$ and the curl-free $v = \nabla_x \phi$ requirement.

It turns out that the inner product

$$\langle v_1, v_2 \rangle_\rho := \int_{\mathbb{R}^n} \langle v_1(t, x), v_2(t, x) \rangle \rho(t, x) dx,$$

⁴ This metric is also known as Monge–Kantorovich, or earth mover’s distance. The particular version that we use is based on quadratic transportation cost, noted in the subscript W_2 .

between tangent velocity fields has elegant geometric properties and intrinsic physical significance. Firstly, it induces a Riemannian⁵ structure with norm-squared

$$\left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2 := \int_{\mathbb{R}^n} \|v(t, x)\|^2 \rho(t, x) dx,$$

interpreted as (twice the) kinetic energy of the ensemble (mass \times velocity²). Secondly, the length of a path

$$\ell_{\rho_0:t_f} := \int_0^{t_f} \left(\left\| \frac{\partial \rho}{\partial t} \right\|_{W_2} \right) dt$$

(integral of velocity over time), traversed by the thermodynamic ensemble between the end-point distributions ρ_0 and ρ_f , is precisely $W_2(\rho_0, \rho_f)$; that is, $W_2(\rho_0, \rho_f)$ is a geodesic distance (Villani, 2003, Ch. 8). Thirdly, the action integral

$$\mathcal{A}_{\rho_0:t_f} := \int_0^{t_f} \left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2 dt \quad (8)$$

of kinetic energy along any thermodynamic transition $\{\rho(t, \cdot); t \in [0, t_f]\}$ turns out to quantify precisely dissipation (entropy production) along the path. Finally, a useful relationship that follows readily from the Cauchy–Schwartz inequality is that

$$\mathcal{A}_{\rho_0:t_f} \geq \frac{1}{t_f} \ell_{\rho_0:t_f}^2, \quad (9)$$

with the bound achieved when the velocity remains constant along the path ($\|\frac{\partial \rho}{\partial t}\|_{W_2} = \text{constant}$).

3.2. Energetics over a cycle

We now consider the overdamped model (1) and assume that the temperature $T(t)$ is a periodic function of time, independent of the state of the system, with period t_f . As before, it is seen to represent the dynamics of any single particle of an ensemble whose distribution $\rho(t, \cdot)$ obeys the Fokker–Planck equation (2a). Thence, $\rho(t, \cdot)$ is the state of the ensemble and traverses over a period of duration t_f a closed orbit on the thermodynamic manifold \mathcal{P}_2 .

The key in quantifying energy exchange between the system and the environment is the free energy (6b), which is a function $\mathcal{F}(\rho(t, \cdot), U(t, \cdot), T(t))$ of the ensemble state, the potential and the temperature. Since all of the entries are periodic with the same period t_f , the change $\Delta\mathcal{F}$ in the free energy of the system over a cycle is zero, i.e.,

$$\underbrace{\mathcal{F}(\rho(t_f, \cdot), U(t_f, \cdot), T(t_f)) - \mathcal{F}(\rho(0, \cdot), U(0, \cdot), T(0))}_{\Delta\mathcal{F}} = 0,$$

and, in general, $\Delta\mathcal{F} = \int_0^{t_f^+} \dot{\mathcal{F}} dt = 0$. On the other hand, expanding the rate of change $\dot{\mathcal{F}} = d\mathcal{F}/dt$ along the cycle allows separating the contributions of heat and work that come in and out of the ensemble during that time period. To this end, we compute

$$\frac{d\mathcal{F}}{dt} = \int \frac{\partial U}{\partial t} \rho dx + \int \left[(U + k_B T \log \rho) \frac{\partial \rho}{\partial t} \right] dx - \dot{S}(\rho), \quad (10)$$

where we used the fact that $\frac{\partial \rho}{\partial t}$ integrates to zero; spatial integrals from here on are understood as being over \mathbb{R}^n unless made explicit otherwise. Following Aurell et al. (2011) (see also Chen

⁵ As \mathcal{P}_2 can be thought to contain measures, it is often referred to as almost-Riemannian due to the fact that vector fields about singular points/measures cannot effect flow in all directions, a technical point of no interest here.

et al., 2019), the second term in (10) can be rewritten as

$$\begin{aligned} & \int \left[(U + k_B T(t) \log \rho) \frac{\partial \rho}{\partial t} \right] dx \\ &= - \int (U + k_B T(t) \log \rho) \nabla_x \cdot (\rho v) dx \\ &= \int \langle \nabla_x U + k_B T(t) \nabla_x \log \rho, v \rangle \rho dx \\ &= -\gamma \int \|v\|^2 \rho dx = -\gamma \left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2, \end{aligned}$$

where the first equality utilizes the Fokker–Planck equation (2a), the second equality follows using integration by parts,⁶ the third equality utilizes (2b), and the final equality is a re-write that uses the norm $\|\cdot\|_{W_2}$ in the tangent space of \mathcal{P}_2 .

From (10) and (4b), the important equation

$$\frac{d\mathcal{F}}{dt} = \frac{d\mathcal{W}}{dt} - \gamma \left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2 - \dot{T}(t)S(\rho) \quad (11)$$

follows. In this we recognize three contributions. The first term on the right represents work delivered to the system as explained earlier, the second and third terms represent heat exchange with the environment. Of those, the integral along a cycle of the one that involves a quadratic expression of the velocity $\partial \rho / \partial t$, is always negative and vanishes for quasi-static ($t_f \rightarrow \infty$) operation. Thus, it represents dissipation, i.e., it represents heat being released to the environment that cannot be recovered in the reverse direction. The last term on the right represents again heat, but this time the flow is reversible with time and the integral over time is independent of the velocity of the ensemble, thus, representing quasi-static heat transference.

We are now in a position to give an expression for

$$\mathcal{P} := \frac{1}{t_f} \int_{\text{period}} d\mathcal{W},$$

the (average) power delivered over a cycle.

Proposition 1. *The power output over a cycle is*

$$\mathcal{P} = -\frac{1}{t_f} \int_0^{t_f} \left[\gamma \left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2 \right] dt - \frac{1}{t_f} \int_0^{t_f} [\dot{T}(t)S(\rho)] dt. \quad (12)$$

Proof. In view of (11) and the fact that $\Delta\mathcal{F} = 0$ over a cycle, we obtain that work output over a cycle is

$$-\int_0^{t_f} \frac{d\mathcal{W}}{dt} dt = -\gamma \int_0^{t_f} \left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2 dt - \int_0^{t_f} \dot{T}(t)S(\rho) dt$$

which concludes (12). \square

As noted, the first term is always negative and represents work that is being dissipated and lost as heat to the environment. Thus, we denote dissipative losses

$$\mathcal{W}_{\text{diss}} := \gamma \int_0^{t_f} \left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2 dt.$$

The average of $-\dot{T}S$ over a period can be both, positive or negative, depending on the control protocol U and relates to the “useful” portion of the work that is being extracted (when positive, and contributed, when negative). It is independent of the speed of traversing the cycle, and thereby we refer to it as quasi-static,

$$\mathcal{W}_{\text{qs}} := - \int_0^{t_f} \dot{T}(t)S(\rho) dt. \quad (13)$$

⁶ Under the assumption that the controlling potential $U(t, x)$ grows sufficiently fast for large x , the state $\rho(t, x)$ vanishes at infinity – a condition that is needed in applying the well-known integration by parts formula.

It can also be expressed in geometric terms as

$$\mathcal{W}_{\text{qs}} = -k_B \int_0^{t_f} T(t) \int \langle \nabla_x \log(\rho), v \rangle \rho dx dt, \quad (14)$$

where we have integrated (13) by parts and utilized

$$\frac{d}{dt} S(\rho) = -k_B \int \langle \nabla_x \log(\rho), v \rangle \rho dx.$$

To recap, the power delivered over a cycle is

$$\mathcal{P} = \frac{1}{t_f} (\mathcal{W}_{\text{qs}} - \mathcal{W}_{\text{diss}}). \quad (15)$$

The problem to maximize power by a suitable choice of regulating potential $U(t, \cdot)$, reduces to selecting a closed curve $\{\rho(t, \cdot) \mid t \in [0, t_f]\}$ in the thermodynamic manifold \mathcal{P}_2 , such that

$$\begin{aligned} \mathcal{P}^* &:= \max_{\rho(t, \cdot)} -\frac{1}{t_f} \int_0^{t_f} \left[\gamma \left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2 + \dot{T}(t)S(\rho) \right] dt, \\ \text{s.t. } &\rho(0, \cdot) = \rho(t_f, \cdot). \end{aligned} \quad (16)$$

Remark 1. The quasi-static work over a cycle can be written as an area integral as long as the state of the system has a finite dimensional parametrization (Miangolarra, Taghvaei, Chen, & Georgiou, 2022). On the other hand, the dissipation $\mathcal{W}_{\text{diss}}$ over a cycle can achieve the lower bound

$$\mathcal{W}_{\text{diss}} \geq \frac{\gamma}{t_f} \ell_{\rho_0: t_f}^2, \quad (17)$$

when the velocity $\left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}$ is constant along the curve that the system traverses on \mathcal{P}_2 . Thus, ensuring constant velocity, the maximal power is

$$\mathcal{P} = \frac{1}{t_f} \left(\mathcal{W}_{\text{qs}} - \frac{\gamma}{t_f} \ell_{\rho_0: t_f}^2 \right). \quad (18)$$

In the quasi-static limit, as $t_f \rightarrow \infty$, the contribution from dissipation vanishes. \square

Remark 2. The traditional definition of efficiency, where the work generated is compared to the heat drawn out of the heat bath of highest temperature, does not apply in the present case of a single heat bath with piecewise continuous temperature profile; *heat is drawn out of this single heat bath, taking advantage of temperature gradients, as the temperature fluctuates.* Remark 1 motivates the following new definition for the efficiency of a thermodynamic cycle in the present context:

$$\eta := \frac{\mathcal{W}_{\text{qs}} - \mathcal{W}_{\text{diss}}}{\mathcal{W}_{\text{qs}}}. \quad (19)$$

It is readily seen that $\eta \leq 1$, with equality achieved in the quasi-static limit, when the dissipation vanishes. \square

3.3. Illustrative examples

We next discuss two special cases for which the expression for power can be made explicit. This will not only prove useful later on, but also shed some light into the problem of maximizing power.

3.3.1. Carnot-like cycle

Consider the one-dimensional system (1) of overdamped particles and assume that the temperature is piecewise constant. That is, we consider Carnot-like operating conditions where the system is brought in contact, alternatingly, with two heat baths of different temperatures. In this case,

$$T(t) = \begin{cases} T_h, & t \in (0, t_{1/2}), \\ T_c, & t \in (t_{1/2}, t_f), \end{cases} \quad (20)$$

over a period t_f , with $t_{1/2}$ to be determined. The power delivered is now

$$\mathcal{P} = -\frac{1}{t_f} \left(\gamma \int_0^{t_f} \left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2 dt - \Delta T (S(\rho_{1/2}) - S(\rho_0)) \right),$$

where $\Delta T := T_h - T_c$, and the thermodynamic state is $\rho_0(\cdot) = \rho(t_0, \cdot)$ and $\rho_{1/2}(\cdot) = \rho(t_{1/2}, \cdot)$, at times $t = 0$ and $t = t_{1/2}$, respectively. Maximizing power over a choice of control potential $U(t, \cdot)$ and $t_{1/2}$, gives $t_{1/2} = t_f/2$ and

$$\mathcal{P}^* = -\frac{\gamma}{t_{1/2}(t_f - t_{1/2})} W_2(\rho_0, \rho_{1/2})^2 + \frac{1}{t_f} \Delta T \Delta S, \quad (21)$$

where $\Delta S = S(\rho_{1/2}) - S(\rho_0)$, see Fu et al. (2021) for more details.

Remark 3. When the control action $(-\nabla_x U(t, x))$ is strong enough to localize the thermodynamic state at some point in time, e.g., at $t = 0$ with $\rho(0, \cdot)$ being close to a Dirac, then $S(\rho_0) \approx -\infty$. As a consequence, $\Delta S \approx \infty$, and limitless power can be drawn as \mathcal{P} in (21) is not bounded from above. This phenomenon is not particular to the Carnot cycle and can be traced to unreasonable demands on ∇U to bring the thermodynamic state to a very low entropy condition. Below we highlight that the same is true for a quadratic potential when the thermodynamic state remains Gaussian.

3.3.2. Gaussian states:

We consider once again the dynamics in (1) of overdamped particles subject now to a quadratic controlling potential, and further specialize to one degree of freedom, i.e., $n = 1$ and $x \in \mathbb{R}$. We assume that the thermodynamic state $\rho(t, \cdot)$ of the ensemble is Gaussian with mean zero and variance $\sigma(t)^2$, i.e., $\rho(t, \cdot) = N(0, \sigma(t)^2)$.

If $q(t)$ denotes the “spring constant” of the potential, i.e., $U(t, x) = \frac{1}{2} q(t) x^2$, $\sigma(t)$ is governed by the Lyapunov equation

$$\gamma \frac{d}{dt} (\sigma(t)^2) = -2q(t)\sigma(t)^2 + 2k_B T(t). \quad (22)$$

The effective velocity field is

$$v(t, x) = -\frac{1}{\gamma} (q(t)x - k_B T(t) \frac{x}{\sigma(t)^2}) = \frac{\dot{\sigma}(t)}{\sigma(t)} x,$$

where the last identity follows from Lyapunov equation. Hence,

$$\left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2 = \frac{1}{\gamma^2} \left(q(t)\sigma(t) - \frac{k_B T(t)}{\sigma(t)} \right)^2 = \gamma \dot{\sigma}(t)^2.$$

In addition, the entropy of the Gaussian distribution is

$$S(\rho) = \frac{k_B}{2} \log(2\pi e \sigma(t)^2). \quad (23)$$

Using these identities the expression for the power delivered (12) simplifies to

$$\mathcal{P} = -\frac{1}{t_f} \int_0^{t_f} [\gamma \dot{\sigma}(t)^2 + k_B \dot{T}(t) \log(\sigma(t))] dt. \quad (24)$$

It is now intuitively clear that, as long as the temperature does not remain constant (and thus, there is nontrivial temperature gradient), one can apply a similar strategy as the one utilized in the Carnot-like cycle and extract unbounded power from this system. Specifically, with a suitable control protocol $\sigma(t)$ can be made arbitrarily small at the time when the temperature of the heat bath is at its lowest, thereby allowing unbounded power to be extracted as the heat bath moves to higher temperatures. For completeness, we detail such a strategy in the appendix (see the Appendix).

Remark 4. It is apparent that without any restrictions on the allowable control $U(t, x)$, infinite power can be drawn from a temperature varying heat bath. The reason is that the quasi-static instantaneous power $k_B \dot{T} \log(\sigma)$ can increase without bound for a choice of control U that drives the ensemble to a low entropy state, e.g., close to a Dirac. While this is highly desirable, it is physically unreasonable. Large gradients of $U(t, x)$ that are needed to localize the thermodynamic state amount to excessive forces being applied to the particles of the ensemble. Thus, on physical grounds it is reasonable to impose suitable constraints on the gradients of U or ρ , along any thermodynamic transition. This is done next.

4. Maximizing power under constraints

It is insightful to view the Fokker Planck equation (2a) as a continuity equation $\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho v) = 0$, for a vector field $v = \nabla_x \phi$, where the “effective” potential $\phi = \frac{1}{\gamma}(R - U)$ is composed of two terms, U , that provides control action and a probabilistic potential

$$R(t, x) = -k_B T(t) \log(\rho(t, x)).$$

The gradient of U represents a physical force that drives the ensemble. On the other hand, large values for the gradient of R (seen as some sort of entropic force) also seem physically unrealistic in the context of overdamped (colloidal) particles, where diffusion dominates inertial effects. Below we proceed by postulating and imposing suitable quadratic bounds, and explore the consequences with regard to maximizing power.

Specifically, we postulate that the control mechanism that generates $U(t, x)$, tasked to steer the thermodynamic system along a closed orbit, is restricted in its ability to generate forces. Similarly, that it is restricted in its ability to localize the state to approximate a Dirac. Either of these reasonable constraints can be cast as bounds on the size of the gradients, such as

$$\int_{\mathbb{R}^n} \|\nabla_x R\|^2 \rho dx, \text{ or } \int_{\mathbb{R}^n} \|\nabla_x U\|^2 \rho dx. \quad (25)$$

The first of the two square-norms relates directly to the Fisher information of the thermodynamic state

$$I(\rho) := \int_{\mathbb{R}^n} \|\nabla_x \log(\rho)\|^2 \rho dx, \quad (26)$$

since $(k_B T(t))^2 I(\rho) = \int \|\nabla_x R\|^2 \rho dx$. Therefore, bounding the L_2 norm of $\nabla_x R$ is equivalent to bounding the Fisher information (as long as the temperature is finite and nonzero) and it is the latter that we will impose in the sequel. In passing, we note that the quadratic expression quantifying dissipation, namely,

$$\int_{\mathbb{R}^n} \|\nabla_x R - \nabla_x U\|^2 \rho dx = \gamma \left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2,$$

relates the two gradients.

In the next two subsections we obtain optimal control protocols for generating power under suitable bounds on control and information on the thermodynamic state.

4.1. Maximal power with bounded Fisher information

We now determine an expression for the maximal power that can be extracted under the assumption that

$$I(\rho) \leq I_{\max}, \quad (27)$$

or, equivalently, a corresponding bound on $\int \|\nabla_x R\|^2 \rho dx$. As before, we consider the optimization problem (16) for power generated by the over-damped model (1) over a cycle. In what

follows,

$$\bar{T} := \frac{1}{t_f} \int_0^{t_f} T(t) dt,$$

$$\text{Var}(T(t)) := \frac{1}{t_f} \int_0^{t_f} (T(t) - \bar{T})^2 dt,$$

denote the mean and variance of the temperature profile.

Proposition 2. Under the constraint (27) on thermodynamic paths $\rho(t, x)$ over a closed cycle, the maximal power expressed in (16) satisfies

$$\mathcal{P}^* \leq \frac{k_B^2 I_{\max}}{4\gamma} \text{Var}(T(t)). \quad (28)$$

Proof. Over one cycle, the change of entropy is

$$\int_0^{t_f} \dot{S}(\rho) dt = S(\rho_f) - S(\rho_0) = 0 \quad (29)$$

due to the periodic conditions. Multiplying (29) by a constant C and adding to the expression in (12) yields

$$\begin{aligned} \mathcal{P} &= -\frac{1}{t_f} \int_0^{t_f} \int [\gamma \|v\|^2 + k_B(T(t) - C)v \cdot \nabla_x \log(\rho)] \rho dx dt \\ &= -\frac{1}{t_f} \int_0^{t_f} \int \left[\sqrt{\gamma} v + \frac{1}{2\sqrt{\gamma}} k_B(T(t) - C) \nabla_x \log(\rho) \right]^2 \rho dx dt \\ &\quad + \frac{k_B^2}{4\gamma t_f} \int_0^{t_f} (T(t) - C)^2 I(\rho) dt \\ &\leq \frac{k_B^2 I_{\max}}{4\gamma t_f} \int_0^{t_f} (T(t) - C)^2 dt, \end{aligned}$$

where we use the positivity of the first term and $I(\rho) \leq I_{\max}$. The best bound over all constants C is obtained by letting $C = \bar{T}$ concluding the result. \square

Remark 5. The upper bound of the power extracted from one complete cycle under the Fisher constraint is proportional to the average fluctuations in the temperature profile (27). For the Carnot-like temperature profile (20), the maximal power satisfies

$$\mathcal{P}^* \leq \frac{k_B^2 I_{\max}}{4\gamma} \frac{(T_h - T_c)^2}{4},$$

where $T_h := \max_t \{T(t)\}$ and $T_c := \min_t \{T(t)\}$ are the maximal and minimal temperatures over the cycle, which is consistent with the result in Fu et al. (2021) that deals with piecewise constant temperature profile and fast adiabatic transitions (Carnot-like). \square

We now show that the above bound is tight by constructing a protocol that achieves the upper bound (28) as $t_f \rightarrow 0$, that is, in the limit of “fast operation” (Blaber, Louwerse, & Sivak, 2021; Schmiedl & Seifert, 2007a). To this end, we consider

$$\rho(t, x) = N(0, \sigma(t)^2),$$

once again specializing to $n = 1$. The Fisher information is $I(\rho) = \sigma(t)^{-2}$. We select the following variance

$$\sigma(t) = \sigma_{\min} \exp \left(\frac{\kappa}{2\gamma} \left(\int_{t_0}^t (T(s) - \bar{T}) ds \right) \right), \quad (30)$$

where $\kappa := k_B/\sigma_{\min}^2$, $\sigma_{\min} := \min_t \sigma(t)$, and where t_0 is selected so that

$$\int_{t_0}^t (T(s) - \bar{T}) ds \geq 0, \quad (31)$$

for all t . The profile (30) can be achieved by the quadratic control protocol $U(t, x) = \frac{1}{2} q(t) x^2$, where

$$q(t) = \frac{\kappa \bar{T}}{2} + \frac{\kappa T(t)}{2} \left(2e^{-\frac{\kappa}{\gamma} \left(\int_{t_0}^t T(s) - \bar{T} ds \right)} - 1 \right), \quad (32)$$

together with $\sigma(t)^2$, satisfy the Lyapunov equation (22). Under these conditions we have the following:

Proposition 3. Under the control protocol (32),

$$\mathcal{P} \rightarrow \frac{k_B^2 I_{\max}}{4\gamma} \text{Var}(T(\cdot)), \text{ as } t_f \rightarrow 0.$$

Proof. We first note that $\sigma(t)$ is periodic and satisfies the constraint $I(\rho) \leq I_{\max}$, since $\sigma(t) \geq \sigma_{\min}$ following the definition of t_0 . The expression for power in (24) gives

$$\begin{aligned} \mathcal{P} &= -\frac{1}{t_f} \int_0^{t_f} [\gamma \sigma_{\min}^2 \dot{r}(t)^2 e^{2r(t)} + k_B \dot{T}(t) r(t)] dt \\ &= -\frac{k_B}{t_f} \int_0^{t_f} \left[\frac{\gamma \sigma_{\min}^2}{k_B} \dot{r}(t)^2 e^{2r(t)} - T(t) \dot{r}(t) \right] dt, \end{aligned} \quad (33)$$

for r representing the logarithmic ratio

$$r(t) := \log \left(\frac{\sigma(t)}{\sigma_{\min}} \right) = \frac{\kappa}{2\gamma} \int_{t_0}^t (T(s) - \bar{T}) ds.$$

The equality in (33) follows using integration by parts and the periodic boundary conditions. Then,

$$\begin{aligned} \mathcal{P} &\geq -\frac{k_B}{t_f} \int_0^{t_f} \left[\frac{\gamma \sigma_{\min}^2}{k_B} \dot{r}(t)^2 e^{2r_{\max}} - T(t) \dot{r}(t) \right] dt \\ &= \frac{k_B^2}{4\gamma t_f \sigma_{\min}^2} (2 - e^{2r_{\max}}) \int_0^{t_f} (T(t) - \bar{T})^2 dt \\ &= (2 - e^{2r_{\max}}) \frac{k_B^2}{4\gamma \sigma_{\min}^2} \text{Var}(T(t)), \text{ for} \end{aligned} \quad (34)$$

$$\begin{aligned} 0 \leq r_{\max} &:= \max_t r(t) \leq \frac{\kappa}{2\gamma} \int_{t_0}^t (T(s) - \bar{T}) ds \\ &\leq \frac{\kappa t_f}{2\gamma} (T_h - T_c). \end{aligned}$$

As $t_f \rightarrow 0$, $e^{2r_{\max}} \searrow 1$ and the lower bound in (34) approaches the bound in (28) completing the proof. \square

Remark 6. To get insight on the tradeoff between efficiency and power, we evaluate the efficiency of the proposed protocol (32). Using the expression (30) for the variance in the definition for quasi-static work (13) yields

$$\begin{aligned} \mathcal{W}_{\text{qs}} &= \int_0^{t_f} T(t) \dot{S}(\rho) dt = k_B \int_0^{t_f} T(t) \frac{\dot{\sigma}(t)}{\sigma(t)} dt \\ &= \frac{k_B^2}{2\gamma \sigma_{\min}^2} \int_0^{t_f} T(t) (T(t) - \bar{T}) dt \\ &= \frac{k_B^2 t_f}{2\gamma \sigma_{\min}^2} \text{Var}(T(t)), \end{aligned}$$

while $\mathcal{W}_{\text{qs}} - \mathcal{W}_{\text{diss}} = t_f \mathcal{P} \rightarrow \frac{k_B^2 t_f}{4\gamma \sigma_{\min}^2} \text{Var}(T(t))$ as $t_f \rightarrow 0$, according to Proposition 3. Therefore,

$$\eta = \frac{\mathcal{W}_{\text{qs}} - \mathcal{W}_{\text{diss}}}{\mathcal{W}_{\text{qs}}} \rightarrow \frac{1}{2}$$

as $t_f \rightarrow 0$. This is consistent with the observation made in the underdamped limit (Miangolarra et al., 2021) and the linear response regime (Van den Broeck, 2005), where it was shown that the efficiency at maximum power is $\frac{1}{2}$. \square

4.2. Maximal power with an L_2 -bound on $\nabla_x U(t, x)$

We now determine an expression for the maximal power that can be extracted under the bound

$$\frac{1}{\gamma} \int \|\nabla_x U(t, x)\|^2 \rho(x) dx \leq M \quad (35)$$

on control action. As before, we consider the optimization problem (16) and derive a bound on maximal power.

Proposition 4. *Under the constraint (35), the maximal power in (16) is bounded as follows,*

$$\mathcal{P}^* \leq \frac{M}{4} \frac{1}{t_f} \int_0^{t_f} \frac{T_h - T(t)}{T(t)} dt. \quad (36)$$

Proof. Over a cycle, the rate of change of the entropy is

$$\begin{aligned} \dot{S}(\rho) &= -k_B \int v \cdot \nabla_x \log \rho \rho dx \\ &= \frac{k_B}{\gamma} \int [\nabla_x U \cdot \nabla_x \log(\rho) + k_B T(t) \|\nabla_x \log(\rho)\|^2] \rho dx \\ &\geq -\frac{k_B}{\gamma} \left(\int \|\nabla_x U\|^2 \rho dx \right)^{\frac{1}{2}} \left(\int \|\nabla_x \log(\rho)\|^2 \rho dx \right)^{\frac{1}{2}} \\ &\quad + \frac{k_B^2}{\gamma} T(t) \int \|\nabla_x \log(\rho)\|^2 \rho dx \\ &\geq \frac{k_B}{\gamma} \left[-\sqrt{\gamma M} \sqrt{I(\rho)} + k_B T(t) I(\rho) \right] \\ &\geq -\frac{M}{4T(t)}, \end{aligned}$$

where the first inequality follows by Cauchy–Schwartz, the second is due to the constraint (35), and the last inequality is obtained by minimizing over $I(\rho)$. Thus,

$$\begin{aligned} \mathcal{P} &= \frac{1}{t_f} \int_0^{t_f} \left[-\gamma \left\| \frac{\partial \rho}{\partial t} \right\|_{W_2}^2 + T(t) \dot{S}(\rho) \right] dt \\ &\leq \frac{1}{t_f} \int_0^{t_f} T(t) \dot{S}(\rho) dt, \end{aligned}$$

where we neglected the dissipation term and used integration by parts and cyclic boundary conditions. In order to apply the bound $\dot{S}(\rho) \geq -\frac{M}{4T(t)}$, we need to ensure $\dot{S}(\rho)$ is multiplied by a negative factor. This is achieved using the periodic boundary condition and subtracting the zero term $-T_h \int_0^{t_f} \dot{S}(\rho) dt = 0$. Therefore, \mathcal{P} is bounded above by $\frac{1}{t_f} \int_0^{t_f} (T(t) - T_h) \dot{S}(\rho) dt$, which in turn is bounded above by

$$\frac{M}{4} \frac{1}{t_f} \int_0^{t_f} \frac{T_h - T(t)}{T(t)} dt,$$

completing the proof. \square

Remark 7. For a Carnot-like piece-wise constant temperature profile,

$$\begin{aligned} \mathcal{P}^* &\leq \frac{M}{4} \frac{1}{t_f} \left(\int_0^{t_{1/2}} \frac{T_h - T_h}{T_h} dt + \int_{t_{1/2}}^{t_f} \frac{T_h - T_c}{T_c} dt \right) \\ &= \frac{M}{8} \left(\frac{T_h}{T_c} - 1 \right), \end{aligned}$$

which is consistent with the result in Fu et al. (2021, Theorem 2) that were derived for this special case. \square

Remark 8. Unlike the case constrained by Fisher information, it is not known whether the bound (36) is tight.

5. Conclusions

The present work quantifies the maximal power and the efficiency at maximal power that can be drawn out from a thermodynamic engine in contact with a single heat bath with arbitrary periodic temperature profile. This is contrast to earlier work on rigid Carnot-like alternating thermal excitation, using two heat baths. The formulation of the optimization problem falls within the scope of stochastic control, utilizing Langevin models for thermal mesoscopic systems (Sekimoto, 2010).

We motivate and consider two natural constraints on control actuation. The first constrains the Fisher information of the thermodynamic states ρ , and the second constrains the averaged quadratic control effort (average of the control $-\nabla_x U$ over states). In each case, we obtain insightful bounds for the maximal power and efficiency at maximal power achievable. Specifically, for the case where the Fisher information is constrained, we show that the maximal power is nearly fully determined by the variance of the temperature profile. Of particular interest is that the efficiency at maximal power approaches $\frac{1}{2}$ when the period tends to zero. An important direction for future work pertains to connections between this observation and the universal bound on efficiency at maximal power output (Van den Broeck, 2005) being one half of the Carnot efficiency. The role of closed-loop control in energy harvesting, and in optimizing control strategies for maximizing power, is another challenging and potentially impactful direction (Sandberg, Delvenne, Newton, & Mitter, 2014; Taghvaei, Miangolarra, Fu, Chen, & Georgiou, 2021).

It will be amiss if we did not draw attention to a long line of works in the control literature, aimed at shedding light into the second law and its implications. In fact, the stochastic framework of stochastic energetics (Sekimoto, 2010) adapted herein is akin to the stochastic control approach that goes back to Brockett and Willems (Brockett & Willems, 1979). More recent accounts within the control community diverged, exploring a range of links between classical dissipativity theory, information theory and filtering, and the differential geometry of thermodynamic manifolds (Delvenne & Sandberg, 2015, 2017; Delvenne, Sandberg, & Doyle, 2007; Van Der Schaft, 2021). It is the authors' hope that the present work points to fruitful new directions.

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Appendix

Limitless power under arbitrary protocol.

We herein explain that, as long as the temperature does not remain constant and there are no restrictions on the control potential in (1), the power that can be extracted through the ensemble is arbitrarily large.

Since $T(t)$ varies over the cycle, one of the following two cases must hold:

- (i) There exists an interval $(a, b) \subset [0, t_f]$ such that $\dot{T}(t) > 0$ for $t \in (a, b)$.
- (ii) The derivative $\dot{T}(t)$ is never positive and there exists $t_{1/2} \in [0, t_f]$ where $T(t)$ is discontinuous, with $T(t_{1/2}^-) < T(t_{1/2}^+)$.

In either case, the mechanism for extracting arbitrarily large power is similar. It takes advantage of a localized thermodynamic state (with entropy $\simeq -\infty$) at a point of the cycle when the temperature starts increasing.

Let us first consider case (i). Let ρ be Gaussian $N(0, \sigma(t)^2)$ and choose $\delta > 0$ such that $(a + \delta, b - \delta) \subset (a, b)$. Then, let $\sigma(t)$ be according to

$$\sigma(t) = \begin{cases} \sigma_{\max}, & t \in (0, a] \cup (b, t_f] \\ k_1 t + b_1, & t \in (a, a + \delta] \\ \sigma_{\min}, & t \in (a + \delta, b - \delta] \\ k_2 t + b_2, & t \in (b - \delta, b] \end{cases}$$

where $k_1 < 0$, $k_2 > 0$, b_1 , and b_2 are constants such that $\sigma(t)$ is continuous. From the above, $|k_1|, k_2 < \sigma_{\max}/\delta$. The dissipation term in the expression for power (24) satisfies $-\frac{1}{t_f} \int_0^{t_f} \gamma \dot{\sigma}(t)^2 dt > -2\gamma \sigma_{\max}^2/t_f \delta$. The second term of (24) decomposes into four parts, following $\sigma(t)$,

$$\begin{aligned} \int_{(0,a] \cup (b,t_f]} k_B \dot{T}(t) \log(\sigma(t)) dt &= k_B(T(a) - T(b)) \log(\sigma_{\max}) \\ \int_{(a,a+\delta]} k_B \dot{T}(t) \log(\sigma(t)) dt &\leq k_B(T(a + \delta) - T(a)) \log(\sigma_{\max}) \\ \int_{(b-\delta,b]} k_B \dot{T}(t) \log(\sigma(t)) dt &\leq k_B(T(b) - T(b - \delta)) \log(\sigma_{\max}) \\ \int_{(a+\delta,b-\delta]} k_B \dot{T}(t) \log(\sigma(t)) dt &= k_B(T(b - \delta) - T(a + \delta)) \log(\sigma_{\min}), \end{aligned}$$

where the fact that $\dot{T}(t) > 0$ is used for the inequalities. Combining the above, we have

$$\mathcal{P} \geq -2\gamma \frac{\sigma_{\max}^2}{t_f \delta} - \frac{k_B}{t_f} \Delta T_1 \log\left(\frac{\sigma_{\min}}{\sigma_{\max}}\right) \quad (37)$$

where $\Delta T_1 := T(b - \delta) - T(a + \delta) > 0$. As $\sigma_{\min} \rightarrow 0$, the lower bound for the power tends to ∞ .

For the second case, select $\sigma(t)$ as before where the interval (a, b) and δ are chosen such that the point of discontinuity $t_{1/2} \in (a + \delta, b - \delta) \subset (a, b)$ and $\Delta T_2 := T(b) - T(a) > 0$. As a result

$$\begin{aligned} \int_{(0,a] \cup (b,t_f]} k_B \dot{T}(t) \log(\sigma(t)) dt &= k_B(T(a) - T(b)) \log(\sigma_{\max}) \\ \int_{(a,a+\delta]} k_B \dot{T}(t) \log(\sigma(t)) dt &\leq k_B(T(a + \delta) - T(a)) \log(\sigma_{\min}) \\ \int_{(b-\delta,b]} k_B \dot{T}(t) \log(\sigma(t)) dt &\leq k_B(T(b) - T(b - \delta)) \log(\sigma_{\min}) \\ \int_{(a+\delta,b-\delta]} k_B \dot{T}(t) \log(\sigma(t)) dt &= k_B(T(b - \delta) - T(a + \delta)) \log(\sigma_{\min}) \end{aligned}$$

where the fact that $\dot{T}(t) < 0$ is used for the inequalities. Combining these terms concludes a bound similar to (37), with ΔT_1 replaced by ΔT_2 , which grows to ∞ as $\sigma_{\min} \rightarrow 0$.

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