Underdamped stochastic heat engine at maximum efficiency

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Abstract – We investigate the performance of an underdamped stochastic heat engine, using the paradigmatic model of a harmonic oscillator with time-dependent frequency. We analytically determine the optimal protocol that maximizes the efficiency at fixed power. The maximum efficiency reduces to the Curzon-Ahlborn formula at maximum power and to the Carnot formula at zero power. We establish that the efficiency at maximum power is universally given by the Curzon-Ahlborn efficiency for weak damping. We further show that even small deviations from operation at maximum power results in a significantly increased efficiency.

Introduction. – The universal upper bound on the efficiency of any heat engine operating between two equilibrium baths at temperatures $T_c$ and $T_h$ ($T_c < T_h$) is given by the Carnot formula, $\eta_C = 1 - T_c/T_h$ [1]. The Carnot efficiency is however only reachable in the reversible limit, for ideal engines that run infinitely slowly and thus have zero power. It is hence customary to consider the efficiency at maximum power $\eta^*$, popularized by Curzon and Ahlborn [2], which yields a better estimate for the performance of real engines. For low-dissipation machines, generic bounds on $\eta^*$ have been obtained in refs. [3,4]. They reduce to the Curzon-Ahlborn efficiency, $\eta_{CA} = 1 - \sqrt{T_c/T_h}$, for symmetric coupling to the cold and hot baths. The existence of these general bounds is of fundamental importance. Yet, they do not address the crucial question of how to actually reach them, as they do not provide information about optimal engine cycles. It has recently been shown that seeking the efficiency at maximum power may not always be the best strategy [5,6]. To achieve engines with high efficiency and high power one may rather want to maximize the efficiency at a given power. A motor working at maximum efficiency may, for instance, attain higher efficiency and power than motors working at their maximum power. At the same time, devices that supply a fixed power, with the highest possible efficiency, are often required in practical engineering applications. The efficiency at given power output, as opposed to maximum power output, further offers a direct method to compare the performance of different engines.

In this paper, we compute the maximum efficiency at fixed power $\bar{\eta}$ for an underdamped harmonic stochastic heat engine and determine the corresponding optimal driving protocols. Such a system may be viewed as a minimal model for a piston engine with a microscopic particle as the working medium: Increasing and decreasing the strength of the harmonic potential corresponds to the compression and expansion phases of the cycle. Heating and cooling is accomplished by changing the effective temperature experienced by the center-of-mass motion of the particle. In the overdamped limit, the optimization problem has been solved by Schmiedl and Seifert [7]: they calculated the optimal protocols that lead to maximal power output and derived the corresponding efficiency at maximum power. Interestingly, they found that $\eta^*$ may surpass the Curzon-Ahlborn efficiency $\eta_{CA}$. Experimental realizations of underdamped Brownian engines in colloidal systems have been reported in refs. [8-10]. As the medium typically prevents the implementation of optimized engine cycles due to limited control over its temperature, an externally applied noisy force has been demonstrated to allow mimicking a thermal bath [10]. Our analysis generalizes these studies to underdamped heat engines. Optimization of the engine cycle in the underdamped regime is significantly more difficult, owing to the coupling between position and velocity dynamics [11-13], and thus has been little explored so far.

Recent advances in optomechanics have lead to the development of optically controlled mechanical resonators with large quality factors, $Q = \omega/\gamma$, where $\omega$ is the
frequency and $\gamma$ the damping rate [14]. First demonstrated by Ashkin [15] in the late 1970s, optical levitation has recently been rediscovered for optomechanics. The approach enables quality factors up to $Q \sim 10^8$ [16] and highly tunable resonator frequencies. In essence, optical levitation can provide an analogue to optically controlled colloidal systems, which allows to investigate strongly underdamped Brownian motion [17,18]. A proposal to implement an underdamped stochastic heat engine in such a setup has been put forward in ref. [19]. While underdamped mechanical resonators are omnipresent [20] and have recently been used to realize engine cycles [21], optical levitation is particularly suited to demonstrate the optimal protocols presented here, due to the flexible tunability of the corresponding resonator frequency.

We finally discuss a possible experimental verification of the efficiency of the engine by sacrificing relatively little power. We show that it is possible to considerably enhance the efficiency at maximum power in the underdamped regime, in contrast to the overdamped limit. We further demonstrate that the optimal protocols presented here, due to the flexibility of the corresponding resonator frequency, allow for different bath couplings $\gamma_h$ and $\gamma_c$. During this procedure, the frequency $\omega$ is varied with time to compress or expand the system. After time $\tau_h + \tau_c$, the particle is again coupled to the hot bath and the cycle starts anew. In the underdamped regime, the heat exchanged with any of the two baths $(i = h,c)$ is given by [22,23],

$$Q_i = \gamma_i \int \left[ \tau_i T_i - m \int_0^{\tau_i} dt \sigma_v(t) \right] ,$$

where $\sigma_v(t)$ is the solution of eq. (3) with the appropriate boundary conditions. Here we define heat such that it is positive if the particle absorbs energy from the bath. The energy change, $\Delta U = Q + W$, vanishes over one cycle and the extracted work is equal to the total heat, $-W = Q_h + Q_c$. As a result, power output $P$ and efficiency $\eta$ of the Brownian heat engine may be written as

$$P = \frac{Q_h + Q_c}{\tau_h + \tau_c}, \quad \eta = \frac{Q_h + Q_c}{Q_h} .$$

### Optimal protocols

We now fix the power at a given value, $P = P_0$, and seek the optimal protocol $\omega(t)$ that maximizes the efficiency $\eta$. According to eq. (5), we need to simultaneously minimize $-Q_c$, the heat dissipated to the cold bath, and maximize $Q_h$, the heat uptake from the hot bath. In a first step, we fix the coupling times $\tau_h$ and $\tau_c$. In the underdamped regime, we have to maximize eq. (4) with the constraint (3) imposed on $\sigma_v$. The effective Lagrangian for this optimization problem is

$$\mathcal{L}(\sigma_v, \dot{\sigma}_v, \omega, \dot{\omega}, \psi) = \sigma_v + \dot{\sigma}_v + \left( \frac{\gamma - \omega}{\omega} \right) \sigma_v - \frac{\gamma T}{m} .$$

In the underdamped limit, $\omega \gg \gamma$, the particle completes many oscillations in the potential before its energy is significantly changed through the interaction with the bath. By virtue of the virial theorem, we may take kinetic and potential energies to be equal, $m \sigma_x/2 = m \omega^2 \sigma_x/2$ (averaged over one oscillation period). Replacing $\sigma_x/\omega^2$ in (2a) and keeping in mind that $\omega$ may be time dependent,

$$\dot{\sigma}_v + \left( \frac{\gamma - \omega}{\omega} \right) \sigma_v = \frac{\gamma T}{m} .$$

Whereas the system adjusts instantly to the bath in the overdamped limit, it adjusts immediately to changes of the external potential in the underdamped limit. During an engine cycle, the particle is coupled to the hot bath at temperature $T_h$ for a time $\tau_h$, and then to the cold bath at temperature $T_c < T_h$ for a time $\tau_c$. We assume the switch between the baths to be quasi-instantaneous, as in the experiment [8]. Note that these instantaneous switches do not spoil the validity of the underdamped approximation, since the small damping rate $\gamma$ (compared to the oscillation frequency $\omega$) means that the system only reacts slowly to changes in the bath temperature. We further allow for different bath couplings $\gamma_h$ and $\gamma_c$. During this procedure, the frequency $\omega$ is varied with time to compress or expand the system. After time $\tau_h + \tau_c$, the particle is again coupled to the hot bath and the cycle starts anew.

In the underdamped regime, the heat exchanged with any of the two baths $(i = h,c)$ is given by [22,23],

$$Q_i = \gamma_i \int \left[ \tau_i T_i - m \int_0^{\tau_i} dt \sigma_v(t) \right] ,$$
The corresponding Euler-Lagrange equations read
\[ \begin{align*}
1 + \psi' \left( \gamma - \frac{\dot{\omega}}{\omega} \right) - \psi &= 0, \\
\frac{1}{\omega} d \frac{d}{dt} \left( \psi \sigma_v \right) &= 0, \\
\sigma_v + \left( \gamma - \frac{\dot{\omega}}{\omega} \right) \sigma_v - \frac{\gamma T}{m} &= 0.
\end{align*} \tag{7a-7c} \]

We provide a detailed solution of the above equations in the Supplemental Material Supplementary material.pdf (SM). In particular, we establish that a nontrivial solution of the optimization problem requires discontinuities in both \( \omega(t) \) and \( \sigma_v(t) \) at the transitions between cold and hot baths. We note that in the underdamped limit, a discontinuous variance \( \sigma_v \) is permitted, since we assume that the system instantaneously adjusts to the potential. From the condition \( \sigma_{+} \omega_{+} = \sigma_{-} \omega_{-} \) at time \( t = \tau_h \) and a similar condition at time \( t = \tau_h + \tau_c \) (\( \omega_{\pm} \) and \( \sigma_{\pm} \) being the respective frequencies and variances before/after a jump), we find,
\[ \omega(t) = \omega_0 \begin{cases} \frac{\sigma_{+} \alpha}{\sigma_{+} - \sigma_{-}} \left( \gamma - \frac{T_h}{m \sigma_{+}} \right) \left( 1 - \tau_{+} \right), & \text{for } 0 < t < \tau_h, \\
\frac{\sigma_{-} \alpha}{\sigma_{-} - \sigma_{+}} \left( \gamma - \frac{T_c}{m \sigma_{+}} \right) \left( 1 - \tau_{-} \right), & \text{for } 0 < t - \tau_h < \tau_c. \end{cases} \tag{8a} \]
\[ \gamma_{+} \tau_h \left( 1 - \frac{T_h}{m \sigma_{+}} \right) + \gamma_{-} \tau_c \left( 1 - \frac{T_c}{m \sigma_{-}} \right) = 0. \tag{8b} \]

The above equations completely specify the optimal frequency protocol \( \omega(t) \) that leads to extremal values of the heats \( Q_h \) and \( Q_c \) for fixed \( \tau_c \) and \( \tau_h \). Here, the overall frequency \( \omega_0 \) is arbitrary, however, it needs to be chosen such that the underdamped approximation \( \omega_e \gg 1 \) is valid. The constants \( \sigma_e \) and \( \sigma_0 \) are fixed by the target of the optimization, i.e., maximizing the efficiency or power (see below). The optimal protocols eq. (8a) are our first main result. In contrast to the parabolic protocols for the overdamped case [7], the time dependence of the frequency protocols for the underdamped limit is exponential.

**Maximum efficiency at fixed power.** – In order to determine the maximum efficiency of the stochastic engine, \( \eta = 1 + \gamma_{+} \tau_h \left( T_c - m \sigma_{+} \right) \left( 1 - \tau_{+} \right) \left( 1 - \tau_{-} \right) \left( 1 - \tau_h \right) \), we eliminate \( \sigma_h \) and \( \sigma_c \) using eq. (5), with \( P = P_0 \), and eq. (8b). Maximizing the efficiency \( \eta \) with respect to \( \tau_h \), \( \tau_c \), \( \gamma_{+} \), \( \gamma_{-} \), \( \eta = 0 \), we obtain a relation between the two coupling times,
\[ \frac{\tau_h}{\tau_c} = \sqrt{\frac{\gamma_{+}}{\gamma_{-}}} \tag{9} \]

Using eq. (9), we arrive after some algebra at an explicit expression for the maximum efficiency \( \eta^{\star} \),
\[ \eta^{\star} = \frac{2y(1 - \sqrt{\alpha})^2}{1 - \alpha + y(1 - \sqrt{\alpha})^2} \left( 1 - y \right) \left( 1 - \alpha \right)^2 \left( 1 - y \right) \left( 1 - \sqrt{\alpha} \right)^4 \tag{10} \]

where we have defined \( \alpha = T_c / T_h \) and \( y = P / P^{\star} \). The maximum power \( P^{\star} \) is given by
\[ P^{\star} = \frac{\gamma_{+} \gamma_{-}}{\left( \sqrt{\gamma_{+}} + \sqrt{\gamma_{-}} \right)^2} \left[ T_h + T_c - 2 \sqrt{T_h T_c} \right]. \tag{11} \]

Equation (10) is our second main result. It expresses the maximum efficiency \( \eta^{\star} \) as a function of the output power \( P_0 \) (relative to the maximal value \( P^{\star} \)) and the temperature ratio \( \alpha \). For vanishing power, \( y = 0 \), \( \eta^{\star} \) reduces to the Carnot efficiency, \( \eta^{\star} = 1 - T_c / T_h \). On the other hand, for maximal power, \( y = 1 \), we obtain the Curzon-Ahlborn efficiency, \( \eta^{\star} = 1 - \sqrt{T_c / T_h} \). For intermediate power, \( 0 < P_0 < P^{\star} \), eq. (10) interpolates between the Carnot and Curzon-Ahlborn efficiencies, see fig. 1. Close to maximum power, we may expand around \( y = 1 \) to find \( \eta^{\star} \approx y^{\star} \left( 1 + (T_c / T_h)^{1/4} \sqrt{1 - y} \right) \). The efficiency is thus non-analytic with a diverging slope at this point. The physical consequence of this behavior is that even slightly reducing the power below the maximal value will yield disproportionately large gains in efficiency. This effect is most pronounced for small temperature differences, \( T_c / T_h \approx 1 \). This situation, where the overall efficiency is small, is often encountered in practice, since large temperature gradients are hard to maintain in microscopic systems. In this regime, it is thus possible to significantly increase the efficiency of the heat engine by sacrificing a relatively small amount of power.

Figure 2 presents the optimal protocols (8a) for fixed power \( P_0 \) and maximum power \( P^{\star} \). Their qualitative behavior may be easily understood. During the coupling to the hot bath (red shaded area), the frequency \( \omega \) of the harmonic potential is reduced exponentially. This step allows the particle to explore a larger space, similar to the expansion phase of a standard heat engine. The continuous exponential expansion is followed by an instantaneous

Fig. 1: Maximum efficiency \( \eta \) at constant power \( P_0 = y P^{\star} \) as a function of \( y \) for a temperature ratio of \( \alpha = T_c / T_h = 0.25 \).

The line is the analytic underdamped result (10), the dots are obtained by numerically solving the exact dynamics (2) for \( \omega / \gamma = 100 \) (full symbols) and \( \omega / \gamma = 2000 \) (empty symbols).

At maximum power, \( P_0 = P^{\star} \), the efficiency reduces to the Curzon-Ahlborn formula \( \eta^{\star} = 1 - \sqrt{T_c / T_h} \). Even slightly reducing the power yields a significantly enhanced efficiency.
The solid line is the protocol leading to maximum power output. The shaded background shows the coupling to the hot (cold) bath. Remarkably, we have $\tilde{\eta}/\eta^* > 1.34$; the increase in efficiency is therefore larger than the reduction in power.

expansion step (jump) immediately after the coupling to the cold bath. During the cold phase (blue shaded area), the frequency increases exponentially, again followed by an instantaneous compression step. This behavior is the same irregardless of the power. However, the precise values $\omega_i$ of the trap frequency do depend on the power. The discontinuities in the optimal protocols also occur in the overdamped regime [7]. They have their physical origin in the sudden temperature change when switching between the heat baths.

Universality of Curzon-Ahlborn efficiency. – Equation (10) indicates that the Curzon-Ahlborn formula provides an upper bound to the efficiency at maximum power of the harmonic Brownian engine in the underdamped regime. This can be understood by noting that i) owing to the vanishingly small dissipation, the only source of irreversibility is the heat exchanged with the baths—the engine is thus endoreversible [2]; ii) additionally, heat transfer is linear in the temperature difference, $\delta Q = \gamma_i (T_i - T_{\text{eff}}) dt$ with $T_{\text{eff}} = m \langle \sigma_v \rangle$, as seen from eq. (5). This expression is independent of the potential\(^1\). The above results will hold true for any physical dynamics for sufficiently small bath coupling. The limit of weak damping is thus equivalent to the linear response regime, implying that the Curzon-Ahlborn efficiency is here the universal upper bound at maximum power [24]. This constitutes our third main result.

Discussion. – In the underdamped regime, the particle is assumed to adjust instantaneously to changes of the frequency $\omega$. This is of course an approximation for any real system. In order to verify its validity, we numerically solve the full dynamics (2), for arbitrary $\gamma$, using the optimal protocols obtained in the underdamped limit, as shown in fig. 3 (black squares). For comparison, we also include the overdamped results (red dots) obtained by Schmiedl and Seifert [7] (see also the SM). We take into account the fact that the rate of change of the frequency cannot be arbitrary fast, $\dot{\omega}/\omega \ll 1$, by replacing the instantaneous jumps at $\tau_i$ and $\tau_i + \tau_i$ with a linear variation of length $\tau_{\Delta}$, such that $\dot{\omega}/\omega < 0.1/10$. We observe that the underdamped optimal protocol (8) then leads to values of efficiency and power that are in good agreement with the analytical expressions (10) and (11) for $\omega > 0.1$. At the same time, the overdamped optimal protocol yields a power output which approaches the predicted maximum value for $\omega \leq 0.1\gamma$. By contrast, the actual efficiency at maximum power remains smaller than the theoretical value (dashed line), even for very small ratios of $\omega/\gamma$. While the dynamics of the particle’s position is well described by the overdamped approximation in the limit of large damping, the contribution of the velocity degree of freedom to the heat exchange does not vanish in this limit [7,9,25–29]. Taking the contribution to heat from the velocity degree of freedom explicitly into account, we find that the efficiency at maximum power $\tilde{\eta}^*$ is modified to

\[ \tilde{\eta}^* = \frac{\eta^*}{1 + 2\eta^*/\ln(\sigma_v/\sigma_h)}. \]  

\(^1\)In the overdamped limit, the heat is related to the variance of the position and thus depends explicitly on the time-dependent driving. Although, a linear Fourier law also holds for the heat flow in this case, the time-dependence of the driving violates endoreversibility [7].
see eq. (S9) in the SM. The overdamped result $\eta^*$ is accordingly only recovered in the limit $\sigma_c \gg \sigma_h$, that is, when the particle is more strongly confined when coupled to the hot bath. In this limit of a stiff oscillator, the dynamics of the particle can be more tightly controlled, thus improving efficiency [27]. Excellent agreement with eq. (12) is seen in fig. 3 (dotted line). The overdamped efficiency at maximum power $\eta^*$ might be difficult to reach in practice owing to the logarithmic dependence $\ln (\sigma_c/\sigma_h)$. In the intermediate regime, $\gamma \sim \omega$, where the coupling to the baths is neither weak nor strong, our numerical analysis shows that the optimal protocols derived in both underdamped and overdamped limits fail. The explicit optimal protocols are in this case not known owing to the increased complexity of the optimization procedure [11–13].

Coming back to fig. 1, we find excellent agreement close to maximum power between the underdamped approximation (line) obtained for $\omega/\gamma \to \infty$ and the actual dynamics (2) with large but finite $\omega/\gamma$ (dots). However, as we approach zero power, the efficiency of the engine is significantly reduced compared to the theoretical Carnot efficiency. This can be understood by noting that the underdamped optimal protocols (8a) are independent of the total cycle time $\tau = \tau_0 + \tau_c$. However, for a finite damping rate $\gamma$, a finite-time protocol will be accompanied by a non-zero dissipation due to the irreversibility of the dynamics. While close to maximum power, this additional dissipation is negligible at large $\omega/\gamma$, it becomes dominant as the power tends to zero. Here the system stops operating as an engine and instead dissipates work into the medium. Mathematically speaking, while the underdamped protocols correctly optimize the leading order (in terms of $\omega/\gamma$) heat exchanges, as one approaches the theoretical Carnot regime, the leading order contributions tend to zero and sub-leading terms have to be taken into account.

Experimental considerations. — An experimental demonstration of our theoretical findings seems feasible with state-of-the-art technology. Optically trapped nano- and micrometer particles provide harmonic oscillators that allow for sufficiently fast control of the frequency. They have been experimentally investigated both in the strongly overdamped [8,9] and in the strongly underdamped regime [15,17,30,31]. In addition, nearly instantaneous changes of the temperature of the optically trapped particle are possible in both regimes when an external parameter is used to control the force noise or damping experienced by the particle. In the strongly underdamped regime, we have recently proposed levitated cavity optomechanics as a feasible route to an underdamped Stirling engine that would meet all the requirements discussed above [19]. Here, large temperature ratios and fast temperature switches are feasible via cavity cooling. To demonstrate the performance of such an engine in the transition from the underdamped to the overdamped regime (fig. 3), optical levitation is also suitable [32]. However, to reach large temperature differences in this case the technique recently used by Martinez et al. [9] is more suitable. Here, the change in temperature is emulated by driving a charged nanoparticle with additional force noise applied using an electric field. This force noise can be switched on and off quasi-instantaneously. For example, the relevant regime would be covered using silica spheres with radius 70 nm. When trapped at feasible frequencies around 50 kHz, $Q = 100$ is reached at a pressure of 4 Pa, while $Q = 1$ is reached at room pressure (see, e.g., ref. [30]).

Conclusions. — We have optimized an underdamped stochastic harmonic heat engine for maximum efficiency at fixed power. We have analytically determined the optimal driving protocols for all values of the power. They differ from those obtained in the overdamped limit, but like the former they exhibit jumps that mirror the sudden change in temperature. We have demonstrated that the Curzon-Ahlborn efficiency is the universal efficiency at maximum power due to the linear heat transport implicit in the weak coupling limit. We have further shown that reducing the power slightly below its maximum value leads to disproportionately large gains in efficiency. Our findings confirm that maximizing the efficiency at maximum power is not always the best way to design machines with both high efficiency and high power. Both from a theoretical and experimental point of view, it would be interesting to extend these results to include feedback control, as has been done for the overdamped system in refs. [33,34].

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