Optimizing the Classical Heat Engine

A. E. Allahverdyan[1,3] and Th. M. Nieuwenhuizen[2]
[1]*Institute for Theoretical Physics, University of Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands*
[2]*Department of Physics and Astronomy, University of Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands*
[3]*Yerevan Physics Institute, Alikhanian Brothers Street 2, Yerevan 375036, Armenia*
(Received 10 January 2000)

A pair of systems at different temperatures is a classic environment for a heat engine, which produces work during the relaxation to a common equilibrium. It is generally believed that a direct interaction between the two systems will always decrease the amount of the obtainable work, due to inevitable dissipation. Here a situation is reported where, in some time window, work can be gained due to the direct coupling, while dissipation is relevant only for much larger times. Thus, the amount of extracted work *increases,* at the cost of a change of the final state.

PACS numbers: 05.70.Ln, 05.20.–y, 05.70.Ce

The classical problem of thermodynamics is the determination of the maximal amount of work that can be extracted from a nonequilibrium system, during the relaxation to the equilibrium state [1–4]. In recent years the interest in this time-honored problem was renewed (see [4] for review). In many cases the limits proposed by the founders of the classic thermodynamics have appeared as too idealistic, and attention was focused on the study of dissipative effects, which restrict the abilities of realistic heat engines [4]. One of the most popular examples of that kind is a direct interaction between the thermal baths that drive the standard heat engine [5]. Evidently, this is a way to dissipate energy. The common opinion, expressed in textbooks [1–3], is that dissipation is the main, if not the only, effect of any direct interaction.

The purpose of the present paper is to show that a direct interaction between the baths may have energy transfer, rather than energy dissipation, as its main physical effect. The reason is that the relevant time scale of the transfer arising from the direct coupling can be widely separated from the dissipative time scale. This leads to an optimization of the classical heat engine, in a certain time window. As a result, the final equilibrium state of the heat baths is changed. The mechanism arises from the recently proposed steady adiabatic state [6] (see also [7,8] in the related context).

First, we shall reproduce the classical discussion of the maximal amount of work that can be extracted from a nonequilibrium system. The underlying ideas are, of course, well known, and we shall need them for a careful interpretation of our main result.

The classical analysis.—Consider two subsystems which have different temperatures T_1 and T_2. Depending on the concrete relaxation process, the whole thermally isolated system will produce different amounts of work. This model is well known and described in textbooks on thermodynamics [1–3]. We shall assume that the total volume of the system is unchanged by the relaxation (although it can vary during the process), since we wish to take into account only the work that can be done due to the nonequilibrium initial state, and not due to the general expansion. Denoting by U_i, S_i the initial energy and entropy of the system, we get the following expression for the work W performed by the system:

$$W = U_i - U(S), \qquad (1)$$

where $U(S)$ is energy of the final equilibrium state as a function of its entropy. Because the temperature is positive, U is a monotone function of S ($\partial U/\partial S|_V = T > 0$ in equilibrium). Therefore, W is maximal when S is as small as possible. Since the whole system is thermally isolated, the second law demands $S \geq S_i$. The maximal amount of work is attained for $S = S_i$, i.e., for a *reversible* process towards equilibrium. It is believed that for obtaining the maximal amount of work any direct interaction between subsystems should be removed, because it would induce *irreversible* relaxation. Thus, a third body ("engine") should operate between our subsystems to perform the work. At the end of the relaxation process the working body must return to its initial state. The expression of the total amount W of the extracted work can be given as

$$W = U_1(T_1) + U_2(T_2) - U_1(T_0) - U_2(T_0), \qquad (2)$$

where the final temperature T_0 is determined by the reversibility condition

$$S_1(T_1) + S_2(T_2) = S_1(T_0) + S_2(T_0), \qquad (3)$$

and U_k, S_k ($k = 1, 2$) are energy and entropy of the corresponding subsystems. The reversible relaxation process consists of an infinite amount of elementary cycles of the third body. The famous Carnot process is the most representative example for such a cycle. The local efficiency η of the optimal cycle, defined as the maximal extracted work during the cycle divided by the input energy, depends *only* on the conditions of reversibility and conservation of energy: $\eta = 1 - (T_1/T_2)$, if $T_1 < T_2$ [1–3]. This efficiency is universal and system independent, emphasizing the power of thermodynamics. In contrast, the maximal amount of the extracted work (2) is not universal, and can vary from one system to another.

The steady adiabatic state.—Steady adiabatic systems have two distinctive properties [6]: (1) different subsystems are not in the mutual equilibrium, but possess different temperatures; (2) the local characteristic relaxation times of these subsystems are very well separated. Let us consider a statistical system which has two subsystems with coordinates x_1 and x_2. (x_1 and x_2 can thus also code a set of variables; we will not denote that explicitly.)

The corresponding relaxation times are denoted by Γ_1 and Γ_2. The condition of well-separated time scales is ensured by $\gamma = \Gamma_1/\Gamma_2 \ll 1$. The stationary distribution of this system can be found from the following heuristic arguments (for a more rigorous presentation, see [6]). Because of the large difference between relaxation times the x_1 subsystem comes to an equilibrium while the x_2 variable is almost unchanged. The corresponding Gibbs stationary distribution reads

$$P(x_1\,|\,x_2) = \frac{1}{Z(x_2)}\exp[-\beta_1 H(x_1,x_2)], \tag{4}$$

where

$$H(x_1,x_2) = H_1(x_1) + H_2(x_2) + gH_{\rm int}(x_1,x_2) \tag{5}$$

is the total system's Hamiltonian, $T_1 = 1/\beta_1$ is the temperature of the x_1 subsystem, and $Z(x_2)$ is the partition sum at fixed x_2. For obtaining the coarse-grained distribution $P(x_2)$ notice that, after integrating out of the vast variable x_1, the effective Hamiltonian for the slow variable x_2 is just $-T_1 \ln Z(x_2)$, the free energy of the x_1 subsystem at fixed x_2. The stationary distribution of x_2 then reads

$$P(x_2) = \frac{Z^{T_1/T_2}(x_2)}{\mathcal{Z}}, \qquad \mathcal{Z} = \int dx_2 Z^{T_1/T_2}(x_2). \tag{6}$$

The complete stationary distribution can now be written as $P(x_1,x_2) = P(x_2)P(x_1|x_2)$. The mean energy and entropy of the system are given by the following general definitions:

$$U = \int dx_1\,dx_2\,H(x_1,x_2)P(x_1,x_2), \tag{7}$$

$$S = -\int dx_1\,dx_2\,P(x_1,x_2)\ln P(x_1,x_2), \tag{8}$$

S can be decomposed as the sum of the entropies of the slow and fast subsystems, $S = S_1 + S_2$, with

$$S_1 = \int dx_2\,P(x_2)\left(-\int dx_1\,P(x_1\,|\,x_2)\ln P(x_1\,|\,x_2)\right), \qquad S_2 = -\int dx_2\,P(x_2)\ln P(x_2). \tag{9}$$

S_1 is the entropy of the fast variable x_1 at x_2, averaged x_2, while S_2 is the entropy of this slow variable itself. As was shown in [6] the considered system admits a *thermodynamical* description. In particular, defining the free energy as $F = -T_2 \ln \mathcal{Z}$, we get

$$F = U - T_1S_1 - T_2S_2, \tag{10}$$

where the entropies can also be obtained by the standard relations

$$S_1 = -\frac{\partial F}{\partial T_1}\bigg|_{T_2}, \qquad S_2 = -\frac{\partial F}{\partial T_2}\bigg|_{T_1}. \tag{11}$$

The energy and entropies are constant in the steady state, but a direct coupling induces a steady entropy production at rate $\dot{S}$ and an energy dissipation at rate $\dot{\Pi}$. These quantities were analyzed in Ref. [6], and the obtained formulas read $\dot{\Pi} = T_2\dot{S} + \mathcal{O}(\gamma^2)$, with

$$\dot{S} = \gamma g^2 \frac{(T_1 - T_2)^2}{\Gamma_1 T_1^2 T_2}\int dx_2\,dx_1\,P(x_1,x_2) \times \left[\frac{\partial H_{\rm int}(x_1,x_2)}{\partial x_2} - \int dy\,P(y\,|\,x_2)\,\frac{\partial H_{\rm int}(y,x_2)}{\partial x_2}\right]^2 + \mathcal{O}(\gamma^2). \tag{12}$$

Although these results were obtained for the strictly steady state, they can be applied also in the time-dependent case, if the characteristic time of this *quasistationary* process is much larger than the largest relaxation time Γ_2. For instance, to obtain the time-dependent distribution function for the case of slowly (adiabatically) changing temperatures or other parameters, one just inserts these time-dependent values directly in Eqs. (4) and (6). In this context, the change of free energy (10) can be shown to be the adiabatic work $\mathcal{W}_{\rm ad}$ done on the system, when varying a parameter α (for example, the width of the potential, or a coupling constant) from the initial value α_i to final value α_f at constant temperatures:

$$\mathcal{W}_{\rm ad} = \int_{\alpha_i}^{\alpha_f} d\alpha \int dx_1\,dx_2\,P(x_1,x_2,\alpha)\,\frac{\partial H(x_1,x_2,\alpha)}{\partial\alpha} = F(T_1,T_2;\alpha_f) - F(T_1,T_2;\alpha_i). \tag{13}$$

This is fully analogous to the property of the usual (single-temperature) free energy.

The dissipative effects [given by Eq. (12)] are small for small γ, g. Let us neglect them for the moment; later we shall show that this is allowed in a certain time window.

The maximal amount of work extracted from the steady adiabatic state.—Certainly, we can apply the above-mentioned general analysis, concerning the maximal work, to our adiabatic system. In fact, this analysis does not use any concrete property of the initial nonequilibrium state, but we should take into account that our subsystems interact directly, and not only through the third body. As compared to the case without direct coupling, the system will now relax to a different equilibrium state, and this is the reason why one can get more work done by it. The total amount of the gained work can be again written as

$$W(g) = U(T_1,T_2) - U(T_g,T_g), \tag{14}$$

and the temperature T_g of the final equilibrium state is defined from the condition of reversibility,

$$S(T_1, T_2) = S(T_g, T_g)\,. \tag{15}$$

This condition involves the total entropy of the interacting subsystems, and now assumes that there are no additional sources of dissipation besides (12).

We shall investigate Eqs. (14) and (15) to first order in the small parameter g. Hereafter quantities of the order g^0 and g^1 will be indicated by the index 0 and 1, respectively. It is evident from (5) that to order g^1 it holds that

$$F = F^{(0)} + gV_0\,, \tag{16}$$

where

$$V_0(T_1, T_2) = \int dx_1\, dx_2\, P(x_1, x_2) H_{\mathrm{int}}(x_1, x_2)\,. \tag{17}$$

Using Eqs. (7)–(11), one gets

$$S_1 = S_1^{(0)} + gS_1^{(1)} = S_1^{(0)} - g\partial_{T_1} V_0\,, \tag{18}$$

$$S_2 = S_2^{(0)} + gS_2^{(1)} = S_2^{(0)} - g\partial_{T_2} V_0\,, \tag{19}$$

$$S = S^{(0)} + gS^{(1)} = S^{(0)} - g\{\partial_{T_1} + \partial_{T_2}\} V_0\,, \tag{20}$$

$$U = U^{(0)} + gU^{(1)} = U^{(0)} + g\{1 - T_1\partial_{T_1} - T_2\partial_{T_2}\} V_0\,. \tag{21}$$

Let us now obtain from Eq. (15) an expression for the final temperature T_g to order g, given the value of T_0, the final temperature for $g = 0$,

$$T_g = T_0\left[1 + g\,\frac{S^{(1)}(T_1, T_2) - S^{(1)}(T_0, T_0)}{C_1 + C_2}\right]. \tag{22}$$

Here $C_k = T_k \partial S_k^{(0)}/\partial T_k|_V = \partial U_k^{(0)}/\partial T_k|_V$, with $k = 1, 2$, are the heat capacities of the subsystems when they are uncoupled. Starting from Eq. (14) and using Eqs. (18)–(21), we finally derive the excess work at order g,

$$\begin{aligned} W^{(1)} &= \lim_{g\to 0} \frac{W(g) - W(0)}{g} \\ &= V_0(T_1, T_2) - V_0(T_0, T_0) \\ &\quad + \sum_{k=1}^{2} (T_0 - T_k)\partial_{T_k} V_0(T_1, T_2)\,. \end{aligned} \tag{23}$$

This is the first main result of our work. It remains to be shown in a specific example that this quantity can be positive. Let us first point out that further simplifications occur when T_1 is close to T_2. To first order in the parameter $T_1 - T_2$ Eq. (3) gives us

$$T_0 = \frac{C_1 + C_2}{C_1 T_1 + C_2 T_2}\, T_1 T_2\,, \tag{24}$$

while Eq. (23) can be approximated by

$$W^{(1)} = \sum_{k=1}^{2} (T_0 - T_k)\,(\partial_{T_k} V_0 - \{\partial_{T_k} V_0\}|_{T_1 = T_2 = T_0})\,. \tag{25}$$

To illustrate the general results let us present a concrete model, where the direct interaction increases the total amount of work: $W(g) > W(0)$. One of the most popular models of the thermal bath is a set of harmonic oscillators [9], which is frequently used to derive kinetic equations or to gain fundamental insight. Following this well-established tradition, we shall model our first (second) thermal bath by $N_1(N_2)$ oscillators at temperature T_1 (T_2), and weakly anharmonic interaction:

$$H = \frac{1}{2}\sum_{i=1}^{N_1} x_{1,i}^2 + \frac{1}{2}\sum_{i=1}^{N_2} x_{2,i}^2 + g\sum_{i=1}^{N} x_{1,i}^2 x_{2,i}^2\,, \tag{26}$$

where $g > 0$, and $N_1, N_2 \geq N$. It is straightforward to show that to order g one has the partial partition sum

$$Z(x_2) = T_1^{N_1/2} \exp\!\left(-\frac{1}{2}\beta_1 \sum_{i=1}^{N_2} x_{2,i}^2 - g\sum_{i=1}^{N} x_{2,i}^2\right) \tag{27}$$

and the full partition sum

$$\mathcal{Z} = T_1^{(1/2)N_1 T_1/T_2}\, T_2^{(1/2)N_2} (1 + 2gT_1)^{-(1/2)N}\,. \tag{28}$$

The latter result yields the free energy $F = -T_2 \ln \mathcal{Z}$,

$$F = -\frac{1}{2} N_1 T_1 \ln T_1 - \frac{1}{2} N_2 T_2 \ln T_2 + gNT_1T_2\,, \tag{29}$$

in agreement with the fact that $V_0 = NT_1T_2$. According to previous rules we derive

$$S_1 = \frac{1}{2} N_1(\ln T_1 + 1) - gNT_2\,, \tag{30}$$

$$S_2 = \frac{1}{2} N_2(\ln T_2 + 1) - gNT_1\,. \tag{31}$$

The internal energy follows as $U = F + T_1S_1 + T_2S_2$,

$$U = \frac{1}{2} N_1 T_1 + \frac{1}{2} N_2 T_2 - gNT_1T_2\,. \tag{32}$$

Notice that the sign of the order g correction is negative, due to entropic effects. To determine T_0 from Eq. (3) we need entropies $S_1^{(0)}$, $S_2^{(0)}$, that can be read of from Eqs. (30) and (31) at $g = 0$. One obtains $T_0 = T_1^{\nu_1} T_2^{\nu_2}$ and then from Eq. (22)

$$T_g = T_1^{\nu_1} T_2^{\nu_2} [1 + 2g\nu(2T_1^{\nu_1} T_2^{\nu_2} - T_1 - T_2)]\,, \tag{33}$$

where $\nu = N/(N_1 + N_2)$, $\nu_k = N_k/(N_1 + N_2)$, $k = 1, 2$. According to Eq. (1) and using $U_k^{(0)} = N_k T_k/2$, one gets for $g = 0$ the maximal amount of work,

$$W(0) = \frac{1}{2} N_1(T_1 - T_1^{\nu_1} T_2^{\nu_2}) + \frac{1}{2} N_2(T_2 - T_1^{\nu_1} T_2^{\nu_2})\,. \tag{34}$$

Taking into account that $V_0(T_1, T_2) = NT_1T_2$, one gets from Eq. (23) a non-negative shift in the maximal of amount of work,

$$gW^{(1)} = gN(T_1^{\nu_1} T_2^{\nu_2} - T_1)(T_2 - T_1^{\nu_1} T_2^{\nu_2}) \geq 0\,. \tag{35}$$

The equality is realized in the trivial case $T_1 = T_2$. Only for $g < 0$ this mechanism would reduce the work.

Equation (23), and especially our model-dependent result (35), show that the full amount of the extracted work can *increase* due the direct coupling. Let us now return to the dissipative effects. For the considered model the energy dissipated per unit of time $\dot{\Pi} = T_2 \dot{S}$ can be derived from Eq. (12). It reads [6]

$$\dot{\Pi} = \frac{8g^2N}{\Gamma_1} \gamma T_2 (T_1 - T_2)^2 + \mathcal{O}(\gamma^2) . \tag{36}$$

Our aim is now to obtain the characteristic time $\mathcal{T}$, after which the energy dissipated due to the direct coupling is comparable with the energy $gW^{(1)}$ gained according to Eq. (35). For the dissipated energy an upper estimate can be given as $\dot{\Pi}\mathcal{T}$, and we get, from $\dot{\Pi}\mathcal{T} = gW^{(1)}$,

$$\mathcal{T} = \frac{\Gamma_2}{8g} \frac{(T_1^{\nu_1} T_2^{\nu_2} - T_1)(T_2 - T_1^{\nu_1} T_2^{\nu_2})}{(T_1 - T_2)^2} . \tag{37}$$

To be able to neglect the dissipated energy, the duration of our process t must be much smaller than $\mathcal{T}$. On the other hand, since we are getting the work in the relaxation process, its duration t must be much higher than the largest relaxation time Γ_2. Thus, for times

$$\Gamma_2 \ll t \ll \mathcal{T} \tag{38}$$

it is possible to perform more work due to the presence of the direct coupling. The necessary condition $\Gamma_2 \ll \mathcal{T}$ is realized mainly when g is small. If one were not able to complete the relaxation in the time window (38), then for $t \sim \mathcal{T}$ the gained work would be equal to that without any direct coupling. The same analysis can be applied for the general case.

So far we have compared the efficiencies of two systems with the same initial temperatures T_1, T_2, and different values of g. One can also compare cases of identical initial energies, $(T_1, T_2, g = 0)$ and $(\bar{T}_1, \bar{T}_2, g > 0)$, where the temperatures $\bar{T}_1, \bar{T}_2$ are defined by $U(T_1, T_2, g = 0) = U(\bar{T}_1, \bar{T}_2, g > 0)$. The analysis is very similar to that given above, and indicates that our main result remains valid also in this case. There are examples of $(\bar{T}_1, \bar{T}_2)$, for which the direct coupling enhances the work.

In the context of our main result it is useful to investigate which amount of work $\mathcal{W}(0 \to g)$ should be spent by external sources to switch on the small coupling g, starting from the state with $g = 0$. We shall consider the two extremes, very slow and very fast switching, which happen to give the same answer for small g. In the first case one uses Eqs. (13) and (16) to obtain (T_1, T_2 are constant)

$$\mathcal{W}_{\mathrm{ad}}(0 \to g) = gV_0 . \tag{39}$$

For the very fast switching the initial state does not change, and the main change comes from the Hamiltonian (5): $\mathcal{W}_{\mathrm{fast}}(0 \to g) = \langle H(g) - H(0) \rangle_0$, which for small g leads to the same result as in Eq. (39). Using Eqs. (23), (35), and (39) one readily notices that there are temperatures, for which $\mathcal{W}_{\mathrm{ad}}(0 \to g) < gW^{(1)}$, implying that the cost for the switching is less than the gain due to coupling: $W(0) + \mathcal{W}_{\mathrm{ad}}(0 \to g) < W(g)$.

Until now it was believed that the presence of a direct interaction between the baths of a heat engine reduces its efficiency [1–5,10]. The purpose of the present paper is to demonstrate that it can enhance the efficiency. Having changed the initial and final states, a direct coupling introduces, of course, both a change in work and dissipation. We show that the characteristic times of these two quantities can be well separated. For times in the window (38) the work can be enhanced, though the dissipation is not yet relevant. This additional amount of work, which can be obtained from Eqs. (23), (25), and (35), is provided by the modified final state of the baths.

Finally, we will briefly discuss related studies. References [10,11] consider the local thermodynamic efficiency of brownian motors and related models. The statement of this problem differs from the one considered by us, but it is interesting to mention that the role of a direct interaction between baths was studied also in this context [11].

[1] H. B. Callen, *Thermodynamics* (John Wiley, New York, 1966); *Thermodynamics* (John Wiley, New York, 1985).
[2] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon Press, New York, 1980), Part 1.
[3] S.-K. Ma, *Statistical Mechanics* (World Scientific, Singapore, 1985).
[4] B. Andresen, P. Salamon, and R. S. Berry, Phys. Today **37**, No. 9, 62 (1984); B. Andresen, R. S. Berry, M. J. Ondrechen, and P. Salamon, Acc. Chem. Res. **17**, 266 (1984).
[5] P. Salamon, A. Nitzan, B. Andresen, and R. Berry, Phys. Rev. A **21**, 2115 (1980).
[6] A. E. Allahverdyan and Th. M. Nieuwenhuizen, Phys. Rev. E (to be published).
[7] Th. M. Nieuwenhuizen, Phys. Rev. Lett. **80**, 5580 (1998).
[8] Th. M. Nieuwenhuizen, Phys. Rev. E **61**, 267 (2000).
[9] C. Gardiner, *Handbook of Stochastic Methods* (Springer-Verlag, Berlin, 1982); G. W. Ford, M. Kac, and P. Mazur, J. Math. Phys. **6**, 504 (1965).
[10] J. M. R. Parrondo and P. Espanol, Am. J. Phys. **64**, 1125 (1996); K. Sekimoto, J. Phys. Soc. Jp. **66**, 1234 (1997); I. Derenyi and R. D. Astumian, Phys. Rev. E **59**, 6219 (1999).
[11] I. M. Sokolov, Europhys. Lett. **44**, 278 (1998); Phys. Rev. E **60**, 4946 (1999); cond-mat/0002251.